Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 12:01 AM EDT

PDB ID	:	3IE1
Title	:	Crystal structure of H380A mutant TTHA0252 from Thermus thermophilus HB8 complexed with RNA
Authors	:	Ishikawa, H.; Nakagawa, N.; Kuramitsu, S.; Yokoyama, S.; Masui, R.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2009-07-22
Resolution	:	2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

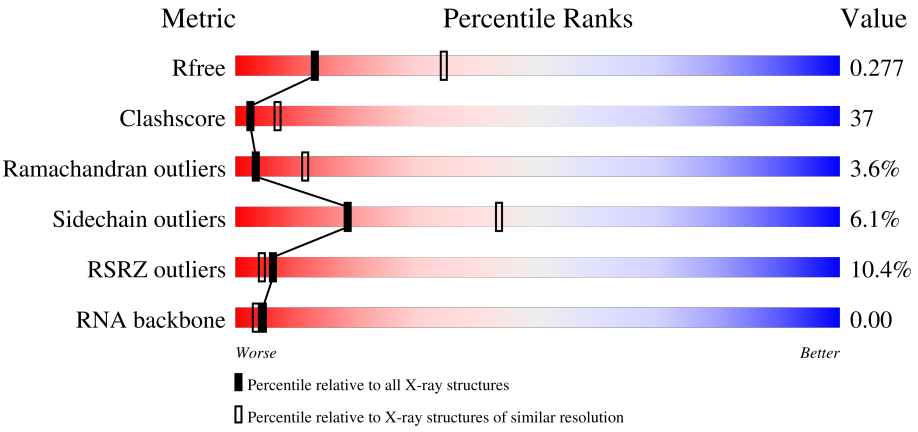
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)
RNA backbone	3102	1088 (3.12-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	52% 43% .
1	B	431	2% 53% 42% .
1	C	431	21% 37% 55% 7% .
1	D	431	18% 37% 56% 6%

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Mol	Chain	Length	Quality of chain
2	E	4	25% 75% 25%
2	F	4	75% 25%
2	G	4	50% 50%
2	H	4	50% 75% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	444	-	-	-	X
3	SO4	D	437	-	-	X	-
4	FLC	A	451	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13910 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ribonuclease TTHA0252.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3321	2124	595	594	8			
1	B	431	Total	C	N	O	S	0	0	0
			3321	2124	595	594	8			
1	C	431	Total	C	N	O	S	0	0	0
			3321	2124	595	594	8			
1	D	431	Total	C	N	O	S	0	0	0
			3321	2124	595	594	8			

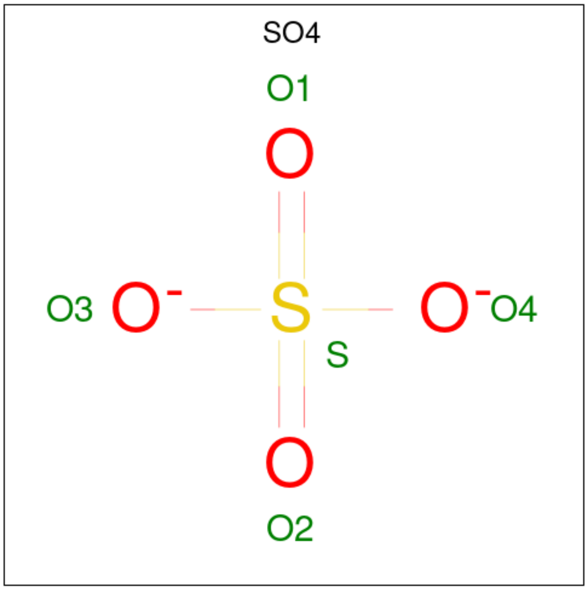
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ALA	HIS	engineered mutation	UNP Q5SLP1
B	380	ALA	HIS	engineered mutation	UNP Q5SLP1
C	380	ALA	HIS	engineered mutation	UNP Q5SLP1
D	380	ALA	HIS	engineered mutation	UNP Q5SLP1

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	P	0	0	0
			81	36	8	33	4			
2	F	4	Total	C	N	O	P	0	0	0
			81	36	8	33	4			
2	G	2	Total	C	N	O	P	0	0	0
			41	18	4	17	2			
2	H	4	Total	C	N	O	P	0	0	0
			81	36	8	33	4			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

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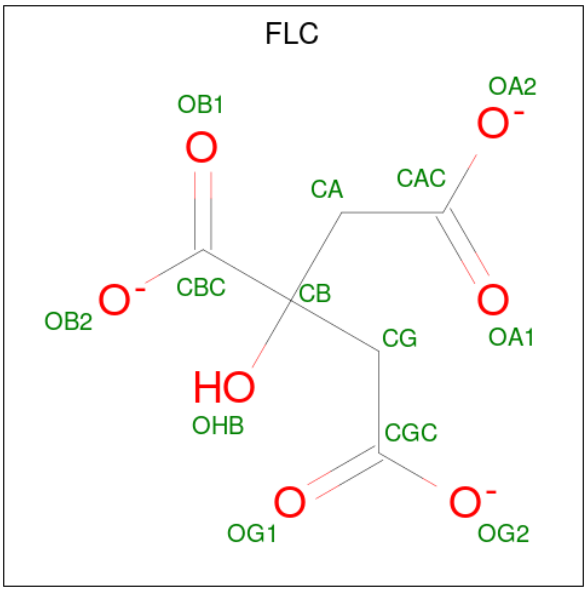
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	A	1	Total C O 13 6 7	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Zn 2 2	0	0
5	B	2	Total Zn 2 2	0	0
5	C	2	Total Zn 2 2	0	0
5	D	2	Total Zn 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	14	Total O 14 14	0	0
6	B	11	Total O 11 11	0	0
6	C	4	Total O 4 4	0	0

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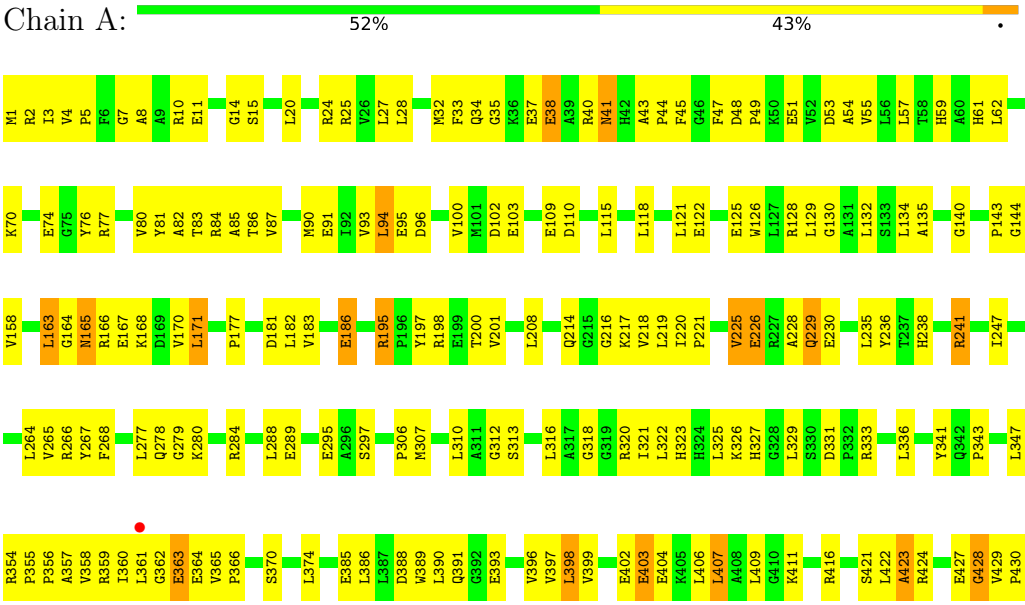
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	7	Total O 7 7	0	0
6	E	1	Total O 1 1	0	0
6	G	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

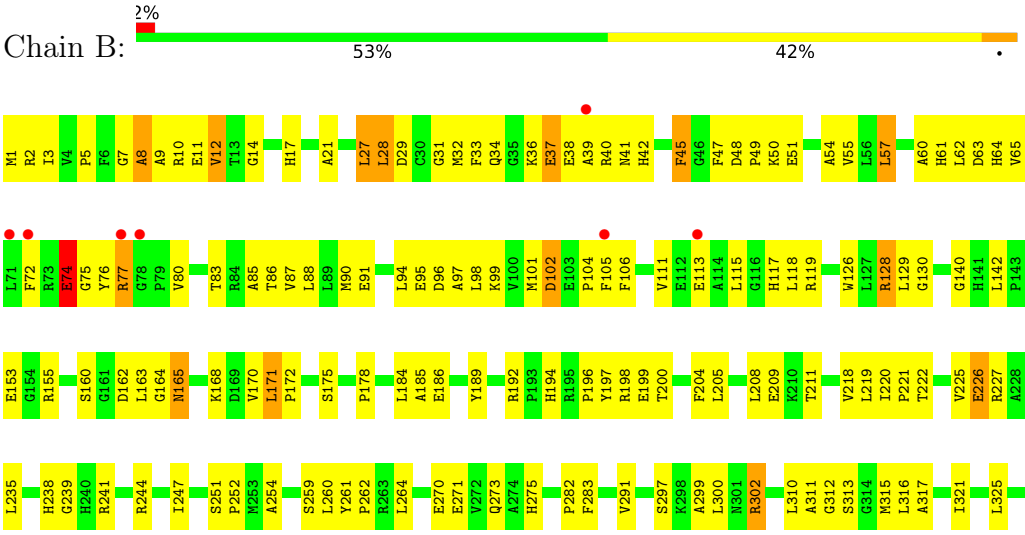
• Molecule 1: Ribonuclease TTHA0252

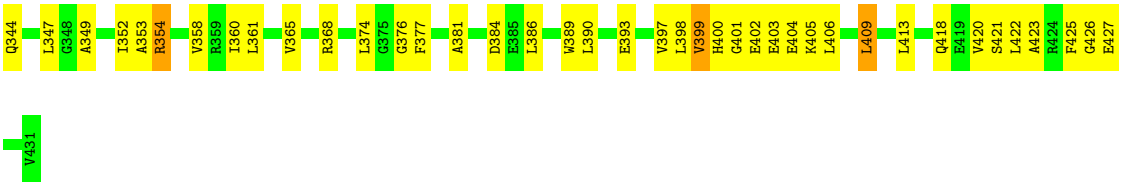
Chain A:



• Molecule 1: Ribonuclease TTHA0252

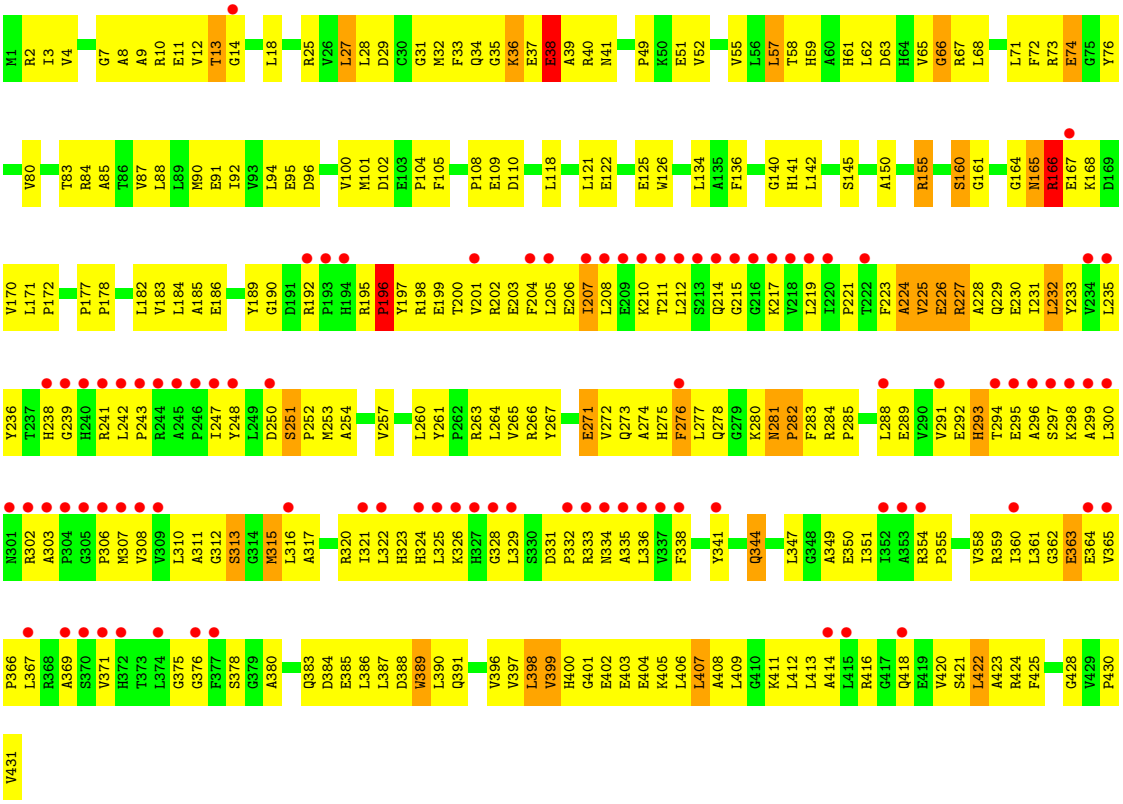
Chain B:





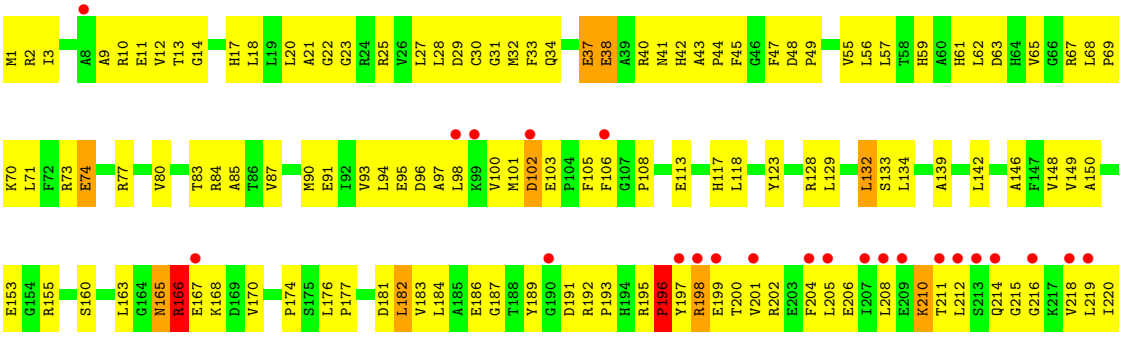
• Molecule 1: Ribonuclease TTHA0252

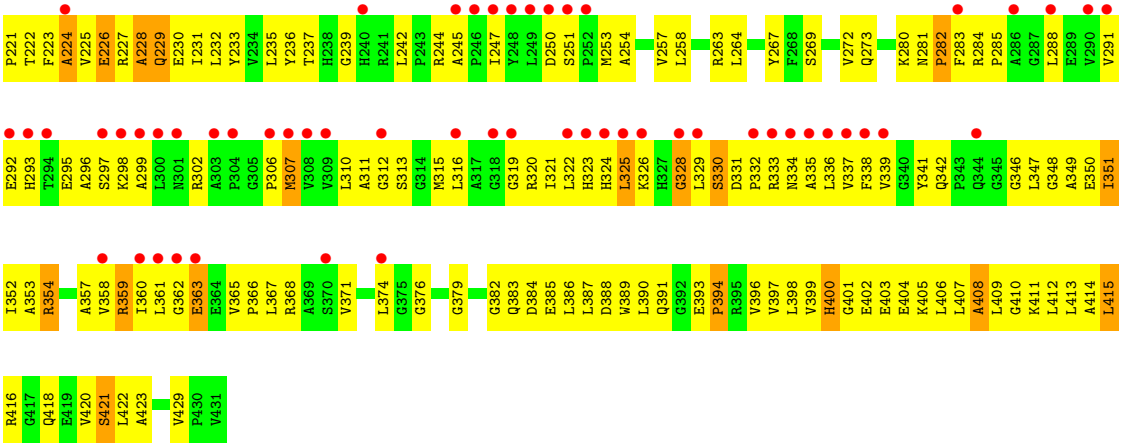
Chain C:



