



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 09:22 PM EST

PDB ID : 1WYV
Title : Crystal structure of glycine decarboxylase (P-protein) of the glycine cleavage system, in inhibitor-bound form
Authors : Nakai, T.; Nakagawa, N.; Maoka, N.; Masui, R.; Kuramitsu, S.; Kamiya, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-02-17
Resolution : 2.40 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

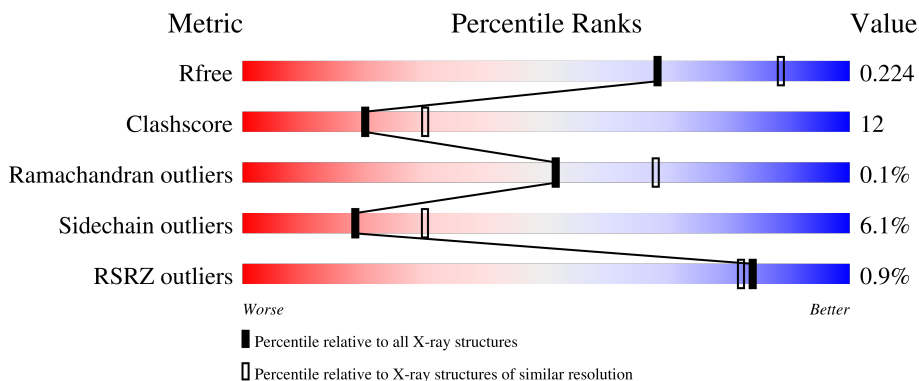
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	438	 77% 19% .
1	C	438	 77% 20% .
1	E	438	 77% 20% .
1	G	438	 79% 18% .
2	B	474	 % 72% 25% .

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Mol	Chain	Length	Quality of chain
2	D	474	
2	F	474	
2	H	474	

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
4	AOA	B	1476	-	-	-	X
4	AOA	D	2476	-	-	X	X
4	AOA	F	3476	-	-	X	X
4	AOA	H	4476	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 29408 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 glycine dehydrogenase (decarboxylating) subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	3320	2129	575	607	9	0	0	0
1	C	437	3320	2129	575	607	9	0	0	0
1	E	437	3320	2129	575	607	9	0	0	0
1	G	437	3320	2129	575	607	9	0	0	0

- Molecule 2 is a protein called glycine dehydrogenase subunit 2 (P-protein).

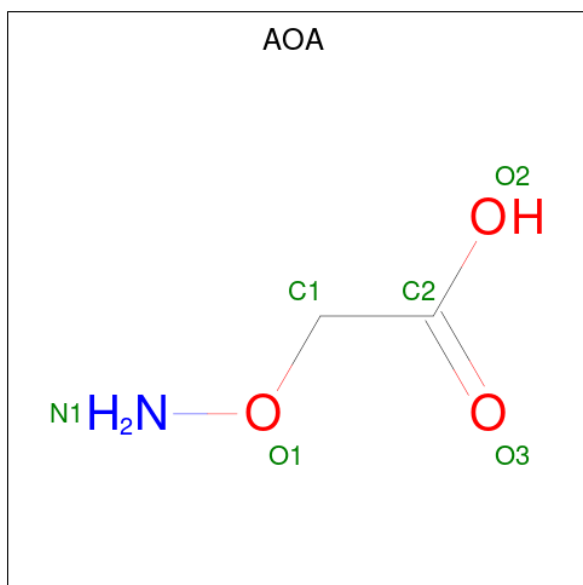
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	473	3713	2380	655	666	12	0	0	0
2	D	473	3713	2380	655	666	12	0	0	0
2	F	473	3713	2380	655	666	12	0	0	0
2	H	473	3713	2380	655	666	12	0	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is (AMINOXY)ACETIC ACID (three-letter code: AOA) (formula: $C_2H_5NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			6	2	1	3		
4	D	1	Total	C	N	O	0	0
			6	2	1	3		
4	F	1	Total	C	N	O	0	0
			6	2	1	3		
4	H	1	Total	C	N	O	0	0
			6	2	1	3		

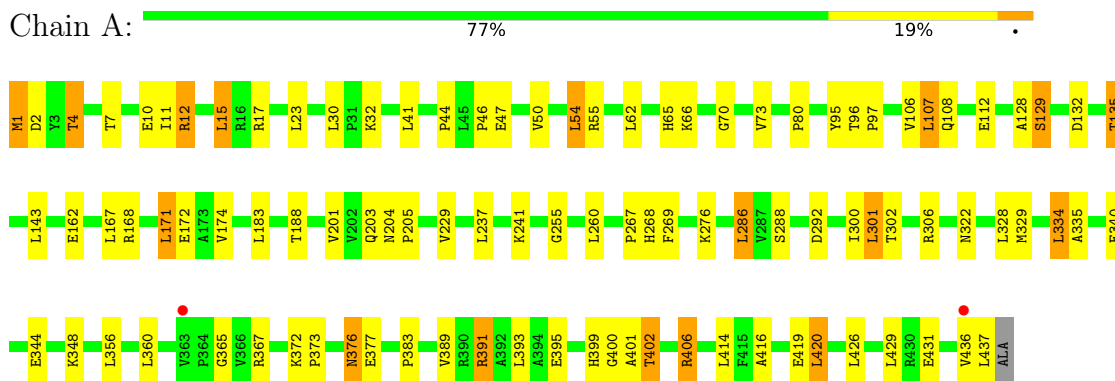
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	162	Total	O	0	0
			162	162		
5	B	182	Total	O	0	0
			182	182		
5	C	145	Total	O	0	0
			145	145		
5	D	117	Total	O	0	0
			117	117		
5	E	152	Total	O	0	0
			152	152		
5	F	159	Total	O	0	0
			159	159		
5	G	150	Total	O	0	0
			150	150		
5	H	125	Total	O	0	0
			125	125		

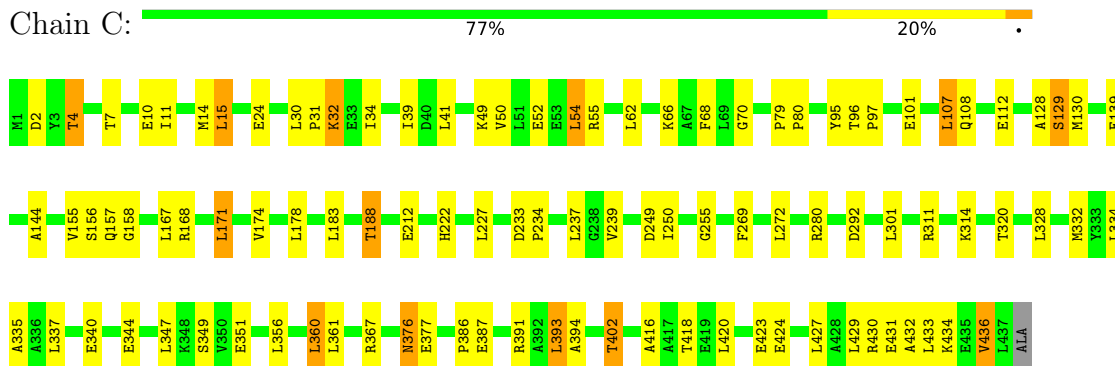
3 Residue-property plots [i](#)

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.

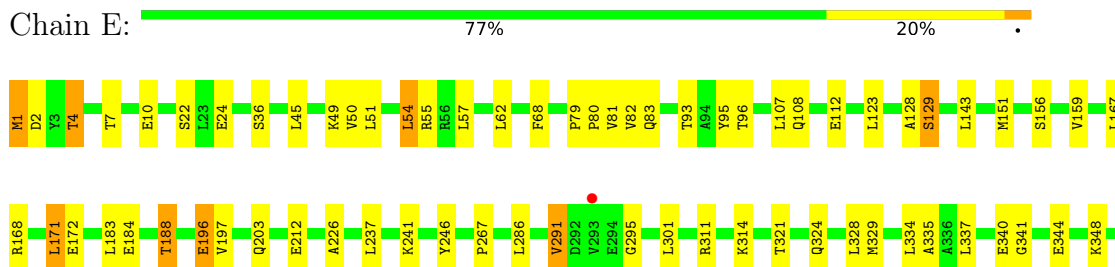
- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1

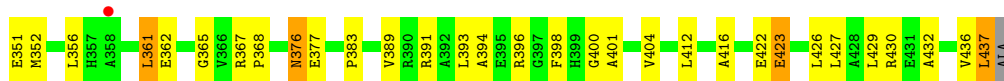


- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1

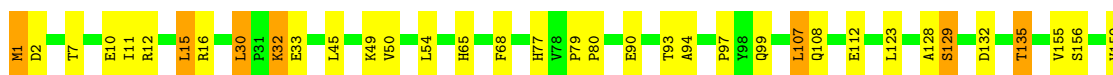
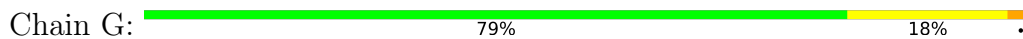


- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1

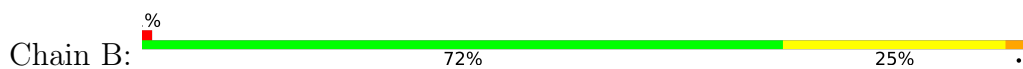




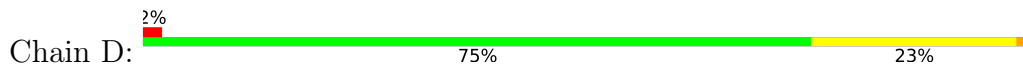
- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1



- Molecule 2: glycine dehydrogenase subunit 2 (P-protein)

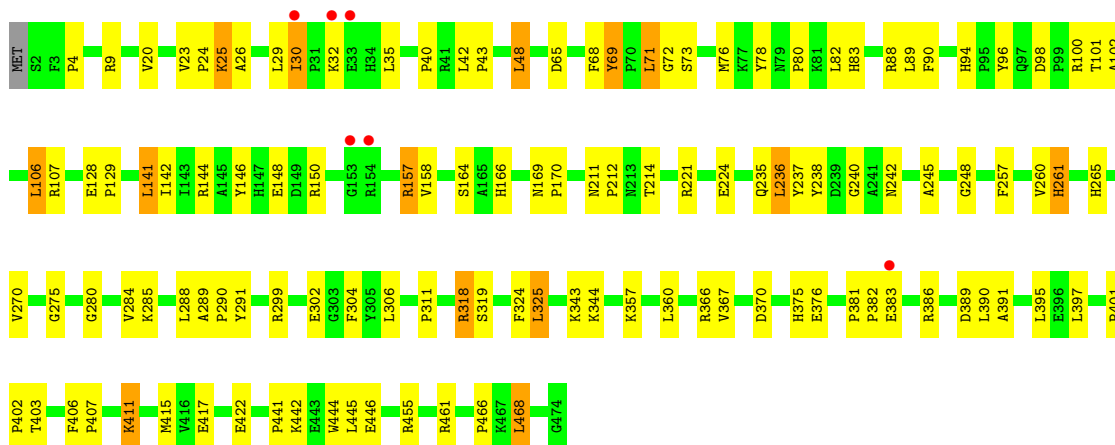
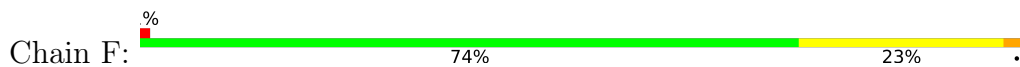


