



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:06 am BST

PDB ID : 3WOD
Title : RNA polymerase-gp39 complex
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Deposited on : 2013-12-26
Resolution : 3.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

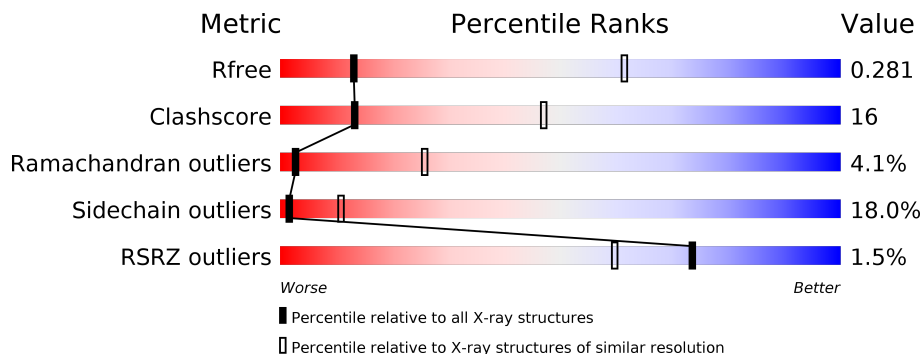
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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.




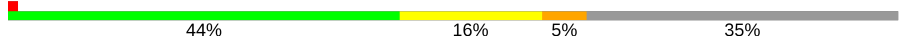
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 on 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 $\leq 5\%$. 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	315	
1	B	315	
2	C	1119	
3	D	1524	
4	E	99	
5	F	423	

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Mol	Chain	Length	Quality of chain
6	G	141	 <p>65% 23% 10%</p>
6	H	141	 <p>44% 16% 5% 35%</p>

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 28954 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	225	Total	C	N	O	S	0	0	0
			1772	1132	308	330	2			
1	B	232	Total	C	N	O	S	0	0	0
			1814	1158	316	338	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1118	Total	C	N	O	S	0	0	0
			8817	5575	1573	1645	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1488	Total	C	N	O	S	0	0	0
			11752	7450	2069	2197	36			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	61	GLU	VAL	SEE REMARK 999	UNP Q8RQE7
E	92	ILE	LEU	SEE REMARK 999	UNP Q8RQE7
E	95	GLY	VAL	SEE REMARK 999	UNP Q8RQE7

- Molecule 5 is a protein called RNA polymerase sigma factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	278	2242	1421	399	420	2	0	0	0

- Molecule 6 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	G	127	1035	673	175	184	3	0	0	0
6	H	91	752	495	125	131	1	0	0	0

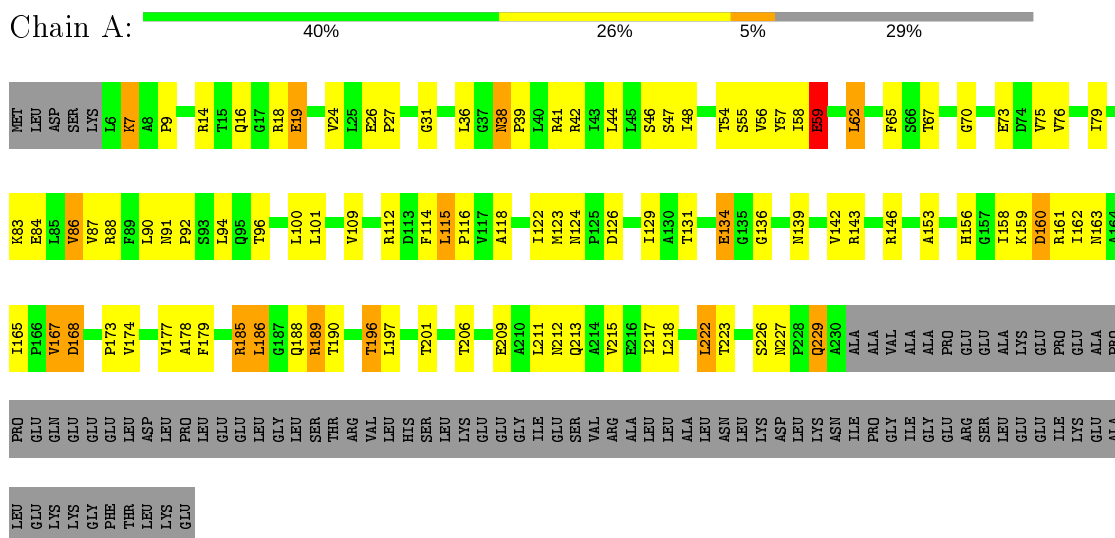
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Zn	0	0
			1	1		

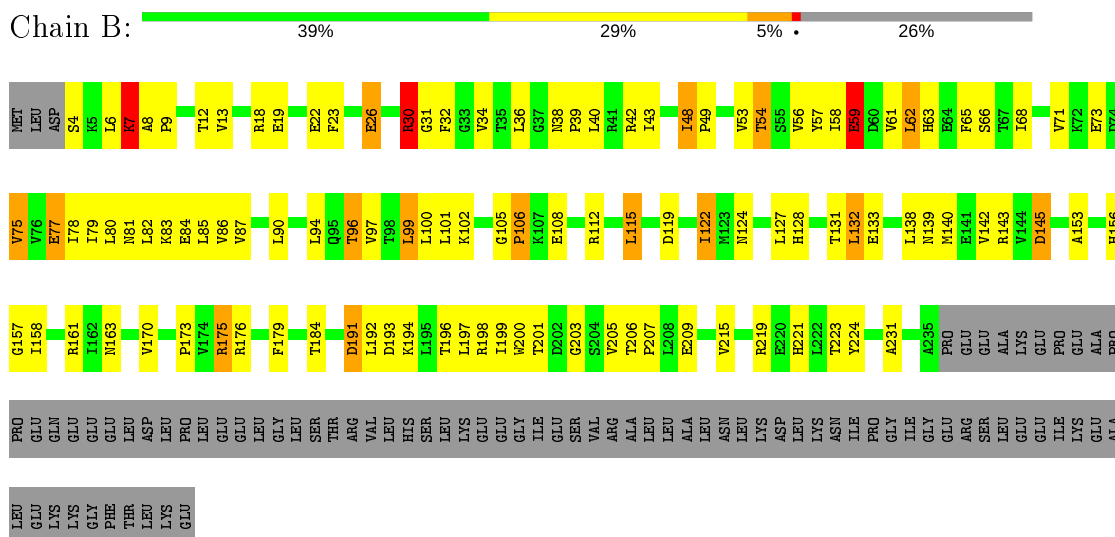
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

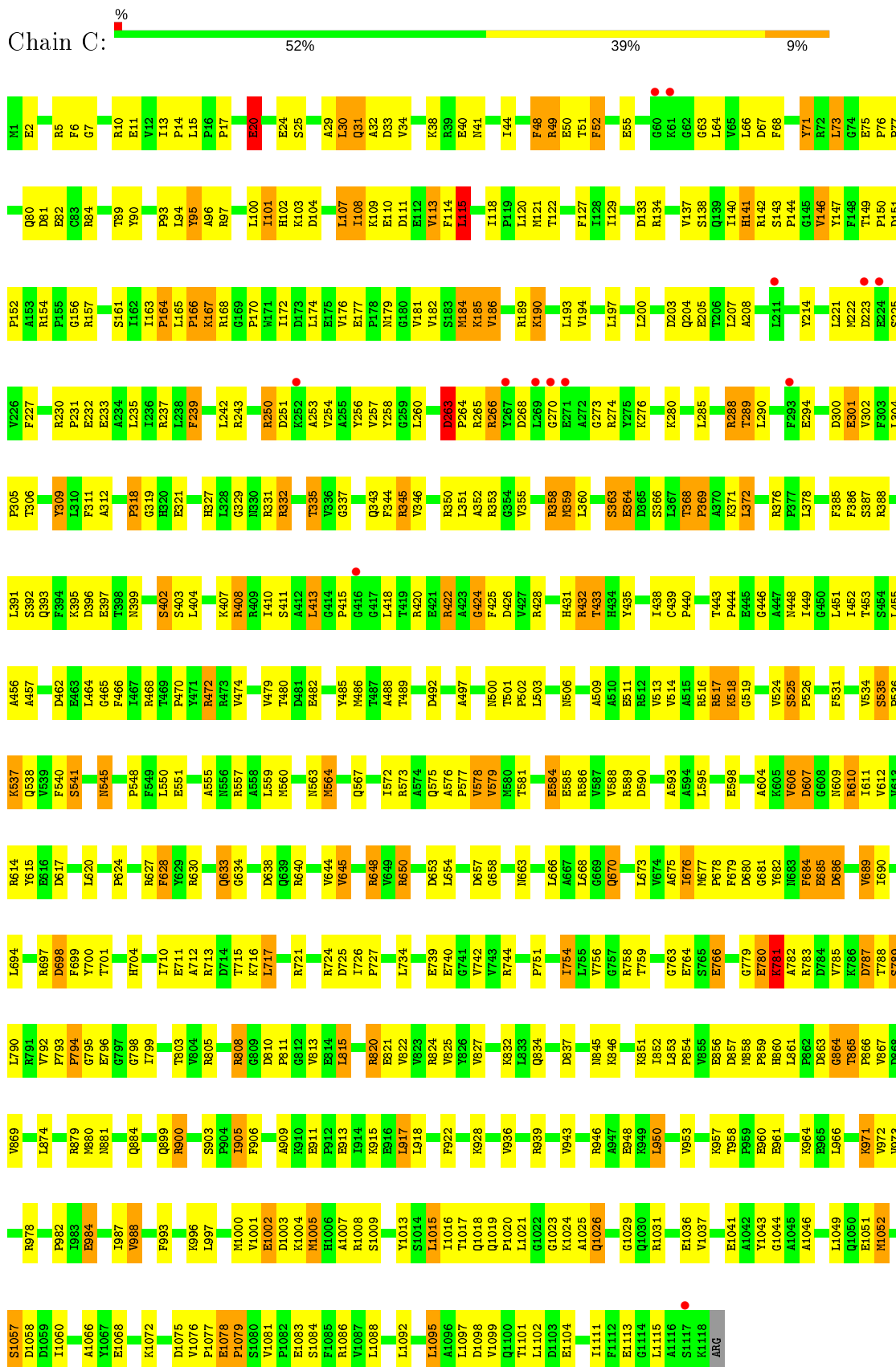
- Molecule 1: DNA-directed RNA polymerase subunit alpha



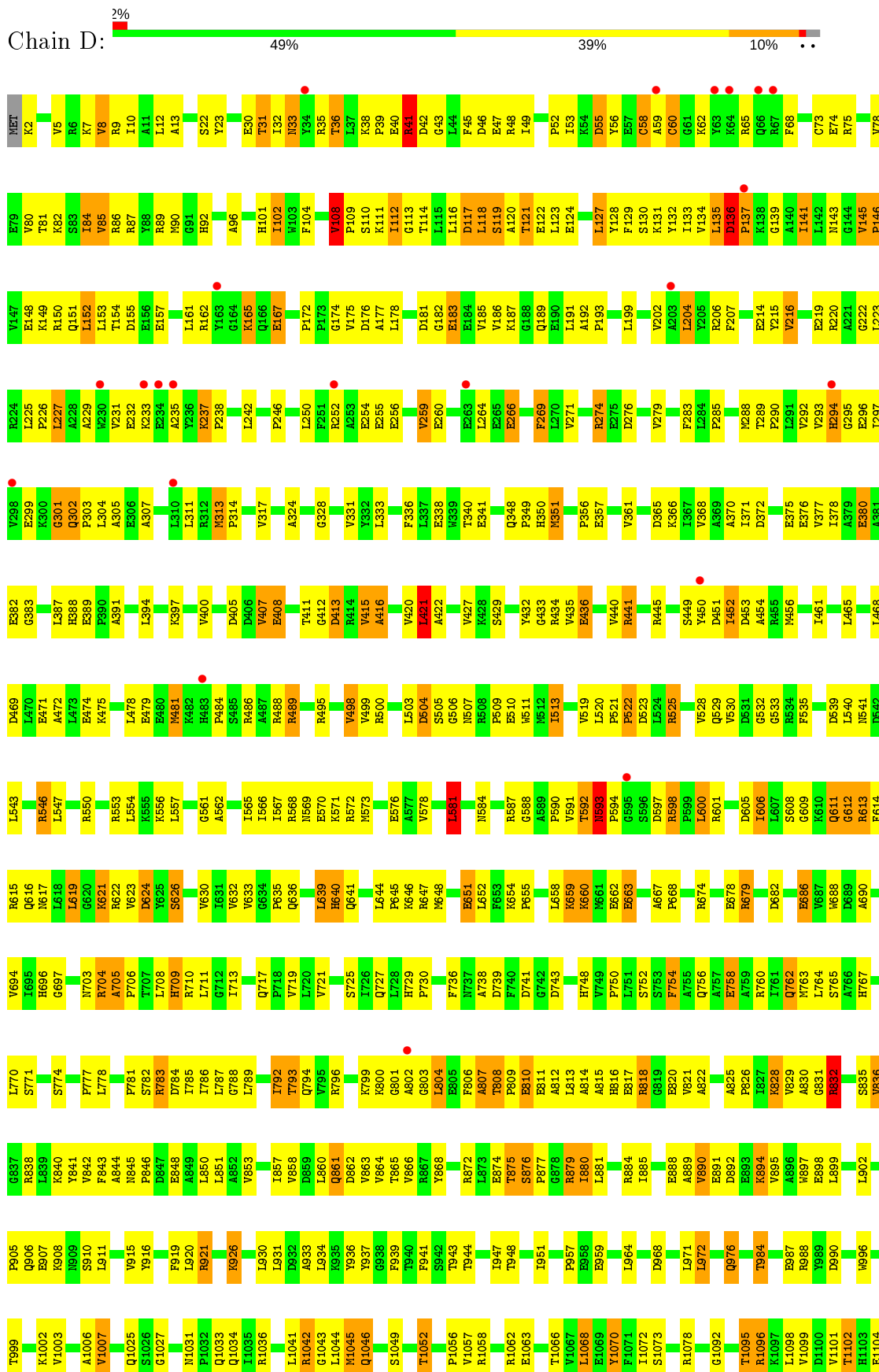
- Molecule 1: DNA-directed RNA polymerase subunit alpha