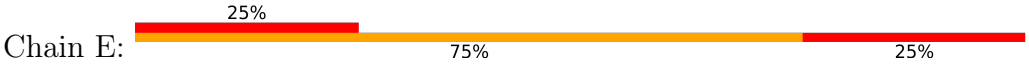
• Molecule 1: Ribonuclease TTHA0252

Chain D:





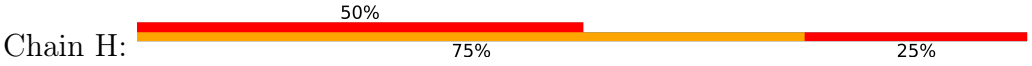
• Molecule 2: RNA (5'-R(P*UP*UP*UP*U)-3')



• Molecule 2: RNA (5'-R(P*UP*UP*UP*U)-3')

• Molecule 2: RNA (5'-R(P*UP*UP*UP*U)-3')

• Molecule 2: RNA (5'-R(P*UP*UP*UP*U)-3')



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.42Å 148.16Å 120.84Å 90.00° 109.61° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 49.92 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-2.85) 97.5 (49.92-2.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.11 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.291 0.220 , 0.277	Depositor DCC
R_{free} test set	5592 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å^2)	65.4	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 59.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13910	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FLC, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.44	0/3401	0.70	0/4613
1	B	0.44	0/3401	0.71	0/4613
1	C	0.33	0/3401	0.59	1/4613 (0.0%)
1	D	0.33	0/3401	0.58	0/4613
2	E	0.94	1/88 (1.1%)	0.85	0/132
2	F	1.03	1/88 (1.1%)	0.87	0/132
2	G	1.32	1/44 (2.3%)	0.82	0/64
2	H	0.97	1/88 (1.1%)	0.84	0/132
All	All	0.41	4/13912 (0.0%)	0.65	1/18912 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	U	OP3-P	-7.19	1.52	1.61
2	F	1	U	OP3-P	-7.16	1.52	1.61
2	G	1	U	OP3-P	-7.11	1.52	1.61
2	E	1	U	OP3-P	-6.32	1.53	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	161	GLY	N-CA-C	-5.33	99.79	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	1	U	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3321	0	3349	192	0
1	B	3321	0	3349	196	0
1	C	3321	0	3349	322	0
1	D	3321	0	3349	313	0
2	E	81	0	41	6	0
2	F	81	0	41	8	0
2	G	41	0	21	5	0
2	H	81	0	41	16	0
3	A	90	0	0	2	0
3	B	85	0	0	3	0
3	C	50	0	0	1	0
3	D	45	0	0	5	0
4	A	26	0	10	6	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	14	0	0	0	0
6	B	11	0	0	0	0
6	C	4	0	0	0	0
6	D	7	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
All	All	13910	0	13550	1026	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (1026) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:GLU:HG2	1:C:364:GLU:H	1.26	0.99
1:D:37:GLU:HG3	1:D:40:ARG:HH11	1.26	0.99
1:C:359:ARG:HH12	1:C:362:GLY:HA2	1.25	0.99
1:D:1:MET:HG3	1:D:21:ALA:HB2	1.40	0.98
1:C:250:ASP:HB3	1:C:311:ALA:HB2	1.45	0.98
1:B:33:PHE:H	1:B:41:ASN:HD21	0.98	0.97
1:A:195:ARG:HB2	3:A:432:SO4:O3	1.64	0.96
1:A:220:ILE:HB	1:A:310:LEU:HD23	1.48	0.96
1:C:235:LEU:HD13	1:C:247:ILE:HD13	1.48	0.96
1:C:33:PHE:H	1:C:41:ASN:HD21	1.00	0.95
1:C:205:LEU:HA	1:C:208:LEU:HD12	1.49	0.92
1:D:33:PHE:H	1:D:41:ASN:HD21	1.11	0.92
1:D:359:ARG:HH12	1:D:362:GLY:HA2	1.37	0.90
1:A:228:ALA:HB3	1:A:229:GLN:NE2	1.86	0.90
1:C:403:GLU:O	1:C:407:LEU:HD13	1.71	0.90
1:B:238:HIS:O	1:B:241:ARG:HG2	1.75	0.86
1:B:360:ILE:HG22	1:B:361:LEU:HD13	1.55	0.86
1:C:359:ARG:HH12	1:C:362:GLY:CA	1.89	0.86
1:D:420:VAL:HG22	1:D:421:SER:H	1.42	0.85
1:D:57:LEU:HD21	1:D:80:VAL:CG1	2.07	0.85
1:C:62:LEU:HD22	2:G:2:U:H3'	1.59	0.85
1:C:420:VAL:HG22	1:C:421:SER:H	1.41	0.85
1:D:98:LEU:HD11	1:D:108:PRO:HA	1.58	0.84
1:A:10:ARG:HG3	1:A:10:ARG:HH11	1.42	0.84
1:C:250:ASP:HA	1:C:291:VAL:HB	1.57	0.84
1:D:258:LEU:HD11	1:D:283:PHE:HB3	1.58	0.84
1:B:401:GLY:HA3	1:B:406:LEU:HD11	1.60	0.84
1:D:191:ASP:OD2	1:D:192:ARG:HG2	1.77	0.83
1:B:349:ALA:HA	1:B:352:ILE:HD12	1.62	0.82
1:A:33:PHE:HB3	1:A:37:GLU:HB2	1.61	0.82
1:A:235:LEU:HD13	1:A:247:ILE:HD13	1.61	0.82
1:D:330:SER:O	1:D:368:ARG:HB2	1.80	0.82
1:A:20:LEU:HD22	1:A:25:ARG:HH11	1.43	0.81
1:B:33:PHE:N	1:B:41:ASN:HD21	1.77	0.81
1:D:168:LYS:HE2	1:D:230:GLU:OE2	1.79	0.81
1:C:221:PRO:HB3	1:C:321:ILE:HG12	1.62	0.81
1:D:165:ASN:HB3	1:D:168:LYS:HG3	1.62	0.81
1:A:411:LYS:HB2	4:A:451:FLC:OB2	1.80	0.81
1:C:88:LEU:HB3	1:C:260:LEU:HD21	1.61	0.81
1:D:45:PHE:HB3	1:D:47:PHE:CE1	2.14	0.81
1:C:420:VAL:HG22	1:C:421:SER:N	1.96	0.80
1:B:88:LEU:HD12	1:B:264:LEU:HD11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:GLU:HB2	1:D:40:ARG:HE	1.48	0.78
1:B:221:PRO:HB3	1:B:321:ILE:HG12	1.65	0.78
1:C:200:THR:HG21	1:C:376:GLY:HA3	1.65	0.78
1:B:27:LEU:HB3	1:B:55:VAL:HG12	1.67	0.77
1:C:192:ARG:HH12	1:C:405:LYS:NZ	1.82	0.77
1:D:211:THR:HG21	1:D:335:ALA:HB2	1.66	0.77
1:D:316:LEU:HB3	1:D:347:LEU:HD23	1.66	0.77
1:D:73:ARG:NH2	1:D:106:PHE:HA	1.98	0.77
1:D:57:LEU:HD21	1:D:80:VAL:HG12	1.67	0.77
1:D:284:ARG:HA	1:D:288:LEU:HD22	1.65	0.77
1:A:84:ARG:HG2	1:A:84:ARG:HH11	1.50	0.77
1:C:168:LYS:HE2	1:C:230:GLU:OE1	1.84	0.77
1:C:336:LEU:HB3	1:C:371:VAL:HG22	1.67	0.76
1:B:37:GLU:HG2	1:B:40:ARG:HH11	1.50	0.76
1:C:57:LEU:HD23	1:C:90:MET:HE2	1.66	0.76
1:D:55:VAL:CG2	1:D:80:VAL:HG13	2.15	0.76
1:C:197:TYR:O	1:C:201:VAL:HG23	1.85	0.76
1:A:348:GLY:O	1:A:352:ILE:HG13	1.86	0.76
1:B:33:PHE:H	1:B:41:ASN:ND2	1.81	0.75
1:D:200:THR:HG21	1:D:376:GLY:HA3	1.68	0.75
1:D:215:GLY:HA2	1:D:306:PRO:HD3	1.67	0.75
1:D:399:VAL:HG12	1:D:400:HIS:H	1.51	0.75
1:C:192:ARG:HH12	1:C:405:LYS:HZ1	1.34	0.75
1:C:211:THR:HG21	1:C:335:ALA:HB2	1.68	0.75
1:C:351:ILE:HG23	1:C:367:LEU:HD11	1.67	0.74
1:B:153:GLU:O	1:B:155:ARG:HG2	1.86	0.74
1:C:57:LEU:HD23	1:C:90:MET:CE	2.18	0.74
1:C:383:GLN:O	1:C:387:LEU:HG	1.86	0.74
1:A:228:ALA:HB3	1:A:229:GLN:HE22	1.50	0.74
1:C:227:ARG:HH21	1:C:378:SER:HA	1.51	0.74
1:C:232:LEU:HD21	1:C:288:LEU:HD13	1.70	0.73
1:D:222:THR:HG22	1:D:339:VAL:HG21	1.69	0.73
1:C:402:GLU:OE1	1:C:405:LYS:HE2	1.88	0.73
1:A:225:VAL:O	1:A:229:GLN:NE2	2.22	0.73
1:A:76:TYR:O	1:A:77:ARG:HD2	1.87	0.73
1:B:61:HIS:CD2	1:B:142:LEU:HD11	2.23	0.73
1:C:293:HIS:HB2	1:C:295:GLU:HG2	1.70	0.73
1:B:97:ALA:O	1:B:101:MET:HB2	1.89	0.73
1:A:347:LEU:HD11	1:A:358:VAL:HG11	1.70	0.73
1:D:84:ARG:HB3	1:D:267:TYR:OH	1.87	0.73
1:C:387:LEU:HB3	1:C:416:ARG:HH12	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLU:O	1:A:95:GLU:HG2	1.90	0.72
1:B:229:GLN:HA	1:B:232:LEU:HD12	1.72	0.72
1:C:215:GLY:HA2	1:C:306:PRO:HD3	1.72	0.72
1:A:10:ARG:HG3	1:A:10:ARG:NH1	2.04	0.72
1:B:196:PRO:HB2	1:B:199:GLU:HG2	1.72	0.72
1:D:170:VAL:HA	1:D:272:VAL:HG21	1.70	0.71
1:A:122:GLU:O	1:A:125:GLU:HB2	1.90	0.71
1:D:91:GLU:O	1:D:95:GLU:HG2	1.91	0.71
1:B:259:SER:O	1:B:262:PRO:HD2	1.91	0.71
1:D:128:ARG:O	1:D:129:LEU:HD23	1.91	0.71
1:D:403:GLU:O	1:D:407:LEU:HB2	1.91	0.71
1:A:208:LEU:HD23	1:A:218:VAL:HG21	1.72	0.71
1:C:49:PRO:HG3	1:C:74:GLU:HB3	1.73	0.70
1:A:183:VAL:HG21	1:A:393:GLU:HG3	1.72	0.70
1:D:102:ASP:CG	1:D:103:GLU:H	1.95	0.70
1:A:411:LYS:HD2	4:A:451:FLC:HG2	1.74	0.70
1:C:360:ILE:HG22	1:C:361:LEU:HD13	1.73	0.70
1:D:299:ALA:HA	1:D:302:ARG:HD3	1.74	0.70
1:A:200:THR:HG23	1:A:374:LEU:HB3	1.74	0.69
1:A:168:LYS:HE3	1:A:230:GLU:OE2	1.90	0.69
1:C:387:LEU:HB3	1:C:416:ARG:NH1	2.06	0.69
1:C:325:LEU:O	1:C:329:LEU:HD13	1.92	0.69
1:D:55:VAL:HG23	1:D:80:VAL:HG13	1.74	0.69
1:A:229:GLN:NE2	1:A:229:GLN:H	1.90	0.69
1:B:34:GLN:OE1	1:B:62:LEU:HD23	1.93	0.69
1:B:76:TYR:C	1:B:77:ARG:HD2	2.12	0.69
1:C:363:GLU:HG2	1:C:364:GLU:N	2.05	0.69
1:D:360:ILE:HG22	1:D:361:LEU:HD13	1.76	0.68
1:D:410:GLY:HA2	1:D:420:VAL:HG21	1.76	0.68
1:D:84:ARG:NH2	1:D:263:ARG:HH21	1.89	0.68
1:B:55:VAL:HG23	1:B:80:VAL:HG13	1.75	0.68
1:B:68:LEU:N	1:B:69:PRO:HD2	2.09	0.68
1:C:91:GLU:O	1:C:95:GLU:HG2	1.92	0.68
1:C:235:LEU:O	1:C:239:GLY:N	2.26	0.68
1:C:402:GLU:HB2	1:C:405:LYS:HG2	1.75	0.68
1:A:166:ARG:HG2	1:A:385:GLU:OE2	1.94	0.68
1:B:192:ARG:HG2	1:B:192:ARG:HH11	1.57	0.68
1:B:229:GLN:CD	1:B:229:GLN:H	1.97	0.68
1:C:13:THR:HG21	1:C:34:GLN:H	1.57	0.68
1:D:1:MET:HE2	1:D:21:ALA:HB1	1.75	0.68
1:A:407:LEU:HG	4:A:451:FLC:OB1	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LEU:O	1:C:55:VAL:HG23	1.93	0.68
1:B:95:GLU:O	1:B:98:LEU:HB2	1.94	0.68
1:C:420:VAL:CG2	1:C:421:SER:H	2.07	0.68
1:A:134:LEU:HD23	1:A:150:ALA:HA	1.75	0.68
1:D:62:LEU:HD13	1:D:93:VAL:HG12	1.75	0.68
1:A:37:GLU:HB3	1:A:40:ARG:HD3	1.76	0.67
1:D:321:ILE:HG13	1:D:325:LEU:HD13	1.75	0.67
1:D:37:GLU:CG	1:D:40:ARG:HH11	2.05	0.67
1:C:49:PRO:HB3	1:C:71:LEU:HD12	1.77	0.67
1:D:14:GLY:HA2	1:D:31:GLY:O	1.95	0.66
1:A:220:ILE:HB	1:A:310:LEU:CD2	2.24	0.66
1:A:45:PHE:HB3	1:A:47:PHE:CE1	2.31	0.66
1:D:199:GLU:HA	1:D:202:ARG:HE	1.60	0.66
1:A:128:ARG:O	1:A:129:LEU:HD23	1.95	0.66
1:D:139:ALA:O	1:D:174:PRO:HG3	1.95	0.66
1:D:206:GLU:O	1:D:210:LYS:HD3	1.94	0.66
1:B:163:LEU:HD21	1:B:389:TRP:CD2	2.31	0.66
1:C:87:VAL:HG13	1:C:118:LEU:CD1	2.25	0.66
1:C:182:LEU:HD23	1:C:431:VAL:HG22	1.76	0.66
1:C:208:LEU:HD13	1:C:242:LEU:HD13	1.76	0.66
1:D:166:ARG:O	1:D:166:ARG:HG3	1.95	0.66
1:D:331:ASP:HB2	1:D:334:ASN:ND2	2.11	0.66
1:D:359:ARG:HH12	1:D:362:GLY:CA	2.09	0.66
1:B:313:SER:HB3	2:F:3:U:C6	2.30	0.65
1:D:177:PRO:HD3	1:D:389:TRP:NE1	2.10	0.65
1:D:229:GLN:H	1:D:229:GLN:NE2	1.93	0.65
1:C:233:TYR:CE1	1:C:282:PRO:HB2	2.32	0.65
1:D:383:GLN:O	1:D:387:LEU:HG	1.96	0.65
1:A:217:LYS:HE2	1:A:307:MET:HE2	1.78	0.65
1:D:336:LEU:HD13	1:D:371:VAL:HG22	1.79	0.65
1:A:96:ASP:O	1:A:100:VAL:HG23	1.97	0.65
1:B:48:ASP:OD2	1:B:51:GLU:HG2	1.97	0.65
1:D:90:MET:HE3	1:D:118:LEU:HD13	1.78	0.64
1:B:225:VAL:O	1:B:229:GLN:NE2	2.30	0.64
1:D:2:ARG:NH1	3:D:437:SO4:S	2.70	0.64
1:C:87:VAL:HG13	1:C:118:LEU:HD13	1.78	0.64
1:B:7:GLY:HA3	1:B:14:GLY:O	1.97	0.64
1:D:224:ALA:HB3	1:D:253:MET:CE	2.27	0.64
1:D:224:ALA:HB3	1:D:253:MET:HE2	1.80	0.64
1:D:212:LEU:HD22	1:D:306:PRO:HB2	1.80	0.64
1:D:37:GLU:HG3	1:D:40:ARG:NH1	2.07	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:ARG:HH21	1:D:106:PHE:HA	1.61	0.64
1:D:9:ALA:O	1:D:11:GLU:HG2	1.98	0.64
1:C:280:LYS:O	1:C:282:PRO:HD3	1.98	0.63
1:B:330:SER:O	1:B:368:ARG:HB2	1.98	0.63
1:C:211:THR:HG21	1:C:335:ALA:CB	2.28	0.63
2:H:3:U:H2'	2:H:4:U:C5'	2.27	0.63
1:C:3:ILE:HD12	1:C:18:LEU:O	1.99	0.63
1:A:1:MET:HG2	1:A:431:VAL:HG21	1.79	0.63
1:B:12:VAL:HG12	1:B:401:GLY:CA	2.28	0.63
1:C:416:ARG:HD2	1:C:418:GLN:OE1	1.98	0.63
1:C:207:ILE:O	1:C:207:ILE:HG22	1.99	0.63
1:C:316:LEU:HD11	1:C:338:PHE:CE1	2.34	0.63
1:D:87:VAL:HG13	1:D:118:LEU:HD13	1.80	0.63
1:C:232:LEU:O	1:C:283:PHE:HA	1.99	0.63
1:C:224:ALA:HA	1:C:254:ALA:HB2	1.80	0.63
1:D:396:VAL:HG12	1:D:398:LEU:HD12	1.81	0.63
1:D:236:TYR:CA	1:D:285:PRO:HB3	2.27	0.62
1:D:10:ARG:HG3	1:D:10:ARG:HH11	1.64	0.62
1:D:420:VAL:HG22	1:D:421:SER:N	2.13	0.62
1:C:351:ILE:HG22	1:C:371:VAL:HG21	1.81	0.62
1:C:359:ARG:NH1	1:C:362:GLY:HA2	2.07	0.62
1:D:10:ARG:NH1	1:D:422:LEU:HB3	2.15	0.62
1:D:57:LEU:CD2	1:D:80:VAL:HG12	2.29	0.62
1:C:236:TYR:N	1:C:285:PRO:HB3	2.14	0.62
1:A:85:ALA:HB2	1:A:267:TYR:CE2	2.34	0.62
1:A:358:VAL:HG12	1:A:359:ARG:N	2.15	0.62
1:B:3:ILE:HD11	1:B:17:HIS:HB3	1.82	0.62
1:D:177:PRO:HD3	1:D:389:TRP:CE2	2.33	0.62
1:C:384:ASP:HA	1:C:387:LEU:HD12	1.82	0.62
1:B:37:GLU:CG	1:B:40:ARG:HE	2.13	0.61
1:B:347:LEU:HD11	1:B:358:VAL:HG11	1.82	0.61
1:C:92:ILE:HD11	1:C:260:LEU:HD22	1.82	0.61
1:A:59:HIS:CD2	1:A:61:HIS:HB2	2.36	0.61
1:B:72:PHE:HE2	1:B:117:HIS:ND1	1.99	0.61
1:B:111:VAL:O	1:B:115:LEU:HG	2.01	0.61
1:D:18:LEU:HD11	1:D:25:ARG:HB3	1.83	0.61
1:D:236:TYR:HA	1:D:285:PRO:HB3	1.83	0.61
1:B:401:GLY:HA3	1:B:406:LEU:CD1	2.30	0.61
1:C:233:TYR:HE1	1:C:282:PRO:HB2	1.63	0.61
1:B:7:GLY:O	1:B:9:ALA:N	2.34	0.61
1:D:2:ARG:NH1	3:D:437:SO4:O4	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:GLY:HA2	2:H:3:U:H1'	1.81	0.61
1:A:33:PHE:H	1:A:41:ASN:HD21	1.47	0.60
1:B:204:PHE:HB2	1:B:374:LEU:HD13	1.83	0.60
1:D:325:LEU:O	1:D:329:LEU:HD13	2.01	0.60
1:B:31:GLY:HA3	1:B:63:ASP:C	2.21	0.60
1:C:32:MET:HA	1:C:67:ARG:HG3	1.83	0.60
1:D:1:MET:HG3	1:D:21:ALA:CB	2.25	0.60
1:B:208:LEU:CD2	1:B:218:VAL:HG11	2.32	0.60
1:C:12:VAL:HG12	1:C:400:HIS:C	2.22	0.60
1:A:325:LEU:O	1:A:329:LEU:HB2	2.01	0.60
1:B:299:ALA:O	1:B:302:ARG:HD2	2.01	0.60