- Molecule 2: glycine dehydrogenase subunit 2 (P-protein)

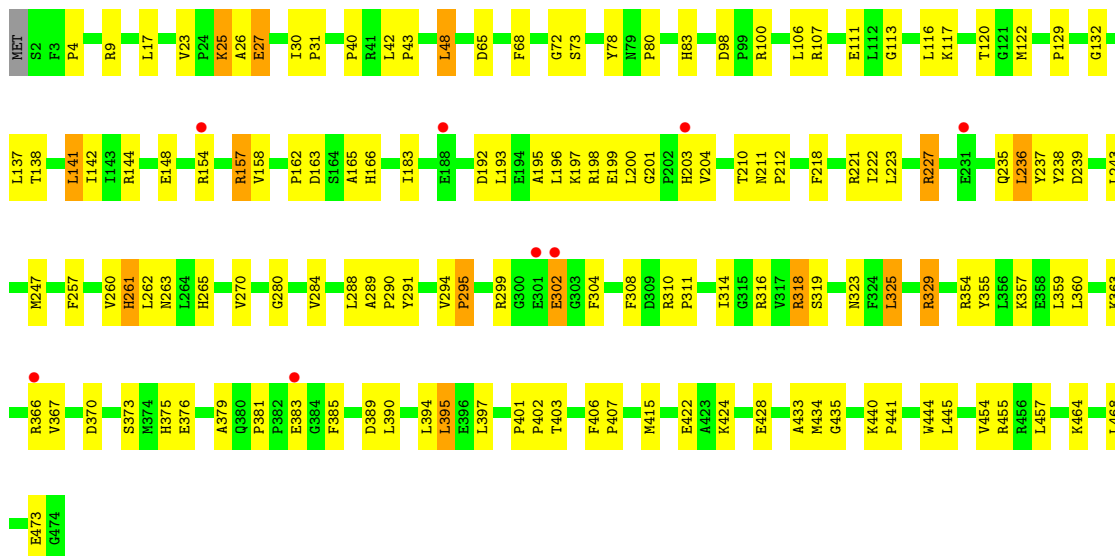




- Molecule 2: glycine dehydrogenase subunit 2 (P-protein)



- Molecule 2: glycine dehydrogenase subunit 2 (P-protein)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.17Å 166.32Å 190.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.90 – 2.40 47.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.90-2.40) 99.5 (47.90-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.39Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.230 0.183 , 0.224	Depositor DCC
R_{free} test set	8362 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtrriage
Anisotropy	0.349	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29408	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.91% 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: AOA, PLP

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	0/3395	0.59	0/4617
1	C	0.34	0/3395	0.59	0/4617
1	E	0.34	0/3395	0.58	0/4617
1	G	0.33	0/3395	0.59	0/4617
2	B	0.36	0/3808	0.61	0/5162
2	D	0.33	0/3808	0.60	0/5162
2	F	0.35	0/3808	0.60	0/5162
2	H	0.33	0/3808	0.60	0/5162
All	All	0.34	0/28812	0.60	0/39116

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3320	0	3363	78	0
1	C	3320	0	3363	88	0
1	E	3320	0	3363	67	0
1	G	3320	0	3363	74	0
2	B	3713	0	3745	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3713	0	3745	111	0
2	F	3713	0	3745	110	0
2	H	3713	0	3745	120	0
3	B	15	0	7	0	0
3	D	15	0	7	0	0
3	F	15	0	6	0	0
3	H	15	0	7	0	0
4	B	6	0	3	3	0
4	D	6	0	2	6	0
4	F	6	0	3	4	0
4	H	6	0	2	2	0
5	A	162	0	0	0	0
5	B	182	0	0	5	0
5	C	145	0	0	6	0
5	D	117	0	0	1	0
5	E	152	0	0	4	0
5	F	159	0	0	3	0
5	G	150	0	0	4	0
5	H	125	0	0	2	0
All	All	29408	0	28469	707	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 12.