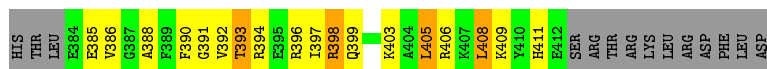


- Molecule 2: DNA-directed RNA polymerase subunit beta



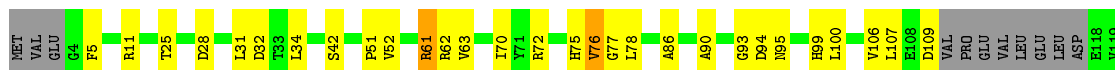
- Molecule 3: DNA-directed RNA polymerase subunit beta'





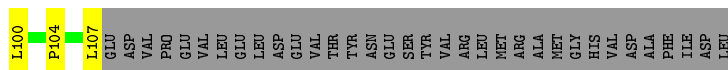
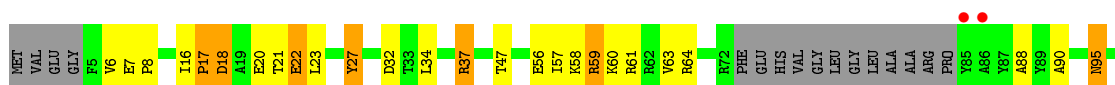
- Molecule 6: Putative uncharacterized protein

Chain G: 65% 23% 10%



- Molecule 6: Putative uncharacterized protein

Chain H: % 44% 16% 5% 35%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	294.44Å 294.44Å 223.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.88 – 3.60 19.88 – 3.58	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.88-3.60) 99.3 (19.88-3.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.61Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.250 , 0.279 0.255 , 0.281	Depositor DCC
R_{free} test set	6487 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtrriage
Anisotropy	0.443	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , -23.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtrriage
Estimated twinning fraction	0.166 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	28954	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.35	0/1804	0.63	1/2454 (0.0%)
1	B	0.32	0/1846	0.59	0/2511
2	C	0.33	0/8985	0.61	2/12150 (0.0%)
3	D	0.32	0/11958	0.60	4/16166 (0.0%)
4	E	0.31	0/783	0.66	0/1054
5	F	0.33	0/2276	0.59	3/3058 (0.1%)
6	G	0.27	0/1065	0.53	0/1449
6	H	0.27	0/775	0.48	0/1057
All	All	0.32	0/29492	0.60	10/39899 (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	C	0	3
3	D	0	3
4	E	0	3
5	F	0	1
All	All	0	10

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	795	GLY	N-CA-C	-6.48	96.90	113.10
1	A	115	LEU	CA-CB-CG	6.18	129.51	115.30
3	D	581	LEU	CA-CB-CG	5.89	128.84	115.30
5	F	174	LEU	CA-CB-CG	5.88	128.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	804	LEU	CA-CB-CG	5.79	128.61	115.30
3	D	136	ASP	C-N-CD	5.49	139.92	128.40
3	D	108	VAL	C-N-CD	5.48	139.91	128.40
5	F	358	LEU	CA-CB-CG	5.48	127.91	115.30
5	F	187	LEU	CA-CB-CG	5.48	127.90	115.30
2	C	455	LEU	CA-CB-CG	5.12	127.08	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	260	LEU	Peptide
2	C	685	GLU	Peptide
2	C	794	PRO	Peptide
3	D	1196	THR	Peptide
3	D	1207	TYR	Peptide
3	D	561	GLY	Peptide
4	E	40	LEU	Peptide
4	E	49	GLN	Peptide
4	E	53	GLY	Peptide
5	F	376	ILE	Peptide

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	1772	0	1821	63	0
1	B	1814	0	1868	73	0
2	C	8817	0	8920	305	0
3	D	11752	0	11990	447	0
4	E	769	0	775	29	0
5	F	2242	0	2305	62	0
6	G	1035	0	1013	19	0
6	H	752	0	748	20	0
7	D	1	0	0	0	0
All	All	28954	0	29440	943	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 16.