1:D:232:LEU:HD22	1:D:288:LEU:HD13	1.83	0.60
1:D:382:GLY:O	1:D:386:LEU:HD13	2.02	0.60
2:H:3:U:H2'	2:H:4:U:H5"	1.83	0.60
1:C:83:THR:O	1:C:87:VAL:HG23	2.01	0.60
1:A:24:ARG:HA	1:A:53:ASP:OD2	2.02	0.60
1:C:278:GLN:O	1:C:280:LYS:HG3	2.02	0.60
1:D:100:VAL:HG13	2:H:3:U:C4	2.37	0.60
1:D:399:VAL:HG12	1:D:400:HIS:N	2.15	0.60
2:G:1:U:O2'	2:G:2:U:H5"	2.01	0.60
1:A:221:PRO:HB3	1:A:321:ILE:HG12	1.82	0.60
1:B:192:ARG:HG2	1:B:192:ARG:NH1	2.16	0.60
1:D:325:LEU:O	1:D:329:LEU:HB2	2.02	0.60
1:A:411:LYS:HA	4:A:451:FLC:HA2	1.81	0.59
1:A:20:LEU:HD22	1:A:25:ARG:NH1	2.15	0.59
1:A:200:THR:CG2	1:A:374:LEU:HB3	2.31	0.59
1:B:91:GLU:O	1:B:95:GLU:HG2	2.01	0.59
1:B:353:ALA:O	1:B:354:ARG:CB	2.51	0.59
1:D:250:ASP:HB3	1:D:311:ALA:HB2	1.84	0.59
2:G:2:U:H2'	2:G:2:U:O2	2.01	0.59
1:D:322:LEU:HD13	1:D:361:LEU:HD11	1.84	0.59
1:D:399:VAL:HG22	1:D:423:ALA:CB	2.33	0.59
1:C:14:GLY:HA2	1:C:31:GLY:C	2.23	0.59
1:A:198:ARG:NH2	1:A:198:ARG:HG3	2.16	0.59
1:C:336:LEU:CB	1:C:371:VAL:HG22	2.32	0.59
1:D:299:ALA:HA	1:D:302:ARG:CD	2.32	0.59
1:A:68:LEU:N	1:A:69:PRO:HD2	2.18	0.58
1:B:381:ALA:HB3	1:B:386:LEU:HD13	1.85	0.58
1:C:217:LYS:HG2	1:C:307:MET:HG2	1.85	0.58
1:A:157:LEU:HG	1:A:158:VAL:N	2.15	0.58
1:B:200:THR:OG1	1:B:376:GLY:HA3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:PRO:HD2	2:F:4:U:OP1	2.03	0.58
1:C:90:MET:SD	1:C:118:LEU:HD11	2.42	0.58
1:C:252:PRO:HD2	3:C:436:SO4:S	2.43	0.58
1:D:163:LEU:N	1:D:163:LEU:HD12	2.18	0.58
1:C:413:LEU:HD22	1:C:418:GLN:NE2	2.19	0.58
1:D:61:HIS:HA	2:H:2:U:OP2	2.03	0.58
2:H:1:U:O2'	2:H:2:U:H4'	2.03	0.58
1:C:33:PHE:CD2	1:C:40:ARG:HB2	2.38	0.58
1:D:13:THR:HG21	1:D:34:GLN:HB2	1.84	0.58
1:D:208:LEU:HD23	1:D:218:VAL:HG11	1.85	0.58
1:D:332:PRO:HA	1:D:368:ARG:O	2.03	0.58
1:A:3:ILE:O	1:A:428:GLY:HA2	2.03	0.58
1:A:186:GLU:HA	1:A:399:VAL:O	2.03	0.58
1:B:33:PHE:HB3	1:B:37:GLU:HB2	1.85	0.58
1:C:232:LEU:HD13	1:C:288:LEU:HD22	1.86	0.58
1:D:239:GLY:HA2	1:D:242:LEU:HD12	1.86	0.58
1:D:297:SER:HB2	1:D:320:ARG:HH11	1.69	0.58
1:D:350:GLU:HG3	1:D:351:ILE:N	2.19	0.58
1:A:217:LYS:HE2	1:A:307:MET:CE	2.34	0.58
1:A:404:GLU:H	1:A:404:GLU:CD	2.06	0.58
1:D:229:GLN:H	1:D:229:GLN:CD	2.08	0.58
1:C:61:HIS:CD2	1:C:142:LEU:HD11	2.38	0.57
1:C:182:LEU:HD12	1:C:183:VAL:N	2.19	0.57
1:C:299:ALA:O	1:C:303:ALA:HB2	2.04	0.57
1:B:185:ALA:O	1:B:399:VAL:HG22	2.03	0.57
1:D:13:THR:HB	1:D:33:PHE:HA	1.86	0.57
1:D:225:VAL:O	1:D:229:GLN:NE2	2.37	0.57
1:A:266:ARG:NH2	1:D:273:GLN:HE22	2.03	0.57
1:B:220:ILE:HB	1:B:310:LEU:HD23	1.86	0.57
1:C:277:LEU:HB3	1:C:278:GLN:NE2	2.19	0.57
1:A:85:ALA:HB2	1:A:267:TYR:CD2	2.39	0.57
1:B:86:THR:HG22	1:B:90:MET:CE	2.35	0.57
1:B:178:PRO:HB3	1:C:126:TRP:CE3	2.40	0.57
1:C:208:LEU:HD13	1:C:242:LEU:CD1	2.33	0.57
1:D:32:MET:HE1	1:D:105:PHE:CZ	2.39	0.57
1:B:168:LYS:HG2	1:B:197:TYR:CD2	2.39	0.57
1:B:221:PRO:HA	1:B:311:ALA:O	2.04	0.57
1:C:336:LEU:O	1:C:371:VAL:HA	2.04	0.57
1:C:388:ASP:O	1:C:391:GLN:HB2	2.04	0.57
1:D:68:LEU:N	1:D:69:PRO:HD2	2.19	0.57
1:D:269:SER:OG	1:D:272:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:VAL:HG13	1:C:80:VAL:HG13	1.87	0.57
1:D:83:THR:O	1:D:87:VAL:HG23	2.04	0.57
1:D:321:ILE:O	1:D:325:LEU:HB2	2.04	0.57
1:A:170:VAL:HG21	1:A:230:GLU:HG3	1.86	0.57
1:D:186:GLU:HA	1:D:399:VAL:O	2.04	0.57
2:F:1:U:H2'	2:F:2:U:O5'	2.04	0.57
1:A:32:MET:HE3	1:A:66:GLY:HA3	1.87	0.57
1:C:34:GLN:NE2	1:C:62:LEU:HD23	2.18	0.57
1:A:360:ILE:HG22	1:A:361:LEU:HD13	1.87	0.57
1:B:10:ARG:HD3	1:B:403:GLU:OE2	2.04	0.57
1:B:252:PRO:HD2	2:F:4:U:P	2.45	0.57
1:C:170:VAL:HG12	1:C:171:LEU:HD12	1.87	0.57
1:C:204:PHE:CE1	1:C:208:LEU:HD11	2.39	0.57
1:D:31:GLY:O	1:D:67:ARG:HD3	2.04	0.57
1:D:235:LEU:HD13	1:D:247:ILE:HD13	1.87	0.57
1:A:65:VAL:HG12	1:A:94:LEU:HD11	1.87	0.56
1:B:172:PRO:HA	3:B:440:SO4:O1	2.05	0.56
1:B:220:ILE:HG22	1:B:222:THR:HG23	1.88	0.56
1:C:228:ALA:HB3	1:C:229:GLN:HE21	1.69	0.56
1:D:399:VAL:HG22	1:D:423:ALA:HB2	1.87	0.56
1:B:349:ALA:CA	1:B:352:ILE:HD12	2.35	0.56
1:C:236:TYR:OH	1:C:280:LYS:HE2	2.05	0.56
1:C:250:ASP:OD1	1:C:320:ARG:HD2	2.05	0.56
1:C:312:GLY:HA2	1:C:313:SER:O	2.05	0.56
1:D:251:SER:HB3	1:D:254:ALA:HB3	1.86	0.56
1:B:65:VAL:HG11	1:B:90:MET:SD	2.45	0.56
1:C:59:HIS:HB3	1:C:145:SER:HA	1.87	0.56
1:D:204:PHE:CE1	1:D:208:LEU:HD11	2.41	0.56
1:C:10:ARG:HH21	1:C:424:ARG:HG2	1.70	0.56
1:C:224:ALA:HB3	1:C:253:MET:CE	2.36	0.56
1:D:224:ALA:O	1:D:257:VAL:HG21	2.05	0.56
1:D:337:VAL:CG1	1:D:374:LEU:HD12	2.36	0.56
1:B:32:MET:SD	1:B:62:LEU:HD21	2.46	0.56
1:B:142:LEU:CD2	1:B:226:GLU:HB2	2.35	0.56
1:C:142:LEU:CD2	1:C:226:GLU:HB2	2.36	0.56
1:D:315:MET:HA	1:D:342:GLN:HE22	1.69	0.56
1:B:315:MET:O	1:B:317:ALA:N	2.39	0.56
1:C:250:ASP:OD2	1:C:291:VAL:HG11	2.06	0.56
1:A:360:ILE:CG2	1:A:361:LEU:HD13	2.35	0.56
1:A:235:LEU:CD1	1:A:247:ILE:HD13	2.35	0.55
1:C:121:LEU:HD23	1:C:136:PHE:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:THR:HG22	1:C:298:LYS:HG2	1.87	0.55
1:D:123:TYR:HE1	1:D:146:ALA:HB2	1.70	0.55
1:C:336:LEU:HD13	1:C:351:ILE:HG21	1.89	0.55
1:D:224:ALA:HB1	1:D:254:ALA:CA	2.36	0.55
1:D:353:ALA:O	1:D:354:ARG:HB2	2.05	0.55
1:B:128:ARG:HD3	1:C:177:PRO:O	2.06	0.55
1:D:307:MET:O	1:D:307:MET:HG3	2.04	0.55
1:B:90:MET:O	1:B:94:LEU:HB2	2.07	0.55
1:C:65:VAL:HG12	1:C:94:LEU:HD11	1.89	0.55
1:C:316:LEU:HD11	1:C:338:PHE:CZ	2.42	0.55
1:C:171:LEU:HB3	1:C:172:PRO:HD2	1.87	0.55
1:B:88:LEU:HD13	1:B:260:LEU:HD11	1.87	0.55
1:D:59:HIS:CD2	1:D:61:HIS:H	2.25	0.55
1:C:221:PRO:HA	1:C:311:ALA:O	2.07	0.55
1:D:224:ALA:HB1	1:D:254:ALA:HA	1.87	0.55
1:C:277:LEU:HB3	1:C:278:GLN:HE21	1.71	0.55
1:B:330:SER:O	1:B:368:ARG:HD2	2.07	0.55
1:A:163:LEU:HD21	1:A:389:TRP:CD2	2.41	0.55
1:A:165:ASN:HD21	1:A:167:GLU:HB2	1.71	0.55
1:C:214:GLN:HE21	1:C:333:ARG:HB3	1.70	0.55
1:C:350:GLU:CD	1:C:358:VAL:HG13	2.27	0.55
1:C:404:GLU:CD	1:C:404:GLU:H	2.10	0.55
1:B:251:SER:HB3	1:B:254:ALA:HB3	1.89	0.54
1:B:404:GLU:H	1:B:404:GLU:CD	2.11	0.54
1:C:274:ALA:O	1:C:278:GLN:HG2	2.06	0.54
1:D:31:GLY:HA3	1:D:63:ASP:C	2.27	0.54
1:D:390:LEU:HD12	1:D:390:LEU:N	2.23	0.54
1:C:12:VAL:HG12	1:C:401:GLY:N	2.22	0.54
1:D:221:PRO:HD2	1:D:337:VAL:O	2.06	0.54
1:A:128:ARG:C	1:A:129:LEU:HD23	2.28	0.54
1:A:126:TRP:HB2	1:D:176:LEU:O	2.08	0.54
1:D:65:VAL:CG1	1:D:94:LEU:HD11	2.38	0.54
1:A:182:LEU:HD11	1:A:397:VAL:HG23	1.90	0.54
1:B:401:GLY:CA	1:B:406:LEU:HD11	2.36	0.54
1:D:402:GLU:O	1:D:406:LEU:HD13	2.07	0.54
1:A:24:ARG:HE	1:A:130:GLY:HA3	1.73	0.54
1:B:8:ALA:HB1	1:B:400:HIS:HA	1.90	0.54
1:D:59:HIS:NE2	1:D:61:HIS:HB2	2.23	0.54
1:D:331:ASP:HB2	1:D:334:ASN:HD22	1.72	0.54
1:A:177:PRO:HD3	1:A:389:TRP:CE2	2.43	0.54
1:C:55:VAL:HG22	1:C:57:LEU:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:LEU:HD12	1:D:183:VAL:N	2.23	0.54
1:C:362:GLY:O	1:C:363:GLU:HB2	2.07	0.54
1:A:197:TYR:O	1:A:201:VAL:HG23	2.07	0.53
1:B:3:ILE:HG12	1:B:184:LEU:HD22	1.90	0.53
1:B:204:PHE:HB2	1:B:374:LEU:CD1	2.39	0.53
1:A:347:LEU:CD1	1:A:358:VAL:HG11	2.37	0.53
2:H:1:U:O4'	2:H:1:U:O2	2.27	0.53
1:B:12:VAL:HG12	1:B:401:GLY:HA2	1.88	0.53
1:B:422:LEU:HD12	1:B:422:LEU:N	2.23	0.53
1:C:224:ALA:O	1:C:257:VAL:HG21	2.08	0.53
1:C:102:ASP:O	1:C:104:PRO:HD3	2.08	0.53
1:C:232:LEU:HD22	1:C:285:PRO:HD2	1.89	0.53
1:D:332:PRO:HB3	1:D:368:ARG:HB3	1.90	0.53
1:B:55:VAL:CG2	1:B:80:VAL:HG13	2.39	0.53
1:C:202:ARG:HG3	1:C:203:GLU:N	2.23	0.53
1:C:231:ILE:C	1:C:233:TYR:H	2.12	0.53
1:C:351:ILE:CG2	1:C:371:VAL:HG21	2.39	0.53
1:D:338:PHE:O	1:D:374:LEU:HB2	2.09	0.53
1:D:411:LYS:O	1:D:415:LEU:HB2	2.07	0.53
1:B:402:GLU:O	1:B:405:LYS:N	2.40	0.53
1:C:360:ILE:CG2	1:C:361:LEU:HD13	2.39	0.53
1:C:420:VAL:CG2	1:C:421:SER:N	2.64	0.53
1:D:291:VAL:CG1	1:D:296:ALA:HB3	2.39	0.53
1:B:32:MET:HE3	1:B:62:LEU:HD11	1.90	0.53
1:B:37:GLU:HG3	1:B:40:ARG:NE	2.23	0.53
1:A:397:VAL:HG12	1:A:423:ALA:HB2	1.90	0.53
1:C:398:LEU:H	1:C:398:LEU:CD1	2.21	0.53
1:C:406:LEU:HB3	1:C:422:LEU:CD2	2.38	0.53
1:A:357:ALA:HB2	1:A:366:PRO:HA	1.91	0.53
1:B:54:ALA:HA	1:B:76:TYR:OH	2.08	0.53
1:C:398:LEU:H	1:C:398:LEU:HD13	1.74	0.53
1:C:406:LEU:HD23	1:C:422:LEU:HD23	1.90	0.53
1:D:231:ILE:HG21	1:D:310:LEU:HD21	1.91	0.53
1:A:32:MET:HA	1:A:67:ARG:HG3	1.91	0.52
1:C:250:ASP:HB3	1:C:311:ALA:CB	2.31	0.52
1:C:409:LEU:HD23	1:C:413:LEU:HG	1.90	0.52
1:D:13:THR:HG21	1:D:34:GLN:H	1.74	0.52
1:D:168:LYS:HA	1:D:197:TYR:CD1	2.44	0.52
1:C:224:ALA:HB3	1:C:253:MET:HE3	1.91	0.52
1:C:235:LEU:HD12	1:C:285:PRO:HG3	1.91	0.52
1:C:238:HIS:O	1:C:241:ARG:HG2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LEU:HD22	1:D:57:LEU:N	2.25	0.52
1:D:85:ALA:HB2	1:D:267:TYR:CD2	2.44	0.52
1:A:216:GLY:O	1:A:306:PRO:HA	2.08	0.52
1:D:32:MET:HA	1:D:67:ARG:HD2	1.91	0.52
1:D:299:ALA:O	1:D:302:ARG:HG2	2.08	0.52
1:A:2:ARG:NH1	3:A:446:SO4:O3	2.43	0.52
1:A:14:GLY:HA3	1:A:33:PHE:CE1	2.44	0.52
1:A:102:ASP:CG	1:A:103:GLU:H	2.13	0.52
1:D:367:LEU:HG	1:D:367:LEU:O	2.10	0.52
1:B:37:GLU:CG	1:B:40:ARG:NE	2.73	0.52
1:C:266:ARG:HA	1:C:273:GLN:NE2	2.24	0.52
2:F:1:U:C2'	2:F:2:U:O5'	2.57	0.52
1:A:355:PRO:HB2	1:A:356:PRO:HD2	1.91	0.52
1:A:411:LYS:CD	4:A:451:FLC:HG2	2.38	0.52
1:C:182:LEU:HD12	1:C:183:VAL:H	1.75	0.52
1:D:228:ALA:HB3	1:D:229:GLN:NE2	2.25	0.52
1:D:291:VAL:HG13	1:D:296:ALA:HB3	1.92	0.52
1:B:325:LEU:O	1:B:329:LEU:HD22	2.10	0.52
1:D:90:MET:HE3	1:D:118:LEU:CD1	2.39	0.52
1:A:115:LEU:HD23	1:A:118:LEU:HD11	1.92	0.52
1:B:37:GLU:O	1:B:39:ALA:N	2.42	0.52
1:D:227:ARG:NH1	1:D:379:GLY:H	2.08	0.52
1:B:27:LEU:CB	1:B:55:VAL:HG12	2.39	0.52
1:D:214:GLN:HE21	1:D:333:ARG:HG2	1.73	0.52
1:B:325:LEU:HG	1:B:329:LEU:HD21	1.92	0.52
1:C:12:VAL:CG1	1:C:401:GLY:HA2	2.40	0.52
1:A:393:GLU:HA	1:A:393:GLU:OE2	2.11	0.51
1:B:271:GLU:O	1:B:275:HIS:HD2	1.94	0.51
1:D:41:ASN:HB3	1:D:105:PHE:CE2	2.44	0.51
1:C:166:ARG:HD3	1:C:166:ARG:O	2.10	0.51
1:C:326:LYS:HA	1:C:365:VAL:HG11	1.92	0.51
1:B:198:ARG:HH21	1:B:198:ARG:HB2	1.75	0.51
1:B:360:ILE:CG2	1:B:361:LEU:HD13	2.34	0.51
1:C:233:TYR:C	1:C:235:LEU:H	2.12	0.51
1:C:409:LEU:HD23	1:C:409:LEU:O	2.10	0.51
2:E:4:U:O4'	2:E:4:U:O2	2.29	0.51
1:A:322:LEU:HB3	1:A:361:LEU:HD11	1.92	0.51
1:D:160:SER:HB2	1:D:163:LEU:HD11	1.91	0.51
1:D:170:VAL:HA	1:D:272:VAL:CG2	2.40	0.51
1:A:165:ASN:C	1:A:165:ASN:HD22	2.14	0.51
1:A:170:VAL:CG2	1:A:230:GLU:HG3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:GLU:O	1:C:125:GLU:HG3	2.10	0.51
1:C:288:LEU:HD12	1:C:289:GLU:H	1.76	0.51
1:A:54:ALA:HA	1:A:76:TYR:OH	2.10	0.51
1:A:289:GLU:OE2	1:B:291:VAL:HA	2.10	0.51
1:D:3:ILE:HD11	1:D:17:HIS:CB	2.41	0.51
1:D:85:ALA:HB2	1:D:267:TYR:CE2	2.46	0.51
1:D:87:VAL:HG13	1:D:118:LEU:CD1	2.41	0.51
1:B:353:ALA:O	1:B:354:ARG:HB3	2.11	0.51
1:C:288:LEU:HD12	1:C:289:GLU:N	2.26	0.51
1:A:397:VAL:CG1	1:A:423:ALA:HB2	2.41	0.51
1:C:2:ARG:HH22	1:C:430:PRO:HB3	1.76	0.51
1:D:216:GLY:O	1:D:306:PRO:HA	2.11	0.51
1:D:222:THR:CG2	1:D:339:VAL:HG21	2.40	0.51
1:A:84:ARG:HG2	1:A:84:ARG:NH1	2.20	0.51
1:B:128:ARG:O	1:B:129:LEU:HD23	2.10	0.51
1:B:398:LEU:CD1	1:B:398:LEU:N	2.74	0.51
1:D:386:LEU:HD23	1:D:409:LEU:HD11	1.92	0.51
1:A:421:SER:OG	1:A:422:LEU:N	2.45	0.50
1:B:57:LEU:HG	1:B:65:VAL:HG22	1.92	0.50
1:B:88:LEU:HD12	1:B:264:LEU:CD1	2.38	0.50
1:C:236:TYR:CE2	1:C:282:PRO:HA	2.46	0.50
1:D:295:GLU:OE2	1:D:295:GLU:N	2.25	0.50
1:A:198:ARG:HG3	1:A:198:ARG:HH21	1.76	0.50
1:B:86:THR:O	1:B:90:MET:HB2	2.10	0.50
1:C:85:ALA:HB2	1:C:267:TYR:CD2	2.46	0.50
1:C:134:LEU:HD23	1:C:150:ALA:HB2	1.93	0.50
1:D:132:LEU:HD22	1:D:134:LEU:HG	1.92	0.50
1:A:87:VAL:HA	1:A:90:MET:CE	2.42	0.50
1:C:28:LEU:O	1:C:29:ASP:HB2	2.11	0.50
1:D:397:VAL:HG21	1:D:429:VAL:HG11	1.92	0.50
1:C:52:VAL:HG12	1:C:76:TYR:CE2	2.47	0.50
1:C:354:ARG:HA	1:C:367:LEU:HD23	1.93	0.50
1:D:227:ARG:NH1	1:D:379:GLY:N	2.60	0.50
1:B:142:LEU:H	1:B:145:SER:HB3	1.76	0.50
1:C:184:LEU:HD11	1:C:399:VAL:HG11	1.94	0.50