All (707) 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)
2:F:30:ILE:HD11	2:F:35:LEU:HD21	1.49	0.94
1:C:32:LYS:H	1:C:32:LYS:HD2	1.33	0.93
1:C:70:GLY:H	1:C:402:THR:HG21	1.38	0.89
2:D:386:ARG:H	2:D:386:ARG:HE	1.23	0.86
2:D:386:ARG:H	2:D:386:ARG:NE	1.75	0.85
2:F:265:HIS:HA	2:F:270:VAL:HB	1.57	0.84
2:H:227:ARG:HH11	2:H:227:ARG:HB3	1.38	0.84
2:H:265:HIS:HA	2:H:270:VAL:HB	1.58	0.84
1:A:66:LYS:HG2	1:A:420:LEU:HD13	1.63	0.81
1:E:335:ALA:HA	2:F:43:PRO:HG2	1.62	0.81
2:D:210:THR:HG22	2:D:239:ASP:HB3	1.63	0.81
1:G:32:LYS:HD3	1:G:32:LYS:H	1.45	0.81
2:H:25:LYS:HE3	2:H:26:ALA:H	1.45	0.81
2:F:72:GLY:HA3	2:F:415:MET:HG2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:366:ARG:NH1	2:F:382:PRO:HA	1.97	0.79
2:B:25:LYS:HE3	2:B:26:ALA:H	1.46	0.78
2:H:157:ARG:HE	2:H:157:ARG:HA	1.47	0.78
1:G:12:ARG:NE	1:G:16:ARG:HH21	1.81	0.78
2:D:265:HIS:HA	2:D:270:VAL:HB	1.66	0.77
1:A:70:GLY:H	1:A:402:THR:HG21	1.50	0.76
2:D:25:LYS:HE3	2:D:26:ALA:H	1.51	0.76
2:B:357:LYS:NZ	2:B:370:ASP:HB2	2.01	0.75
2:D:166:HIS:NE2	4:D:2476:AOA:H1C1	2.02	0.75
2:F:4:PRO:HG2	2:F:9:ARG:NH2	2.02	0.74
1:G:132:ASP:OD1	1:G:135:THR:HB	1.88	0.74
1:C:32:LYS:HD2	1:C:32:LYS:N	2.03	0.74
2:B:80:PRO:HG2	2:B:83:HIS:CE1	2.23	0.74
2:B:444:TRP:HE3	2:B:445:LEU:HD12	1.52	0.73
2:B:367:VAL:CG1	2:B:370:ASP:HB3	2.18	0.73
2:F:26:ALA:HB1	2:F:35:LEU:HD21	1.71	0.73
1:G:97:PRO:HG2	1:G:301:LEU:HD21	1.69	0.73
1:G:311:ARG:HG3	1:G:314:LYS:HB2	1.69	0.73
2:B:403:THR:HB	2:B:415:MET:HB3	1.70	0.72
1:A:436:VAL:HG23	1:A:437:LEU:HD13	1.69	0.72
1:E:83:GLN:HE22	1:E:329:MET:CE	2.03	0.72
1:C:234:PRO:HA	1:C:237:LEU:HD23	1.71	0.72
2:B:395:LEU:HD13	2:B:401:PRO:HD3	1.71	0.72
1:G:377:GLU:HG2	1:G:416:ALA:HB2	1.72	0.72
2:F:466:PRO:HB2	2:F:468:LEU:HD11	1.70	0.71
1:G:188:THR:HG23	1:G:212:GLU:CD	2.11	0.71
1:C:158:GLY:N	1:C:183:LEU:HD11	2.06	0.71
1:E:432:ALA:O	1:E:436:VAL:HG13	1.91	0.71
2:F:25:LYS:HE3	5:F:3599:HOH:O	1.89	0.71
2:D:442:LYS:H	2:D:442:LYS:HD2	1.55	0.71
2:B:294:VAL:CG2	2:B:308:PHE:HA	2.22	0.70
2:F:284:VAL:HG13	2:F:288:LEU:HB2	1.72	0.70
1:C:335:ALA:HA	2:D:43:PRO:HG2	1.74	0.70
1:C:95:TYR:HB2	2:D:76:MET:CE	2.22	0.69
1:G:107:LEU:HD11	1:G:301:LEU:HD22	1.72	0.69
2:D:25:LYS:HE3	2:D:26:ALA:N	2.06	0.69
1:E:2:ASP:OD2	1:E:4:THR:HB	1.92	0.69
2:H:403:THR:HB	2:H:415:MET:HB3	1.74	0.69
2:F:366:ARG:HH12	2:F:383:GLU:N	1.90	0.68
1:G:32:LYS:H	1:G:32:LYS:CD	2.05	0.68
2:H:454:VAL:HG11	2:H:457:LEU:HD21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:ARG:HG3	1:E:391:ARG:HH11	1.59	0.68
2:B:265:HIS:HA	2:B:270:VAL:HB	1.75	0.67
2:D:395:LEU:HD13	2:D:401:PRO:HD3	1.77	0.67
2:F:144:ARG:O	2:F:148:GLU:HG3	1.95	0.67
2:H:284:VAL:CG2	2:H:288:LEU:HB2	2.24	0.67
1:G:99:GLN:HG3	2:H:395:LEU:HD21	1.76	0.67
2:F:367:VAL:CG1	2:F:370:ASP:HB3	2.24	0.67
2:D:31:PRO:HB2	2:D:33:GLU:OE2	1.95	0.66
1:E:376:ASN:HD22	1:E:376:ASN:H	1.42	0.66
1:G:335:ALA:HA	2:H:43:PRO:HG2	1.76	0.66
1:C:188:THR:HG23	1:C:212:GLU:CD	2.15	0.66
2:D:294:VAL:CG2	2:D:308:PHE:HA	2.25	0.66
2:H:294:VAL:CG2	2:H:308:PHE:HA	2.25	0.66
2:D:221:ARG:NH2	2:D:224:GLU:HG3	2.12	0.65
2:D:166:HIS:NE2	4:D:2476:AOA:N1	2.45	0.65
2:D:367:VAL:CG1	2:D:370:ASP:HB3	2.26	0.65
1:E:4:THR:HG21	2:F:344:LYS:HE2	1.78	0.65
1:E:156:SER:OG	1:E:188:THR:HG21	1.96	0.65
1:G:436:VAL:HG23	1:G:437:LEU:HD13	1.78	0.65
2:H:25:LYS:HE3	2:H:26:ALA:N	2.11	0.65
1:A:4:THR:HG21	2:B:344:LYS:HE2	1.78	0.65
2:F:466:PRO:HB2	2:F:468:LEU:CD1	2.27	0.65
1:C:156:SER:OG	1:C:188:THR:HG21	1.97	0.65
1:E:83:GLN:HE22	1:E:329:MET:HE1	1.60	0.65
2:B:158:VAL:HG13	2:B:204:VAL:HA	1.78	0.64
2:H:238:TYR:HD2	2:H:260:VAL:HG13	1.61	0.64
2:D:72:GLY:HA2	2:D:417:GLU:HB2	1.78	0.64
2:D:238:TYR:HD2	2:D:260:VAL:HG13	1.60	0.64
1:G:12:ARG:HE	1:G:16:ARG:HH21	1.43	0.64
2:B:78:TYR:HB2	2:D:48:LEU:HG	1.79	0.64
2:B:375:HIS:CE1	2:B:376:GLU:HG2	2.33	0.64
2:B:442:LYS:H	2:B:442:LYS:HD2	1.61	0.64
2:D:302:GLU:CD	2:D:302:GLU:H	2.01	0.64
1:A:128:ALA:O	1:A:129:SER:HB3	1.96	0.64
2:D:4:PRO:HG2	2:D:9:ARG:CZ	2.28	0.64
1:A:12:ARG:HG2	1:A:12:ARG:HH11	1.63	0.64
2:D:106:LEU:HD11	2:D:306:LEU:HD21	1.80	0.63
1:E:340:GLU:O	1:E:344:GLU:HG3	1.98	0.63
1:C:66:LYS:HG2	1:C:420:LEU:HD13	1.81	0.63
2:F:318:ARG:HD3	2:F:319:SER:O	1.97	0.63
1:C:391:ARG:HG3	1:C:391:ARG:HH11	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:ARG:O	2:D:148:GLU:HG3	1.98	0.63
1:C:432:ALA:O	1:C:436:VAL:HG12	1.99	0.63
2:F:236:LEU:HD22	2:F:257:PHE:CE1	2.34	0.63
1:A:2:ASP:OD2	1:A:4:THR:HB	1.99	0.62
2:B:68:PHE:CE1	2:B:422:GLU:HG3	2.33	0.62
1:C:95:TYR:HB2	2:D:76:MET:HE1	1.81	0.62
2:B:137:LEU:O	2:B:141:LEU:HD22	1.99	0.62
1:C:387:GLU:HG3	5:C:577:HOH:O	1.98	0.62
2:H:238:TYR:HB3	2:H:260:VAL:HG22	1.80	0.62
2:D:188:GLU:HB2	5:D:2565:HOH:O	2.00	0.62
2:H:367:VAL:CG1	2:H:370:ASP:HB3	2.28	0.62
1:C:233:ASP:O	1:C:237:LEU:HD22	2.00	0.62
2:D:120:THR:HG23	2:D:122:MET:HG2	1.80	0.62
2:D:129:PRO:HG2	2:D:280:GLY:O	2.00	0.62
1:E:68:PHE:CD2	1:E:429:LEU:HD22	2.36	0.61
2:H:193:LEU:O	2:H:197:LYS:HG3	2.00	0.61
2:B:30:ILE:HB	2:B:35:LEU:HD21	1.82	0.61
1:A:1:MET:HG3	1:A:46:PRO:HA	1.82	0.61
2:B:88:ARG:HD3	5:B:1580:HOH:O	1.99	0.61
2:B:316:ARG:HG2	2:B:316:ARG:HH11	1.65	0.61
1:C:144:ALA:HA	1:C:227:LEU:HD12	1.83	0.61
1:A:32:LYS:H	1:A:32:LYS:HD3	1.66	0.61
1:A:32:LYS:H	1:A:32:LYS:CD	2.13	0.60
1:C:49:LYS:HE3	1:C:52:GLU:OE1	1.99	0.60
1:E:128:ALA:O	1:E:129:SER:HB3	2.00	0.60
2:F:80:PRO:HG2	2:F:83:HIS:CE1	2.36	0.60
1:E:188:THR:HG23	1:E:212:GLU:CD	2.21	0.60
1:C:4:THR:HG21	2:D:344:LYS:HE2	1.84	0.60
2:F:383:GLU:CD	2:F:383:GLU:H	2.04	0.60
2:H:80:PRO:HG2	2:H:83:HIS:CE1	2.37	0.60
2:H:284:VAL:HG22	2:H:288:LEU:HB2	1.83	0.60
2:B:25:LYS:HG3	2:B:27:GLU:HG2	1.84	0.60
2:B:166:HIS:CD2	4:B:1476:AOA:H1N1	2.20	0.59
1:E:324:GLN:HE21	1:E:328:LEU:HD13	1.67	0.59
1:G:77:HIS:HB2	1:G:420:LEU:HD21	1.83	0.59
1:G:97:PRO:HB2	1:G:107:LEU:HD22	1.84	0.59
1:C:130:MET:HE3	1:C:139:GLU:HB2	1.84	0.59
2:D:80:PRO:HG2	2:D:83:HIS:CE1	2.36	0.59
2:D:411:LYS:NZ	2:D:411:LYS:HB3	2.17	0.59
2:F:411:LYS:HB2	2:F:411:LYS:NZ	2.17	0.59
2:H:83:HIS:HB3	2:H:329:ARG:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:THR:CG2	4:D:2476:AOA:H1C2	2.33	0.59
1:G:50:VAL:O	1:G:54:LEU:HD23	2.03	0.59
2:B:210:THR:HG22	2:B:239:ASP:HB3	1.84	0.59
2:F:68:PHE:CE1	2:F:422:GLU:HG3	2.37	0.59
2:F:78:TYR:HB2	2:H:48:LEU:HG	1.85	0.59
2:B:442:LYS:HD2	2:B:442:LYS:N	2.17	0.59
2:B:31:PRO:HG2	2:B:34:HIS:HD2	1.67	0.59
2:H:72:GLY:O	2:H:73:SER:HB2	2.03	0.59
2:H:107:ARG:O	2:H:111:GLU:HG3	2.02	0.59
2:F:4:PRO:HG2	2:F:9:ARG:CZ	2.32	0.59
2:B:129:PRO:HG2	2:B:280:GLY:O	2.02	0.59
2:H:154:ARG:HG3	2:H:154:ARG:HH11	1.68	0.59
2:F:26:ALA:O	2:F:30:ILE:HD13	2.03	0.58
2:B:40:PRO:HG2	2:B:42:LEU:HD22	1.85	0.58
1:E:376:ASN:H	1:E:376:ASN:ND2	2.00	0.58
2:B:370:ASP:HA	5:B:1554:HOH:O	2.02	0.58
2:B:442:LYS:O	2:B:446:GLU:HG3	2.03	0.58
2:D:30:ILE:HD11	2:D:35:LEU:HD21	1.86	0.58
1:A:32:LYS:HD3	1:A:32:LYS:N	2.19	0.58
2:D:442:LYS:HD2	2:D:442:LYS:N	2.18	0.58
2:B:158:VAL:HG12	2:B:203:HIS:O	2.04	0.58
2:H:211:ASN:HA	2:H:212:PRO:C	2.24	0.58
2:H:236:LEU:HD22	2:H:257:PHE:CE1	2.38	0.58
2:D:83:HIS:HB3	2:D:329:ARG:HD2	1.85	0.58
1:A:70:GLY:H	1:A:402:THR:CG2	2.16	0.57
1:A:132:ASP:OD1	1:A:135:THR:HB	2.04	0.57
1:A:286:LEU:HB2	1:A:306:ARG:NH2	2.20	0.57
2:D:291:TYR:O	2:D:314:ILE:HG23	2.05	0.57
2:H:210:THR:HG22	2:H:239:ASP:HB3	1.86	0.57
2:B:442:LYS:H	2:B:442:LYS:CD	2.16	0.57
1:G:33:GLU:H	1:G:33:GLU:CD	2.06	0.57
2:H:318:ARG:HD3	2:H:319:SER:O	2.04	0.57
2:F:455:ARG:HB3	5:F:3565:HOH:O	2.03	0.57
2:B:4:PRO:HG2	2:B:9:ARG:NH2	2.19	0.57
2:B:221:ARG:NH2	2:B:224:GLU:HG3	2.20	0.57
1:E:351:GLU:OE1	2:F:24:PRO:HB3	2.05	0.57
1:G:45:LEU:HD22	1:G:49:LYS:HG2	1.87	0.57
2:H:243:LEU:CD1	2:H:247:MET:HG2	2.34	0.57
1:E:168:ARG:O	1:E:172:GLU:HG3	2.05	0.57
1:C:68:PHE:CD2	1:C:429:LEU:HD22	2.40	0.56
2:B:166:HIS:NE2	4:B:1476:AOA:H1C2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:THR:HG22	5:C:565:HOH:O	2.04	0.56
1:A:108:GLN:O	1:A:112:GLU:HG3	2.05	0.56
2:B:32:LYS:HE3	2:B:32:LYS:HA	1.86	0.56
2:D:442:LYS:H	2:D:442:LYS:CD	2.14	0.56
1:G:128:ALA:O	1:G:129:SER:HB3	2.05	0.56
2:H:129:PRO:HG2	2:H:280:GLY:O	2.05	0.56
2:B:68:PHE:HE1	2:B:422:GLU:HG3	1.69	0.56
1:C:377:GLU:HG2	1:C:416:ALA:HB2	1.87	0.56
2:D:424:LYS:O	2:D:428:GLU:HG3	2.04	0.56
1:C:391:ARG:NH1	2:D:100:ARG:HD2	2.20	0.56
1:A:372:LYS:N	1:A:372:LYS:HD2	2.21	0.56
2:B:243:LEU:HD13	2:B:247:MET:HB3	1.86	0.56
2:H:262:LEU:O	2:H:280:GLY:HA2	2.05	0.56
2:D:4:PRO:HG2	2:D:9:ARG:NH2	2.20	0.56
2:F:166:HIS:NE2	4:F:3476:AOA:C1	2.69	0.56
2:B:25:LYS:HE3	2:B:26:ALA:N	2.16	0.56
2:D:117:LYS:HA	2:D:120:THR:HG22	1.88	0.56
2:B:367:VAL:HG11	2:B:370:ASP:HB3	1.88	0.56
1:E:128:ALA:O	1:E:129:SER:CB	2.53	0.55
1:E:365:GLY:H	1:E:367:ARG:NH1	2.04	0.55
1:A:335:ALA:HA	2:B:43:PRO:HG2	1.89	0.55
1:C:301:LEU:N	1:C:301:LEU:HD22	2.21	0.55
2:H:375:HIS:CE1	2:H:376:GLU:HG2	2.41	0.55
2:B:238:TYR:HB3	2:B:260:VAL:HG22	1.86	0.55
1:A:128:ALA:O	1:A:129:SER:CB	2.54	0.55
2:H:237:TYR:OH	2:H:261:HIS:HB3	2.06	0.55
1:C:130:MET:CE	1:C:139:GLU:HB2	2.36	0.55
1:A:62:LEU:HD22	1:A:399:HIS:NE2	2.22	0.55
2:F:284:VAL:CG1	2:F:288:LEU:HB2	2.37	0.54
2:H:116:LEU:O	2:H:120:THR:HG22	2.07	0.54
1:E:7:THR:OG1	1:E:10:GLU:HG3	2.08	0.54
2:B:383:GLU:H	2:B:383:GLU:CD	2.10	0.54
1:A:7:THR:OG1	1:A:10:GLU:HG3	2.08	0.54
1:A:167:LEU:HG	1:A:171:LEU:HD22	1.89	0.54
2:F:248:GLY:HA3	2:F:343:LYS:HG2	1.89	0.54
1:C:222:HIS:HE1	1:C:249:ASP:OD2	1.89	0.54
2:H:289:ALA:N	2:H:290:PRO:HD2	2.23	0.54
1:C:128:ALA:O	1:C:129:SER:CB	2.54	0.54
1:G:156:SER:OG	1:G:188:THR:HG21	2.08	0.54
2:B:146:TYR:O	2:B:150:ARG:HG3	2.06	0.54
2:D:107:ARG:NH1	2:D:111:GLU:OE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:376:ASN:HD22	1:E:376:ASN:N	2.01	0.54
2:D:210:THR:OG1	2:D:213:ASN:HA	2.08	0.54
2:F:30:ILE:HD13	2:F:30:ILE:H	1.71	0.54
2:H:395:LEU:HD13	2:H:401:PRO:HD3	1.90	0.54
2:F:26:ALA:HB1	2:F:30:ILE:HD11	1.90	0.53
2:H:40:PRO:HB2	2:H:42:LEU:HD13	1.89	0.53
2:H:265:HIS:CA	2:H:270:VAL:HB	2.35	0.53
2:B:134:HIS:HE1	2:B:318:ARG:HB3	1.72	0.53
2:H:120:THR:HG23	2:H:122:MET:H	1.72	0.53
2:H:235:GLN:HE21	2:H:288:LEU:HD11	1.74	0.53
2:B:318:ARG:HD3	2:B:319:SER:O	2.07	0.53
1:C:50:VAL:O	1:C:54:LEU:HD22	2.08	0.53
2:H:302:GLU:OE1	2:H:302:GLU:N	2.36	0.53
2:F:25:LYS:HE2	2:F:26:ALA:H	1.73	0.53
1:A:276:LYS:HD3	2:B:474:GLY:O	2.08	0.53
2:B:444:TRP:CE3	2:B:445:LEU:HD12	2.40	0.53
1:G:328:LEU:O	1:G:332:MET:HG3	2.09	0.53
2:B:357:LYS:CE	2:B:370:ASP:HB2	2.39	0.53
2:B:357:LYS:HZ3	2:B:370:ASP:HB2	1.73	0.53
2:F:32:LYS:O	2:F:32:LYS:HD3	2.08	0.53
1:C:167:LEU:HG	1:C:171:LEU:HD22	1.91	0.52