All (943) 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)
3:D:820:GLU:HG3	3:D:836:VAL:HG21	1.51	0.92
2:C:164:PRO:HA	2:C:266:ARG:HH22	1.36	0.90
4:E:54:LEU:HA	4:E:58:PRO:HD2	1.57	0.85
2:C:63:GLY:HA3	2:C:103:LYS:HG2	1.58	0.83
3:D:133:ILE:HG21	3:D:454:ALA:HB1	1.60	0.83
1:A:27:PRO:HG3	1:A:186:LEU:HD13	1.60	0.82
3:D:225:LEU:HD13	3:D:231:VAL:HG23	1.63	0.81
3:D:678:GLU:HG3	3:D:679:ARG:HD3	1.64	0.79
3:D:295:GLY:HA2	3:D:302:GLN:HB3	1.65	0.79
1:B:18:ARG:NH1	1:B:203:GLY:O	2.16	0.79
3:D:116:LEU:O	3:D:118:LEU:N	2.14	0.79
2:C:679:PHE:O	2:C:681:GLY:N	2.14	0.79
1:A:18:ARG:HH22	1:A:88:ARG:HH21	1.31	0.78
1:A:18:ARG:HH12	1:A:88:ARG:HE	1.32	0.78
3:D:697:GLY:O	3:D:760:ARG:NH1	2.18	0.77
3:D:252:ARG:HA	3:D:301:GLY:HA3	1.67	0.77
2:C:716:LYS:HG3	3:D:533:GLY:HA3	1.68	0.76
2:C:289:THR:HG22	2:C:290:LEU:HD23	1.67	0.76
3:D:181:ASP:O	3:D:183:GLU:N	2.18	0.76
3:D:1488:ASP:N	3:D:1488:ASP:OD1	2.20	0.75
3:D:711:LEU:HD12	3:D:778:LEU:HD23	1.68	0.75
3:D:591:VAL:HG13	3:D:597:ASP:HA	1.69	0.74
2:C:874:LEU:HD13	3:D:783:ARG:HB2	1.68	0.74
3:D:1045:MET:HG2	3:D:1073:SER:HA	1.67	0.74
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.69	0.73
2:C:576:ALA:O	2:C:900:ARG:NH2	2.21	0.73
3:D:815:ALA:O	3:D:818:ARG:HG3	1.89	0.72
5:F:109:GLY:HA2	5:F:177:ALA:HA	1.71	0.72
5:F:385:GLU:HA	5:F:388:ALA:HB2	1.71	0.72
2:C:1078:GLU:HG3	2:C:1079:PRO:HD3	1.71	0.72
3:D:1155:VAL:O	3:D:1157:GLY:N	2.22	0.72
6:H:20:GLU:HA	6:H:61:ARG:HD2	1.71	0.72
2:C:650:ARG:HG2	2:C:653:ASP:HB2	1.72	0.71
3:D:520:LEU:O	3:D:525:ARG:NH1	2.23	0.71
2:C:34:VAL:HB	2:C:38:LYS:HG3	1.71	0.71
2:C:555:ALA:HB2	3:D:1070:TYR:HE1	1.56	0.71
5:F:85:LEU:HD22	5:F:193:ARG:HD3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:O	1:A:146:ARG:NH1	2.23	0.71
3:D:617:ASN:ND2	3:D:1466:VAL:O	2.23	0.71
5:F:403:LYS:HA	5:F:406:ARG:HD2	1.72	0.71
3:D:640:HIS:HB3	3:D:641:GLN:HG3	1.71	0.70
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.73	0.70
2:C:1083:GLU:OE1	3:D:87:ARG:NH1	2.24	0.70
1:B:34:VAL:HG11	2:C:978:ARG:HB2	1.73	0.70
2:C:1099:VAL:HG12	3:D:10:ILE:HG12	1.73	0.70
3:D:1209:LEU:HD13	3:D:1215:VAL:HA	1.72	0.70
2:C:464:LEU:O	2:C:466:PHE:N	2.25	0.70
1:A:160:ASP:N	1:A:160:ASP:OD1	2.26	0.69
6:G:90:ALA:HB2	6:G:100:LEU:HD23	1.74	0.69
6:H:90:ALA:HB2	6:H:100:LEU:HD23	1.74	0.69
1:A:41:ARG:NH1	1:A:177:VAL:O	2.25	0.69
3:D:1098:LEU:O	3:D:1102:THR:OG1	2.10	0.69
1:B:77:GLU:HB2	3:D:872:ARG:HH21	1.57	0.69
3:D:1194:CYS:SG	3:D:1195:GLN:N	2.65	0.69
3:D:810:GLU:O	3:D:813:LEU:HG	1.92	0.69
2:C:573:ARG:O	2:C:670:GLN:NE2	2.26	0.69
3:D:119:SER:H	3:D:123:LEU:HD12	1.57	0.69
3:D:1476:THR:HG23	4:E:21:VAL:HG22	1.75	0.69
6:G:124:SER:HA	6:G:127:ARG:HG3	1.74	0.69
3:D:127:LEU:HD11	3:D:461:ILE:HD11	1.74	0.68
2:C:432:ARG:HG3	2:C:519:GLY:HA2	1.73	0.68
3:D:119:SER:O	3:D:121:THR:N	2.23	0.68
2:C:607:ASP:HB3	2:C:609:ASN:H	1.57	0.68
2:C:41:ASN:ND2	2:C:268:ASP:OD1	2.26	0.68
3:D:422:ALA:HB3	3:D:427:VAL:HB	1.75	0.68
2:C:391:LEU:HD13	2:C:415:PRO:HD3	1.75	0.67
2:C:31:GLN:NE2	2:C:40:GLU:O	2.28	0.66
3:D:615:ARG:HH22	3:D:1441:GLN:HA	1.60	0.66
3:D:153:LEU:HB2	3:D:157:GLU:HG3	1.76	0.66
1:B:96:THR:OG1	1:B:97:VAL:N	2.29	0.66
3:D:906:GLN:HB3	3:D:911:LEU:HD11	1.77	0.66
2:C:939:ARG:HD2	2:C:982:PRO:HD3	1.78	0.66
3:D:226:PRO:HB2	3:D:229:ALA:HB3	1.78	0.66
5:F:123:ASP:H	5:F:126:LEU:HD23	1.61	0.66
1:A:31:GLY:O	1:B:42:ARG:NH2	2.29	0.65
2:C:30:LEU:O	2:C:32:ALA:N	2.29	0.65
3:D:591:VAL:HG12	3:D:592:THR:O	1.96	0.65
3:D:679:ARG:NE	3:D:682:ASP:OD2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:288:MET:HG3	3:D:305:ALA:HB1	1.77	0.65
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.78	0.65
2:C:689:VAL:HG13	2:C:851:LYS:HB3	1.79	0.65
1:A:24:VAL:HG22	1:A:196:THR:HB	1.78	0.65
2:C:164:PRO:CA	2:C:266:ARG:HH22	2.10	0.65
3:D:540:LEU:HD11	3:D:606:ILE:HD11	1.77	0.65
2:C:327:HIS:HD2	2:C:329:GLY:H	1.44	0.65
3:D:407:VAL:HG22	3:D:408:GLU:H	1.61	0.65
3:D:139:GLY:HA3	3:D:452:ILE:HD12	1.78	0.65
2:C:948:GLU:HB3	2:C:953:VAL:HG23	1.79	0.64
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.78	0.64
1:B:100:LEU:HB2	1:B:115:LEU:HD11	1.80	0.64
4:E:41:GLU:HA	4:E:45:ARG:HG3	1.79	0.64
3:D:1101:VAL:HG21	3:D:1424:VAL:HG13	1.79	0.64
3:D:368:VAL:HB	3:D:377:VAL:HB	1.78	0.63
3:D:23:TYR:O	3:D:49:ILE:HG23	1.99	0.63
2:C:550:LEU:HD23	2:C:905:ILE:HD11	1.79	0.63
3:D:238:PRO:HA	3:D:313:MET:HG2	1.80	0.63
3:D:216:VAL:HG22	3:D:340:THR:HG22	1.81	0.63
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.79	0.63
3:D:1400:VAL:HG12	3:D:1401:GLU:HG2	1.79	0.63
5:F:408:LEU:O	6:G:122:ASN:ND2	2.31	0.62
2:C:274:ARG:HG3	2:C:285:LEU:HB3	1.82	0.62
3:D:1290:LEU:HB2	3:D:1305:LEU:HB2	1.81	0.62
3:D:504:ASP:C	3:D:506:GLY:H	2.02	0.62
1:B:77:GLU:O	1:B:81:ASN:ND2	2.32	0.62
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.82	0.62
2:C:97:ARG:HH21	2:C:109:LYS:HD2	1.65	0.62
5:F:364:ARG:O	5:F:368:VAL:HG23	1.99	0.62
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.82	0.62
3:D:10:ILE:HG13	3:D:1434:TRP:CZ2	2.35	0.62
2:C:673:LEU:HD23	2:C:867:VAL:HA	1.80	0.61
2:C:905:ILE:HG23	2:C:906:PHE:H	1.65	0.61
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	1.81	0.61
3:D:789:LEU:O	3:D:793:THR:OG1	2.15	0.61
3:D:124:GLU:OE2	3:D:124:GLU:N	2.28	0.61
3:D:407:VAL:HG11	5:F:171:LYS:HD3	1.82	0.61
6:H:21:THR:HG22	6:H:22:GLU:H	1.65	0.61
1:A:42:ARG:NH1	2:C:857:ASP:HB3	2.15	0.61
3:D:58:CYS:SG	3:D:59:ALA:N	2.74	0.61
2:C:100:LEU:HD21	2:C:368:THR:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1378:TYR:HE2	3:D:1394:VAL:HG22	1.65	0.61
3:D:504:ASP:O	3:D:506:GLY:N	2.30	0.61
3:D:655:PRO:HA	3:D:658:LEU:HD12	1.82	0.61
3:D:704:ARG:NH1	3:D:743:ASP:OD2	2.30	0.61
5:F:209:PHE:HA	5:F:212:LEU:HD12	1.83	0.61
2:C:141:HIS:CE1	2:C:165:LEU:HD11	2.36	0.61
2:C:424:GLY:HA3	2:C:428:ARG:HE	1.65	0.61
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.83	0.61
3:D:274:ARG:HB2	3:D:279:VAL:HG21	1.82	0.61
3:D:1104:GLU:OE1	3:D:1374:GLN:NE2	2.33	0.61
1:A:86:VAL:HG13	1:A:124:ASN:HB2	1.83	0.61
2:C:270:GLY:H	2:C:288:ARG:NH2	1.99	0.61
3:D:593:ASN:OD1	3:D:593:ASN:N	2.34	0.61
3:D:215:TYR:HE1	3:D:380:GLU:HB3	1.66	0.60
3:D:416:ALA:HB2	3:D:432:TYR:HA	1.83	0.60
3:D:781:PRO:HG2	3:D:911:LEU:HD23	1.83	0.60
3:D:800:LYS:HE2	3:D:830:ALA:HB3	1.82	0.60
3:D:660:LYS:HA	3:D:663:GLU:HG3	1.84	0.60
2:C:101:ILE:HG23	2:C:107:LEU:HB3	1.83	0.60
2:C:399:ASN:OD1	2:C:402:SER:OG	2.19	0.60
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.84	0.60
3:D:42:ASP:OD2	3:D:48:ARG:NH2	2.34	0.60
2:C:676:ILE:HG23	2:C:988:VAL:HG13	1.82	0.60
3:D:73:CYS:SG	3:D:74:GLU:N	2.75	0.60
3:D:782:SER:O	3:D:786:ILE:HD12	2.02	0.60
3:D:846:PRO:HB3	3:D:880:ILE:HD12	1.83	0.60
1:B:48:ILE:HG23	1:B:173:PRO:HD2	1.84	0.59
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.84	0.59
1:A:206:THR:HG23	1:A:209:GLU:H	1.66	0.59
2:C:141:HIS:HE1	2:C:165:LEU:HD11	1.67	0.59
5:F:353:GLU:HG2	6:G:127:ARG:HB3	1.84	0.59
3:D:484:PRO:O	3:D:489:ARG:NH1	2.34	0.59
3:D:756:GLN:O	3:D:760:ARG:HG2	2.01	0.59
3:D:972:LEU:HD23	3:D:976:GLN:HE21	1.66	0.59
5:F:80:PRO:HA	5:F:83:GLN:HB2	1.84	0.59
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.02	0.59
6:H:56:GLU:HG3	6:H:64:ARG:HD2	1.83	0.59
1:B:143:ARG:NE	1:B:145:ASP:OD1	2.33	0.59
2:C:690:ILE:HD13	2:C:869:VAL:HG23	1.83	0.59
3:D:313:MET:HG3	3:D:314:PRO:HD2	1.85	0.59
2:C:1013:TYR:HA	2:C:1020:PRO:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:THR:HG23	1:B:209:GLU:H	1.68	0.59
2:C:185:LYS:HA	2:C:189:ARG:O	2.02	0.59
3:D:259:VAL:HG11	3:D:293:VAL:HG12	1.84	0.59
3:D:238:PRO:HB3	3:D:317:VAL:O	2.02	0.59
3:D:569:ASN:ND2	5:F:84:TYR:OH	2.34	0.59
2:C:686:ASP:OD1	2:C:879:ARG:NH2	2.36	0.59
3:D:1154:GLU:HG2	3:D:1159:ARG:HG2	1.85	0.59
2:C:288:ARG:NE	2:C:288:ARG:HA	2.18	0.58
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.35	0.58
3:D:1152:GLU:OE1	3:D:1159:ARG:NH2	2.32	0.58
2:C:1076:VAL:HG22	3:D:752:SER:HB2	1.83	0.58
4:E:40:LEU:HD13	4:E:45:ARG:HD2	1.85	0.58
1:A:156:HIS:CD2	1:A:158:ILE:HG12	2.39	0.58
2:C:751:PRO:HG3	2:C:796:GLU:HA	1.84	0.58
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.38	0.58
1:A:168:ASP:N	1:A:168:ASP:OD1	2.36	0.58
3:D:1129:THR:HG23	3:D:1131:SER:HB3	1.85	0.58
2:C:285:LEU:HD12	2:C:301:GLU:HG2	1.85	0.58
3:D:902:LEU:H	3:D:902:LEU:HD23	1.68	0.58
3:D:1278:ASP:N	3:D:1278:ASP:OD1	2.36	0.58
3:D:1379:VAL:O	3:D:1392:GLY:HA2	2.04	0.58
3:D:58:CYS:SG	3:D:60:CYS:N	2.76	0.58
3:D:84:ILE:HA	3:D:87:ARG:HG2	1.85	0.58
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.84	0.58
1:B:65:PHE:HE1	3:D:813:LEU:HD13	1.69	0.58
3:D:39:PRO:HG2	3:D:47:GLU:HG2	1.85	0.58
1:A:14:ARG:HG2	1:B:231:ALA:HB3	1.85	0.58
3:D:812:ALA:O	3:D:816:HIS:HB2	2.04	0.58
2:C:711:GLU:HG2	2:C:822:VAL:HG12	1.86	0.57
2:C:721:ARG:NH2	6:G:95:ASN:OD1	2.37	0.57
2:C:1044:GLY:O	2:C:1046:ALA:N	2.37	0.57
3:D:841:TYR:HB2	3:D:864:VAL:HG13	1.86	0.57
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.86	0.57
3:D:786:ILE:HG21	3:D:1027:GLY:H	1.69	0.57
2:C:197:LEU:HA	2:C:200:LEU:HD12	1.86	0.57
2:C:266:ARG:HD3	2:C:273:GLY:HA3	1.86	0.57
3:D:804:LEU:O	3:D:831:GLY:HA2	2.04	0.57
1:B:86:VAL:HG13	1:B:124:ASN:HB2	1.85	0.57
2:C:567:GLN:HB2	2:C:997:LEU:HD12	1.86	0.57
3:D:1135:ARG:NH2	3:D:1350:GLU:OE2	2.37	0.57
3:D:357:GLU:HA	3:D:387:LEU:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:OD2	2:C:832:LYS:NZ	2.34	0.57
3:D:547:LEU:HD11	3:D:578:VAL:HG23	1.86	0.57
3:D:1462:LEU:O	3:D:1466:VAL:HG23	2.05	0.57
3:D:1472:ILE:O	3:D:1477:GLY:HA3	2.05	0.57
3:D:242:LEU:HD22	3:D:285:PRO:HG3	1.86	0.57
2:C:1005:MET:HG3	2:C:1005:MET:O	2.02	0.57
2:C:1092:LEU:HD13	2:C:1099:VAL:HG11	1.86	0.57
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.87	0.57
3:D:539:ASP:OD2	3:D:598:ARG:NH2	2.38	0.57
2:C:861:LEU:HB2	2:C:865:THR:HG23	1.87	0.57
1:B:68:ILE:HB	1:B:71:VAL:HB	1.85	0.57
2:C:165:LEU:HA	2:C:166:PRO:O	2.05	0.57
3:D:1096:ARG:HB2	3:D:1096:ARG:HH11	1.70	0.56
2:C:604:ALA:HB3	2:C:612:VAL:HG12	1.87	0.56
1:A:178:ALA:HB2	2:C:864:GLY:H	1.70	0.56
3:D:892:ASP:OD2	3:D:894:LYS:HG2	2.06	0.56
1:A:56:VAL:HG13	1:A:142:VAL:HG12	1.87	0.56
2:C:290:LEU:HB2	2:C:300:ASP:HA	1.87	0.56
2:C:846:LYS:HB3	3:D:741:ASP:HB2	1.88	0.56
3:D:1472:ILE:HG22	3:D:1474:ALA:H	1.71	0.56
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.86	0.56
2:C:134:ARG:NH1	2:C:392:SER:OG	2.38	0.56
3:D:1207:TYR:HA	3:D:1214:PRO:HA	1.88	0.56
3:D:465:LEU:HD22	3:D:509:PRO:HB2	1.88	0.56
3:D:131:LYS:HG3	3:D:568:ARG:HG2	1.88	0.56
2:C:369:PRO:O	2:C:372:LEU:N	2.30	0.56
3:D:908:LYS:HB3	3:D:1027:GLY:HA3	1.88	0.56
3:D:1205:TYR:CE1	3:D:1366:LYS:HD3	2.41	0.56
4:E:46:PRO:HB3	4:E:54:LEU:HD13	1.88	0.56
2:C:89:THR:HG23	2:C:129:ILE:HA	1.88	0.56
1:A:38:ASN:H	1:A:39:PRO:HD2	1.70	0.55
1:A:48:ILE:HG22	1:A:173:PRO:HD2	1.88	0.55
3:D:843:PHE:HB2	3:D:866:VAL:HG13	1.88	0.55
4:E:54:LEU:HD22	4:E:63:TRP:HE1	1.71	0.55
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.88	0.55
2:C:606:VAL:HG12	2:C:611:ILE:HG12	1.89	0.55
3:D:207:PHE:O	3:D:391:ALA:N	2.39	0.55
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.88	0.55
2:C:1084:SER:HB2	3:D:613:ARG:HH12	1.72	0.55
1:A:156:HIS:HD2	1:A:158:ILE:HG12	1.70	0.55
1:B:58:ILE:HD13	1:B:140:MET:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.42	0.55
3:D:215:TYR:CE1	3:D:380:GLU:HB3	2.42	0.55
3:D:207:PHE:HB2	3:D:391:ALA:HB3	1.89	0.55
5:F:392:VAL:HG12	5:F:393:THR:H	1.72	0.55
1:A:156:HIS:HE1	1:A:167:VAL:O	1.89	0.55
3:D:186:VAL:N	3:D:189:GLN:OE1	2.36	0.55
3:D:562:ALA:HB1	3:D:567:ILE:HD11	1.89	0.55
3:D:1137:ARG:H	3:D:1137:ARG:HD2	1.72	0.54
3:D:324:ALA:HB1	3:D:331:VAL:HG11	1.89	0.54
3:D:1486:VAL:HG11	4:E:22:VAL:HG13	1.89	0.54
5:F:394:ARG:O	5:F:397:ILE:HG13	2.07	0.54
3:D:1462:LEU:HD21	3:D:1472:ILE:HG23	1.89	0.54
2:C:95:TYR:HD2	2:C:114:PHE:HB3	1.72	0.54
3:D:539:ASP:OD1	5:F:316:SER:OG	2.14	0.54
3:D:820:GLU:HG2	3:D:825:ALA:O	2.08	0.54
2:C:358:ARG:HG2	2:C:371:LYS:O	2.07	0.54
2:C:143:SER:O	2:C:147:TYR:OH	2.17	0.54
5:F:223:ALA:HB2	5:F:242:TRP:HB2	1.90	0.54
2:C:25:SER:OG	2:C:337:GLY:N	2.38	0.54
2:C:598:GLU:HB2	2:C:615:TYR:HE1	1.71	0.54
2:C:794:PRO:HG3	2:C:1025:ALA:HA	1.89	0.54
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.41	0.54
3:D:112:ILE:HG13	3:D:113:GLY:N	2.22	0.54
3:D:782:SER:H	3:D:785:ILE:HD13	1.72	0.54
3:D:807:ALA:HB2	3:D:832:ARG:HB3	1.89	0.54
5:F:126:LEU:O	5:F:130:VAL:HG23	2.08	0.54
3:D:408:GLU:HG2	3:D:421:LEU:O	2.07	0.54
3:D:465:LEU:HD12	3:D:513:ILE:HD11	1.89	0.54
3:D:811:GLU:O	3:D:815:ALA:HB3	2.06	0.54
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.43	0.54
4:E:33:HIS:O	4:E:37:ASN:ND2	2.41	0.54
3:D:206:ARG:HE	3:D:394:LEU:HB2	1.72	0.54
1:B:65:PHE:CE1	3:D:813:LEU:HD13	2.43	0.54
3:D:911:LEU:O	3:D:915:VAL:HG23	2.07	0.54
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.43	0.54
2:C:1041:GLU:HB3	3:D:1223:ILE:HD13	1.90	0.53
2:C:115:LEU:HD12	2:C:378:LEU:HD22	1.89	0.53
2:C:557:ARG:HA	2:C:560:MET:HG3	1.89	0.53
3:D:1003:VAL:O	3:D:1007:VAL:HG13	2.06	0.53
1:A:185:ARG:HB3	1:A:190:THR:HG23	1.91	0.53
2:C:1068:GLU:O	2:C:1072:LYS:HG2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1263:PHE:HE2	3:D:1371:VAL:HG11	1.74	0.53
3:D:1404:ASN:O	3:D:1409:ALA:HB3	2.08	0.53
3:D:412:GLY:N	3:D:435:VAL:O	2.39	0.53
2:C:1007:ALA:HB2	3:D:648:MET:HG3	1.90	0.53
3:D:785:ILE:HG13	3:D:939:PHE:CE2	2.44	0.53
2:C:627:ARG:HG3	2:C:628:PHE:N	2.24	0.53
5:F:79:ASP:HB3	5:F:80:PRO:HD3	1.90	0.53
1:B:161:ARG:HG3	1:B:163:ASN:H	1.73	0.53
2:C:863:ASP:N	2:C:863:ASP:OD1	2.41	0.53
3:D:1292:VAL:HG23	3:D:1305:LEU:HD11	1.90	0.53
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.91	0.53
3:D:568:ARG:HH11	3:D:571:LYS:HD2	1.74	0.53
3:D:792:ILE:HG21	3:D:941:PHE:CD1	2.44	0.53
2:C:410:ILE:HB	2:C:453:THR:O	2.08	0.53
3:D:237:LYS:HB3	3:D:238:PRO:HD2	1.91	0.53
5:F:371:LEU:HD22	5:F:375:LEU:HB2	1.91	0.53
2:C:41:ASN:OD1	2:C:41:ASN:N	2.39	0.52
3:D:1233:GLY:HA2	3:D:1236:LEU:HD12	1.91	0.52
3:D:86:ARG:HG2	3:D:522:PRO:HG2	1.89	0.52
1:A:229:GLN:HB3	1:B:12:THR:HG22	1.91	0.52
2:C:84:ARG:NH2	2:C:133:ASP:OD1	2.35	0.52
2:C:276:LYS:HE3	2:C:464:LEU:HD21	1.91	0.52
2:C:50:GLU:OE2	2:C:345:ARG:NH1	2.42	0.52
2:C:71:TYR:HA	2:C:96:ALA:HA	1.92	0.52
3:D:1164:ARG:NH2	3:D:1170:ASP:OD1	2.43	0.52
1:B:59:GLU:HG2	1:B:139:ASN:HB3	1.91	0.52
3:D:957:PRO:HG2	3:D:1007:VAL:HG12	1.90	0.52
3:D:12:LEU:HD21	3:D:104:PHE:HZ	1.73	0.52
3:D:546:ARG:NH2	3:D:576:GLU:OE2	2.42	0.52