1:C:190:GLY:HA3	1:C:409:LEU:HB2	1.93	0.50
1:C:424:ARG:HB3	1:C:424:ARG:NH1	2.25	0.50
1:D:233:TYR:O	1:D:237:THR:HG23	2.12	0.50
1:B:170:VAL:HG12	1:B:171:LEU:HD13	1.94	0.50
1:C:165:ASN:ND2	1:C:385:GLU:OE1	2.45	0.50
1:A:365:VAL:O	1:A:365:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:PRO:HG3	1:D:74:GLU:HG2	1.94	0.50
1:A:85:ALA:HB3	1:A:144:GLY:HA3	1.94	0.50
1:A:87:VAL:HA	1:A:90:MET:HE2	1.94	0.50
1:B:1:MET:HG3	1:B:21:ALA:HB2	1.94	0.50
1:C:101:MET:SD	1:C:104:PRO:HA	2.52	0.50
1:C:250:ASP:O	1:C:251:SER:HB2	2.11	0.50
1:A:295:GLU:OE1	1:B:244:ARG:HB2	2.11	0.50
1:C:225:VAL:HG12	1:C:226:GLU:N	2.26	0.50
1:C:302:ARG:HH21	1:C:302:ARG:HG3	1.77	0.50
1:D:84:ARG:NH2	1:D:263:ARG:NH2	2.57	0.50
1:A:32:MET:HE3	1:A:66:GLY:CA	2.42	0.49
1:A:404:GLU:OE2	1:A:404:GLU:N	2.25	0.49
1:B:10:ARG:HG3	1:B:10:ARG:HH11	1.77	0.49
1:B:147:PHE:HB3	1:B:160:SER:O	2.12	0.49
1:C:236:TYR:CD2	1:C:282:PRO:HA	2.45	0.49
1:D:312:GLY:HA2	1:D:313:SER:O	2.12	0.49
1:D:358:VAL:O	1:D:365:VAL:N	2.44	0.49
1:A:20:LEU:HD22	1:A:25:ARG:HG2	1.94	0.49
1:B:347:LEU:HD11	1:B:358:VAL:CG1	2.42	0.49
1:C:322:LEU:HD22	1:C:347:LEU:HD23	1.93	0.49
1:B:41:ASN:HB3	1:B:105:PHE:CE2	2.47	0.49
1:B:398:LEU:HD23	1:B:406:LEU:O	2.12	0.49
1:C:170:VAL:HG21	1:C:230:GLU:HG3	1.94	0.49
1:C:210:LYS:O	1:C:210:LYS:HD3	2.12	0.49
1:C:406:LEU:O	1:C:408:ALA:N	2.45	0.49
1:A:129:LEU:O	1:A:132:LEU:HB3	2.13	0.49
1:A:217:LYS:HG2	1:A:307:MET:HG2	1.95	0.49
1:A:362:GLY:O	1:A:363:GLU:HB2	2.11	0.49
1:B:40:ARG:C	1:B:42:HIS:H	2.16	0.49
1:C:155:ARG:HD2	1:C:431:VAL:O	2.12	0.49
1:A:76:TYR:O	1:A:77:ARG:CD	2.57	0.49
1:B:7:GLY:O	1:B:8:ALA:C	2.50	0.49
1:C:203:GLU:O	1:C:207:ILE:HG13	2.12	0.49
1:C:284:ARG:HA	1:C:288:LEU:CD2	2.43	0.49
1:C:386:LEU:O	1:C:390:LEU:HD13	2.12	0.49
1:A:1:MET:SD	1:A:431:VAL:HG11	2.51	0.49
1:C:387:LEU:CB	1:C:416:ARG:HH12	2.23	0.49
1:A:220:ILE:HD12	1:A:310:LEU:HD21	1.94	0.49
1:B:37:GLU:N	1:B:37:GLU:OE2	2.45	0.49
1:B:80:VAL:HB	1:B:118:LEU:HD23	1.95	0.49
1:C:236:TYR:OH	1:C:280:LYS:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:VAL:HG11	1:D:94:LEU:HD11	1.94	0.49
1:D:225:VAL:HG12	1:D:226:GLU:N	2.27	0.49
1:D:358:VAL:O	1:D:365:VAL:HG22	2.11	0.49
1:A:396:VAL:HG12	1:A:398:LEU:HD13	1.94	0.49
1:C:248:TYR:CD2	1:C:300:LEU:HD21	2.48	0.49
1:D:55:VAL:HG22	1:D:80:VAL:HA	1.95	0.49
1:D:61:HIS:O	1:D:65:VAL:HG23	2.13	0.49
1:A:321:ILE:O	1:A:325:LEU:HD13	2.13	0.49
1:C:202:ARG:O	1:C:206:GLU:HG3	2.13	0.49
1:D:269:SER:HB2	3:D:436:SO4:O3	2.13	0.49
1:C:9:ALA:O	1:C:11:GLU:HG2	2.12	0.49
1:C:206:GLU:C	1:C:208:LEU:H	2.17	0.49
1:D:32:MET:HE1	1:D:105:PHE:HZ	1.77	0.49
1:D:219:LEU:HD23	1:D:325:LEU:CD1	2.42	0.49
1:A:250:ASP:OD2	1:A:297:SER:OG	2.30	0.48
1:B:409:LEU:HD22	1:B:413:LEU:HG	1.95	0.48
1:C:265:VAL:HG13	1:C:266:ARG:H	1.78	0.48
1:A:82:ALA:HB1	1:A:86:THR:HB	1.95	0.48
1:A:83:THR:O	1:A:87:VAL:HG23	2.12	0.48
1:A:318:GLY:HA2	1:A:322:LEU:HD12	1.95	0.48
1:B:235:LEU:HD13	1:B:247:ILE:HD13	1.95	0.48
1:B:299:ALA:HA	1:B:302:ARG:HH21	1.78	0.48
1:C:409:LEU:HA	1:C:412:LEU:HD12	1.95	0.48
1:C:424:ARG:HB3	1:C:424:ARG:HH11	1.78	0.48
1:A:167:GLU:HB3	1:A:197:TYR:HB2	1.95	0.48
1:A:214:GLN:NE2	1:A:333:ARG:HA	2.28	0.48
1:A:391:GLN:HA	1:A:416:ARG:NH2	2.29	0.48
1:B:48:ASP:OD2	1:B:50:LYS:HB2	2.13	0.48
1:C:224:ALA:HB1	1:C:254:ALA:N	2.28	0.48
1:A:252:PRO:HD2	2:E:4:U:OP1	2.13	0.48
1:C:141:HIS:HB3	1:C:145:SER:HB2	1.94	0.48
1:C:165:ASN:C	1:C:167:GLU:H	2.17	0.48
1:C:331:ASP:O	1:C:334:ASN:OD1	2.31	0.48
1:D:214:GLN:NE2	1:D:333:ARG:HG2	2.28	0.48
1:D:402:GLU:HB2	1:D:405:LYS:CG	2.43	0.48
1:B:239:GLY:C	1:B:241:ARG:N	2.67	0.48
1:C:25:ARG:NH1	1:C:51:GLU:HB3	2.28	0.48
1:C:80:VAL:HB	1:C:118:LEU:HD23	1.96	0.48
1:C:184:LEU:HD12	1:C:397:VAL:O	2.14	0.48
1:D:28:LEU:O	1:D:29:ASP:HB2	2.13	0.48
1:A:43:ALA:HB1	1:A:44:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HD13	1:A:93:VAL:HG12	1.95	0.48
1:D:219:LEU:HD23	1:D:325:LEU:HD12	1.95	0.48
1:A:318:GLY:HA2	1:A:322:LEU:CD1	2.43	0.48
1:B:37:GLU:HG2	1:B:40:ARG:NH1	2.21	0.48
1:C:398:LEU:CD1	1:C:398:LEU:N	2.76	0.48
1:D:102:ASP:CG	1:D:103:GLU:N	2.64	0.48
1:A:177:PRO:HD3	1:A:389:TRP:NE1	2.28	0.48
1:A:229:GLN:HG3	1:A:261:TYR:CE1	2.49	0.48
1:C:28:LEU:N	1:C:28:LEU:HD12	2.29	0.48
1:C:65:VAL:CG1	1:C:94:LEU:HD11	2.44	0.48
1:D:61:HIS:CD2	2:H:2:U:OP2	2.67	0.48
1:D:165:ASN:C	1:D:167:GLU:H	2.17	0.48
1:D:319:GLY:CA	2:H:3:U:H1'	2.44	0.48
1:A:62:LEU:N	2:E:2:U:OP2	2.32	0.48
1:A:102:ASP:CG	1:A:103:GLU:N	2.67	0.48
1:A:313:SER:HB3	2:E:3:U:C6	2.49	0.48
1:C:57:LEU:HD21	1:C:68:LEU:HD22	1.96	0.48
1:C:275:HIS:N	1:C:275:HIS:CD2	2.82	0.48
1:D:43:ALA:HB1	1:D:44:PRO:HD2	1.95	0.48
1:D:55:VAL:HG21	1:D:80:VAL:HG13	1.93	0.48
1:C:219:LEU:HD21	1:C:324:HIS:O	2.14	0.48
1:C:351:ILE:HG23	1:C:367:LEU:CD1	2.40	0.48
1:D:61:HIS:ND1	2:H:1:U:H5'	2.29	0.48
1:D:383:GLN:NE2	1:D:412:LEU:HD11	2.29	0.48
1:A:357:ALA:CB	1:A:366:PRO:HA	2.44	0.47
1:A:358:VAL:CG1	1:A:359:ARG:N	2.76	0.47
1:C:189:TYR:OH	1:C:341:TYR:HB2	2.14	0.47
1:D:168:LYS:HA	1:D:197:TYR:CE1	2.48	0.47
1:D:212:LEU:HA	1:D:306:PRO:HB3	1.95	0.47
1:A:170:VAL:HG12	1:A:171:LEU:HD13	1.95	0.47
1:C:177:PRO:HD3	1:C:389:TRP:CE2	2.49	0.47
1:C:242:LEU:HB3	1:C:243:PRO:HD2	1.96	0.47
1:D:192:ARG:HH21	1:D:405:LYS:NZ	2.12	0.47
2:F:1:U:O2'	2:F:2:U:OP1	2.32	0.47
1:A:1:MET:HA	1:A:20:LEU:O	2.14	0.47
1:A:229:GLN:H	1:A:229:GLN:HE21	1.60	0.47
1:A:265:VAL:HA	1:A:268:PHE:HD2	1.79	0.47
1:C:13:THR:HB	1:C:33:PHE:HA	1.96	0.47
1:A:225:VAL:HG12	1:A:226:GLU:N	2.29	0.47
1:B:88:LEU:HB3	1:B:260:LEU:HD21	1.96	0.47
1:B:297:SER:O	1:B:300:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:GLY:HA3	1:C:14:GLY:O	2.14	0.47
1:C:37:GLU:O	1:C:39:ALA:N	2.47	0.47
1:C:360:ILE:O	1:C:361:LEU:HB2	2.14	0.47
1:D:91:GLU:O	1:D:95:GLU:CG	2.61	0.47
1:B:33:PHE:HD2	1:B:41:ASN:ND2	2.12	0.47
1:C:225:VAL:HG21	2:G:2:U:OP1	2.14	0.47
1:C:236:TYR:CA	1:C:285:PRO:HB3	2.44	0.47
1:D:357:ALA:HB1	1:D:365:VAL:O	2.15	0.47
1:A:156:THR:N	1:A:181:ASP:OD1	2.42	0.47
1:B:229:GLN:H	1:B:229:GLN:NE2	2.12	0.47
1:B:233:TYR:CE1	1:B:282:PRO:HB2	2.49	0.47
1:C:141:HIS:HB3	1:C:145:SER:CB	2.45	0.47
2:E:2:U:H1'	2:E:3:U:C5	2.49	0.47
1:A:351:ILE:HG12	1:A:358:VAL:HG21	1.96	0.47
1:B:33:PHE:HD2	1:B:41:ASN:HD22	1.61	0.47
1:D:37:GLU:N	1:D:37:GLU:CD	2.68	0.47
1:D:166:ARG:O	1:D:166:ARG:CG	2.61	0.47
1:C:214:GLN:HE21	1:C:333:ARG:CB	2.28	0.47
1:C:322:LEU:HD22	1:C:347:LEU:CD2	2.45	0.47
1:D:315:MET:O	1:D:316:LEU:HB2	2.14	0.47
1:A:121:LEU:HD12	1:A:125:GLU:HB3	1.97	0.47
1:B:9:ALA:O	1:B:10:ARG:HB2	2.15	0.47
1:C:170:VAL:HG13	1:C:283:PHE:HZ	1.79	0.47
1:C:232:LEU:CD2	1:C:288:LEU:HD13	2.42	0.47
1:D:42:HIS:CE1	1:D:105:PHE:HB3	2.50	0.47
1:D:219:LEU:HB2	1:D:336:LEU:HA	1.97	0.47
1:A:7:GLY:HA3	1:A:14:GLY:O	2.15	0.47
1:A:143:PRO:HD3	1:A:226:GLU:HG2	1.96	0.47
1:D:153:GLU:O	1:D:155:ARG:HG2	2.15	0.47
1:D:184:LEU:HD21	1:D:399:VAL:HG21	1.97	0.47
1:A:4:VAL:HA	1:A:428:GLY:HA2	1.97	0.46
1:C:2:ARG:NH2	1:C:430:PRO:HB3	2.30	0.46
1:C:166:ARG:HH21	1:C:166:ARG:HG3	1.80	0.46
1:C:166:ARG:HG3	1:C:166:ARG:NH2	2.29	0.46
1:C:281:ASN:C	1:C:283:PHE:H	2.19	0.46
1:D:420:VAL:O	1:D:421:SER:HB3	2.15	0.46
1:A:24:ARG:HH11	1:A:130:GLY:HA2	1.79	0.46
1:A:297:SER:OG	1:A:320:ARG:HD3	2.16	0.46
1:A:321:ILE:HG13	1:A:325:LEU:HD13	1.98	0.46
1:C:227:ARG:HG2	1:C:227:ARG:HH11	1.80	0.46
1:C:401:GLY:HA3	1:C:406:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PRO:HG2	1:A:423:ALA:HB1	1.97	0.46
1:C:140:GLY:O	1:C:164:GLY:HA3	2.15	0.46
1:C:225:VAL:HG12	1:C:226:GLU:H	1.80	0.46
1:D:220:ILE:HB	1:D:310:LEU:HD23	1.97	0.46
1:C:58:THR:O	1:C:59:HIS:HB3	2.15	0.46
1:B:32:MET:HA	1:B:67:ARG:HG3	1.96	0.46
1:C:11:GLU:O	1:C:401:GLY:N	2.48	0.46
1:C:108:PRO:HD2	1:C:109:GLU:OE2	2.15	0.46
1:C:272:VAL:O	1:C:276:PHE:HD2	1.97	0.46
1:D:55:VAL:CG2	1:D:80:VAL:HA	2.46	0.46
1:D:228:ALA:O	1:D:231:ILE:HB	2.15	0.46
1:B:45:PHE:HB3	1:B:47:PHE:CE1	2.51	0.46
1:D:177:PRO:HD3	1:D:389:TRP:CD1	2.51	0.46
1:A:28:LEU:N	1:A:28:LEU:CD1	2.78	0.46
1:A:38:GLU:O	1:A:41:ASN:HB2	2.16	0.46
1:B:1:MET:HG3	1:B:21:ALA:CB	2.46	0.46
1:B:5:PRO:HG2	1:B:423:ALA:HB1	1.98	0.46
1:C:329:LEU:HB3	1:C:366:PRO:O	2.15	0.46
1:D:227:ARG:HH11	1:D:379:GLY:N	2.13	0.46
1:D:326:LYS:C	1:D:328:GLY:H	2.19	0.46
1:B:393:GLU:O	1:B:418:GLN:HG2	2.16	0.46
1:C:205:LEU:O	1:C:208:LEU:HB2	2.16	0.46
1:C:232:LEU:HD13	1:C:288:LEU:CD2	2.46	0.46
1:D:77:ARG:HG2	1:D:77:ARG:HH11	1.80	0.46
1:D:165:ASN:HB3	1:D:168:LYS:CG	2.42	0.46
1:A:266:ARG:HH21	1:D:273:GLN:HE22	1.63	0.46
1:B:85:ALA:HB3	1:B:144:GLY:HA3	1.98	0.46
1:C:350:GLU:OE1	1:C:358:VAL:HG13	2.15	0.46
1:C:384:ASP:HA	1:C:387:LEU:CD1	2.44	0.46
1:D:31:GLY:O	1:D:67:ARG:CD	2.64	0.46
1:B:425:PHE:O	1:B:427:GLU:N	2.49	0.45
1:C:221:PRO:HB3	1:C:321:ILE:CG1	2.38	0.45
1:A:10:ARG:NH1	1:A:10:ARG:CG	2.74	0.45
1:A:288:LEU:HD12	1:A:289:GLU:N	2.32	0.45
1:A:354:ARG:NH2	1:A:370:SER:HA	2.31	0.45
1:B:37:GLU:CG	1:B:40:ARG:HH11	2.24	0.45
1:B:229:GLN:HG3	1:B:261:TYR:CE1	2.51	0.45
1:C:32:MET:CE	1:C:105:PHE:HZ	2.29	0.45
1:D:3:ILE:HD11	1:D:17:HIS:HB3	1.98	0.45
1:D:33:PHE:N	1:D:41:ASN:HD21	1.95	0.45
1:D:322:LEU:O	1:D:326:LYS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLN:H	1:A:229:GLN:CD	2.14	0.45
1:A:238:HIS:O	1:A:241:ARG:HG3	2.17	0.45
1:B:117:HIS:O	1:B:119:ARG:HG3	2.17	0.45
1:C:3:ILE:HD12	1:C:18:LEU:C	2.36	0.45
1:C:199:GLU:HA	1:C:202:ARG:HG2	1.98	0.45
1:C:294:THR:HA	1:C:297:SER:HB3	1.98	0.45
1:D:236:TYR:N	1:D:285:PRO:HB3	2.31	0.45
1:B:27:LEU:HD13	1:B:29:ASP:O	2.15	0.45
1:B:47:PHE:HA	3:B:447:SO4:O1	2.16	0.45
1:C:68:LEU:HD11	1:C:72:PHE:HE1	1.82	0.45
1:D:2:ARG:HG2	1:D:20:LEU:HB2	1.99	0.45
1:D:223:PHE:C	1:D:225:VAL:H	2.20	0.45
1:D:297:SER:HB2	1:D:320:ARG:NH1	2.32	0.45
1:A:20:LEU:CD2	1:A:25:ARG:HH11	2.23	0.45
1:A:278:GLN:O	1:A:280:LYS:HG3	2.17	0.45
1:B:62:LEU:O	1:B:62:LEU:HG	2.16	0.45
1:C:88:LEU:HD12	1:C:264:LEU:HD11	1.98	0.45
1:C:354:ARG:NH1	1:C:369:ALA:O	2.42	0.45
1:D:2:ARG:CZ	3:D:437:SO4:O1	2.64	0.45
1:D:214:GLN:HE21	1:D:333:ARG:CG	2.30	0.45
1:B:31:GLY:HA3	1:B:63:ASP:O	2.16	0.45
1:B:226:GLU:C	1:B:229:GLN:HE21	2.20	0.45
1:B:397:VAL:HA	1:B:421:SER:O	2.17	0.45
1:C:7:GLY:O	1:C:9:ALA:N	2.50	0.45
1:C:12:VAL:HG23	1:C:12:VAL:O	2.17	0.45
1:C:248:TYR:CE2	1:C:300:LEU:HD21	2.51	0.45
1:C:320:ARG:O	1:C:320:ARG:HG2	2.15	0.45
1:C:359:ARG:NH1	1:C:359:ARG:HG3	2.31	0.45
1:C:407:LEU:HD12	1:C:422:LEU:CD2	2.47	0.45
1:D:37:GLU:HB2	1:D:40:ARG:NE	2.25	0.45
1:D:73:ARG:NH2	1:D:106:PHE:CA	2.77	0.45
1:B:42:HIS:ND1	1:B:105:PHE:HB3	2.32	0.45
1:B:165:ASN:HD22	1:B:165:ASN:C	2.20	0.45
1:B:384:ASP:OD2	1:B:384:ASP:N	2.49	0.45
1:C:32:MET:HE1	1:C:105:PHE:CZ	2.51	0.45
1:C:212:LEU:O	1:C:306:PRO:HG3	2.16	0.45
1:C:411:LYS:O	1:C:414:ALA:HB3	2.17	0.45
1:D:401:GLY:HA3	1:D:406:LEU:HD11	1.99	0.45
1:A:80:VAL:HB	1:A:118:LEU:HD23	1.98	0.45
1:B:32:MET:HE3	1:B:66:GLY:HA3	1.99	0.45
1:B:126:TRP:CE3	1:C:178:PRO:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:ILE:HA	1:C:308:VAL:HB	1.98	0.45
1:D:235:LEU:O	1:D:239:GLY:N	2.50	0.45
1:C:38:GLU:OE2	1:C:38:GLU:O	2.34	0.45
1:C:355:PRO:HD2	1:C:367:LEU:CD2	2.47	0.45
1:D:2:ARG:NH2	3:D:437:SO4:O2	2.49	0.45
1:D:113:GLU:OE2	1:D:117:HIS:HE1	2.00	0.45
1:D:134:LEU:HD23	1:D:150:ALA:HA	1.99	0.45
1:D:163:LEU:HD21	1:D:389:TRP:CD2	2.52	0.45
1:B:77:ARG:HH11	1:B:77:ARG:HG3	1.81	0.45
1:B:205:LEU:O	1:B:209:GLU:HG3	2.17	0.45
1:B:239:GLY:C	1:B:241:ARG:H	2.19	0.45
1:C:294:THR:O	1:C:297:SER:HB3	2.17	0.45
1:C:359:ARG:HG3	1:C:359:ARG:HH11	1.82	0.45
1:D:347:LEU:O	1:D:351:ILE:HG13	2.17	0.45
1:B:2:ARG:HG2	1:B:2:ARG:HH21	1.82	0.44
1:B:140:GLY:O	1:B:164:GLY:HA3	2.16	0.44
1:C:165:ASN:O	1:C:167:GLU:N	2.50	0.44
1:C:396:VAL:HG12	1:C:398:LEU:HD12	1.98	0.44
1:D:59:HIS:CD2	1:D:142:LEU:HD12	2.52	0.44
1:A:81:TYR:HD2	1:A:121:LEU:HB2	1.82	0.44
1:B:32:MET:HB2	1:B:41:ASN:OD1	2.17	0.44