5:E:586:HOH:O	2:F:461:ARG:HD3	2.09	0.52
1:E:356:LEU:HD13	1:E:426:LEU:HD22	1.91	0.52
2:H:198:ARG:NH1	2:H:198:ARG:HB2	2.25	0.52
2:F:129:PRO:HG2	2:F:280:GLY:O	2.09	0.52
2:H:454:VAL:CG1	2:H:457:LEU:HD21	2.39	0.52
1:E:51:LEU:HG	2:F:82:LEU:HD11	1.91	0.52
2:B:294:VAL:CG2	2:B:295:PRO:HA	2.39	0.52
2:B:394:LEU:HD13	2:B:437:LEU:HD11	1.90	0.52
2:D:68:PHE:CE1	2:D:422:GLU:HG3	2.45	0.52
1:A:143:LEU:C	1:A:143:LEU:HD23	2.30	0.52
1:A:300:ILE:CD1	2:B:459:GLU:HG2	2.40	0.52
2:B:4:PRO:HG2	2:B:9:ARG:CZ	2.40	0.52
2:B:294:VAL:HG22	2:B:295:PRO:HA	1.90	0.52
2:D:294:VAL:CG2	2:D:295:PRO:HA	2.40	0.52
2:H:98:ASP:OD2	2:H:100:ARG:HB2	2.10	0.52
2:F:102:ALA:O	2:F:106:LEU:HD22	2.10	0.52
2:H:238:TYR:HB2	2:H:257:PHE:CD1	2.45	0.52
1:E:93:THR:HG21	2:F:65:ASP:OD1	2.10	0.51
2:B:160:LEU:HD23	2:B:181:ARG:HB3	1.91	0.51
1:C:320:THR:HG23	4:D:2476:AOA:H1C2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:367:VAL:HG11	2:F:370:ASP:HB3	1.93	0.51
1:G:32:LYS:HD3	1:G:32:LYS:N	2.20	0.51
2:H:243:LEU:O	2:H:243:LEU:HD13	2.11	0.51
2:H:290:PRO:HA	2:H:310:ARG:HH21	1.75	0.51
2:H:441:PRO:HG2	2:H:444:TRP:HB2	1.92	0.51
2:B:155:THR:O	2:B:203:HIS:HA	2.09	0.51
2:B:238:TYR:HD2	2:B:260:VAL:HG13	1.74	0.51
1:G:128:ALA:O	1:G:129:SER:CB	2.58	0.51
1:C:30:LEU:HD22	2:D:218:PHE:CG	2.44	0.51
2:D:367:VAL:HG12	2:D:370:ASP:HB3	1.91	0.51
2:H:424:LYS:O	2:H:428:GLU:HG3	2.11	0.51
1:E:57:LEU:CD2	2:F:107:ARG:HD2	2.41	0.51
2:F:375:HIS:CE1	2:F:376:GLU:HG2	2.46	0.51
1:A:383:PRO:HG2	1:A:437:LEU:HG	1.92	0.51
2:B:397:LEU:HD22	2:B:437:LEU:HD21	1.91	0.51
2:D:72:GLY:HA3	2:D:415:MET:HG2	1.93	0.51
2:F:395:LEU:CD1	2:F:401:PRO:HD3	2.41	0.51
1:G:222:HIS:HE1	1:G:249:ASP:OD2	1.93	0.51
2:H:383:GLU:CD	2:H:383:GLU:H	2.14	0.51
1:C:108:GLN:O	1:C:112:GLU:HG3	2.10	0.51
1:G:7:THR:OG1	1:G:10:GLU:HG3	2.11	0.51
2:H:381:PRO:HB3	2:H:390:LEU:CD1	2.40	0.51
2:D:235:GLN:HE21	2:D:288:LEU:HD11	1.74	0.51
2:H:4:PRO:HG2	2:H:9:ARG:CZ	2.41	0.51
2:F:142:ILE:HG23	2:F:291:TYR:HB2	1.91	0.51
2:H:357:LYS:CE	2:H:370:ASP:HB2	2.41	0.51
1:A:406:ARG:HG2	1:A:406:ARG:HH11	1.75	0.50
2:B:236:LEU:HD22	2:B:257:PHE:CE1	2.46	0.50
1:C:430:ARG:O	1:C:434:LYS:HG3	2.11	0.50
2:F:441:PRO:HG2	2:F:444:TRP:HB2	1.94	0.50
2:B:294:VAL:HG21	2:B:308:PHE:HA	1.93	0.50
1:C:95:TYR:CG	1:C:96:THR:N	2.79	0.50
2:D:464:LYS:HE2	2:D:464:LYS:HA	1.93	0.50
2:H:113:GLY:O	2:H:117:LYS:HG3	2.10	0.50
2:B:245:ALA:HB2	2:B:375:HIS:HB3	1.92	0.50
1:C:97:PRO:HG2	1:C:301:LEU:HD21	1.93	0.50
1:C:280:ARG:HG2	1:C:280:ARG:O	2.10	0.50
2:D:289:ALA:N	2:D:290:PRO:HD2	2.26	0.50
2:H:166:HIS:NE2	4:H:4476:AOA:N1	2.59	0.50
1:E:212:GLU:HG3	5:E:562:HOH:O	2.11	0.50
2:H:142:ILE:HG23	2:H:291:TYR:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:377:GLU:HG2	1:E:416:ALA:HB2	1.94	0.50
1:E:383:PRO:HG2	1:E:437:LEU:HG	1.92	0.50
2:H:201:GLY:HA3	2:H:203:HIS:CE1	2.47	0.50
2:F:442:LYS:O	2:F:446:GLU:HG3	2.11	0.50
1:G:430:ARG:O	1:G:434:LYS:HG3	2.11	0.50
1:A:340:GLU:O	1:A:344:GLU:HG3	2.12	0.50
2:B:188:GLU:HB2	5:B:1597:HOH:O	2.12	0.50
2:B:316:ARG:HG2	2:B:316:ARG:NH1	2.27	0.50
1:C:128:ALA:O	1:C:129:SER:HB3	2.12	0.50
2:F:238:TYR:HB2	2:F:257:PHE:CD1	2.46	0.50
1:E:167:LEU:HG	1:E:171:LEU:HD22	1.93	0.50
1:G:1:MET:HG2	1:G:45:LEU:C	2.32	0.49
2:D:210:THR:CG2	2:D:239:ASP:HB3	2.39	0.49
2:H:68:PHE:CE1	2:H:422:GLU:HG3	2.47	0.49
2:H:260:VAL:HG12	2:H:261:HIS:N	2.26	0.49
2:H:406:PHE:HA	2:H:407:PRO:C	2.32	0.49
2:F:30:ILE:HD11	2:F:35:LEU:CD2	2.33	0.49
2:F:69:TYR:HD1	2:F:71:LEU:HD22	1.77	0.49
2:F:166:HIS:HA	2:F:406:PHE:CZ	2.47	0.49
1:G:291:VAL:HG13	1:G:295:GLY:HA2	1.94	0.49
2:D:245:ALA:HB2	2:D:375:HIS:HB3	1.95	0.49
1:A:377:GLU:HG2	1:A:416:ALA:HB2	1.94	0.49
1:G:12:ARG:O	1:G:16:ARG:HG3	2.13	0.49
1:A:356:LEU:HB2	1:A:426:LEU:HD22	1.94	0.49
2:B:394:LEU:HD23	2:B:401:PRO:HA	1.94	0.49
2:F:166:HIS:NE2	4:F:3476:AOA:H1C1	2.27	0.49
2:B:318:ARG:NH2	2:B:323:ASN:OD1	2.46	0.49
2:F:245:ALA:HB2	2:F:375:HIS:HB3	1.94	0.49
2:F:284:VAL:HG12	2:F:285:LYS:O	2.13	0.49
1:G:372:LYS:HB2	1:G:372:LYS:NZ	2.28	0.49
1:A:73:VAL:HG23	2:B:320:PHE:CZ	2.48	0.49
1:C:431:GLU:OE2	1:C:434:LYS:HE2	2.13	0.49
2:D:463:ASN:C	2:D:464:LYS:HE2	2.33	0.49
1:E:151:MET:HG2	5:E:578:HOH:O	2.13	0.49
2:H:294:VAL:CG2	2:H:295:PRO:HA	2.43	0.49
1:G:107:LEU:HD11	1:G:301:LEU:CD2	2.42	0.49
1:G:286:LEU:HD22	2:H:468:LEU:HD12	1.94	0.49
1:A:95:TYR:CG	1:A:96:THR:N	2.80	0.49
2:D:261:HIS:C	2:D:261:HIS:CD2	2.86	0.49
2:F:78:TYR:CZ	2:F:80:PRO:HA	2.48	0.49
2:B:367:VAL:HG12	2:B:370:ASP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:294:VAL:HG21	2:D:308:PHE:HA	1.95	0.48
1:E:108:GLN:O	1:E:112:GLU:HG3	2.13	0.48
2:F:403:THR:HB	2:F:415:MET:HB3	1.94	0.48
2:H:4:PRO:HG2	2:H:9:ARG:NH2	2.28	0.48
2:H:318:ARG:NH2	2:H:323:ASN:OD1	2.46	0.48
1:C:32:LYS:H	1:C:32:LYS:CD	2.03	0.48
2:D:237:TYR:CD1	2:D:259:VAL:HG13	2.48	0.48
2:F:128:GLU:N	2:F:129:PRO:HD2	2.28	0.48
2:H:144:ARG:HG2	2:H:148:GLU:OE1	2.13	0.48
2:F:235:GLN:HE21	2:F:288:LEU:HD11	1.76	0.48
2:F:40:PRO:HB2	2:F:42:LEU:HD13	1.94	0.48
2:D:383:GLU:H	2:D:383:GLU:CD	2.15	0.48
2:H:243:LEU:HD13	2:H:247:MET:HG2	1.96	0.48
2:H:455:ARG:HB3	5:H:4553:HOH:O	2.13	0.48
1:A:11:ILE:HG22	1:A:15:LEU:HD22	1.96	0.48
1:A:376:ASN:H	1:A:376:ASN:HD22	1.62	0.48
1:E:362:GLU:OE1	1:E:430:ARG:NH1	2.47	0.48
2:F:238:TYR:HB3	2:F:260:VAL:HG22	1.95	0.48
1:G:167:LEU:HG	1:G:171:LEU:HD22	1.96	0.48
1:C:320:THR:HG21	4:D:2476:AOA:H1C2	1.96	0.48
1:E:361:LEU:HD21	1:E:368:PRO:HB3	1.96	0.48
2:F:265:HIS:CA	2:F:270:VAL:HB	2.36	0.48
1:A:391:ARG:O	1:A:395:GLU:HG3	2.14	0.48
1:C:255:GLY:HA3	1:C:269:PHE:CE1	2.48	0.48
1:A:300:ILE:HD13	2:B:459:GLU:HG2	1.96	0.47
1:C:2:ASP:OD2	1:C:4:THR:HB	2.14	0.47
2:D:227:ARG:HG2	2:D:227:ARG:HH11	1.79	0.47
2:F:25:LYS:HE2	2:F:25:LYS:HA	1.96	0.47
2:H:198:ARG:CB	2:H:198:ARG:HH11	2.27	0.47
2:D:166:HIS:NE2	4:D:2476:AOA:C1	2.73	0.47
1:E:291:VAL:HG22	1:E:295:GLY:C	2.35	0.47
1:G:311:ARG:HG3	1:G:314:LYS:CB	2.41	0.47
2:H:402:PRO:HB2	2:H:415:MET:O	2.14	0.47
1:A:322:ASN:O	2:B:277:PRO:HA	2.14	0.47
1:G:80:PRO:HG2	5:G:469:HOH:O	2.14	0.47
2:H:316:ARG:HG2	2:H:316:ARG:HH11	1.80	0.47
1:A:260:LEU:HG	1:A:329:MET:CE	2.44	0.47
2:D:221:ARG:O	2:D:225:ILE:HG13	2.14	0.47
1:G:376:ASN:H	1:G:376:ASN:HD22	1.60	0.47
2:H:284:VAL:HG21	2:H:288:LEU:HB2	1.94	0.47
1:A:260:LEU:HG	1:A:329:MET:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:TYR:HB2	2:B:257:PHE:CD1	2.50	0.47
2:F:69:TYR:HB3	2:F:76:MET:HG3	1.96	0.47
2:F:80:PRO:HG2	2:F:83:HIS:ND1	2.29	0.47
2:F:166:HIS:HA	2:F:406:PHE:HZ	1.79	0.47
2:F:169:ASN:HB2	2:F:170:PRO:CD	2.45	0.47
2:F:311:PRO:HG2	5:F:3609:HOH:O	2.14	0.47
2:H:25:LYS:HG3	2:H:27:GLU:CG	2.45	0.47
1:A:32:LYS:H	1:A:32:LYS:CE	2.28	0.47
1:A:168:ARG:O	1:A:172:GLU:HG3	2.14	0.47
2:B:381:PRO:HB3	2:B:390:LEU:CD1	2.45	0.47
1:C:157:GLN:HB3	1:C:183:LEU:HD13	1.95	0.47
2:D:406:PHE:CD1	2:D:407:PRO:HA	2.50	0.47
1:E:50:VAL:O	1:E:54:LEU:HD22	2.15	0.47
1:E:81:VAL:HG13	1:E:82:VAL:N	2.29	0.47
1:A:376:ASN:H	1:A:376:ASN:ND2	2.12	0.47
1:E:348:LYS:HE3	2:F:20:VAL:HG13	1.97	0.47
2:B:301:GLU:H	2:B:301:GLU:HG3	1.47	0.47
2:H:72:GLY:HA3	2:H:415:MET:HG2	1.97	0.47
1:A:32:LYS:CD	1:A:32:LYS:N	2.77	0.47
1:E:143:LEU:HD23	1:E:143:LEU:C	2.36	0.47
1:A:162:GLU:HG2	2:B:316:ARG:NE	2.30	0.46
2:B:136:GLU:O	2:B:140:ILE:HG12	2.15	0.46
2:B:235:GLN:HE21	2:B:288:LEU:HD11	1.80	0.46
1:E:391:ARG:HG3	1:E:391:ARG:NH1	2.29	0.46
1:G:1:MET:HG2	1:G:45:LEU:O	2.15	0.46
1:A:402:THR:HG23	1:A:414:LEU:HB2	1.95	0.46
2:B:466:PRO:HB2	2:B:468:LEU:CD1	2.46	0.46
1:E:55:ARG:NH2	1:G:65:HIS:NE2	2.63	0.46
2:F:468:LEU:CD1	2:F:468:LEU:N	2.78	0.46
2:D:78:TYR:CZ	2:D:80:PRO:HA	2.50	0.46
2:H:138:THR:O	2:H:142:ILE:HG13	2.15	0.46
2:H:157:ARG:HE	2:H:157:ARG:CA	2.21	0.46
2:H:325:LEU:HD12	2:H:325:LEU:HA	1.80	0.46
2:F:72:GLY:HA2	2:F:417:GLU:HB3	1.97	0.46
2:H:227:ARG:HH11	2:H:227:ARG:CB	2.19	0.46
1:C:55:ARG:NH2	5:C:494:HOH:O	2.48	0.46
2:D:106:LEU:HD11	2:D:306:LEU:CD2	2.45	0.46
2:D:263:ASN:HB2	2:D:266:LYS:HB2	1.97	0.46
1:A:376:ASN:HD22	1:A:376:ASN:N	2.13	0.46
1:G:112:GLU:HB2	5:G:482:HOH:O	2.15	0.46
2:B:48:LEU:HG	2:D:78:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:389:VAL:O	1:E:393:LEU:HB2	2.15	0.46
2:F:164:SER:HB2	2:F:214:THR:OG1	2.15	0.46
1:G:384:LYS:HD2	1:G:437:LEU:HD12	1.96	0.46
2:H:30:ILE:HG23	2:H:31:PRO:HD2	1.96	0.46
2:H:354:ARG:O	2:H:357:LYS:HB3	2.15	0.46
2:H:363:LYS:HD2	2:H:435:GLY:HA3	1.98	0.46
1:E:241:LYS:HD3	1:E:246:TYR:CZ	2.50	0.46
2:B:195:ALA:O	2:B:198:ARG:HG2	2.15	0.46
1:C:424:GLU:HG2	5:C:538:HOH:O	2.15	0.46
1:E:95:TYR:CG	1:E:96:THR:N	2.84	0.46
2:H:166:HIS:NE2	4:H:4476:AOA:C1	2.79	0.46
2:H:381:PRO:HB3	2:H:390:LEU:HD12	1.98	0.46
1:A:344:GLU:OE1	2:B:15:ARG:NH2	2.47	0.46
1:C:239:VAL:HG21	1:C:347:LEU:HD21	1.97	0.46
1:C:433:LEU:HA	1:C:436:VAL:CG1	2.46	0.46
2:D:245:ALA:HB2	2:D:375:HIS:CG	2.50	0.46
2:F:237:TYR:OH	2:F:261:HIS:HB3	2.16	0.46
1:A:292:ASP:HB3	2:B:454:VAL:HG22	1.98	0.45
1:E:391:ARG:HA	2:F:98:ASP:OD2	2.16	0.45
2:F:221:ARG:NH2	2:F:224:GLU:HG3	2.32	0.45
2:F:238:TYR:CE2	2:F:240:GLY:HA2	2.51	0.45
2:H:4:PRO:HB3	5:H:4548:HOH:O	2.16	0.45
2:H:195:ALA:HA	2:H:198:ARG:NH2	2.31	0.45
2:B:98:ASP:OD2	2:B:100:ARG:HB2	2.17	0.45
1:G:436:VAL:CG2	1:G:437:LEU:HD13	2.46	0.45
2:H:196:LEU:HG	2:H:200:LEU:HD13	1.98	0.45
1:A:46:PRO:HD3	2:D:21:LYS:HG2	1.96	0.45
1:E:45:LEU:HD13	1:E:49:LYS:HG3	1.98	0.45
1:G:97:PRO:HB2	1:G:107:LEU:CD2	2.46	0.45
1:G:311:ARG:HG2	1:G:311:ARG:HH11	1.80	0.45
2:H:162:PRO:HG2	2:H:165:ALA:HB2	1.97	0.45
2:B:262:LEU:O	2:B:280:GLY:HA2	2.16	0.45
1:E:83:GLN:HE22	1:E:329:MET:HE3	1.80	0.45
2:F:25:LYS:HE2	2:F:26:ALA:N	2.31	0.45
2:F:211:ASN:HA	2:F:212:PRO:C	2.37	0.45
2:F:381:PRO:HB3	2:F:390:LEU:CD1	2.46	0.45
1:G:30:LEU:HD13	2:H:218:PHE:CE1	2.52	0.45
1:G:387:GLU:HG3	5:G:550:HOH:O	2.15	0.45
2:B:31:PRO:HG2	2:B:34:HIS:CD2	2.50	0.45
1:G:68:PHE:CD2	1:G:429:LEU:HD22	2.51	0.45
1:C:107:LEU:HD11	1:C:301:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:LEU:O	1:C:332:MET:HG3	2.16	0.45
2:D:143:ILE:HD11	2:D:259:VAL:HG11	1.98	0.45
2:B:289:ALA:N	2:B:290:PRO:HD2	2.32	0.45
2:D:169:ASN:HB2	2:D:170:PRO:CD	2.47	0.45
2:D:316:ARG:HG2	2:D:316:ARG:HH11	1.82	0.45
2:H:440:LYS:HB2	2:H:445:LEU:HD21	1.98	0.45
1:A:11:ILE:O	1:A:15:LEU:HB2	2.17	0.45
2:B:211:ASN:HA	2:B:212:PRO:C	2.36	0.45
2:B:325:LEU:HD12	2:B:325:LEU:HA	1.84	0.45
1:C:337:LEU:HD13	2:D:17:LEU:HB2	1.99	0.45
2:D:237:TYR:HD1	2:D:259:VAL:CG1	2.29	0.45
1:E:196:GLU:H	1:E:196:GLU:CD	2.21	0.45
2:F:48:LEU:HG	2:H:78:TYR:HB2	1.97	0.45
2:F:411:LYS:HB2	2:F:411:LYS:HZ3	1.80	0.45
2:F:391:ALA:O	2:F:395:LEU:HD13	2.16	0.45