2:C:1088:LEU:O	2:C:1092:LEU:HB2	2.10	0.52
2:C:1086:ARG:HG2	2:C:1111:ILE:HD12	1.91	0.52
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.73	0.52
3:D:1486:VAL:HA	4:E:74:VAL:O	2.09	0.52
2:C:100:LEU:HD22	2:C:372:LEU:HD21	1.91	0.52
3:D:214:GLU:O	3:D:383:GLY:HA2	2.10	0.52
3:D:436:GLU:HG3	3:D:445:ARG:HB2	1.92	0.52
1:B:48:ILE:CG2	1:B:173:PRO:HD2	2.40	0.52
2:C:200:LEU:HD22	2:C:300:ASP:HB3	1.92	0.52
2:C:170:PRO:HG2	2:C:258:TYR:CD2	2.45	0.52
2:C:524:VAL:HG22	2:C:525:SER:H	1.75	0.52
2:C:690:ILE:HB	2:C:852:ILE:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:413:ASP:OD1	5:F:178:ARG:NH1	2.36	0.52
2:C:204:GLN:HE22	2:C:225:SER:HB3	1.75	0.51
2:C:94:LEU:O	2:C:114:PHE:HA	2.09	0.51
3:D:1428:ALA:O	3:D:1431:THR:HG23	2.10	0.51
3:D:754:PHE:O	3:D:758:GLU:HG2	2.10	0.51
1:A:153:ALA:HA	1:A:156:HIS:CE1	2.44	0.51
3:D:376:GLU:O	3:D:378:ILE:HG13	2.10	0.51
3:D:611:GLN:O	3:D:616:GLN:HB2	2.10	0.51
2:C:1066:ALA:HA	2:C:1077:PRO:HD2	1.93	0.51
2:C:235:LEU:HD21	2:C:251:ASP:O	2.11	0.51
2:C:312:ALA:HB1	2:C:318:PRO:HG3	1.91	0.51
2:C:368:THR:HB	2:C:369:PRO:HD3	1.93	0.51
3:D:475:LYS:HA	3:D:478:LEU:HD12	1.91	0.51
3:D:835:SER:H	3:D:838:ARG:HE	1.58	0.51
2:C:578:VAL:HG23	2:C:579:VAL:HG12	1.92	0.51
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.45	0.51
3:D:206:ARG:HB3	3:D:207:PHE:CD1	2.46	0.51
3:D:222:GLY:HA2	3:D:333:LEU:O	2.10	0.51
3:D:813:LEU:HD12	3:D:814:ALA:N	2.25	0.51
1:A:188:GLN:HG2	1:A:189:ARG:HG2	1.93	0.51
1:B:4:SER:HA	1:B:7:LYS:HD3	1.93	0.51
2:C:1019:GLN:HB2	3:D:622:ARG:HB2	1.92	0.51
2:C:1101:THR:HG21	2:C:1111:ILE:HG21	1.93	0.51
2:C:17:PRO:O	2:C:20:GLU:HB3	2.11	0.51
3:D:1264:GLU:OE2	3:D:1425:THR:OG1	2.25	0.51
3:D:802:ALA:O	3:D:804:LEU:N	2.44	0.51
6:H:18:ASP:OD1	6:H:60:LYS:NZ	2.36	0.51
3:D:1042:ARG:O	3:D:1057:VAL:HB	2.10	0.51
2:C:1095:LEU:O	2:C:1097:LEU:N	2.41	0.51
3:D:612:GLY:O	3:D:614:PHE:N	2.44	0.51
5:F:132:ARG:O	5:F:136:LEU:HG	2.11	0.51
1:A:7:LYS:HG2	1:A:9:PRO:HD3	1.93	0.51
1:B:124:ASN:HD21	1:B:127:LEU:HD22	1.76	0.51
2:C:540:PHE:HE1	2:C:906:PHE:HE1	1.59	0.51
2:C:726:ILE:HG12	2:C:787:ASP:HB2	1.93	0.51
3:D:165:LYS:HG3	3:D:397:LYS:HB3	1.93	0.51
3:D:931:LEU:HA	3:D:934:LEU:HD12	1.93	0.51
3:D:799:LYS:HE2	3:D:801:GLY:HA3	1.92	0.50
3:D:850:LEU:HA	3:D:853:VAL:HB	1.93	0.50
2:C:73:LEU:HA	2:C:93:PRO:O	2.11	0.50
3:D:90:MET:HG3	3:D:521:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:411:HIS:O	6:G:120:THR:OG1	2.16	0.50
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.11	0.50
3:D:84:ILE:HG12	3:D:85:VAL:N	2.25	0.50
6:G:34:LEU:HD23	6:G:129:MET:HE1	1.92	0.50
1:A:59:GLU:HG2	1:A:139:ASN:HB3	1.94	0.50
2:C:66:LEU:HD13	2:C:100:LEU:HB3	1.93	0.50
3:D:366:LYS:NZ	3:D:376:GLU:OE1	2.39	0.50
1:B:83:LYS:O	1:B:170:VAL:HG21	2.12	0.50
1:B:6:LEU:C	1:B:8:ALA:H	2.15	0.50
2:C:15:LEU:HD11	2:C:457:ALA:HB1	1.93	0.50
2:C:276:LYS:O	2:C:280:LYS:HD2	2.11	0.50
3:D:1125:PRO:HA	3:D:1131:SER:O	2.11	0.50
3:D:1479:ASP:HA	3:D:1482:ARG:HD3	1.94	0.50
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.94	0.50
2:C:575:GLN:HB2	2:C:670:GLN:HA	1.94	0.50
1:B:58:ILE:HB	1:B:61:VAL:HB	1.93	0.49
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.93	0.49
2:C:677:MET:HB3	2:C:987:ILE:HD13	1.94	0.49
3:D:371:ILE:HG13	3:D:372:ASP:H	1.76	0.49
2:C:11:GLU:HG2	2:C:535:SER:HB2	1.94	0.49
4:E:51:LEU:HD12	4:E:53:GLY:H	1.77	0.49
2:C:971:LYS:HA	2:C:988:VAL:HA	1.94	0.49
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.93	0.49
3:D:233:LYS:HD3	3:D:235:ALA:HB3	1.94	0.49
3:D:30:GLU:O	3:D:43:GLY:HA3	2.12	0.49
3:D:475:LYS:O	3:D:479:GLU:HG2	2.11	0.49
3:D:87:ARG:HB3	3:D:523:ASP:HB2	1.94	0.49
3:D:646:LYS:HB3	3:D:688:TRP:CH2	2.47	0.49
3:D:52:PRO:HD3	3:D:78:VAL:HG13	1.93	0.49
2:C:759:THR:HB	2:C:785:VAL:CG2	2.42	0.49
6:G:52:VAL:HG12	6:G:70:ILE:HA	1.94	0.49
1:A:41:ARG:HA	1:A:177:VAL:HG11	1.94	0.49
1:B:94:LEU:HD21	1:B:119:ASP:HB2	1.94	0.49
3:D:176:ASP:OD1	3:D:389:GLU:HG2	2.13	0.49
2:C:146:VAL:HG11	2:C:306:THR:HG22	1.94	0.49
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.95	0.49
3:D:1110:ALA:O	3:D:1202:GLN:HB2	2.12	0.49
3:D:136:ASP:HB3	3:D:137:PRO:CD	2.43	0.49
5:F:346:THR:O	5:F:350:LEU:HB2	2.12	0.49
6:G:86:ALA:HA	6:G:107:LEU:HG	1.95	0.49
1:A:55:SER:HA	1:A:167:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1031:ASN:HB3	3:D:1034:GLN:HG3	1.92	0.49
3:D:1112:CYS:HB2	3:D:1195:GLN:HB3	1.95	0.49
3:D:1286:THR:HB	3:D:1289:LYS:O	2.13	0.49
3:D:303:PRO:O	3:D:305:ALA:N	2.45	0.49
6:G:31:LEU:HA	6:G:51:PRO:HB2	1.95	0.49
1:A:44:LEU:O	1:A:174:VAL:HG21	2.12	0.49
1:A:57:TYR:CE1	1:A:163:ASN:HB2	2.48	0.49
2:C:913:GLU:O	2:C:917:LEU:HD12	2.12	0.49
1:B:86:VAL:CG1	1:B:124:ASN:HB2	2.43	0.49
3:D:764:LEU:HD23	3:D:767:HIS:CE1	2.48	0.49
2:C:725:ASP:HB2	6:G:99:HIS:HE1	1.78	0.49
3:D:959:GLU:HG3	3:D:1006:ALA:HB1	1.95	0.49
2:C:541:SER:O	2:C:545:ASN:HB2	2.13	0.48
3:D:1462:LEU:HD23	3:D:1472:ILE:HD12	1.94	0.48
1:A:213:GLN:O	1:A:217:ILE:HG13	2.14	0.48
1:B:128:HIS:NE2	1:B:131:THR:HG23	2.28	0.48
1:B:73:GLU:CD	1:B:131:THR:H	2.16	0.48
2:C:108:ILE:HB	2:C:368:THR:HG23	1.95	0.48
3:D:254:GLU:O	3:D:255:GLU:HB2	2.13	0.48
3:D:440:VAL:HG23	3:D:441:ARG:H	1.77	0.48
5:F:376:ILE:HG22	5:F:377:ASP:HB2	1.95	0.48
1:B:13:VAL:HG22	1:B:23:PHE:HD1	1.78	0.48
2:C:75:GLU:O	2:C:93:PRO:HD3	2.13	0.48
2:C:922:PHE:CD2	2:C:964:LYS:HD2	2.48	0.48
3:D:1364:HIS:NE2	3:D:1366:LYS:HE3	2.28	0.48
3:D:1349:VAL:HA	3:D:1368:ILE:HG21	1.94	0.48
3:D:41:ARG:HB2	3:D:42:ASP:H	1.53	0.48
3:D:39:PRO:HB3	3:D:45:PHE:O	2.13	0.48
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.94	0.48
5:F:355:GLU:HA	5:F:358:LEU:HB3	1.95	0.48
2:C:2:GLU:O	2:C:899:GLN:HB2	2.14	0.48
2:C:712:ALA:O	2:C:820:ARG:HB2	2.13	0.48
3:D:56:TYR:O	3:D:80:VAL:HG21	2.13	0.48
1:A:122:ILE:HG22	1:A:124:ASN:H	1.78	0.48
1:A:178:ALA:HB2	2:C:864:GLY:N	2.29	0.48
3:D:481:MET:SD	3:D:489:ARG:HB2	2.53	0.48
2:C:350:ARG:HG2	2:C:353:ARG:NH1	2.29	0.48
3:D:351:MET:HG3	3:D:370:ALA:HB2	1.95	0.48
3:D:804:LEU:HD22	3:D:825:ALA:HB1	1.95	0.48
2:C:151:ASP:HB2	2:C:157:ARG:O	2.13	0.48
2:C:266:ARG:HD2	2:C:266:ARG:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1330:ILE:HG21	3:D:1335:LEU:HD12	1.95	0.48
5:F:152:ASP:HB2	5:F:153:PRO:HD3	1.95	0.48
3:D:770:LEU:HA	3:D:777:PRO:HA	1.94	0.48
3:D:838:ARG:HD3	3:D:874:GLU:HB3	1.96	0.48
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.96	0.48
2:C:697:ARG:O	2:C:698:ASP:C	2.51	0.48
4:E:60:ALA:O	4:E:63:TRP:HB2	2.12	0.48
1:B:81:ASN:O	1:B:127:LEU:HD21	2.14	0.48
2:C:151:ASP:HB3	2:C:154:ARG:O	2.13	0.48
2:C:863:ASP:O	2:C:865:THR:N	2.41	0.48
3:D:1381:VAL:HG23	3:D:1391:GLU:HB2	1.95	0.48
2:C:250:ARG:HB3	2:C:250:ARG:HE	1.46	0.47
3:D:1155:VAL:C	3:D:1157:GLY:H	2.16	0.47
3:D:1172:HIS:HA	3:D:1175:ILE:HD12	1.96	0.47
3:D:1192:LEU:HG	3:D:1369:GLU:HB3	1.95	0.47
3:D:45:PHE:HB3	3:D:86:ARG:HH22	1.79	0.47
3:D:764:LEU:HD12	3:D:765:SER:N	2.29	0.47
1:B:30:ARG:HE	2:C:854:PRO:HB3	1.80	0.47
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.96	0.47
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.96	0.47
3:D:817:GLU:O	3:D:821:VAL:HG23	2.13	0.47
3:D:877:PRO:O	3:D:880:ILE:HG22	2.14	0.47
1:A:46:SER:OG	1:A:47:SER:N	2.46	0.47
2:C:346:VAL:O	2:C:350:ARG:HG3	2.14	0.47
5:F:94:LEU:HB3	5:F:97:GLU:HB2	1.96	0.47
2:C:535:SER:OG	2:C:537:LYS:NZ	2.40	0.47
2:C:798:GLY:H	2:C:827:VAL:HG12	1.79	0.47
3:D:117:ASP:HB3	3:D:150:ARG:HD3	1.96	0.47
3:D:413:ASP:OD1	3:D:413:ASP:N	2.47	0.47
5:F:232:ARG:HA	5:F:232:ARG:HD2	1.78	0.47
2:C:433:THR:C	2:C:435:TYR:H	2.17	0.47
2:C:780:GLU:O	2:C:781:LYS:HB3	2.15	0.47
4:E:27:ALA:HB2	4:E:61:GLU:HA	1.96	0.47
4:E:70:THR:HB	4:E:72:ARG:HG3	1.96	0.47
1:A:86:VAL:HG22	1:A:123:MET:HB2	1.96	0.47
3:D:686:GLU:HG3	3:D:686:GLU:H	1.36	0.47
3:D:804:LEU:HD21	3:D:829:VAL:HG21	1.96	0.47
3:D:850:LEU:HD21	3:D:881:LEU:HB2	1.96	0.47
5:F:88:ILE:HD13	5:F:193:ARG:HB2	1.96	0.47
6:G:34:LEU:HD13	6:G:134:HIS:CE1	2.50	0.47
3:D:135:LEU:HD22	3:D:137:PRO:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:348:GLN:HB2	3:D:351:MET:SD	2.54	0.47
3:D:632:VAL:O	3:D:727:GLN:HA	2.14	0.47
3:D:860:LEU:HD23	3:D:877:PRO:HB2	1.96	0.47
6:H:21:THR:HG22	6:H:22:GLU:N	2.30	0.47
2:C:264:PRO:HB2	2:C:289:THR:HG21	1.96	0.47
2:C:717:LEU:O	2:C:783:ARG:NH1	2.37	0.47
3:D:1278:ASP:HA	3:D:1319:VAL:O	2.15	0.47
3:D:62:LYS:HE2	3:D:75:ARG:HD3	1.95	0.47
3:D:800:LYS:HB2	3:D:829:VAL:HB	1.96	0.47
3:D:889:ALA:HB1	3:D:930:LEU:HA	1.96	0.47
2:C:25:SER:OG	2:C:335:THR:HB	2.15	0.47
2:C:584:GLU:O	2:C:588:VAL:HG13	2.15	0.47
2:C:97:ARG:HA	2:C:111:ASP:O	2.15	0.47
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	1.97	0.47
3:D:130:SER:HB3	3:D:132:TYR:HD2	1.79	0.47
3:D:1412:LYS:O	3:D:1414:PRO:HD3	2.15	0.47
3:D:9:ARG:HB2	3:D:1456:LYS:HG2	1.96	0.47
3:D:433:GLY:HA2	3:D:449:SER:H	1.79	0.47
3:D:800:LYS:HG2	3:D:802:ALA:O	2.15	0.47
3:D:892:ASP:OD2	3:D:895:VAL:HG23	2.15	0.47
1:B:62:LEU:HD12	1:B:63:HIS:H	1.79	0.47
3:D:269:PHE:HD1	3:D:283:PHE:HD1	1.63	0.47
3:D:719:VAL:O	3:D:721:VAL:HG13	2.15	0.47
5:F:405:LEU:HA	5:F:408:LEU:HD23	1.96	0.47
2:C:1081:VAL:HG11	2:C:1086:ARG:HG3	1.97	0.47
3:D:1341:PRO:HA	3:D:1376:MET:HE1	1.96	0.47
3:D:259:VAL:HG21	3:D:293:VAL:HG12	1.97	0.47
2:C:1029:GLY:HA3	3:D:623:VAL:O	2.14	0.47
1:A:83:LYS:HE2	1:A:168:ASP:HB2	1.97	0.46
3:D:1106:VAL:HG12	3:D:1107:VAL:H	1.81	0.46
3:D:1481:VAL:HG12	4:E:21:VAL:HG21	1.97	0.46
5:F:93:LEU:HD13	5:F:99:GLU:HG2	1.96	0.46
2:C:149:THR:HG22	2:C:150:PRO:O	2.15	0.46
2:C:302:VAL:O	2:C:305:PRO:HD2	2.14	0.46
2:C:739:GLU:OE1	6:G:61:ARG:HB2	2.15	0.46
3:D:1271:LYS:HE3	3:D:1334:GLN:HE22	1.80	0.46
3:D:546:ARG:O	3:D:550:ARG:HG2	2.15	0.46
3:D:495:ARG:O	3:D:498:VAL:HG13	2.15	0.46
3:D:565:ILE:HD12	3:D:566:ILE:HG13	1.97	0.46
4:E:41:GLU:O	4:E:42:PRO:C	2.53	0.46
6:G:63:VAL:HG12	6:G:93:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:VAL:HA	1:B:78:ILE:HD12	1.97	0.46
2:C:1076:VAL:HA	2:C:1077:PRO:HD3	1.69	0.46
3:D:1282:ARG:HA	3:D:1315:ASP:OD1	2.16	0.46
3:D:635:PRO:HG2	3:D:636:GLN:HG2	1.96	0.46
1:B:54:THR:OG1	1:B:158:ILE:HG13	2.16	0.46
1:B:80:LEU:HG	3:D:844:ALA:HB2	1.98	0.46
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.98	0.46
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.76	0.46
3:D:1493:LYS:O	3:D:1496:GLU:HB3	2.14	0.46
2:C:431:HIS:ND1	2:C:433:THR:OG1	2.42	0.46
2:C:598:GLU:HB2	2:C:615:TYR:CE1	2.50	0.46
3:D:130:SER:O	3:D:568:ARG:NH2	2.49	0.46
3:D:1317:ASP:OD1	3:D:1317:ASP:N	2.48	0.46
3:D:1440:PHE:O	3:D:1442:ASN:N	2.42	0.46
3:D:845:ASN:HB2	3:D:848:GLU:HB2	1.98	0.46
5:F:388:ALA:HB3	5:F:397:ILE:HD13	1.97	0.46
6:H:95:ASN:OD1	6:H:95:ASN:N	2.48	0.46
3:D:90:MET:HG2	3:D:519:VAL:O	2.15	0.46
1:B:191:ASP:N	1:B:191:ASP:OD1	2.42	0.46
2:C:49:ARG:HH11	2:C:49:ARG:HB2	1.81	0.46
2:C:787:ASP:OD1	2:C:789:SER:OG	2.33	0.46
3:D:123:LEU:HD23	3:D:152:LEU:HD13	1.96	0.46
2:C:177:GLU:HG3	2:C:179:ASN:H	1.81	0.46
2:C:424:GLY:O	2:C:428:ARG:HG3	2.16	0.46
2:C:678:PRO:HG2	3:D:943:THR:HA	1.96	0.46
3:D:1271:LYS:HZ1	3:D:1273:VAL:HG12	1.81	0.46
3:D:30:GLU:HB3	3:D:40:GLU:HG2	1.97	0.46
3:D:566:ILE:HD13	5:F:217:ASN:HB3	1.98	0.46
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.99	0.45
3:D:835:SER:H	3:D:838:ARG:NE	2.15	0.45
6:G:11:ARG:HH21	6:H:17:PRO:HG2	1.81	0.45
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.97	0.45
3:D:1118:ILE:HD11	3:D:1346:ARG:HD2	1.98	0.45
3:D:510:GLU:O	3:D:513:ILE:HD12	2.17	0.45
3:D:529:GLN:NE2	3:D:532:GLY:O	2.48	0.45
3:D:729:HIS:HA	3:D:730:PRO:HD2	1.81	0.45
5:F:369:LEU:HD13	5:F:373:LYS:HE3	1.97	0.45
6:H:7:GLU:N	6:H:8:PRO:HD2	2.30	0.45
3:D:1036:ARG:HH21	3:D:1042:ARG:HA	1.82	0.45
3:D:840:LYS:HD3	3:D:841:TYR:CE1	2.52	0.45
3:D:959:GLU:N	3:D:959:GLU:OE1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:23:LEU:HB3	6:H:59:ARG:HH12	1.82	0.45
1:A:18:ARG:HH22	1:A:88:ARG:NH2	2.08	0.45
1:B:175:ARG:N	1:B:200:TRP:O	2.27	0.45
2:C:700:TYR:HD2	2:C:996:LYS:HB2	1.81	0.45
2:C:810:ASP:HA	2:C:811:PRO:HD3	1.79	0.45
1:A:42:ARG:HD2	2:C:978:ARG:HA	1.97	0.45
3:D:102:ILE:O	3:D:102:ILE:HG13	2.17	0.45
3:D:266:GLU:O	3:D:314:PRO:HG3	2.17	0.45
4:E:40:LEU:HG	4:E:67:GLU:HG2	1.97	0.45
1:A:62:LEU:H	1:A:62:LEU:HD12	1.81	0.45
2:C:95:TYR:HA	2:C:113:VAL:O	2.15	0.45
2:C:627:ARG:O	2:C:638:ASP:HB2	2.16	0.45
3:D:1258:ARG:NH1	3:D:1261:GLU:OE2	2.50	0.45
3:D:1432:LYS:HD2	3:D:1433:SER:H	1.82	0.45
3:D:408:GLU:HG3	3:D:422:ALA:HA	1.99	0.45
3:D:161:LEU:O	3:D:449:SER:HB2	2.17	0.45
3:D:612:GLY:O	3:D:615:ARG:N	2.50	0.45
5:F:108:GLU:HB3	5:F:176:ILE:HG23	1.99	0.45
5:F:355:GLU:HG3	5:F:358:LEU:HD22	1.99	0.45
1:B:19:GLU:O	1:B:200:TRP:HA	2.16	0.45
2:C:446:GLY:O	2:C:449:ILE:HG13	2.17	0.45
2:C:627:ARG:HG3	2:C:628:PHE:H	1.80	0.45
2:C:690:ILE:HG23	2:C:694:LEU:HD12	1.99	0.45
2:C:725:ASP:HB2	6:G:99:HIS:CE1	2.51	0.45
2:C:815:LEU:HD21	2:C:821:GLU:HA	1.98	0.45
3:D:1259:VAL:O	3:D:1263:PHE:HD1	1.97	0.45
3:D:8:VAL:HG12	3:D:1434:TRP:CH2	2.51	0.45
3:D:939:PHE:O	3:D:943:THR:HG23	2.16	0.45
2:C:190:LYS:HB3	2:C:190:LYS:HE2	1.66	0.45
2:C:309:TYR:HA	2:C:312:ALA:HB3	1.98	0.45
2:C:439:CYS:HA	2:C:440:PRO:HD3	1.75	0.45
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.98	0.45
3:D:828:LYS:O	3:D:828:LYS:HG2	2.16	0.45
3:D:907:GLU:HG2	3:D:908:LYS:H	1.82	0.45
2:C:782:ALA:HB1	6:G:34:LEU:HD12	1.99	0.45
2:C:1002:GLU:C	2:C:1004:LYS:H	2.19	0.45
2:C:1008:ARG:NH1	3:D:624:ASP:OD1	2.49	0.45
2:C:479:VAL:N	2:C:506:ASN:O	2.42	0.45
3:D:553:ARG:NH1	3:D:570:GLU:OE1	2.49	0.45
1:A:88:ARG:HD3	1:A:90:LEU:HD23	1.99	0.45
1:B:132:LEU:HD12	1:B:132:LEU:HA	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1016:ILE:HG13	2:C:1017:THR:H	1.81	0.45
2:C:593:ALA:HB1	2:C:658:GLY:HA3	1.98	0.45
3:D:709:HIS:HA	3:D:1227:GLN:HB3	1.99	0.45
3:D:177:ALA:HB3	3:D:191:LEU:O	2.17	0.45
3:D:800:LYS:HG3	3:D:804:LEU:HG	1.98	0.45
3:D:809:PRO:O	3:D:812:ALA:HB3	2.17	0.45
3:D:907:GLU:HG3	3:D:1025:GLN:O	2.17	0.45
5:F:399:GLN:O	5:F:403:LYS:HG2	2.17	0.45
1:A:19:GLU:O	1:A:201:THR:N	2.50	0.45
1:A:212:ASN:O	1:A:215:VAL:HG22	2.17	0.45
2:C:1024:LYS:H	2:C:1026:GLN:HE22	1.65	0.45
2:C:1043:TYR:CE1	3:D:710:ARG:HB2	2.52	0.45
2:C:214:TYR:CE1	2:C:311:PHE:HB3	2.52	0.45
2:C:110:GLU:HG2	2:C:369:PRO:HB3	1.99	0.45
2:C:721:ARG:NH2	6:G:94:ASP:OD1	2.50	0.45
3:D:1377:LYS:HE3	3:D:1394:VAL:HG13	1.99	0.45
3:D:879:ARG:NE	3:D:902:LEU:O	2.31	0.45
4:E:26:ARG:O	4:E:30:LEU:HB2	2.16	0.45
2:C:352:ALA:HA	2:C:355:VAL:HG12	2.00	0.44
3:D:1434:TRP:CZ3	3:D:1457:ASP:HB2	2.52	0.44
3:D:202:VAL:HG12	3:D:204:LEU:HD12	1.98	0.44