1:B:270:GLU:O	1:B:273:GLN:N	2.48	0.44
1:C:192:ARG:NH1	1:C:405:LYS:NZ	2.61	0.44
1:C:195:ARG:HB3	1:C:375:GLY:O	2.16	0.44
1:C:232:LEU:HB3	1:C:283:PHE:O	2.17	0.44
1:B:65:VAL:HG12	1:B:65:VAL:O	2.16	0.44
1:C:331:ASP:OD2	1:C:332:PRO:HD2	2.17	0.44
1:D:192:ARG:HH21	1:D:405:LYS:HZ2	1.64	0.44
1:D:229:GLN:HB3	1:D:258:LEU:HD13	1.99	0.44
1:D:306:PRO:O	1:D:307:MET:HB3	2.17	0.44
1:D:410:GLY:CA	1:D:420:VAL:HG21	2.45	0.44
2:H:3:U:HO2'	2:H:4:U:P	2.40	0.44
1:D:13:THR:CB	1:D:34:GLN:H	2.30	0.44
1:A:171:LEU:HD21	1:A:226:GLU:HG3	1.98	0.44
1:B:130:GLY:N	3:B:441:SO4:O3	2.50	0.44
1:D:350:GLU:HG3	1:D:351:ILE:H	1.82	0.44
1:D:406:LEU:O	1:D:407:LEU:C	2.56	0.44
1:A:28:LEU:N	1:A:28:LEU:HD12	2.33	0.44
1:A:168:LYS:HA	1:A:197:TYR:CD1	2.53	0.44
1:C:49:PRO:HB3	1:C:71:LEU:CD1	2.47	0.44
1:C:233:TYR:C	1:C:235:LEU:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:LEU:N	1:C:386:LEU:HD12	2.32	0.44
1:D:195:ARG:O	1:D:196:PRO:C	2.56	0.44
1:D:204:PHE:HD2	1:D:374:LEU:CD1	2.31	0.44
1:D:384:ASP:OD2	1:D:384:ASP:N	2.50	0.44
1:A:284:ARG:NH2	4:A:450:FLC:HA1	2.33	0.44
1:B:312:GLY:CA	1:B:313:SER:C	2.85	0.44
1:C:275:HIS:CD2	1:C:275:HIS:H	2.35	0.44
1:C:386:LEU:HD12	1:C:386:LEU:H	1.83	0.44
1:C:407:LEU:HD12	1:C:422:LEU:HD21	1.99	0.44
1:D:55:VAL:C	1:D:56:LEU:HD12	2.37	0.44
1:D:97:ALA:HA	2:H:2:U:H5	1.81	0.44
1:D:197:TYR:O	1:D:201:VAL:HG23	2.16	0.44
1:D:297:SER:O	1:D:324:HIS:HE1	2.01	0.44
1:B:49:PRO:HG3	1:B:74:GLU:HB3	1.99	0.44
1:B:101:MET:HG2	1:B:104:PRO:HA	2.00	0.44
1:C:12:VAL:CG1	1:C:401:GLY:CA	2.95	0.44
1:C:232:LEU:HD13	1:C:283:PHE:O	2.17	0.44
1:C:405:LYS:O	1:C:408:ALA:HB3	2.17	0.44
1:B:37:GLU:CD	1:B:37:GLU:H	2.21	0.44
1:B:104:PRO:C	1:B:106:PHE:H	2.20	0.44
1:D:61:HIS:CG	2:H:1:U:H5'	2.53	0.44
1:A:429:VAL:HG13	1:A:430:PRO:HD2	2.00	0.43
1:B:37:GLU:CG	1:B:40:ARG:NH1	2.81	0.43
1:B:77:ARG:NH1	1:B:113:GLU:OE1	2.42	0.43
1:B:313:SER:HB3	2:F:3:U:C5	2.53	0.43
1:C:62:LEU:O	1:C:66:GLY:N	2.46	0.43
1:C:401:GLY:HA3	1:C:406:LEU:HD11	2.00	0.43
1:A:90:MET:HE1	1:A:118:LEU:HD22	2.01	0.43
1:A:35:GLY:O	1:A:38:GLU:HB2	2.17	0.43
1:A:70:LYS:O	1:A:74:GLU:HG3	2.18	0.43
1:A:236:TYR:CD2	1:A:236:TYR:C	2.91	0.43
1:A:341:TYR:CE1	1:A:343:PRO:HA	2.53	0.43
1:D:3:ILE:HG12	1:D:184:LEU:HD12	1.99	0.43
1:D:284:ARG:HA	1:D:288:LEU:CD2	2.43	0.43
1:D:298:LYS:HE2	1:D:323:HIS:ND1	2.32	0.43
1:D:350:GLU:C	1:D:352:ILE:H	2.21	0.43
1:D:358:VAL:HG12	1:D:359:ARG:N	2.33	0.43
1:D:404:GLU:H	1:D:404:GLU:CD	2.20	0.43
1:C:297:SER:OG	1:C:320:ARG:HD3	2.18	0.43
1:D:1:MET:HE2	1:D:21:ALA:CB	2.46	0.43
1:D:128:ARG:C	1:D:129:LEU:HD23	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:TYR:CE1	1:D:282:PRO:HB2	2.53	0.43
1:A:48:ASP:HA	1:A:49:PRO:HD2	1.81	0.43
1:A:126:TRP:CE3	1:A:135:ALA:HB2	2.54	0.43
1:A:128:ARG:HH21	1:D:177:PRO:HG2	1.83	0.43
1:B:60:ALA:O	1:B:61:HIS:C	2.57	0.43
1:B:422:LEU:N	1:B:422:LEU:CD1	2.82	0.43
1:C:231:ILE:HG21	1:C:310:LEU:HD11	2.01	0.43
1:C:233:TYR:OH	1:C:271:GLU:HG2	2.19	0.43
1:A:61:HIS:CG	2:E:1:U:H5'	2.53	0.43
1:A:90:MET:HE3	1:A:118:LEU:HD13	2.00	0.43
1:B:64:HIS:NE2	1:B:162:ASP:OD1	2.51	0.43
1:C:214:GLN:NE2	1:C:333:ARG:HA	2.34	0.43
1:C:251:SER:HB3	1:C:254:ALA:HB3	2.01	0.43
1:C:344:GLN:HA	1:C:349:ALA:HB2	2.01	0.43
1:C:390:LEU:HD23	1:C:396:VAL:HG21	2.01	0.43
1:D:148:VAL:HG12	1:D:149:VAL:N	2.34	0.43
1:D:223:PHE:O	1:D:225:VAL:N	2.46	0.43
1:D:362:GLY:O	1:D:363:GLU:HB2	2.18	0.43
1:B:200:THR:HG23	1:B:374:LEU:HB3	2.00	0.43
1:B:261:TYR:HD1	1:B:283:PHE:CE2	2.35	0.43
1:C:27:LEU:HD13	1:C:29:ASP:O	2.18	0.43
1:C:96:ASP:OD1	1:C:96:ASP:O	2.36	0.43
1:D:212:LEU:HD13	1:D:245:ALA:HB3	2.00	0.43
1:D:389:TRP:HB3	1:D:390:LEU:HD12	2.00	0.43
1:D:34:GLN:HA	1:D:38:GLU:HG2	1.99	0.43
1:D:62:LEU:CD1	1:D:93:VAL:HG12	2.47	0.43
1:D:269:SER:O	1:D:273:GLN:HG3	2.19	0.43
1:A:235:LEU:HD13	1:A:247:ILE:CD1	2.41	0.43
1:B:69:PRO:HB2	1:B:106:PHE:CD2	2.54	0.43
1:B:163:LEU:HD21	1:B:389:TRP:CG	2.53	0.43
1:B:398:LEU:O	1:B:399:VAL:HG13	2.18	0.43
1:C:202:ARG:CG	1:C:203:GLU:N	2.82	0.43
1:C:250:ASP:HA	1:C:291:VAL:CB	2.38	0.43
1:D:223:PHE:HA	2:H:3:U:OP1	2.19	0.43
1:D:236:TYR:OH	1:D:280:LYS:HE2	2.19	0.43
1:A:25:ARG:HH11	1:A:25:ARG:HG2	1.82	0.43
1:B:102:ASP:C	1:B:104:PRO:HD3	2.39	0.43
1:C:10:ARG:HH12	1:C:422:LEU:HD13	1.84	0.43
1:C:84:ARG:HB3	1:C:267:TYR:OH	2.19	0.43
1:D:197:TYR:O	1:D:198:ARG:C	2.58	0.43
1:D:251:SER:HB3	1:D:254:ALA:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:HH11	1:A:84:ARG:CG	2.26	0.42
1:C:350:GLU:O	1:C:355:PRO:HD3	2.19	0.42
1:D:155:ARG:CZ	1:D:181:ASP:OD1	2.67	0.42
1:D:168:LYS:CE	1:D:230:GLU:OE2	2.58	0.42
1:D:351:ILE:HG22	1:D:351:ILE:O	2.18	0.42
2:F:1:U:O2'	2:F:2:U:P	2.76	0.42
1:A:316:LEU:C	1:A:318:GLY:H	2.22	0.42
1:B:36:LYS:HB2	1:B:37:GLU:OE2	2.19	0.42
1:C:14:GLY:HA2	1:C:31:GLY:O	2.19	0.42
1:A:163:LEU:HD21	1:A:389:TRP:CE2	2.54	0.42
1:C:227:ARG:NH2	1:C:378:SER:HA	2.24	0.42
1:C:257:VAL:HG12	1:C:261:TYR:CD2	2.55	0.42
1:D:90:MET:HE1	1:D:118:LEU:HD22	2.02	0.42
1:D:90:MET:O	1:D:94:LEU:HD13	2.19	0.42
1:D:281:ASN:O	1:D:283:PHE:N	2.51	0.42
1:D:323:HIS:CD2	1:D:323:HIS:N	2.87	0.42
1:A:109:GLU:HG2	1:A:110:ASP:N	2.34	0.42
1:A:424:ARG:NE	1:A:427:GLU:OE2	2.52	0.42
1:C:235:LEU:CD1	1:C:247:ILE:HD13	2.34	0.42
1:C:347:LEU:HD21	1:C:360:ILE:CD1	2.50	0.42
1:D:12:VAL:HG23	1:D:13:THR:N	2.33	0.42
1:A:57:LEU:CD2	1:A:65:VAL:HG22	2.49	0.42
1:B:8:ALA:HA	1:B:11:GLU:HG3	2.01	0.42
1:B:86:THR:HG22	1:B:90:MET:HE3	2.00	0.42
1:C:406:LEU:O	1:C:407:LEU:C	2.58	0.42
1:D:201:VAL:O	1:D:205:LEU:HG	2.20	0.42
1:D:408:ALA:O	1:D:409:LEU:C	2.58	0.42
1:A:24:ARG:NH1	1:A:130:GLY:HA2	2.34	0.42
1:A:312:GLY:O	1:A:321:ILE:HG22	2.19	0.42
1:B:96:ASP:O	1:B:99:LYS:N	2.48	0.42
1:B:189:TYR:CD2	1:B:194:HIS:HE1	2.37	0.42
1:C:399:VAL:HG12	1:C:423:ALA:HB3	2.00	0.42
1:D:77:ARG:HG2	1:D:77:ARG:NH1	2.35	0.42
1:D:133:SER:C	1:D:134:LEU:HG	2.39	0.42
1:D:281:ASN:C	1:D:283:PHE:H	2.22	0.42
1:D:398:LEU:HD12	1:D:398:LEU:N	2.34	0.42
1:D:414:ALA:C	1:D:416:ARG:H	2.22	0.42
1:C:33:PHE:O	1:C:38:GLU:HA	2.20	0.42
1:C:100:VAL:HG12	1:C:100:VAL:O	2.19	0.42
1:C:253:MET:O	1:C:257:VAL:HG23	2.20	0.42
1:D:48:ASP:HA	1:D:49:PRO:HD2	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:ASP:OD1	1:D:405:LYS:HD3	2.19	0.42
1:A:41:ASN:HD22	1:A:41:ASN:HA	1.53	0.42
1:A:265:VAL:HA	1:A:268:PHE:CD2	2.55	0.42
1:B:42:HIS:CE1	1:B:105:PHE:HB3	2.55	0.42
1:C:4:VAL:HG22	1:C:428:GLY:HA3	2.02	0.42
1:D:325:LEU:HG	1:D:329:LEU:CD1	2.50	0.42
1:D:346:GLY:H	1:D:349:ALA:HB3	1.85	0.42
2:G:2:U:O2	2:G:2:U:C2'	2.68	0.42
1:C:165:ASN:HB2	1:C:380:ALA:O	2.19	0.42
1:C:260:LEU:CD1	1:C:263:ARG:HH21	2.33	0.42
1:D:59:HIS:HD2	1:D:61:HIS:H	1.67	0.42
1:D:212:LEU:CD2	1:D:306:PRO:HB2	2.48	0.42
1:A:361:LEU:HD12	1:A:361:LEU:N	2.35	0.42
1:B:3:ILE:HG23	1:B:3:ILE:O	2.20	0.42
1:B:68:LEU:N	1:B:69:PRO:CD	2.79	0.42
1:B:102:ASP:C	1:B:104:PRO:CD	2.88	0.42
1:C:323:HIS:HD2	1:C:361:LEU:HD21	1.83	0.42
1:D:21:ALA:O	1:D:23:GLY:N	2.53	0.42
1:D:208:LEU:CD2	1:D:218:VAL:HG11	2.48	0.42
1:D:224:ALA:HB3	1:D:253:MET:HE3	1.99	0.42
1:D:360:ILE:O	1:D:361:LEU:HB2	2.18	0.42
1:D:413:LEU:HD22	1:D:418:GLN:OE1	2.19	0.41
1:B:229:GLN:O	1:B:232:LEU:HB2	2.20	0.41
1:C:73:ARG:NH2	1:C:110:ASP:OD2	2.50	0.41
1:C:235:LEU:HD13	1:C:247:ILE:CD1	2.34	0.41
1:C:388:ASP:O	1:C:391:GLN:CB	2.67	0.41
1:D:181:ASP:O	1:D:182:LEU:HB2	2.20	0.41
1:D:312:GLY:HA2	1:D:313:SER:C	2.40	0.41
1:A:25:ARG:HD2	1:A:51:GLU:O	2.21	0.41
1:B:77:ARG:HD2	1:B:77:ARG:N	2.34	0.41
1:B:196:PRO:HD2	1:B:199:GLU:CD	2.40	0.41
1:C:236:TYR:HB2	1:C:285:PRO:CA	2.51	0.41
1:C:322:LEU:CD2	1:C:347:LEU:HD23	2.49	0.41
1:D:211:THR:HG21	1:D:335:ALA:CB	2.44	0.41
1:D:250:ASP:OD1	1:D:320:ARG:NH1	2.54	0.41
1:D:348:GLY:O	1:D:352:ILE:HG13	2.20	0.41
1:B:77:ARG:HG3	1:B:77:ARG:NH1	2.36	0.41
1:B:425:PHE:C	1:B:427:GLU:H	2.24	0.41
1:C:224:ALA:HA	1:C:254:ALA:CB	2.50	0.41
1:C:231:ILE:O	1:C:233:TYR:N	2.50	0.41
1:C:341:TYR:CD1	1:C:341:TYR:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:HIS:CD2	1:D:142:LEU:HD11	2.56	0.41
1:A:8:ALA:HA	1:A:11:GLU:HG3	2.02	0.41
1:A:424:ARG:HH11	1:A:424:ARG:HG2	1.84	0.41
1:B:75:GLY:O	1:B:77:ARG:CD	2.69	0.41
1:C:202:ARG:HG3	1:C:203:GLU:H	1.86	0.41
1:C:273:GLN:HA	1:C:276:PHE:HB2	2.02	0.41
1:D:12:VAL:HG12	1:D:401:GLY:HA2	2.02	0.41
1:D:321:ILE:O	1:D:325:LEU:HD13	2.19	0.41
1:A:140:GLY:O	1:A:164:GLY:HA3	2.21	0.41
1:A:329:LEU:HD12	1:A:329:LEU:HA	1.87	0.41
1:A:331:ASP:OD2	1:A:331:ASP:C	2.58	0.41
1:B:72:PHE:CE2	1:B:117:HIS:ND1	2.84	0.41
1:B:398:LEU:HD13	1:B:420:VAL:HG23	2.02	0.41
1:C:186:GLU:HA	1:C:399:VAL:O	2.21	0.41
1:C:295:GLU:HG3	1:C:296:ALA:N	2.36	0.41
1:C:425:PHE:CD2	1:C:425:PHE:C	2.93	0.41
1:A:422:LEU:O	1:A:423:ALA:C	2.58	0.41
1:C:36:LYS:O	1:C:37:GLU:HG2	2.20	0.41
1:C:302:ARG:HB2	1:C:302:ARG:CZ	2.51	0.41
1:C:347:LEU:O	1:C:351:ILE:HG13	2.20	0.41
1:D:385:GLU:O	1:D:388:ASP:HB2	2.20	0.41
1:A:323:HIS:O	1:A:327:HIS:HD2	2.04	0.41
1:C:35:GLY:C	1:C:37:GLU:H	2.24	0.41
1:A:10:ARG:HH11	1:A:10:ARG:CG	2.18	0.41
1:A:165:ASN:C	1:A:165:ASN:ND2	2.73	0.41
1:A:326:LYS:O	1:A:326:LYS:HG2	2.21	0.41
1:B:261:TYR:HD1	1:B:283:PHE:CD2	2.38	0.41
1:B:420:VAL:HG22	1:B:421:SER:N	2.35	0.41
1:C:160:SER:HB3	1:C:185:ALA:HA	2.02	0.41
1:C:190:GLY:HA2	1:C:409:LEU:HD12	2.02	0.41
1:C:221:PRO:HG3	1:C:316:LEU:HD21	2.01	0.41
1:C:223:PHE:C	1:C:225:VAL:H	2.24	0.41
1:C:280:LYS:O	1:C:282:PRO:CD	2.68	0.41
1:C:321:ILE:O	1:C:325:LEU:HD13	2.21	0.41
1:D:210:LYS:H	1:D:210:LYS:CD	2.34	0.41
1:D:224:ALA:HB1	1:D:254:ALA:N	2.35	0.41
1:D:293:HIS:HB3	1:D:295:GLU:OE2	2.20	0.41
1:D:312:GLY:O	1:D:320:ARG:N	2.54	0.41
1:D:360:ILE:CG2	1:D:361:LEU:HD13	2.48	0.41
1:B:28:LEU:O	1:B:29:ASP:HB2	2.20	0.41
1:B:36:LYS:HB2	1:B:36:LYS:HE3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:THR:O	1:B:87:VAL:HG23	2.21	0.41
1:C:32:MET:HB3	1:C:32:MET:HE2	1.92	0.41
1:C:413:LEU:HD22	1:C:418:GLN:HE22	1.86	0.41
1:D:165:ASN:HD22	1:D:165:ASN:HA	1.55	0.41
1:D:244:ARG:O	1:D:245:ALA:HB2	2.21	0.41
1:A:403:GLU:O	1:A:407:LEU:HB2	2.21	0.40
1:B:165:ASN:C	1:B:165:ASN:ND2	2.74	0.40
1:B:178:PRO:HB3	1:C:126:TRP:CD2	2.56	0.40
1:B:226:GLU:O	1:B:229:GLN:HG2	2.21	0.40
1:C:31:GLY:HA3	1:C:63:ASP:C	2.42	0.40
1:C:312:GLY:HA2	1:C:313:SER:C	2.41	0.40
1:D:399:VAL:HG22	1:D:423:ALA:HB3	2.03	0.40
1:B:312:GLY:O	1:B:321:ILE:HG22	2.21	0.40
1:C:32:MET:HE1	1:C:105:PHE:HZ	1.84	0.40
1:C:88:LEU:CD1	1:C:264:LEU:HD11	2.51	0.40
1:D:97:ALA:HA	2:H:2:U:C5	2.56	0.40
1:D:97:ALA:O	1:D:101:MET:N	2.39	0.40
1:D:100:VAL:HG13	2:H:3:U:O4	2.21	0.40
1:D:235:LEU:CD1	1:D:247:ILE:HD13	2.50	0.40
1:D:402:GLU:HB2	1:D:405:LYS:HG3	2.02	0.40
1:A:163:LEU:HA	1:A:163:LEU:HD12	1.70	0.40
1:A:402:GLU:O	1:A:403:GLU:C	2.58	0.40
1:B:48:ASP:HB3	1:B:51:GLU:CG	2.51	0.40
1:C:231:ILE:HG21	1:C:310:LEU:HD21	2.03	0.40
1:C:336:LEU:CD1	1:C:351:ILE:HG21	2.51	0.40
1:C:354:ARG:HA	1:C:367:LEU:CD2	2.51	0.40
1:C:387:LEU:O	1:C:416:ARG:NH2	2.49	0.40
1:D:189:TYR:OH	1:D:341:TYR:HB2	2.21	0.40
1:D:393:GLU:HA	1:D:394:PRO:HD2	1.92	0.40
1:A:266:ARG:NH2	1:D:273:GLN:NE2	2.68	0.40
1:C:207:ILE:O	1:C:207:ILE:CG2	2.69	0.40
1:D:45:PHE:CE2	1:D:70:LYS:HG2	2.57	0.40
1:D:258:LEU:HD21	1:D:283:PHE:O	2.21	0.40
1:D:358:VAL:CG1	1:D:359:ARG:N	2.84	0.40
1:D:420:VAL:CG2	1:D:421:SER:H	2.22	0.40
1:A:277:LEU:C	1:A:279:GLY:H	2.24	0.40
1:C:195:ARG:O	1:C:196:PRO:C	2.60	0.40
1:C:197:TYR:O	1:C:198:ARG:C	2.60	0.40
1:C:315:MET:HE3	1:C:317:ALA:HB3	2.03	0.40
1:D:49:PRO:HB3	1:D:71:LEU:HD12	2.03	0.40
1:D:396:VAL:HG12	1:D:397:VAL:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	429/431 (100%)	393 (92%)	31 (7%)	5 (1%)	13 35
1	B	429/431 (100%)	374 (87%)	46 (11%)	9 (2%)	7 22
1	C	429/431 (100%)	334 (78%)	73 (17%)	22 (5%)	2 5
1	D	429/431 (100%)	345 (80%)	58 (14%)	26 (6%)	1 3
All	All	1716/1724 (100%)	1446 (84%)	208 (12%)	62 (4%)	3 11