2:F:261:HIS:CD2	2:F:261:HIS:C	2.91	0.45
1:C:311:ARG:NH1	1:C:314:LYS:HD3	2.32	0.44
1:C:356:LEU:HG	1:C:360:LEU:HD22	1.99	0.44
2:D:33:GLU:CD	2:D:33:GLU:H	2.20	0.44
2:F:80:PRO:CG	2:F:83:HIS:CE1	3.00	0.44
1:A:356:LEU:HD11	1:A:429:LEU:HD23	1.99	0.44
1:A:406:ARG:HG2	1:A:406:ARG:NH1	2.32	0.44
1:C:31:PRO:HG2	1:C:34:ILE:CD1	2.48	0.44
2:D:395:LEU:CD1	2:D:401:PRO:HD3	2.45	0.44
2:H:210:THR:CG2	2:H:239:ASP:HB3	2.46	0.44
1:C:7:THR:OG1	1:C:10:GLU:HG3	2.16	0.44
1:E:352:MET:HE2	1:E:422:GLU:HA	1.99	0.44
2:F:141:LEU:HD12	2:F:141:LEU:HA	1.80	0.44
2:H:316:ARG:HG2	2:H:316:ARG:NH1	2.32	0.44
1:A:50:VAL:O	1:A:54:LEU:HD22	2.17	0.44
1:A:373:PRO:HG3	2:B:31:PRO:HG3	1.98	0.44
2:D:464:LYS:HE2	2:D:464:LYS:CA	2.47	0.44
1:E:36:SER:HA	5:E:560:HOH:O	2.17	0.44
1:E:197:VAL:O	1:E:226:ALA:HB2	2.18	0.44
2:F:299:ARG:HB3	2:F:304:PHE:CE1	2.53	0.44
2:H:137:LEU:O	2:H:141:LEU:HB2	2.18	0.44
1:C:30:LEU:HD22	2:D:218:PHE:CD1	2.52	0.44
1:C:250:ILE:HG23	1:C:272:LEU:HD11	1.99	0.44
2:D:157:ARG:HA	2:D:157:ARG:HE	1.83	0.44
2:D:238:TYR:HB2	2:D:257:PHE:CD1	2.53	0.44
1:G:50:VAL:O	1:G:54:LEU:CD2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:192:ASP:HB3	2:H:195:ALA:HB3	1.99	0.44
2:B:243:LEU:CD1	2:B:247:MET:HB3	2.46	0.44
2:B:245:ALA:HB2	2:B:375:HIS:CG	2.53	0.44
2:B:261:HIS:HA	2:B:281:PRO:O	2.18	0.44
2:F:357:LYS:NZ	2:F:370:ASP:HB2	2.33	0.44
1:G:255:GLY:HA3	1:G:269:PHE:CE1	2.52	0.44
2:H:163:ASP:N	2:H:163:ASP:OD1	2.49	0.44
2:H:355:TYR:CE2	2:H:359:LEU:HD11	2.53	0.44
2:H:397:LEU:HD23	2:H:433:ALA:HB1	2.00	0.44
1:C:433:LEU:O	1:C:436:VAL:HG13	2.18	0.44
1:A:201:VAL:HG22	1:A:229:VAL:HB	2.00	0.44
2:D:72:GLY:O	2:D:73:SER:HB2	2.18	0.44
1:E:57:LEU:HD21	2:F:107:ARG:HD2	2.00	0.44
2:F:157:ARG:HG2	2:F:157:ARG:HH11	1.83	0.44
1:G:376:ASN:H	1:G:376:ASN:ND2	2.16	0.44
2:H:117:LYS:HA	2:H:120:THR:HG22	1.99	0.44
2:H:183:ILE:HG22	2:H:199:GLU:HG3	1.99	0.44
2:B:394:LEU:HD13	2:B:437:LEU:CD1	2.47	0.43
2:H:25:LYS:HG3	2:H:27:GLU:HG3	2.00	0.43
2:H:158:VAL:HG13	2:H:204:VAL:HA	2.00	0.43
2:B:132:GLY:HA3	2:B:263:ASN:ND2	2.33	0.43
2:D:264:LEU:HD22	2:D:279:SER:HB3	2.00	0.43
1:E:321:THR:HG23	2:F:275:GLY:O	2.18	0.43
2:B:264:LEU:HB2	2:B:279:SER:HB3	1.99	0.43
2:D:107:ARG:O	2:D:111:GLU:HG3	2.17	0.43
2:D:406:PHE:HA	2:D:407:PRO:C	2.37	0.43
1:G:159:VAL:HG22	1:G:203:GLN:HB2	2.01	0.43
2:D:80:PRO:HG2	2:D:83:HIS:ND1	2.34	0.43
1:G:97:PRO:HG3	1:G:107:LEU:HD13	2.00	0.43
1:G:311:ARG:HE	1:G:314:LYS:HE3	1.82	0.43
1:A:30:LEU:HD22	2:B:218:PHE:CD2	2.53	0.43
1:E:396:ARG:HG3	1:E:396:ARG:HH11	1.83	0.43
2:F:24:PRO:HB2	2:F:29:LEU:HD21	2.00	0.43
1:G:11:ILE:HG22	1:G:15:LEU:HD22	2.00	0.43
2:B:357:LYS:HE3	2:B:367:VAL:HG11	1.99	0.43
1:C:391:ARG:HG3	1:C:391:ARG:NH1	2.32	0.43
2:D:201:GLY:HA3	2:D:203:HIS:CE1	2.53	0.43
2:D:394:LEU:HD23	2:D:401:PRO:HA	2.01	0.43
2:B:376:GLU:HB3	2:B:417:GLU:HB2	2.01	0.43
1:C:157:GLN:HB3	1:C:183:LEU:CD1	2.49	0.43
2:F:146:TYR:O	2:F:150:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:THR:HG21	2:H:65:ASP:OD1	2.18	0.43
1:C:391:ARG:HH11	1:C:391:ARG:CG	2.31	0.43
2:D:136:GLU:O	2:D:140:ILE:HG12	2.19	0.43
2:D:265:HIS:CA	2:D:270:VAL:HB	2.42	0.43
1:E:311:ARG:HG3	1:E:314:LYS:HB2	2.00	0.43
1:G:79:PRO:HA	1:G:80:PRO:HD2	1.89	0.43
1:G:329:MET:HE1	5:G:575:HOH:O	2.19	0.43
1:G:337:LEU:HD13	2:H:17:LEU:HB2	2.01	0.43
1:A:47:GLU:OE2	2:D:17:LEU:HD22	2.19	0.43
1:A:203:GLN:HG2	1:A:205:PRO:O	2.19	0.43
2:B:210:THR:CG2	2:B:239:ASP:HB3	2.46	0.43
1:C:340:GLU:O	1:C:344:GLU:HG3	2.18	0.43
1:G:90:GLU:O	1:G:94:ALA:HB2	2.18	0.43
2:B:25:LYS:HE2	5:B:1657:HOH:O	2.18	0.43
1:C:301:LEU:HD22	1:C:301:LEU:H	1.83	0.43
1:G:391:ARG:NH1	1:G:391:ARG:HG3	2.34	0.43
2:F:94:HIS:CE1	2:F:96:TYR:HB2	2.54	0.42
1:A:348:LYS:HG3	1:A:419:GLU:HA	2.02	0.42
2:B:466:PRO:HB2	2:B:468:LEU:HD11	2.00	0.42
1:E:1:MET:HG2	1:E:45:LEU:C	2.39	0.42
2:H:294:VAL:HG22	2:H:308:PHE:CD1	2.54	0.42
2:H:294:VAL:HG21	2:H:308:PHE:HA	1.97	0.42
2:H:366:ARG:O	2:H:379:ALA:HA	2.20	0.42
1:A:106:VAL:HG23	2:B:61:GLN:CD	2.40	0.42
2:B:242:ASN:HB3	2:B:375:HIS:CE1	2.54	0.42
1:C:107:LEU:HD11	1:C:301:LEU:CD2	2.49	0.42
1:C:155:VAL:CG1	1:C:178:LEU:HD11	2.49	0.42
2:F:30:ILE:HD13	2:F:30:ILE:N	2.34	0.42
2:F:106:LEU:HD11	2:F:306:LEU:HD21	2.01	0.42
2:F:242:ASN:HB3	2:F:375:HIS:CE1	2.55	0.42
2:H:299:ARG:HA	2:H:304:PHE:HA	2.01	0.42
1:A:30:LEU:HD22	2:B:218:PHE:CG	2.54	0.42
1:C:311:ARG:HG3	1:C:314:LYS:HB2	2.00	0.42
2:F:25:LYS:HA	2:F:25:LYS:CE	2.50	0.42
1:A:204:ASN:HA	1:A:205:PRO:C	2.40	0.42
1:A:389:VAL:O	1:A:393:LEU:HB2	2.19	0.42
2:B:40:PRO:CG	2:B:42:LEU:HD22	2.48	0.42
2:F:402:PRO:HB2	2:F:415:MET:O	2.19	0.42
1:G:185:GLY:O	1:G:371:PRO:HG3	2.20	0.42
1:A:97:PRO:HG3	1:A:107:LEU:HD13	2.01	0.42
1:C:15:LEU:HD12	1:C:15:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:PRO:O	1:C:34:ILE:HG12	2.20	0.42
1:G:311:ARG:HG2	1:G:311:ARG:NH1	2.35	0.42
1:G:400:GLY:O	1:G:401:ALA:HB3	2.19	0.42
2:B:5:LEU:HD13	2:B:470:TYR:HD1	1.83	0.42
2:B:360:LEU:HD21	2:B:434:MET:CE	2.50	0.42
1:C:49:LYS:HD2	1:C:49:LYS:HA	1.77	0.42
1:C:174:VAL:HG22	1:C:174:VAL:O	2.20	0.42
2:F:166:HIS:NE2	4:F:3476:AOA:N1	2.55	0.42
1:G:291:VAL:CG1	1:G:295:GLY:HA2	2.50	0.42
1:G:171:LEU:HD12	1:G:171:LEU:HA	1.89	0.42
2:H:381:PRO:HB2	2:H:385:PHE:HB2	2.02	0.42
2:H:394:LEU:HD12	2:H:394:LEU:HA	1.93	0.42
2:B:226:SER:OG	2:B:256:GLY:HA3	2.19	0.42
1:C:79:PRO:HA	1:C:80:PRO:HD2	1.88	0.42
1:C:349:SER:CB	1:C:418:THR:HA	2.50	0.42
2:D:160:LEU:HD23	2:D:181:ARG:HB2	2.02	0.42
1:G:108:GLN:O	1:G:112:GLU:HG3	2.19	0.42
1:A:255:GLY:HA3	1:A:269:PHE:CZ	2.55	0.41
2:D:128:GLU:N	2:D:129:PRO:HD2	2.35	0.41
2:D:237:TYR:HD1	2:D:259:VAL:HG13	1.85	0.41
2:D:329:ARG:HG2	2:D:329:ARG:HH11	1.85	0.41
1:E:267:PRO:HD2	2:F:325:LEU:HB2	2.02	0.41
1:E:337:LEU:O	1:E:341:GLY:HA3	2.20	0.41
1:G:241:LYS:HD3	1:G:246:TYR:CZ	2.55	0.41
2:H:132:GLY:HA3	2:H:263:ASN:HD21	1.85	0.41
1:A:65:HIS:O	1:A:66:LYS:HB2	2.20	0.41
1:C:24:GLU:H	1:C:24:GLU:CD	2.23	0.41
2:D:262:LEU:O	2:D:280:GLY:HA2	2.21	0.41
2:H:78:TYR:CE2	2:H:80:PRO:HA	2.55	0.41
1:C:11:ILE:O	1:C:15:LEU:HB2	2.20	0.41
1:C:351:GLU:HB2	2:D:29:LEU:HD21	2.02	0.41
1:E:394:ALA:HA	1:E:398:PHE:O	2.20	0.41
2:F:166:HIS:CD2	4:F:3476:AOA:H1N1	2.35	0.41
1:G:155:VAL:CG1	1:G:178:LEU:HD11	2.50	0.41
2:H:222:ILE:HG23	2:H:223:LEU:N	2.34	0.41
2:H:284:VAL:HG21	2:H:288:LEU:CB	2.50	0.41
1:A:365:GLY:H	1:A:367:ARG:NH1	2.17	0.41
1:A:400:GLY:O	1:A:401:ALA:HB3	2.20	0.41
1:C:157:GLN:HG2	1:C:157:GLN:O	2.20	0.41
2:D:447:ASN:HB2	2:D:450:TYR:OH	2.19	0.41
2:F:406:PHE:HA	2:F:407:PRO:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:404:VAL:HB	1:G:412:LEU:HB2	2.02	0.41
2:H:310:ARG:HA	2:H:311:PRO:HD2	1.85	0.41
2:F:284:VAL:CG1	2:F:285:LYS:O	2.68	0.41
2:F:367:VAL:HG12	2:F:370:ASP:HB3	2.01	0.41
2:B:166:HIS:NE2	4:B:1476:AOA:C1	2.83	0.41
2:B:395:LEU:CD1	2:B:401:PRO:HD3	2.43	0.41
1:C:39:ILE:HD12	2:D:248:GLY:HA2	2.02	0.41
2:D:80:PRO:HD2	2:D:269:THR:HB	2.01	0.41
2:D:157:ARG:HA	2:D:157:ARG:NE	2.35	0.41
1:E:143:LEU:HD23	1:E:143:LEU:O	2.20	0.41
1:E:400:GLY:O	1:E:401:ALA:HB3	2.21	0.41
2:F:90:PHE:HB3	2:F:324:PHE:HE2	1.85	0.41
2:H:260:VAL:CG1	2:H:261:HIS:N	2.83	0.41
1:A:80:PRO:HG2	5:C:489:HOH:O	2.20	0.41
1:A:288:SER:HB2	1:A:302:THR:HG21	2.03	0.41
2:B:65:ASP:O	2:D:52:ARG:HG2	2.20	0.41
2:B:260:VAL:HG12	2:B:261:HIS:N	2.35	0.41
2:B:294:VAL:HG22	2:B:295:PRO:CA	2.51	0.41
2:D:30:ILE:HD13	2:D:30:ILE:N	2.36	0.41
2:F:366:ARG:HH12	2:F:382:PRO:HA	1.79	0.41
2:H:291:TYR:O	2:H:314:ILE:HG23	2.21	0.41
1:A:17:ARG:HH21	2:B:362:GLU:CD	2.24	0.41
1:A:241:LYS:HE3	1:A:241:LYS:HB2	1.95	0.41
2:B:5:LEU:HD13	2:B:470:TYR:CD1	2.56	0.41
2:D:261:HIS:HA	2:D:281:PRO:O	2.21	0.41
1:A:62:LEU:HD22	1:A:399:HIS:HE2	1.85	0.41
1:A:174:VAL:HG13	5:B:1613:HOH:O	2.20	0.41
1:C:101:GLU:HA	2:D:454:VAL:HG12	2.03	0.41
1:C:158:GLY:CA	1:C:183:LEU:HD11	2.50	0.41
1:C:171:LEU:HD12	1:C:171:LEU:HA	1.81	0.41
1:C:393:LEU:HD13	1:C:436:VAL:HG11	2.02	0.41
2:D:80:PRO:CG	2:D:83:HIS:CE1	3.04	0.41
2:D:136:GLU:HA	2:D:237:TYR:OH	2.21	0.41
1:E:423:GLU:HA	1:E:423:GLU:OE1	2.21	0.41
2:F:357:LYS:HZ1	2:F:370:ASP:HB2	1.85	0.41
2:F:386:ARG:HD3	2:F:389:ASP:OD2	2.20	0.41
1:G:159:VAL:O	1:G:160:HIS:C	2.59	0.41
1:G:267:PRO:HD2	2:H:325:LEU:HB2	2.03	0.41
1:G:432:ALA:O	1:G:436:VAL:HG13	2.21	0.41
2:H:289:ALA:N	2:H:290:PRO:CD	2.84	0.41
1:A:431:GLU:HA	1:A:431:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:PRO:HG2	5:C:577:HOH:O	2.20	0.41
2:D:227:ARG:HG2	2:D:227:ARG:NH1	2.36	0.41
1:E:22:SER:OG	1:E:24:GLU:HG2	2.21	0.41
2:H:357:LYS:HD2	2:H:373:SER:OG	2.21	0.41
2:B:462:ALA:O	2:B:466:PRO:HB3	2.22	0.40
1:C:314:LYS:NZ	1:C:314:LYS:HB3	2.36	0.40
1:C:394:ALA:HB1	2:D:101:THR:HG21	2.03	0.40
2:H:30:ILE:CG2	2:H:31:PRO:HD2	2.51	0.40
2:H:367:VAL:HG12	2:H:370:ASP:HB3	2.02	0.40
2:H:394:LEU:HD23	2:H:401:PRO:HA	2.02	0.40
1:A:1:MET:HE2	1:A:44:PRO:HB2	2.02	0.40
1:C:95:TYR:HB2	2:D:76:MET:HE2	2.02	0.40
1:C:376:ASN:H	1:C:376:ASN:ND2	2.19	0.40
1:E:79:PRO:HA	1:E:80:PRO:HD2	1.89	0.40
1:E:404:VAL:HB	1:E:412:LEU:HB2	2.03	0.40
1:A:260:LEU:HD23	1:A:268:HIS:HA	2.03	0.40
1:A:334:LEU:HD12	1:A:334:LEU:HA	1.92	0.40
2:D:134:HIS:HE1	2:D:318:ARG:HB3	1.86	0.40
2:D:294:VAL:HG22	2:D:295:PRO:HA	2.01	0.40
2:D:302:GLU:CD	2:D:302:GLU:N	2.71	0.40
2:F:289:ALA:N	2:F:290:PRO:HD2	2.37	0.40
2:B:128:GLU:N	2:B:129:PRO:HD2	2.36	0.40
2:D:243:LEU:CD1	2:D:247:MET:HG2	2.51	0.40
2:F:366:ARG:HH12	2:F:382:PRO:C	2.25	0.40
2:F:366:ARG:HH11	2:F:382:PRO:HA	1.81	0.40
1:G:234:PRO:HG3	1:G:255:GLY:HA2	2.03	0.40
1:G:324:GLN:HE21	1:G:328:LEU:HD13	1.86	0.40
2:H:389:ASP:HB3	2:H:445:LEU:HB3	2.03	0.40
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.91	0.40
2:B:299:ARG:HB3	2:B:304:PHE:CD1	2.57	0.40
1:C:10:GLU:O	1:C:14:MET:HG3	2.21	0.40
1:C:168:ARG:HG3	1:C:168:ARG:HH11	1.87	0.40
2:D:394:LEU:HD12	2:D:394:LEU:HA	1.88	0.40
1:E:62:LEU:HB3	2:F:101:THR:HB	2.04	0.40
1:E:159:VAL:HG22	1:E:203:GLN:HB2	2.04	0.40
1:E:391:ARG:HD3	2:F:100:ARG:NH1	2.36	0.40
1:G:190:LEU:HD12	1:G:191:PRO:HD2	2.04	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	435/438 (99%)	416 (96%)	18 (4%)	1 (0%)	47	62
1	C	435/438 (99%)	415 (95%)	19 (4%)	1 (0%)	47	62
1	E	435/438 (99%)	417 (96%)	17 (4%)	1 (0%)	47	62
1	G	435/438 (99%)	416 (96%)	18 (4%)	1 (0%)	47	62
2	B	471/474 (99%)	456 (97%)	15 (3%)	0	100	100
2	D	471/474 (99%)	456 (97%)	15 (3%)	0	100	100
2	F	471/474 (99%)	452 (96%)	19 (4%)	0	100	100
2	H	471/474 (99%)	452 (96%)	19 (4%)	0	100	100
All	All	3624/3648 (99%)	3480 (96%)	140 (4%)	4 (0%)	51	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	SER
1	C	129	SER
1	E	129	SER
1	G	129	SER