3:D:229:ALA:O	3:D:231:VAL:HG22	2.17	0.44
1:A:70:GLY:HA3	1:A:136:GLY:HA2	1.98	0.44
1:B:153:ALA:HA	1:B:156:HIS:HE1	1.82	0.44
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.82	0.44
3:D:415:VAL:O	3:D:416:ALA:HB2	2.17	0.44
1:A:134:GLU:CD	1:A:134:GLU:H	2.19	0.44
1:B:99:LEU:HA	1:B:99:LEU:HD13	1.85	0.44
2:C:432:ARG:NH1	2:C:492:ASP:OD2	2.49	0.44
5:F:368:VAL:HG12	5:F:369:LEU:N	2.31	0.44
1:B:39:PRO:O	1:B:43:ILE:HG12	2.18	0.44
2:C:1044:GLY:HA2	3:D:1475:GLY:HA3	1.99	0.44
2:C:492:ASP:HB3	2:C:518:LYS:HB3	1.99	0.44
3:D:1412:LYS:HD2	3:D:1414:PRO:HG3	1.99	0.44
6:H:57:ILE:HG22	6:H:58:LYS:HG2	1.99	0.44
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.87	0.44
1:B:87:VAL:HG12	1:B:122:ILE:HG23	1.99	0.44
2:C:411:SER:OG	2:C:413:LEU:HD12	2.17	0.44
2:C:472:ARG:HD3	2:C:534:VAL:HA	2.00	0.44
2:C:444:PRO:HA	2:C:563:ASN:HD21	1.82	0.44
2:C:648:ARG:HG2	2:C:648:ARG:H	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:219:GLU:HG2	3:D:220:ARG:H	1.83	0.44
3:D:7:LYS:HG2	3:D:1458:GLU:OE2	2.17	0.44
1:A:100:LEU:HD13	1:A:115:LEU:HD21	1.98	0.44
2:C:263:ASP:HB2	2:C:264:PRO:HD3	1.98	0.44
2:C:614:ARG:HH11	2:C:620:LEU:HD12	1.83	0.44
3:D:584:ASN:CG	3:D:590:PRO:HD2	2.38	0.44
3:D:601:ARG:NH2	3:D:605:ASP:O	2.51	0.44
1:B:176:ARG:HD3	3:D:884:ARG:HH22	1.83	0.44
6:H:18:ASP:HB3	6:H:61:ARG:NH2	2.33	0.44
1:B:221:HIS:HA	1:B:224:TYR:CD2	2.53	0.44
2:C:170:PRO:HG2	2:C:258:TYR:HD2	1.82	0.44
2:C:363:SER:O	2:C:364:GLU:HG3	2.18	0.44
2:C:560:MET:O	2:C:564:MET:HB2	2.18	0.44
3:D:1123:PHE:HE2	3:D:1184:GLN:HA	1.82	0.44
3:D:136:ASP:HB3	3:D:137:PRO:HD3	2.00	0.44
3:D:46:ASP:OD2	3:D:48:ARG:N	2.51	0.44
3:D:644:LEU:HA	3:D:645:PRO:HD3	1.82	0.44
3:D:875:THR:HG23	3:D:876:SER:O	2.18	0.44
3:D:999:THR:O	3:D:1003:VAL:HG13	2.17	0.44
4:E:30:LEU:HA	4:E:30:LEU:HD12	1.86	0.44
3:D:256:GLU:HG2	3:D:299:GLU:HG2	1.99	0.44
6:H:88:ALA:HB2	6:H:104:PRO:HA	2.00	0.44
1:B:53:VAL:HG21	1:B:82:LEU:HB3	2.00	0.43
2:C:396:ASP:O	2:C:402:SER:HB2	2.18	0.43
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.52	0.43
2:C:946:ARG:NH1	3:D:861:GLN:OE1	2.51	0.43
3:D:256:GLU:HB3	3:D:299:GLU:HG2	2.00	0.43
3:D:825:ALA:HA	3:D:826:PRO:HD3	1.74	0.43
1:B:100:LEU:O	1:B:115:LEU:HG	2.18	0.43
2:C:742:VAL:HG22	2:C:756:VAL:HG22	1.99	0.43
2:C:957:LYS:HG2	2:C:961:GLU:OE1	2.18	0.43
3:D:214:GLU:HA	3:D:341:GLU:O	2.18	0.43
4:E:43:GLU:HG3	4:E:44:GLU:H	1.83	0.43
2:C:397:GLU:N	2:C:633:GLN:OE1	2.51	0.43
2:C:634:GLY:HA3	2:C:704:HIS:NE2	2.33	0.43
2:C:879:ARG:O	2:C:881:ASN:N	2.51	0.43
3:D:503:LEU:HA	3:D:503:LEU:HD23	1.78	0.43
3:D:783:ARG:HG2	3:D:783:ARG:H	1.53	0.43
5:F:369:LEU:HA	5:F:372:ARG:HB3	1.99	0.43
1:A:218:LEU:O	1:A:222:LEU:HD22	2.19	0.43
2:C:1015:LEU:HA	2:C:1015:LEU:HD22	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:121:MET:HB2	2:C:127:PHE:HE2	1.84	0.43
2:C:194:VAL:HG21	2:C:221:LEU:O	2.18	0.43
2:C:200:LEU:HD13	2:C:300:ASP:HB3	2.01	0.43
3:D:135:LEU:HD23	3:D:453:ASP:O	2.18	0.43
3:D:943:THR:OG1	3:D:944:THR:N	2.51	0.43
4:E:33:HIS:C	4:E:37:ASN:HD21	2.21	0.43
3:D:760:ARG:NH1	4:E:61:GLU:OE2	2.52	0.43
1:B:85:LEU:HA	1:B:124:ASN:HD22	1.84	0.43
1:B:23:PHE:HB2	1:B:197:LEU:HD23	2.00	0.43
2:C:227:PHE:CE2	2:C:237:ARG:HD3	2.54	0.43
2:C:20:GLU:O	2:C:24:GLU:HB2	2.18	0.43
3:D:592:THR:O	3:D:593:ASN:C	2.56	0.43
3:D:984:THR:HG23	3:D:987:GLU:H	1.84	0.43
5:F:397:ILE:HG13	5:F:398:ARG:H	1.83	0.43
1:A:65:PHE:CE1	2:C:799:ILE:HD11	2.54	0.43
2:C:1058:ASP:HB2	3:D:621:LYS:HE3	2.01	0.43
2:C:456:ALA:HB1	2:C:538:GLN:O	2.19	0.43
2:C:64:LEU:HD22	2:C:359:MET:HG3	2.01	0.43
3:D:495:ARG:O	3:D:499:VAL:HG23	2.18	0.43
4:E:6:ILE:HD12	4:E:6:ILE:HA	1.83	0.43
5:F:166:LEU:HA	5:F:167:PRO:HD3	1.89	0.43
5:F:253:ASP:N	5:F:253:ASP:OD2	2.51	0.43
1:B:73:GLU:OE2	1:B:131:THR:OG1	2.29	0.43
2:C:1057:SER:OG	2:C:1058:ASP:N	2.51	0.43
3:D:167:GLU:O	3:D:206:ARG:NH2	2.51	0.43
3:D:504:ASP:C	3:D:506:GLY:N	2.67	0.43
3:D:921:ARG:HH11	3:D:921:ARG:HB3	1.84	0.43
4:E:54:LEU:HG	4:E:58:PRO:HB2	2.00	0.43
1:A:179:PHE:HA	1:A:197:LEU:HA	2.01	0.43
1:B:102:LYS:HB2	1:B:139:ASN:OD1	2.19	0.43
2:C:1018:GLN:HG3	2:C:1060:ILE:HD11	2.01	0.43
2:C:165:LEU:HA	2:C:166:PRO:C	2.39	0.43
3:D:289:THR:O	3:D:305:ALA:HA	2.18	0.43
5:F:329:TYR:CE2	5:F:333:ILE:HD11	2.54	0.43
2:C:264:PRO:O	2:C:266:ARG:NH1	2.52	0.43
2:C:288:ARG:CZ	2:C:288:ARG:HA	2.48	0.43
2:C:497:ALA:N	2:C:531:PHE:O	2.44	0.43
2:C:573:ARG:HG3	2:C:698:ASP:O	2.19	0.43
3:D:31:THR:O	3:D:32:ILE:HG13	2.19	0.43
3:D:639:LEU:HD23	3:D:639:LEU:HA	1.84	0.43
3:D:829:VAL:H	3:D:835:SER:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:895:VAL:O	3:D:898:GLU:N	2.52	0.43
1:A:109:VAL:HG12	1:A:129:ILE:HB	2.01	0.43
1:A:75:VAL:O	1:A:79:ILE:HG23	2.18	0.43
2:C:717:LEU:H	2:C:717:LEU:HG	1.62	0.43
2:C:766:GLU:H	2:C:766:GLU:HG3	1.67	0.43
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.85	0.43
1:A:159:LYS:O	6:H:21:THR:HG23	2.18	0.43
6:H:37:ARG:HH11	6:H:37:ARG:HA	1.82	0.43
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.84	0.42
1:B:18:ARG:O	1:B:207:PRO:HD3	2.19	0.42
1:B:40:LEU:HD21	1:B:215:VAL:HG12	2.00	0.42
2:C:13:ILE:HA	2:C:14:PRO:HD3	1.79	0.42
3:D:1389:LEU:HD23	3:D:1389:LEU:H	1.84	0.42
3:D:1394:VAL:HB	3:D:1397:LYS:HB2	2.01	0.42
3:D:778:LEU:HA	3:D:778:LEU:HD12	1.81	0.42
6:H:27:TYR:OH	6:H:34:LEU:O	2.37	0.42
2:C:29:ALA:HB2	2:C:337:GLY:CA	2.49	0.42
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.51	0.42
3:D:469:ASP:HB3	3:D:472:ALA:HB3	2.01	0.42
4:E:54:LEU:CD2	4:E:63:TRP:HE1	2.32	0.42
5:F:147:LEU:HD23	5:F:147:LEU:HA	1.79	0.42
6:H:20:GLU:HA	6:H:61:ARG:CD	2.46	0.42
2:C:540:PHE:CE1	2:C:906:PHE:HE1	2.37	0.42
2:C:1052:MET:HE1	3:D:748:HIS:HB3	2.00	0.42
2:C:1036:GLU:OE1	2:C:1036:GLU:N	2.45	0.42
2:C:448:ASN:HA	2:C:451:LEU:HD12	2.01	0.42
2:C:676:ILE:O	2:C:676:ILE:HG12	2.18	0.42
3:D:227:LEU:HD13	3:D:328:GLY:C	2.40	0.42
3:D:792:ILE:HG13	3:D:793:THR:N	2.33	0.42
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.85	0.42
3:D:1377:LYS:HE2	3:D:1378:TYR:CZ	2.54	0.42
2:C:1098:ASP:HB2	3:D:13:ALA:HB2	2.00	0.42
3:D:39:PRO:HG2	3:D:47:GLU:CG	2.47	0.42
3:D:525:ARG:NE	3:D:541:ASN:OD1	2.47	0.42
3:D:535:PHE:HB2	5:F:314:PRO:HB3	2.02	0.42
1:A:88:ARG:HD2	1:A:123:MET:HE1	2.02	0.42
2:C:881:ASN:OD1	2:C:884:GLN:NE2	2.46	0.42
3:D:1112:CYS:HB3	3:D:1196:THR:HG23	2.02	0.42
3:D:1149:LEU:HD23	3:D:1149:LEU:HA	1.78	0.42
3:D:1170:ASP:O	3:D:1173:LEU:HB3	2.20	0.42
3:D:313:MET:HG3	3:D:314:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:703:ASN:HB2	3:D:713:ILE:HG12	2.01	0.42
5:F:105:LYS:HB3	5:F:180:GLY:HA2	2.02	0.42
5:F:249:ARG:HG3	5:F:250:ALA:N	2.35	0.42
1:B:75:VAL:O	1:B:79:ILE:HG23	2.19	0.42
2:C:404:LEU:O	2:C:408:ARG:HG2	2.19	0.42
2:C:422:ARG:HG3	2:C:422:ARG:H	1.54	0.42
2:C:572:ILE:HG12	2:C:701:THR:O	2.19	0.42
2:C:676:ILE:CG2	2:C:988:VAL:HG13	2.49	0.42
3:D:1171:VAL:O	3:D:1175:ILE:HG13	2.19	0.42
3:D:1209:LEU:HD12	3:D:1209:LEU:HA	1.89	0.42
3:D:1262:LEU:HA	3:D:1262:LEU:HD12	1.89	0.42
3:D:256:GLU:HB2	3:D:296:GLU:CG	2.50	0.42
3:D:667:ALA:HA	3:D:668:PRO:HD3	1.89	0.42
2:C:1051:GLU:OE2	3:D:752:SER:HB3	2.20	0.42
2:C:470:PRO:HA	2:C:485:TYR:HA	2.01	0.42
2:C:717:LEU:HD13	2:C:763:GLY:HA2	2.01	0.42
2:C:988:VAL:HG12	3:D:948:THR:OG1	2.20	0.42
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.35	0.42
3:D:178:LEU:O	3:D:181:ASP:HB2	2.20	0.42
3:D:550:ARG:NH1	3:D:573:MET:HB3	2.35	0.42
3:D:881:LEU:O	3:D:885:ILE:HG13	2.19	0.42
6:G:134:HIS:N	6:G:134:HIS:CD2	2.88	0.42
2:C:143:SER:HB2	2:C:332:ARG:HB2	2.01	0.42
2:C:239:PHE:HZ	2:C:253:ALA:HB3	1.83	0.42
2:C:97:ARG:HE	2:C:97:ARG:HB3	1.72	0.42
3:D:1364:HIS:CE1	3:D:1366:LYS:HB2	2.54	0.42
3:D:250:LEU:HD11	3:D:304:LEU:HB3	2.01	0.42
3:D:36:THR:C	3:D:38:LYS:H	2.23	0.42
3:D:623:VAL:HG12	3:D:626:SER:HB3	2.01	0.42
3:D:764:LEU:HD12	3:D:765:SER:H	1.84	0.42
5:F:82:ARG:O	5:F:86:HIS:HB2	2.19	0.42
3:D:349:PRO:HB3	5:F:96:LEU:HB3	2.02	0.42
1:A:173:PRO:O	1:A:201:THR:HG23	2.20	0.42
1:B:40:LEU:HA	1:B:40:LEU:HD23	1.86	0.42
2:C:30:LEU:HD22	2:C:118:ILE:HD11	2.02	0.42
2:C:576:ALA:HA	2:C:577:PRO:HD3	1.90	0.42
2:C:80:GLN:HG3	2:C:90:TYR:CE1	2.55	0.42
3:D:1463:LYS:O	3:D:1467:ILE:HG13	2.20	0.42
3:D:440:VAL:HG23	3:D:441:ARG:N	2.34	0.42
2:C:684:PHE:HB2	3:D:633:VAL:HG21	2.02	0.42
3:D:690:ALA:O	3:D:694:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:806:PHE:O	3:D:808:THR:N	2.52	0.42
3:D:840:LYS:HD3	3:D:841:TYR:CZ	2.55	0.42
1:A:161:ARG:HG2	1:A:162:ILE:N	2.35	0.41
1:A:42:ARG:NH2	1:B:31:GLY:O	2.53	0.41
2:C:137:VAL:HG12	2:C:138:SER:N	2.35	0.41
2:C:48:PHE:HD1	2:C:48:PHE:HA	1.75	0.41
3:D:1348:LEU:HA	3:D:1348:LEU:HD12	1.85	0.41
3:D:223:LEU:HA	3:D:223:LEU:HD12	1.83	0.41
3:D:808:THR:HB	3:D:809:PRO:HD3	2.01	0.41
5:F:135:ILE:HD11	5:F:178:ARG:HD3	2.02	0.41
2:C:628:PHE:CD2	2:C:638:ASP:HB3	2.55	0.41
2:C:548:PRO:HA	2:C:581:THR:HG22	2.02	0.41
3:D:1396:GLU:O	3:D:1400:VAL:HG23	2.19	0.41
3:D:1403:LEU:HD23	3:D:1407:LEU:HD13	2.01	0.41
3:D:292:VAL:HG12	3:D:293:VAL:HG13	2.02	0.41
3:D:31:THR:HG23	3:D:45:PHE:CD2	2.55	0.41
3:D:33:ASN:HB3	3:D:35:ARG:HG3	2.03	0.41
3:D:758:GLU:O	3:D:762:GLN:HG3	2.19	0.41
3:D:1494:ALA:HB1	4:E:88:GLU:OE2	2.20	0.41
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.55	0.41
1:B:23:PHE:CE2	1:B:199:ILE:HD12	2.55	0.41
2:C:44:ILE:HG23	2:C:344:PHE:CE1	2.55	0.41
2:C:803:THR:HG22	2:C:825:VAL:HG13	2.02	0.41
2:C:943:VAL:HG11	2:C:973:VAL:HG13	2.01	0.41
2:C:670:GLN:O	2:C:993:PHE:HA	2.21	0.41
3:D:104:PHE:CD2	3:D:104:PHE:N	2.88	0.41
3:D:1117:TYR:O	3:D:1193:THR:HG21	2.20	0.41
3:D:450:TYR:O	3:D:452:ILE:N	2.53	0.41
1:B:26:GLU:HB2	1:B:194:LYS:HA	2.01	0.41
1:B:219:ARG:O	1:B:223:THR:HG23	2.21	0.41
2:C:1009:SER:HB2	3:D:651:GLU:O	2.20	0.41
2:C:176:VAL:HG12	2:C:182:VAL:HG22	2.01	0.41
2:C:424:GLY:HA3	2:C:428:ARG:NE	2.34	0.41
2:C:511:GLU:O	2:C:526:PRO:HD3	2.21	0.41
3:D:1209:LEU:HD21	3:D:1216:SER:HB2	2.01	0.41
3:D:543:LEU:HD21	3:D:600:LEU:HD12	2.02	0.41
3:D:654:LYS:HB3	3:D:655:PRO:HD3	2.03	0.41
3:D:786:ILE:HD13	3:D:908:LYS:HB3	2.02	0.41
1:B:99:LEU:HD12	1:B:100:LEU:H	1.86	0.41
2:C:517:ARG:HH21	2:C:524:VAL:CG2	2.33	0.41
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:606:VAL:HG22	2:C:645:VAL:HG13	2.03	0.41
3:D:299:GLU:O	3:D:301:GLY:N	2.50	0.41
3:D:659:LYS:O	3:D:663:GLU:HG2	2.21	0.41
3:D:706:PRO:O	3:D:708:LEU:HG	2.21	0.41
3:D:894:LYS:H	3:D:894:LYS:CD	2.33	0.41
2:C:984:GLU:HG3	3:D:944:THR:O	2.21	0.41
6:H:107:LEU:HA	6:H:107:LEU:HD23	1.92	0.41
1:B:106:PRO:HA	1:B:132:LEU:O	2.20	0.41
1:B:192:LEU:HA	1:B:192:LEU:HD23	1.74	0.41
2:C:273:GLY:HA2	2:C:276:LYS:NZ	2.36	0.41
2:C:319:GLY:N	2:C:321:GLU:OE1	2.38	0.41
2:C:754:ILE:HG12	2:C:754:ILE:H	1.60	0.41
2:C:906:PHE:HZ	3:D:1070:TYR:HD2	1.69	0.41
2:C:950:LEU:HD13	2:C:950:LEU:HA	1.60	0.41
1:A:211:LEU:O	1:A:215:VAL:HG13	2.21	0.41
1:B:36:LEU:O	1:B:39:PRO:HD2	2.21	0.41
2:C:113:VAL:O	2:C:115:LEU:HD23	2.20	0.41
3:D:361:VAL:O	3:D:382:GLU:HA	2.20	0.41
3:D:421:LEU:HD13	3:D:429:SER:H	1.85	0.41
3:D:957:PRO:HB2	3:D:959:GLU:HG2	2.02	0.41
5:F:360:LYS:HA	5:F:360:LYS:HD3	1.87	0.41
2:C:184:MET:HG3	2:C:193:LEU:HD23	2.03	0.41
2:C:227:PHE:CD2	2:C:237:ARG:HD3	2.56	0.41
2:C:274:ARG:HB2	2:C:288:ARG:HH12	1.85	0.41
3:D:172:PRO:O	3:D:174:GLY:N	2.54	0.41
3:D:556:LYS:HE2	3:D:556:LYS:HB3	1.94	0.41
5:F:125:ASP:O	5:F:129:GLU:HG2	2.20	0.41
5:F:188:ILE:O	5:F:192:LEU:HD12	2.21	0.41
1:B:8:ALA:HA	1:B:9:PRO:HD3	1.87	0.41
2:C:263:ASP:OD2	2:C:263:ASP:N	2.54	0.41
2:C:517:ARG:HH21	2:C:524:VAL:HG23	1.85	0.41
2:C:724:ARG:NH2	2:C:734:LEU:O	2.54	0.41
2:C:758:ARG:HB3	2:C:788:THR:O	2.21	0.41
3:D:260:GLU:HB2	3:D:271:VAL:O	2.21	0.41
3:D:890:VAL:HG12	3:D:926:LYS:HG2	2.02	0.41
4:E:42:PRO:HB2	4:E:45:ARG:HH21	1.86	0.41
2:C:1015:LEU:HD23	5:F:334:PRO:O	2.20	0.41
5:F:371:LEU:HD13	5:F:375:LEU:HD22	2.03	0.41
6:H:37:ARG:NH1	6:H:37:ARG:HA	2.36	0.41
6:H:16:ILE:HG21	6:H:63:VAL:HG21	2.03	0.41
2:C:101:ILE:HG22	2:C:102:HIS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:172:ILE:HG23	2:C:186:VAL:HG13	2.03	0.41
2:C:270:GLY:O	2:C:274:ARG:HD3	2.21	0.41
3:D:1148:VAL:HG21	3:D:1203:LYS:HA	2.01	0.41
3:D:162:ARG:HD2	3:D:162:ARG:HA	1.90	0.41
3:D:933:ALA:O	3:D:937:TYR:HD1	2.04	0.41
5:F:228:GLU:HB3	5:F:230:LYS:HE3	2.03	0.41
2:C:911:GLU:O	2:C:915:LYS:HG2	2.21	0.40
3:D:996:TRP:HB2	3:D:1044:LEU:HD11	2.02	0.40
3:D:1485:GLN:O	4:E:75:PHE:HA	2.20	0.40
3:D:41:ARG:H	3:D:41:ARG:HG2	1.56	0.40
3:D:736:PHE:O	3:D:738:ALA:N	2.54	0.40
5:F:181:GLU:O	5:F:184:ARG:HB3	2.21	0.40
2:C:501:THR:HA	2:C:502:PRO:HD3	1.80	0.40
2:C:666:LEU:HG	2:C:668:LEU:HD11	2.03	0.40
2:C:52:PHE:CD1	2:C:68:PHE:HB2	2.56	0.40
3:D:1472:ILE:HA	3:D:1473:PRO:HD3	1.89	0.40
3:D:307:ALA:HB1	3:D:311:LEU:HD11	2.03	0.40
3:D:785:ILE:HD12	3:D:785:ILE:H	1.86	0.40
3:D:828:LYS:HD2	3:D:862:ASP:OD2	2.21	0.40
3:D:920:LEU:HD12	3:D:920:LEU:HA	1.95	0.40
1:A:101:LEU:HB2	1:A:114:PHE:CE2	2.56	0.40
2:C:610:ARG:HB3	2:C:624:PRO:HA	2.03	0.40
2:C:76:PRO:HA	2:C:77:PRO:HD3	1.93	0.40
2:C:953:VAL:HG13	2:C:966:LEU:HD13	2.03	0.40
3:D:1092:GLY:O	3:D:1096:ARG:N	2.52	0.40
3:D:128:TYR:CZ	3:D:461:ILE:HG13	2.57	0.40
5:F:198:ILE:HD11	5:F:240:THR:HA	2.04	0.40
2:C:433:THR:HG21	2:C:488:ALA:HB1	2.02	0.40
3:D:148:GLU:HB3	3:D:151:GLN:HB2	2.04	0.40
3:D:237:LYS:HB3	3:D:238:PRO:CD	2.52	0.40
3:D:421:LEU:HB3	3:D:422:ALA:H	1.78	0.40
3:D:12:LEU:O	3:D:507:ASN:ND2	2.54	0.40
3:D:788:GLY:O	3:D:792:ILE:HG23	2.21	0.40
5:F:174:LEU:HD13	5:F:175:HIS:N	2.37	0.40
5:F:323:ASP:O	5:F:325:LYS:N	2.54	0.40
5:F:365:GLU:HG3	5:F:365:GLU:H	1.59	0.40
2:C:208:ALA:HB2	2:C:222:MET:SD	2.62	0.40
2:C:129:ILE:HD11	2:C:386:PHE:HD2	1.87	0.40
2:C:860:HIS:HA	2:C:866:PRO:HA	2.03	0.40
3:D:1096:ARG:HB2	3:D:1096:ARG:NH1	2.34	0.40
3:D:129:PHE:O	3:D:572:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:471:GLU:O	3:D:474:GLU:HB3	2.22	0.40
3:D:771:SER:OG	3:D:774:SER:O	2.30	0.40
3:D:972:LEU:HD23	3:D:976:GLN:NE2	2.35	0.40
5:F:98:GLU:O	5:F:102:LEU:HG	2.22	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	223/315 (71%)	198 (89%)	22 (10%)	3 (1%)	12	50
1	B	230/315 (73%)	207 (90%)	14 (6%)	9 (4%)	3	27
2	C	1116/1119 (100%)	947 (85%)	128 (12%)	41 (4%)	3	28
3	D	1484/1524 (97%)	1209 (82%)	200 (14%)	75 (5%)	2	20
4	E	93/99 (94%)	75 (81%)	12 (13%)	6 (6%)	1	16
5	F	272/423 (64%)	225 (83%)	36 (13%)	11 (4%)	3	26
6	G	123/141 (87%)	116 (94%)	5 (4%)	2 (2%)	9	46
6	H	87/141 (62%)	81 (93%)	4 (5%)	2 (2%)	6	38
All	All	3628/4077 (89%)	3058 (84%)	421 (12%)	149 (4%)	3	26