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	ALA
1	B	38	GLU
1	B	316	LEU
1	B	354	ARG
1	C	166	ARG
1	C	292	GLU
1	A	225	VAL
1	A	423	ALA
1	B	74	GLU
1	C	8	ALA
1	C	38	GLU
1	C	225	VAL
1	C	232	LEU
1	C	363	GLU
1	C	407	LEU
1	D	22	GLY
1	D	166	ARG
1	D	182	LEU
1	D	198	ARG
1	D	228	ALA

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Mol	Chain	Res	Type
1	D	307	MET
1	D	421	SER
1	C	196	PRO
1	C	328	GLY
1	D	196	PRO
1	D	210	LYS
1	D	224	ALA
1	D	328	GLY
1	D	330	SER
1	D	363	GLU
1	D	408	ALA
1	A	363	GLU
1	A	403	GLU
1	A	428	GLY
1	B	426	GLY
1	C	66	GLY
1	C	313	SER
1	D	38	GLU
1	D	102	ASP
1	D	400	HIS
1	B	45	PHE
1	B	399	VAL
1	C	160	SER
1	C	226	GLU
1	C	271	GLU
1	C	344	GLN
1	D	30	CYS
1	D	193	PRO
1	D	282	PRO
1	D	292	GLU
1	D	394	PRO
1	B	377	PHE
1	C	224	ALA
1	C	251	SER
1	C	282	PRO
1	D	366	PRO
1	C	399	VAL
1	D	354	ARG
1	C	281	ASN
1	D	187	GLY
1	C	207	ILE
1	D	351	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	341/341 (100%)	315 (92%)	26 (8%)	13	33
1	B	341/341 (100%)	316 (93%)	25 (7%)	14	35
1	C	341/341 (100%)	324 (95%)	17 (5%)	24	53
1	D	341/341 (100%)	326 (96%)	15 (4%)	28	58
All	All	1364/1364 (100%)	1281 (94%)	83 (6%)	18	43

