Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:01 am GMT

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
http://wwpdb.org/validation/2016/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:
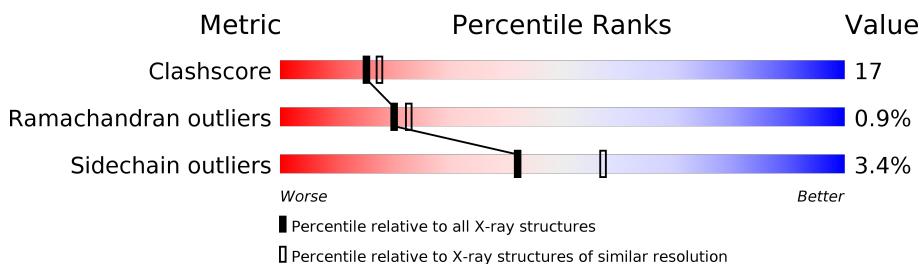
1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.30 Å.
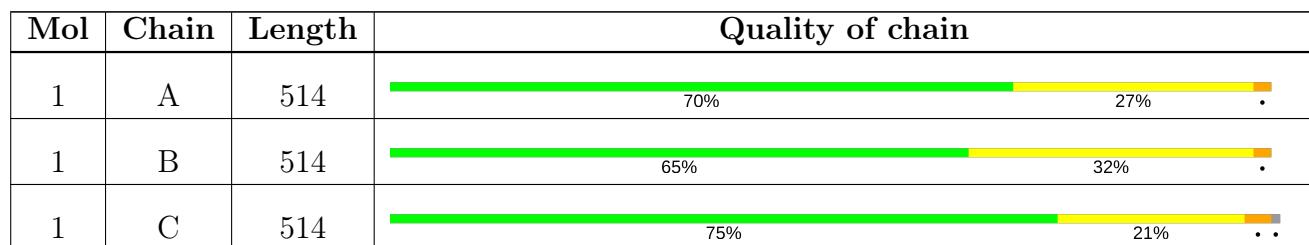
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		17
Ramachandran outliers		0.9%
Sidechain outliers		3.4%

Worse ◾ *Better*

◾ Percentile relative to all X-ray structures

⧠ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	70% 27% •
1	B	514	65% 32% •
1	C	514	75% 21% • •

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 12832 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.
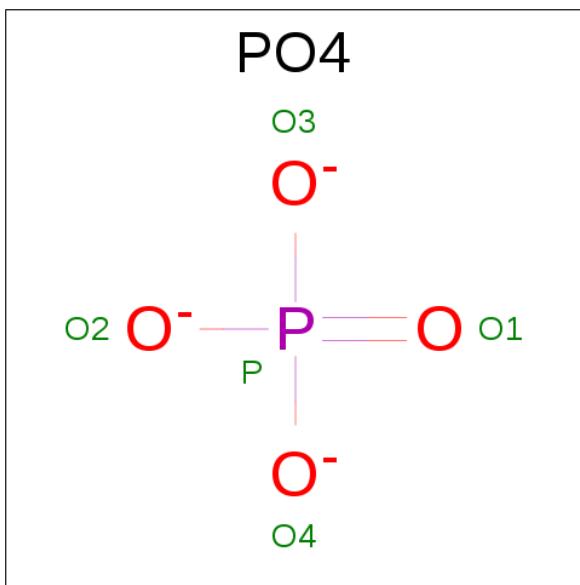
- Molecule 1 is a protein called ATP SULPHURYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			4093	2609	710	768	6			
1	B	512	Total	C	N	O	S	0	0	0
			4093	2609	710	768	6			
1	C	511	Total	C	N	O	S	0	0	0
			4083	2603	707	767	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P08536
A	-1	SER	-	EXPRESSION TAG	UNP P08536
A	0	HIS	-	EXPRESSION TAG	UNP P08536
B	-2	GLY	-	EXPRESSION TAG	UNP P08536
B	-1	SER	-	EXPRESSION TAG	UNP P08536
B	0	HIS	-	EXPRESSION TAG	UNP P08536
C	-2	GLY	-	EXPRESSION TAG	UNP P08536
C	-1	SER	-	EXPRESSION TAG	UNP P08536
C	0	HIS	-	EXPRESSION TAG	UNP P08536

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	A	1	Total 5	O 4	P 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	C	2	Total 2	Na 2	0	0