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	B	7	LYS
1	B	59	GLU
1	B	75	VAL
2	C	31	GLN
2	C	166	PRO

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Mol	Chain	Res	Type
2	C	231	PRO
2	C	369	PRO
2	C	465	GLY
2	C	541	SER
2	C	680	ASP
2	C	698	ASP
2	C	779	GLY
3	D	41	ARG
3	D	82	LYS
3	D	117	ASP
3	D	120	ALA
3	D	136	ASP
3	D	137	PRO
3	D	143	ASN
3	D	182	GLY
3	D	237	LYS
3	D	416	ALA
3	D	421	LEU
3	D	505	SER
3	D	613	ARG
3	D	624	ASP
3	D	640	HIS
3	D	705	ALA
3	D	832	ARG
3	D	1156	LEU
3	D	1207	TYR
3	D	1208	ASP
4	E	42	PRO
5	F	368	VAL
1	B	157	GLY
2	C	7	GLY
2	C	115	LEU
2	C	250	ARG
2	C	265	ARG
2	C	363	SER
2	C	425	PHE
2	C	518	LYS
2	C	684	PHE
2	C	727	PRO
2	C	864	GLY
2	C	1075	ASP
2	C	1079	PRO

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Mol	Chain	Res	Type
3	D	31	THR
3	D	119	SER
3	D	187	LYS
3	D	405	ASP
3	D	451	ASP
3	D	612	GLY
3	D	619	LEU
3	D	803	GLY
3	D	807	ALA
3	D	822	ALA
3	D	905	PRO
3	D	1125	PRO
3	D	1269	LYS
3	D	1407	LEU
3	D	1410	GLU
3	D	1475	GLY
4	E	58	PRO
5	F	97	GLU
5	F	152	ASP
6	G	77	GLY
1	A	118	ALA
1	B	106	PRO
2	C	20	GLU
2	C	318	PRO
2	C	764	GLU
2	C	781	LYS
2	C	808	ARG
2	C	1023	GLY
2	C	1057	SER
3	D	55	ASP
3	D	110	SER
3	D	121	THR
3	D	375	GLU
3	D	587	ARG
3	D	594	PRO
3	D	608	SER
3	D	1286	THR
3	D	1441	GLN
5	F	150	THR
5	F	342	VAL
5	F	375	LEU
1	B	66	SER