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	336/336 (100%)	311 (93%)	25 (7%)	13	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	336/336 (100%)	316 (94%)	20 (6%)	19	31
1	E	336/336 (100%)	316 (94%)	20 (6%)	19	31
1	G	336/336 (100%)	313 (93%)	23 (7%)	16	25
2	B	384/385 (100%)	357 (93%)	27 (7%)	15	24
2	D	384/385 (100%)	366 (95%)	18 (5%)	26	42
2	F	384/385 (100%)	361 (94%)	23 (6%)	19	31
2	H	384/385 (100%)	363 (94%)	21 (6%)	21	35
All	All	2880/2884 (100%)	2703 (94%)	177 (6%)	18	30

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	THR
1	A	12	ARG
1	A	15	LEU
1	A	23	LEU
1	A	41	LEU
1	A	54	LEU
1	A	55	ARG
1	A	107	LEU
1	A	135	THR
1	A	171	LEU
1	A	183	LEU
1	A	188	THR
1	A	237	LEU
1	A	267	PRO
1	A	286	LEU
1	A	301	LEU
1	A	328	LEU
1	A	334	LEU
1	A	360	LEU
1	A	376	ASN
1	A	391	ARG
1	A	402	THR
1	A	406	ARG
1	A	420	LEU
2	B	10	SER
2	B	23	VAL
2	B	25	LYS