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	27	LEU
1	A	34	GLN
1	A	38	GLU
1	A	41	ASN
1	A	55	VAL
1	A	94	LEU
1	A	163	LEU
1	A	165	ASN
1	A	171	LEU
1	A	186	GLU
1	A	195	ARG
1	A	219	LEU
1	A	226	GLU
1	A	229	GLN
1	A	241	ARG
1	A	264	LEU
1	A	336	LEU
1	A	364	GLU
1	A	386	LEU
1	A	388	ASP
1	A	390	LEU
1	A	398	LEU
1	A	406	LEU

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Mol	Chain	Res	Type
1	A	407	LEU
1	A	409	LEU
1	B	12	VAL
1	B	27	LEU
1	B	28	LEU
1	B	37	GLU
1	B	57	LEU
1	B	74	GLU
1	B	77	ARG
1	B	102	ASP
1	B	128	ARG
1	B	165	ASN
1	B	171	LEU
1	B	175	SER
1	B	186	GLU
1	B	211	THR
1	B	219	LEU
1	B	226	GLU
1	B	227	ARG
1	B	229	GLN
1	B	302	ARG
1	B	329	LEU
1	B	336	LEU
1	B	344	GLN
1	B	365	VAL
1	B	390	LEU
1	B	409	LEU
1	C	13	THR
1	C	27	LEU
1	C	36	LYS
1	C	38	GLU
1	C	57	LEU
1	C	74	GLU
1	C	155	ARG
1	C	165	ASN
1	C	166	ARG
1	C	196	PRO
1	C	227	ARG
1	C	276	PHE
1	C	293	HIS
1	C	315	MET
1	C	389	TRP

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Mol	Chain	Res	Type
1	C	398	LEU
1	C	422	LEU
1	D	27	LEU
1	D	37	GLU
1	D	74	GLU
1	D	96	ASP
1	D	132	LEU
1	D	165	ASN
1	D	166	ARG
1	D	196	PRO
1	D	226	GLU
1	D	229	GLN
1	D	264	LEU
1	D	325	LEU
1	D	359	ARG
1	D	391	GLN
1	D	415	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	59	HIS
1	A	151	GLN
1	A	165	ASN
1	A	229	GLN
1	A	301	ASN
1	B	41	ASN
1	B	151	GLN
1	B	165	ASN
1	B	229	GLN
1	B	238	HIS
1	B	275	HIS
1	B	344	GLN
1	B	383	GLN
1	C	41	ASN
1	C	165	ASN
1	C	194	HIS
1	C	214	GLN
1	C	273	GLN
1	C	275	HIS
1	C	278	GLN

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Mol	Chain	Res	Type
1	C	323	HIS
1	C	327	HIS
1	D	34	GLN
1	D	41	ASN
1	D	59	HIS
1	D	117	HIS
1	D	165	ASN
1	D	214	GLN
1	D	229	GLN
1	D	273	GLN
1	D	327	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	3/4 (75%)	3 (100%)	0
2	F	4/4 (100%)	3 (75%)	1 (25%)
2	G	1/4 (25%)	1 (100%)	0
2	H	4/4 (100%)	2 (50%)	2 (50%)
All	All	12/16 (75%)	9 (75%)	3 (25%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	2	U
2	E	3	U
2	E	4	U
2	F	2	U
2	F	3	U
2	F	4	U
2	G	2	U
2	H	2	U
2	H	4	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	F	1	U
2	H	1	U
2	H	3	U