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Mol	Chain	Res	Type
1	B	105	GLY
2	C	167	LYS
2	C	364	GLU
2	C	424	GLY
2	C	880	MET
2	C	1003	ASP
2	C	1113	GLU
3	D	96	ALA
3	D	356	PRO
3	D	593	ASN
3	D	696	HIS
3	D	1205	TYR
3	D	1338	ALA
5	F	141	VAL
5	F	203	THR
1	A	38	ASN
1	B	30	ARG
1	B	191	ASP
2	C	156	GLY
2	C	263	ASP
2	C	905	ILE
3	D	141	ILE
3	D	146	PRO
3	D	183	GLU
3	D	274	ARG
3	D	294	HIS
3	D	302	GLN
3	D	522	PRO
3	D	530	VAL
3	D	1155	VAL
3	D	1211	MET
3	D	1386	ASP
3	D	1390	LEU
4	E	51	LEU
4	E	57	ASP
5	F	324	GLU
3	D	1043	GLY
3	D	1413	THR
4	E	52	GLU
6	H	17	PRO
6	H	18	ASP
3	D	108	VAL

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Mol	Chain	Res	Type
3	D	246	PRO
3	D	588	GLY
3	D	1472	ILE
2	C	152	PRO
3	D	301	GLY
3	D	407	VAL
3	D	609	GLY
3	D	808	THR
5	F	167	PRO
2	C	859	PRO
4	E	41	GLU
5	F	391	GLY
2	C	164	PRO
3	D	216	VAL
2	C	144	PRO
3	D	750	PRO
6	G	76	VAL

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	197/273 (72%)	164 (83%)	33 (17%)	2	14
1	B	200/273 (73%)	172 (86%)	28 (14%)	3	21
2	C	940/941 (100%)	756 (80%)	184 (20%)	1	8
3	D	1254/1279 (98%)	1018 (81%)	236 (19%)	1	9
4	E	83/87 (95%)	70 (84%)	13 (16%)	2	17
5	F	241/371 (65%)	200 (83%)	41 (17%)	2	14
6	G	107/121 (88%)	92 (86%)	15 (14%)	3	21
6	H	79/121 (65%)	71 (90%)	8 (10%)	7	34
All	All	3101/3466 (90%)	2543 (82%)	558 (18%)	1	11

All (558) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	16	GLN
1	A	19	GLU
1	A	26	GLU
1	A	54	THR
1	A	58	ILE
1	A	59	GLU
1	A	62	LEU
1	A	67	THR
1	A	73	GLU
1	A	76	VAL
1	A	84	GLU
1	A	86	VAL
1	A	87	VAL
1	A	96	THR
1	A	112	ARG
1	A	126	ASP
1	A	131	THR
1	A	134	GLU
1	A	143	ARG
1	A	160	ASP
1	A	165	ILE
1	A	167	VAL
1	A	168	ASP
1	A	185	ARG
1	A	186	LEU
1	A	189	ARG
1	A	196	THR
1	A	222	LEU
1	A	223	THR
1	A	226	SER
1	A	227	ASN
1	A	229	GLN
1	B	7	LYS
1	B	26	GLU
1	B	30	ARG
1	B	32	PHE
1	B	48	ILE
1	B	54	THR
1	B	59	GLU
1	B	62	LEU
1	B	77	GLU
1	B	84	GLU

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Mol	Chain	Res	Type
1	B	90	LEU
1	B	96	THR
1	B	99	LEU
1	B	101	LEU
1	B	112	ARG
1	B	115	LEU
1	B	122	ILE
1	B	132	LEU
1	B	133	GLU
1	B	138	LEU
1	B	145	ASP
1	B	175	ARG
1	B	179	PHE
1	B	184	THR
1	B	193	ASP
1	B	196	THR
1	B	201	THR
1	B	205	VAL
2	C	5	ARG
2	C	10	ARG
2	C	20	GLU
2	C	30	LEU
2	C	33	ASP
2	C	48	PHE
2	C	49	ARG
2	C	51	THR
2	C	52	PHE
2	C	55	GLU
2	C	67	ASP
2	C	71	TYR
2	C	73	LEU
2	C	81	ASP
2	C	82	GLU
2	C	95	TYR
2	C	101	ILE
2	C	104	ASP
2	C	107	LEU
2	C	108	ILE
2	C	113	VAL
2	C	115	LEU
2	C	120	LEU
2	C	122	THR