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Mol	Chain	Res	Type
2	B	29	LEU
2	B	42	LEU
2	B	48	LEU
2	B	69	TYR
2	B	73	SER
2	B	89	LEU
2	B	106	LEU
2	B	141	LEU
2	B	236	LEU
2	B	259	VAL
2	B	261	HIS
2	B	301	GLU
2	B	302	GLU
2	B	306	LEU
2	B	318	ARG
2	B	321	TYR
2	B	325	LEU
2	B	360	LEU
2	B	394	LEU
2	B	395	LEU
2	B	397	LEU
2	B	440	LYS
2	B	442	LYS
2	B	468	LEU
1	C	4	THR
1	C	15	LEU
1	C	32	LYS
1	C	41	LEU
1	C	54	LEU
1	C	62	LEU
1	C	107	LEU
1	C	171	LEU
1	C	188	THR
1	C	292	ASP
1	C	334	LEU
1	C	360	LEU
1	C	361	LEU
1	C	367	ARG
1	C	376	ASN
1	C	393	LEU
1	C	402	THR
1	C	423	GLU

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Mol	Chain	Res	Type
1	C	427	LEU
1	C	436	VAL
2	D	25	LYS
2	D	30	ILE
2	D	42	LEU
2	D	48	LEU
2	D	73	SER
2	D	88	ARG
2	D	89	LEU
2	D	158	VAL
2	D	236	LEU
2	D	261	HIS
2	D	318	ARG
2	D	325	LEU
2	D	386	ARG
2	D	395	LEU
2	D	440	LYS
2	D	442	LYS
2	D	445	LEU
2	D	454	VAL
1	E	1	MET
1	E	4	THR
1	E	54	LEU
1	E	107	LEU
1	E	123	LEU
1	E	171	LEU
1	E	183	LEU
1	E	184	GLU
1	E	188	THR
1	E	196	GLU
1	E	237	LEU
1	E	286	LEU
1	E	291	VAL
1	E	301	LEU
1	E	334	LEU
1	E	361	LEU
1	E	376	ASN
1	E	423	GLU
1	E	427	LEU
1	E	437	LEU
2	F	23	VAL
2	F	25	LYS