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 64 ligands modelled in this entry, 8 are monoatomic - leaving 56 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	439	-	4,4,4	1.01	0	6,6,6	0.66	0
3	SO4	A	445	-	4,4,4	1.01	0	6,6,6	0.66	0
3	SO4	A	448	-	4,4,4	1.00	0	6,6,6	0.68	0
3	SO4	B	435	-	4,4,4	1.03	0	6,6,6	0.65	0
3	SO4	D	435	-	4,4,4	1.02	0	6,6,6	0.66	0
3	SO4	A	438	-	4,4,4	0.91	0	6,6,6	0.68	0
3	SO4	C	436	-	4,4,4	1.02	0	6,6,6	0.64	0
4	FLC	A	450	-	12,12,12	1.60	4 (33%)	17,17,17	1.44	1 (5%)
3	SO4	D	432	-	4,4,4	1.03	0	6,6,6	0.65	0
3	SO4	B	432	-	4,4,4	1.00	0	6,6,6	0.65	0
3	SO4	B	443	-	4,4,4	1.04	0	6,6,6	0.65	0
3	SO4	A	441	-	4,4,4	0.98	0	6,6,6	0.68	0
3	SO4	A	433	-	4,4,4	1.00	0	6,6,6	0.68	0
3	SO4	D	440	-	4,4,4	1.00	0	6,6,6	0.67	0
3	SO4	D	434	-	4,4,4	0.99	0	6,6,6	0.66	0
3	SO4	B	434	-	4,4,4	0.99	0	6,6,6	0.68	0
3	SO4	B	437	-	4,4,4	1.02	0	6,6,6	0.66	0
3	SO4	A	435	-	4,4,4	1.01	0	6,6,6	0.65	0
3	SO4	B	446	-	4,4,4	1.03	0	6,6,6	0.67	0
3	SO4	B	436	-	4,4,4	1.04	0	6,6,6	0.64	0
3	SO4	B	444	-	4,4,4	1.07	0	6,6,6	0.63	0
4	FLC	A	451	-	12,12,12	1.73	3 (25%)	17,17,17	1.53	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	A	432	-	4,4,4	1.07	0	6,6,6	0.62	0
3	SO4	B	448	-	4,4,4	1.08	0	6,6,6	0.63	0
3	SO4	D	436	-	4,4,4	1.00	0	6,6,6	0.67	0
3	SO4	C	438	-	4,4,4	1.01	0	6,6,6	0.67	0
3	SO4	A	442	-	4,4,4	1.02	0	6,6,6	0.65	0
3	SO4	B	433	-	4,4,4	1.01	0	6,6,6	0.65	0
3	SO4	C	435	-	4,4,4	1.00	0	6,6,6	0.66	0
3	SO4	C	437	-	4,4,4	0.99	0	6,6,6	0.67	0
3	SO4	A	437	-	4,4,4	1.02	0	6,6,6	0.66	0
3	SO4	A	440	-	4,4,4	1.03	0	6,6,6	0.67	0
3	SO4	A	443	-	4,4,4	0.97	0	6,6,6	0.66	0
3	SO4	A	434	-	4,4,4	1.02	0	6,6,6	0.66	0
3	SO4	A	446	-	4,4,4	1.01	0	6,6,6	0.69	0
3	SO4	A	436	-	4,4,4	1.01	0	6,6,6	0.65	0
3	SO4	A	447	-	4,4,4	0.97	0	6,6,6	0.67	0
3	SO4	C	440	-	4,4,4	1.00	0	6,6,6	0.66	0
3	SO4	B	438	-	4,4,4	1.02	0	6,6,6	0.62	0
3	SO4	C	439	-	4,4,4	1.00	0	6,6,6	0.69	0
3	SO4	C	434	-	4,4,4	1.01	0	6,6,6	0.67	0
3	SO4	D	438	-	4,4,4	1.01	0	6,6,6	0.62	0
3	SO4	B	442	-	4,4,4	0.98	0	6,6,6	0.68	0
3	SO4	A	444	-	4,4,4	1.02	0	6,6,6	0.66	0
3	SO4	C	433	-	4,4,4	0.99	0	6,6,6	0.65	0
3	SO4	C	432	-	4,4,4	1.00	0	6,6,6	0.68	0
3	SO4	D	437	-	4,4,4	1.01	0	6,6,6	0.62	0
3	SO4	B	447	-	4,4,4	0.99	0	6,6,6	0.65	0
3	SO4	A	449	-	4,4,4	1.01	0	6,6,6	0.65	0
3	SO4	B	440	-	4,4,4	0.97	0	6,6,6	0.75	0
3	SO4	B	441	-	4,4,4	1.01	0	6,6,6	0.63	0
3	SO4	D	439	-	4,4,4	1.01	0	6,6,6	0.64	0
3	SO4	B	439	-	4,4,4	0.99	0	6,6,6	0.66	0
3	SO4	C	441	-	4,4,4	1.03	0	6,6,6	0.65	0
3	SO4	D	433	-	4,4,4	1.02	0	6,6,6	0.67	0
3	SO4	B	445	-	4,4,4	1.01	0	6,6,6	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FLC	A	451	-	-	0/16/16/16	-
4	FLC	A	450	-	-	0/16/16/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	451	FLC	OA2-CAC	-2.73	1.21	1.30
4	A	451	FLC	CG-CB	2.53	1.57	1.53
4	A	450	FLC	OG2-CGC	-2.48	1.22	1.30
4	A	451	FLC	OG2-CGC	-2.45	1.22	1.30
4	A	450	FLC	OA2-CAC	-2.43	1.22	1.30
4	A	450	FLC	CA-CB	2.33	1.56	1.53
4	A	450	FLC	CG-CB	2.15	1.56	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	451	FLC	OB2-CBC-CB	4.49	120.85	113.05
4	A	450	FLC	OB2-CBC-CB	4.27	120.47	113.05
4	A	451	FLC	OB1-CBC-CB	-2.03	119.38	122.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	436	SO4	1	0
4	A	450	FLC	1	0
4	A	451	FLC	5	0
3	A	432	SO4	1	0
3	D	436	SO4	1	0
3	A	446	SO4	1	0
3	D	437	SO4	4	0
3	B	447	SO4	1	0
3	B	440	SO4	1	0
3	B	441	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	431/431 (100%)	-0.13	1 (0%) 95 95	25, 46, 69, 83	0
1	B	431/431 (100%)	-0.10	7 (1%) 72 70	24, 46, 84, 103	0
1	C	431/431 (100%)	0.99	90 (20%) 1 0	34, 94, 165, 167	0
1	D	431/431 (100%)	0.88	79 (18%) 1 1	40, 88, 152, 163	0
2	E	4/4 (100%)	1.30	1 (25%) 0 0	70, 76, 81, 95	0
2	F	4/4 (100%)	1.15	0 100 100	83, 90, 98, 100	0
2	G	2/4 (50%)	1.46	0 100 100	145, 145, 145, 151	0
2	H	4/4 (100%)	1.74	2 (50%) 0 0	118, 125, 139, 151	0
All	All	1738/1740 (99%)	0.42	180 (10%) 6 4	24, 62, 155, 167	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	335	ALA	12.3
1	C	322	LEU	8.6
1	C	337	VAL	8.4
1	C	219	LEU	7.8
1	C	329	LEU	7.5
1	C	213	SER	7.3
1	C	218	VAL	6.9
1	C	300	LEU	6.8
1	C	307	MET	6.8
1	C	326	LYS	6.7
1	C	336	LEU	6.7
1	D	294	THR	6.6
1	C	214	GLN	6.6
1	C	242	LEU	6.6
1	D	322	LEU	6.1
1	D	335	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	371	VAL	5.9
1	C	215	GLY	5.7
1	D	208	LEU	5.7
1	D	298	LYS	5.5
1	C	338	PHE	5.5
1	C	205	LEU	5.5
1	D	300	LEU	5.5
1	C	217	LYS	5.5
1	C	301	ASN	5.4
1	D	360	ILE	5.4
1	C	250	ASP	5.2
1	C	297	SER	5.1
1	D	334	ASN	5.0
1	C	209	GLU	5.0
1	D	245	ALA	4.7
1	C	308	VAL	4.7
1	C	309	VAL	4.7
1	D	336	LEU	4.7
1	D	218	VAL	4.6
1	D	324	HIS	4.6
1	C	325	LEU	4.5
1	C	248	TYR	4.5
1	C	245	ALA	4.5
1	C	294	THR	4.5
1	D	308	VAL	4.4
1	C	324	HIS	4.4
1	D	216	GLY	4.4
1	D	291	VAL	4.3
1	C	247	ILE	4.3
1	D	211	THR	4.3
1	C	194	HIS	4.3
1	C	241	ARG	4.3
1	D	212	LEU	4.3
1	C	288	LEU	4.2
1	D	326	LYS	4.2
1	D	363	GLU	4.1
1	C	327	HIS	4.1
1	D	316	LEU	4.1
1	C	204	PHE	4.1
1	D	325	LEU	4.0
1	C	333	ARG	4.0
1	C	376	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	297	SER	4.0
1	C	415	LEU	3.9
1	C	211	THR	3.9
1	D	250	ASP	3.9
1	D	207	ILE	3.8
1	D	249	LEU	3.8
1	C	167	GLU	3.7
1	C	216	GLY	3.7
1	B	78	GLY	3.7
1	C	367	LEU	3.7
1	C	298	LYS	3.6
1	C	208	LEU	3.6
1	C	239	GLY	3.6
1	D	361	LEU	3.6
1	D	307	MET	3.6
1	D	301	ASN	3.6
1	C	418	GLN	3.6
1	D	362	GLY	3.6
1	D	328	GLY	3.6
1	D	283	PHE	3.5
1	B	77	ARG	3.5
1	C	243	PRO	3.5
1	C	235	LEU	3.5
1	C	291	VAL	3.4
1	D	209	GLU	3.4
1	D	290	VAL	3.4
1	D	358	VAL	3.4
1	C	316	LEU	3.4
1	C	377	PHE	3.4
1	D	8	ALA	3.3
1	C	360	ILE	3.3
1	C	306	PRO	3.3
1	C	365	VAL	3.3
1	B	72	PHE	3.2
1	D	333	ARG	3.2
1	D	309	VAL	3.2
1	D	106	PHE	3.2
1	C	303	ALA	3.1
1	C	372	HIS	3.1
1	C	353	ALA	3.1
1	C	302	ARG	3.1
1	D	312	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	247	ILE	3.0
1	D	332	PRO	3.0
1	C	222	THR	3.0
1	C	207	ILE	2.9
1	C	193	PRO	2.9
1	D	240	HIS	2.9
1	D	204	PHE	2.9
1	C	304	PRO	2.9
1	C	370	SER	2.9
1	C	201	VAL	2.9
1	D	288	LEU	2.9
2	H	4	U	2.8
1	C	305	GLY	2.8
1	C	295	GLU	2.8
1	D	219	LEU	2.8
1	C	296	ALA	2.8
1	D	213	SER	2.7
1	D	205	LEU	2.7
1	C	238	HIS	2.7
1	C	192	ARG	2.7
1	D	99	LYS	2.7
1	D	248	TYR	2.7
1	D	306	PRO	2.6
1	D	303	ALA	2.6
1	C	244	ARG	2.6
1	C	364	GLU	2.6
1	D	370	SER	2.6
1	B	39	ALA	2.6
1	D	201	VAL	2.6
1	D	286	ALA	2.6
1	C	234	VAL	2.5
1	C	210	LYS	2.5
1	D	214	GLN	2.5
1	D	246	PRO	2.5
1	D	190	GLY	2.5
1	C	328	GLY	2.4
1	C	352	ILE	2.4
1	D	292	GLU	2.4
1	C	240	HIS	2.4
1	D	98	LEU	2.4
1	D	329	LEU	2.4
2	H	3	U	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	293	HIS	2.4
1	D	374	LEU	2.4
1	C	276	PHE	2.4
1	C	246	PRO	2.4
1	C	334	ASN	2.3
1	B	105	PHE	2.3
1	D	318	GLY	2.3
1	C	212	LEU	2.3
1	D	251	SER	2.3
1	D	252	PRO	2.3
1	C	414	ALA	2.3
1	D	339	VAL	2.3
1	D	197	TYR	2.3
1	D	337	VAL	2.2
1	D	102	ASP	2.2
1	D	299	ALA	2.2
1	C	220	ILE	2.2
1	D	167	GLU	2.2
2	E	2	U	2.2
1	D	338	PHE	2.2
1	C	321	ILE	2.2
1	C	332	PRO	2.1
1	C	299	ALA	2.1
1	D	199	GLU	2.1
1	D	224	ALA	2.1
1	D	323	HIS	2.1
1	C	369	ALA	2.1
1	D	198	ARG	2.1
1	D	319	GLY	2.1
1	C	374	LEU	2.1
1	C	341	TYR	2.0
1	C	14	GLY	2.0
1	B	113	GLU	2.0
1	B	71	LEU	2.0
1	D	344	GLN	2.0
1	C	354	ARG	2.0
1	A	361	LEU	2.0
1	D	304	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	D	435	5/5	0.43	0.33	152,152,153,153	0
3	SO4	A	432	5/5	0.67	0.32	140,140,141,141	0
3	SO4	D	434	5/5	0.68	0.25	139,139,139,140	0
4	FLC	A	450	13/13	0.73	0.38	122,124,126,128	0
3	SO4	A	436	5/5	0.75	0.30	171,171,171,171	0
3	SO4	A	444	5/5	0.78	0.49	134,134,134,135	0
3	SO4	C	441	5/5	0.78	0.19	125,125,126,126	0
3	SO4	D	433	5/5	0.78	0.17	135,136,136,136	0
3	SO4	B	445	5/5	0.80	0.21	130,131,131,131	0
3	SO4	A	442	5/5	0.80	0.23	139,140,140,140	0
3	SO4	A	437	5/5	0.80	0.20	152,152,152,152	0
3	SO4	B	436	5/5	0.82	0.33	143,143,144,144	0
3	SO4	A	446	5/5	0.82	0.26	117,118,118,118	0
3	SO4	C	434	5/5	0.82	0.34	137,137,137,137	0
3	SO4	A	449	5/5	0.82	0.23	124,124,125,125	0
3	SO4	B	438	5/5	0.83	0.24	96,97,97,98	0
3	SO4	A	435	5/5	0.83	0.22	148,148,149,149	0
4	FLC	A	451	13/13	0.83	0.31	71,76,85,86	0
3	SO4	D	440	5/5	0.84	0.17	148,148,148,149	0
3	SO4	A	440	5/5	0.84	0.16	132,132,133,133	0
3	SO4	B	434	5/5	0.84	0.21	129,129,130,130	0
3	SO4	A	445	5/5	0.85	0.24	109,110,110,111	0
3	SO4	B	432	5/5	0.85	0.44	137,138,138,139	0
3	SO4	D	432	5/5	0.85	0.19	130,130,130,130	0
3	SO4	B	442	5/5	0.86	0.26	116,116,117,117	0
3	SO4	A	448	5/5	0.86	0.29	126,126,126,127	0
3	SO4	B	447	5/5	0.86	0.37	153,153,153,153	0
3	SO4	A	439	5/5	0.87	0.17	135,135,136,136	0
3	SO4	D	437	5/5	0.88	0.18	114,114,115,115	0
3	SO4	C	432	5/5	0.88	0.18	131,132,132,132	0
3	SO4	C	435	5/5	0.89	0.19	110,110,110,111	0
3	SO4	A	441	5/5	0.89	0.16	118,118,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	435	5/5	0.90	0.22	116,116,116,117	0
3	SO4	B	437	5/5	0.90	0.12	132,132,132,132	0
3	SO4	C	437	5/5	0.91	0.16	119,119,120,120	0
3	SO4	C	433	5/5	0.91	0.25	95,95,96,96	0
3	SO4	C	440	5/5	0.92	0.11	116,116,117,117	0
3	SO4	B	444	5/5	0.92	0.26	78,79,80,80	0
3	SO4	B	433	5/5	0.93	0.18	105,105,105,106	0
3	SO4	C	438	5/5	0.93	0.14	116,117,118,118	0
5	ZN	C	443	1/1	0.93	0.12	104,104,104,104	0
3	SO4	A	434	5/5	0.94	0.18	94,95,95,95	0
3	SO4	D	438	5/5	0.94	0.17	80,81,83,83	0
3	SO4	D	439	5/5	0.94	0.17	99,99,100,101	0
3	SO4	C	436	5/5	0.94	0.12	128,128,128,128	0
3	SO4	B	439	5/5	0.94	0.16	104,104,104,104	0
3	SO4	B	441	5/5	0.94	0.12	98,98,98,99	0
3	SO4	B	446	5/5	0.94	0.12	104,104,105,105	0
3	SO4	D	436	5/5	0.96	0.19	86,86,87,87	0
3	SO4	B	440	5/5	0.96	0.19	66,67,69,72	0
3	SO4	A	438	5/5	0.96	0.19	61,62,63,65	0
3	SO4	C	439	5/5	0.96	0.14	74,75,76,77	0
5	ZN	D	441	1/1	0.96	0.12	88,88,88,88	0
3	SO4	A	433	5/5	0.97	0.18	53,54,55,58	0
5	ZN	B	449	1/1	0.97	0.05	61,61,61,61	0
5	ZN	B	450	1/1	0.97	0.10	65,65,65,65	0
3	SO4	A	443	5/5	0.97	0.14	88,88,89,89	0
3	SO4	B	443	5/5	0.97	0.15	94,95,95,96	0
3	SO4	B	448	5/5	0.98	0.13	54,59,60,60	0
5	ZN	C	442	1/1	0.98	0.12	109,109,109,109	0
5	ZN	D	442	1/1	0.98	0.11	86,86,86,86	0
3	SO4	A	447	5/5	0.99	0.13	41,41,43,47	0
5	ZN	A	452	1/1	0.99	0.07	58,58,58,58	0
5	ZN	A	453	1/1	0.99	0.09	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.