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Mol	Chain	Res	Type
2	C	140	ILE
2	C	141	HIS
2	C	142	ARG
2	C	146	VAL
2	C	161	SER
2	C	163	ILE
2	C	167	LYS
2	C	168	ARG
2	C	174	LEU
2	C	181	VAL
2	C	184	MET
2	C	185	LYS
2	C	186	VAL
2	C	190	LYS
2	C	203	ASP
2	C	205	GLU
2	C	207	LEU
2	C	223	ASP
2	C	230	ARG
2	C	232	GLU
2	C	233	GLU
2	C	239	PHE
2	C	242	LEU
2	C	243	ARG
2	C	254	VAL
2	C	256	TYR
2	C	257	VAL
2	C	263	ASP
2	C	266	ARG
2	C	288	ARG
2	C	289	THR
2	C	294	GLU
2	C	301	GLU
2	C	309	TYR
2	C	331	ARG
2	C	332	ARG
2	C	335	THR
2	C	345	ARG
2	C	351	LEU
2	C	358	ARG
2	C	359	MET
2	C	360	LEU

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Mol	Chain	Res	Type
2	C	366	SER
2	C	368	THR
2	C	372	LEU
2	C	376	ARG
2	C	387	SER
2	C	388	ARG
2	C	393	GLN
2	C	402	SER
2	C	407	LYS
2	C	408	ARG
2	C	413	LEU
2	C	418	LEU
2	C	420	ARG
2	C	422	ARG
2	C	426	ASP
2	C	432	ARG
2	C	433	THR
2	C	438	ILE
2	C	443	THR
2	C	452	ILE
2	C	472	ARG
2	C	474	VAL
2	C	480	THR
2	C	482	GLU
2	C	486	MET
2	C	489	THR
2	C	500	ASN
2	C	503	LEU
2	C	513	VAL
2	C	514	VAL
2	C	516	ARG
2	C	517	ARG
2	C	525	SER
2	C	535	SER
2	C	536	PRO
2	C	537	LYS
2	C	545	ASN
2	C	551	GLU
2	C	559	LEU
2	C	564	MET
2	C	578	VAL
2	C	579	VAL

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Mol	Chain	Res	Type
2	C	584	GLU
2	C	585	GLU
2	C	586	ARG
2	C	589	ARG
2	C	590	ASP
2	C	595	LEU
2	C	606	VAL
2	C	607	ASP
2	C	610	ARG
2	C	617	ASP
2	C	628	PHE
2	C	630	ARG
2	C	633	GLN
2	C	640	ARG
2	C	644	VAL
2	C	645	VAL
2	C	648	ARG
2	C	650	ARG
2	C	654	LEU
2	C	657	ASP
2	C	663	ASN
2	C	670	GLN
2	C	676	ILE
2	C	682	TYR
2	C	685	GLU
2	C	686	ASP
2	C	689	VAL
2	C	699	PHE
2	C	713	ARG
2	C	715	THR
2	C	717	LEU
2	C	744	ARG
2	C	754	ILE
2	C	766	GLU
2	C	780	GLU
2	C	781	LYS
2	C	787	ASP
2	C	789	SER
2	C	808	ARG
2	C	813	VAL
2	C	815	LEU
2	C	820	ARG

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Mol	Chain	Res	Type
2	C	824	ARG
2	C	834	GLN
2	C	837	ASP
2	C	845	ASN
2	C	853	LEU
2	C	856	GLU
2	C	858	MET
2	C	865	THR
2	C	900	ARG
2	C	903	SER
2	C	917	LEU
2	C	918	LEU
2	C	928	LYS
2	C	936	VAL
2	C	950	LEU
2	C	958	THR
2	C	960	GLU
2	C	971	LYS
2	C	972	VAL
2	C	984	GLU
2	C	988	VAL
2	C	1000	MET
2	C	1001	VAL
2	C	1002	GLU
2	C	1005	MET
2	C	1015	LEU
2	C	1021	LEU
2	C	1026	GLN
2	C	1031	ARG
2	C	1052	MET
2	C	1078	GLU
2	C	1095	LEU
2	C	1104	GLU
2	C	1115	LEU
3	D	2	LYS
3	D	5	VAL
3	D	8	VAL
3	D	33	ASN
3	D	36	THR
3	D	41	ARG
3	D	53	ILE
3	D	55	ASP

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Mol	Chain	Res	Type
3	D	58	CYS
3	D	60	CYS
3	D	65	ARG
3	D	68	PHE
3	D	81	THR
3	D	84	ILE
3	D	85	VAL
3	D	89	ARG
3	D	101	HIS
3	D	102	ILE
3	D	111	LYS
3	D	112	ILE
3	D	114	THR
3	D	118	LEU
3	D	122	GLU
3	D	127	LEU
3	D	134	VAL
3	D	135	LEU
3	D	141	ILE
3	D	145	VAL
3	D	149	LYS
3	D	152	LEU
3	D	154	THR
3	D	155	ASP
3	D	165	LYS
3	D	167	GLU
3	D	175	VAL
3	D	185	VAL
3	D	199	LEU
3	D	204	LEU
3	D	227	LEU
3	D	232	GLU
3	D	259	VAL
3	D	264	LEU
3	D	266	GLU
3	D	269	PHE
3	D	276	ASP
3	D	290	PRO
3	D	294	HIS
3	D	297	ILE
3	D	313	MET
3	D	336	PHE

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Mol	Chain	Res	Type
3	D	338	GLU
3	D	350	HIS
3	D	351	MET
3	D	365	ASP
3	D	380	GLU
3	D	388	HIS
3	D	400	VAL
3	D	408	GLU
3	D	411	THR
3	D	413	ASP
3	D	415	VAL
3	D	420	VAL
3	D	421	LEU
3	D	434	ARG
3	D	436	GLU
3	D	441	ARG
3	D	452	ILE
3	D	456	MET
3	D	468	LEU
3	D	481	MET
3	D	486	ARG
3	D	488	ARG
3	D	489	ARG
3	D	498	VAL
3	D	500	ARG
3	D	504	ASP
3	D	511	TRP
3	D	513	ILE
3	D	525	ARG
3	D	528	VAL
3	D	546	ARG
3	D	554	LEU
3	D	557	LEU
3	D	581	LEU
3	D	592	THR
3	D	593	ASN
3	D	598	ARG
3	D	600	LEU
3	D	606	ILE
3	D	611	GLN
3	D	619	LEU
3	D	621	LYS

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Mol	Chain	Res	Type
3	D	626	SER
3	D	630	VAL
3	D	639	LEU
3	D	647	ARG
3	D	651	GLU
3	D	652	LEU
3	D	659	LYS
3	D	660	LYS
3	D	662	GLU
3	D	663	GLU
3	D	674	ARG
3	D	679	ARG
3	D	686	GLU
3	D	704	ARG
3	D	709	HIS
3	D	717	GLN
3	D	725	SER
3	D	739	ASP
3	D	754	PHE
3	D	758	GLU
3	D	762	GLN
3	D	763	MET
3	D	783	ARG
3	D	784	ASP
3	D	787	LEU
3	D	792	ILE
3	D	793	THR
3	D	794	GLN
3	D	796	ARG
3	D	810	GLU
3	D	818	ARG
3	D	828	LYS
3	D	832	ARG
3	D	836	VAL
3	D	851	LEU
3	D	857	ILE
3	D	858	VAL
3	D	861	GLN
3	D	863	VAL
3	D	865	THR
3	D	868	TYR
3	D	875	THR

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Mol	Chain	Res	Type
3	D	876	SER
3	D	879	ARG
3	D	880	ILE
3	D	888	GLU
3	D	890	VAL
3	D	891	GLU
3	D	894	LYS
3	D	897	TRP
3	D	899	LEU
3	D	910	SER
3	D	916	TYR
3	D	919	PHE
3	D	921	ARG
3	D	926	LYS
3	D	936	TYR
3	D	947	ILE
3	D	951	ILE
3	D	964	LEU
3	D	971	LEU
3	D	972	LEU
3	D	976	GLN
3	D	984	THR
3	D	988	ARG
3	D	990	ASP
3	D	1002	LYS
3	D	1007	VAL
3	D	1033	GLN
3	D	1041	LEU
3	D	1042	ARG
3	D	1045	MET
3	D	1046	GLN
3	D	1049	SER
3	D	1052	THR
3	D	1062	ARG
3	D	1063	GLU
3	D	1066	THR
3	D	1068	LEU
3	D	1070	TYR
3	D	1078	ARG
3	D	1095	THR
3	D	1096	ARG
3	D	1102	THR

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Mol	Chain	Res	Type
3	D	1109	GLU
3	D	1111	ASP
3	D	1115	THR
3	D	1130	ARG
3	D	1135	ARG
3	D	1137	ARG
3	D	1155	VAL
3	D	1161	GLU
3	D	1166	LEU
3	D	1183	ILE
3	D	1194	CYS
3	D	1197	ARG
3	D	1201	CYS
3	D	1209	LEU
3	D	1210	SER
3	D	1211	MET
3	D	1216	SER
3	D	1223	ILE
3	D	1234	THR
3	D	1238	MET
3	D	1258	ARG
3	D	1262	LEU
3	D	1271	LYS
3	D	1278	ASP
3	D	1295	GLU
3	D	1296	SER
3	D	1304	LYS
3	D	1311	LEU
3	D	1314	LYS
3	D	1319	VAL
3	D	1325	LEU
3	D	1335	LEU
3	D	1339	LYS
3	D	1346	ARG
3	D	1359	GLN
3	D	1373	ARG
3	D	1379	VAL
3	D	1381	VAL
3	D	1382	THR
3	D	1388	ARG
3	D	1389	LEU
3	D	1412	LYS

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Mol	Chain	Res	Type
3	D	1415	VAL
3	D	1422	MET
3	D	1424	VAL
3	D	1425	THR
3	D	1426	LYS
3	D	1429	LEU
3	D	1432	LYS
3	D	1434	TRP
3	D	1435	LEU
3	D	1447	LEU
3	D	1457	ASP
3	D	1462	LEU
3	D	1464	GLU
3	D	1465	ASN
3	D	1468	LEU
3	D	1483	PHE
3	D	1486	VAL
3	D	1488	ASP
4	E	31	LEU
4	E	38	THR
4	E	42	PRO
4	E	47	LYS
4	E	48	MET
4	E	51	LEU
4	E	54	LEU
4	E	56	ASP
4	E	62	THR
4	E	70	THR
4	E	74	VAL
4	E	79	LEU
4	E	85	LEU
5	F	77	THR
5	F	85	LEU
5	F	86	HIS
5	F	94	LEU
5	F	108	GLU
5	F	120	THR
5	F	123	ASP
5	F	125	ASP
5	F	126	LEU
5	F	144	ILE
5	F	147	LEU

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Mol	Chain	Res	Type
5	F	157	GLU
5	F	171	LYS
5	F	174	LEU
5	F	176	ILE
5	F	192	LEU
5	F	197	SER
5	F	210	LEU
5	F	211	ASP
5	F	225	GLU
5	F	249	ARG
5	F	253	ASP
5	F	321	ILE
5	F	323	ASP
5	F	335	ASP
5	F	338	LEU
5	F	347	GLN
5	F	355	GLU
5	F	358	LEU
5	F	362	SER
5	F	365	GLU
5	F	367	MET
5	F	375	LEU
5	F	386	VAL
5	F	390	PHE
5	F	393	THR
5	F	396	ARG
5	F	398	ARG
5	F	405	LEU
5	F	408	LEU
5	F	409	LYS
6	G	5	PHE
6	G	25	THR
6	G	28	ASP
6	G	32	ASP
6	G	42	SER
6	G	61	ARG
6	G	62	ARG
6	G	72	ARG
6	G	75	HIS
6	G	76	VAL
6	G	78	LEU
6	G	106	VAL

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Mol	Chain	Res	Type
6	G	109	ASP
6	G	127	ARG
6	G	136	ASP
6	H	6	VAL
6	H	22	GLU
6	H	27	TYR
6	H	32	ASP
6	H	37	ARG
6	H	47	THR
6	H	59	ARG
6	H	95	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	B	124	ASN
2	C	31	GLN
2	C	45	GLN
2	C	327	HIS
3	D	569	ASN
3	D	909	ASN
3	D	1323	GLN
5	F	218	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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	225/315 (71%)	-0.18	0 100 100	11, 37, 83, 144	0
1	B	232/315 (73%)	-0.22	0 100 100	14, 47, 104, 158	0
2	C	1118/1119 (99%)	-0.12	13 (1%) 79 66	8, 59, 151, 222	0
3	D	1488/1524 (97%)	-0.12	25 (1%) 70 55	8, 85, 179, 244	0
4	E	95/99 (95%)	-0.00	3 (3%) 47 32	40, 74, 183, 242	0
5	F	278/423 (65%)	-0.10	10 (3%) 42 28	44, 119, 192, 255	0
6	G	127/141 (90%)	-0.20	0 100 100	27, 73, 137, 179	0
6	H	91/141 (64%)	-0.03	2 (2%) 62 45	73, 113, 161, 175	0
All	All	3654/4077 (89%)	-0.13	53 (1%) 73 60	8, 74, 170, 255	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	323	ASP	7.4
4	E	57	ASP	7.4
5	F	322	GLY	7.0
3	D	294	HIS	6.6
2	C	60	GLY	6.2
4	E	56	ASP	6.2
3	D	1408	ILE	5.4
3	D	230	TRP	5.3
5	F	339	PRO	4.6
2	C	270	GLY	4.6
3	D	233	LYS	3.9
5	F	321	ILE	3.8
3	D	234	GLU	3.7
2	C	252	LYS	3.6
5	F	255	ALA	3.5
3	D	298	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
5	F	145	PRO	3.4
3	D	67	ARG	3.3
2	C	267	TYR	3.3
3	D	235	ALA	3.3
2	C	293	PHE	3.2
2	C	271	GLU	3.2
3	D	252	ARG	3.1
6	H	85	TYR	3.1
3	D	163	TYR	3.1
3	D	63	TYR	3.1
3	D	310	LEU	2.8
4	E	2	ALA	2.8
3	D	137	PRO	2.7
3	D	1505	ALA	2.7
2	C	269	LEU	2.7
6	H	86	ALA	2.7
3	D	263	GLU	2.7
3	D	595	GLY	2.6
2	C	416	GLY	2.6
5	F	313	GLU	2.6
5	F	143	HIS	2.5
5	F	341	PRO	2.5
2	C	223	ASP	2.5
2	C	61	LYS	2.4
2	C	224	GLU	2.3
3	D	1504	GLU	2.3
2	C	1117	SER	2.3
3	D	450	TYR	2.3
3	D	483	HIS	2.3
3	D	203	ALA	2.2
3	D	64	LYS	2.1
3	D	59	ALA	2.1
3	D	66	GLN	2.1
3	D	802	ALA	2.0
2	C	211	LEU	2.0
3	D	34	TYR	2.0
5	F	337	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95th 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(\AA^2)	Q<0.9
7	ZN	D	1601	1/1	0.98	0.20	110,110,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.