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Mol	Chain	Res	Type
2	F	30	ILE
2	F	48	LEU
2	F	69	TYR
2	F	71	LEU
2	F	73	SER
2	F	88	ARG
2	F	89	LEU
2	F	106	LEU
2	F	141	LEU
2	F	157	ARG
2	F	158	VAL
2	F	236	LEU
2	F	261	HIS
2	F	302	GLU
2	F	318	ARG
2	F	325	LEU
2	F	360	LEU
2	F	397	LEU
2	F	411	LYS
2	F	445	LEU
2	F	468	LEU
1	G	1	MET
1	G	2	ASP
1	G	15	LEU
1	G	30	LEU
1	G	32	LYS
1	G	107	LEU
1	G	123	LEU
1	G	135	THR
1	G	171	LEU
1	G	183	LEU
1	G	188	THR
1	G	237	LEU
1	G	286	LEU
1	G	291	VAL
1	G	328	LEU
1	G	334	LEU
1	G	360	LEU
1	G	361	LEU
1	G	376	ASN
1	G	391	ARG
1	G	393	LEU

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Mol	Chain	Res	Type
1	G	423	GLU
1	G	437	LEU
2	H	23	VAL
2	H	25	LYS
2	H	27	GLU
2	H	48	LEU
2	H	106	LEU
2	H	141	LEU
2	H	157	ARG
2	H	221	ARG
2	H	227	ARG
2	H	236	LEU
2	H	261	HIS
2	H	295	PRO
2	H	302	GLU
2	H	318	ARG
2	H	325	LEU
2	H	329	ARG
2	H	360	LEU
2	H	395	LEU
2	H	434	MET
2	H	464	LYS
2	H	473	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	376	ASN
2	B	34	HIS
2	B	235	GLN
2	B	263	ASN
2	B	380	GLN
1	C	83	GLN
1	C	222	HIS
1	C	376	ASN
2	D	179	GLN
2	D	235	GLN
2	D	263	ASN
1	E	60	GLN
1	E	83	GLN
1	E	376	ASN

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Mol	Chain	Res	Type
2	F	179	GLN
2	F	235	GLN
2	F	375	HIS
1	G	60	GLN
1	G	83	GLN
1	G	222	HIS
1	G	354	HIS
1	G	376	ASN
2	H	179	GLN
2	H	235	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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	$\# Z > 2$
4	AOA	H	4476	3	3,5,5	1.17	0	3,5,5	0.94	0
3	PLP	D	2475	4	15,15,16	1.79	3 (20%)	20,22,23	2.02	3 (15%)
4	AOA	D	2476	3	3,5,5	1.13	0	3,5,5	0.95	0
4	AOA	F	3476	3	3,5,5	1.15	0	3,5,5	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AOA	B	1476	3	3,5,5	1.18	0	3,5,5	0.98	0
3	PLP	H	4475	4	15,15,16	1.84	2 (13%)	20,22,23	1.84	3 (15%)
3	PLP	F	3475	4	15,15,16	1.67	3 (20%)	20,22,23	1.90	3 (15%)
3	PLP	B	1475	4	15,15,16	1.76	3 (20%)	20,22,23	1.90	3 (15%)

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	AOA	H	4476	3	-	1/2/3/3	-
3	PLP	D	2475	4	-	2/6/6/8	0/1/1/1
4	AOA	D	2476	3	-	2/2/3/3	-
4	AOA	F	3476	3	-	0/2/3/3	-
4	AOA	B	1476	3	-	0/2/3/3	-
3	PLP	H	4475	4	-	1/6/6/8	0/1/1/1
3	PLP	F	3475	4	-	0/6/6/8	0/1/1/1
3	PLP	B	1475	4	-	1/6/6/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	4475	PLP	C5-C4	4.58	1.45	1.40
3	D	2475	PLP	C5-C4	4.17	1.45	1.40
3	B	1475	PLP	C5-C4	4.15	1.45	1.40
3	F	3475	PLP	C5-C4	3.60	1.44	1.40
3	B	1475	PLP	C2-N1	3.08	1.39	1.33
3	D	2475	PLP	C2-N1	2.98	1.39	1.33
3	H	4475	PLP	C2-N1	2.96	1.39	1.33
3	F	3475	PLP	C2-N1	2.83	1.39	1.33
3	B	1475	PLP	C2A-C2	2.32	1.54	1.50
3	D	2475	PLP	C2A-C2	2.27	1.54	1.50
3	F	3475	PLP	C2A-C2	2.05	1.53	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2475	PLP	O4P-C5A-C5	7.06	122.80	109.35
3	B	1475	PLP	O4P-C5A-C5	6.62	121.97	109.35
3	F	3475	PLP	O4P-C5A-C5	6.49	121.72	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	4475	PLP	O4P-C5A-C5	6.24	121.23	109.35
3	D	2475	PLP	C5A-C5-C6	-2.57	115.14	119.37
3	B	1475	PLP	C5A-C5-C6	-2.51	115.24	119.37
3	H	4475	PLP	C5A-C5-C6	-2.46	115.33	119.37
3	F	3475	PLP	C5A-C5-C6	-2.36	115.49	119.37
3	D	2475	PLP	C5-C6-N1	-2.25	120.07	123.82
3	H	4475	PLP	C5-C6-N1	-2.25	120.08	123.82
3	F	3475	PLP	C5-C6-N1	-2.08	120.35	123.82
3	B	1475	PLP	C5-C6-N1	-2.06	120.39	123.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2475	PLP	C4-C5-C5A-O4P
3	H	4475	PLP	C4-C5-C5A-O4P
4	D	2476	AOA	O1-C1-C2-O2
4	D	2476	AOA	O1-C1-C2-O3
3	D	2475	PLP	C6-C5-C5A-O4P
3	B	1475	PLP	C6-C5-C5A-O4P
4	H	4476	AOA	O1-C1-C2-O3

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	4476	AOA	2	0
4	D	2476	AOA	6	0
4	F	3476	AOA	4	0
4	B	1476	AOA	3	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, 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	437/438 (99%)	-0.19	2 (0%) 91 89	20, 33, 48, 55	0
1	C	437/438 (99%)	-0.26	0 100 100	20, 34, 49, 59	0
1	E	437/438 (99%)	-0.21	2 (0%) 91 89	22, 33, 47, 57	0
1	G	437/438 (99%)	-0.30	0 100 100	23, 33, 48, 57	0
2	B	473/474 (99%)	-0.23	5 (1%) 80 79	20, 30, 49, 61	0
2	D	473/474 (99%)	-0.20	11 (2%) 60 58	24, 36, 56, 72	0
2	F	473/474 (99%)	-0.21	6 (1%) 77 75	19, 32, 49, 62	0
2	H	473/474 (99%)	-0.15	8 (1%) 70 68	25, 38, 58, 69	0
All	All	3640/3648 (99%)	-0.22	34 (0%) 84 82	19, 33, 51, 72	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	301	GLU	4.6
2	H	154	ARG	4.2
2	D	302	GLU	3.7
2	H	383	GLU	3.5
2	D	301	GLU	3.2
2	F	30	ILE	3.1
2	D	300	GLY	3.0
2	B	443	GLU	2.8
1	A	363	VAL	2.8
2	D	181	ARG	2.8
2	H	302	GLU	2.7
2	F	33	GLU	2.6
2	F	32	LYS	2.6
1	E	358	ALA	2.5
2	H	188	GLU	2.6
2	D	386	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	197	LYS	2.5
2	D	383	GLU	2.5
2	B	32	LYS	2.4
2	F	154	ARG	2.4
2	B	301	GLU	2.3
2	B	383	GLU	2.3
2	H	366	ARG	2.2
2	B	326	ALA	2.2
2	D	474	GLY	2.2
2	H	203	HIS	2.1
2	D	154	ARG	2.1
2	H	231	GLU	2.1
2	D	203	HIS	2.1
1	A	436	VAL	2.0
1	E	293	VAL	2.0
2	D	385	PHE	2.0
2	F	383	GLU	2.0
2	F	153	GLY	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, 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
4	AOA	D	2476	6/6	0.58	0.46	63,64,67,68	0
4	AOA	H	4476	6/6	0.58	0.47	61,62,63,64	0
4	AOA	F	3476	6/6	0.65	0.46	57,57,62,63	0
4	AOA	B	1476	6/6	0.65	0.43	54,55,62,63	0
3	PLP	H	4475	15/16	0.93	0.24	37,54,59,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PLP	D	2475	15/16	0.94	0.24	40,60,64,66	0
3	PLP	B	1475	15/16	0.95	0.22	32,53,57,60	0
3	PLP	F	3475	15/16	0.96	0.22	28,51,55,58	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.