- Molecule 4 is water.
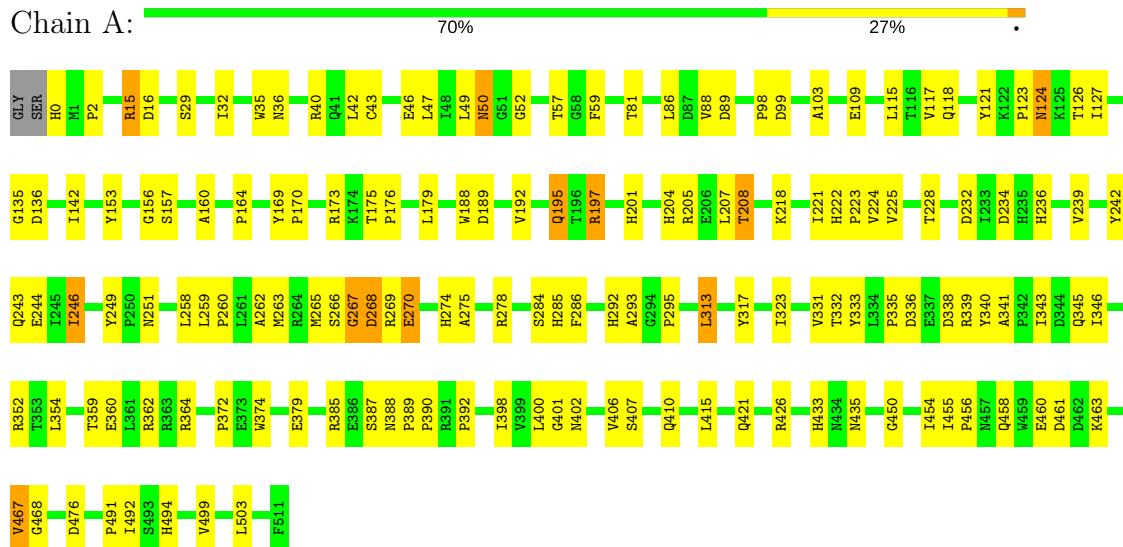
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total 157	O 157	0	0
4	B	119	Total 119	O 119	0	0
4	C	269	Total 269	O 269	0	0

3 Residue-property plots ⓘ
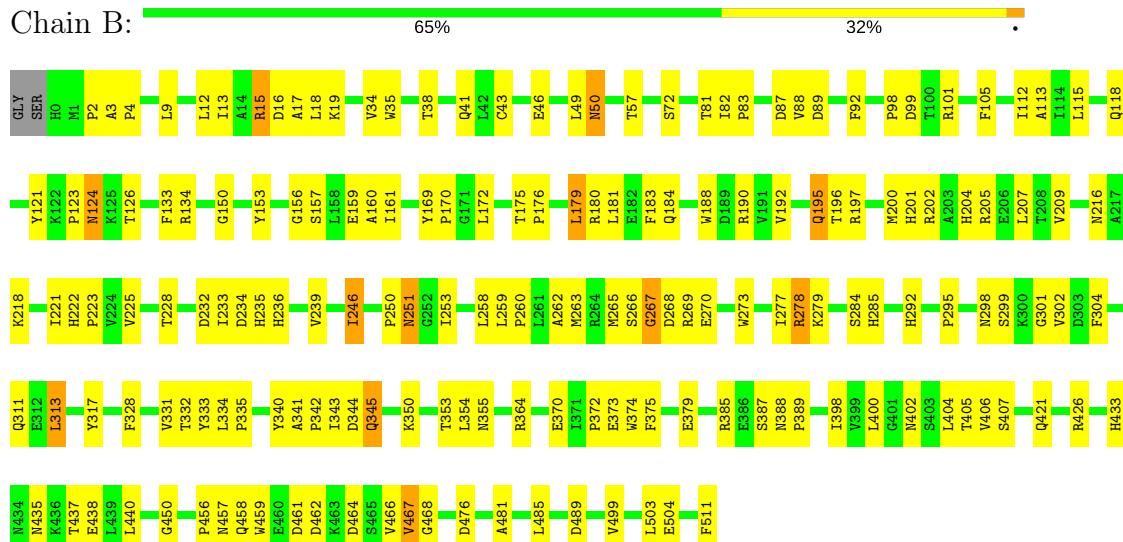
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: ATP SULPHURYLASE
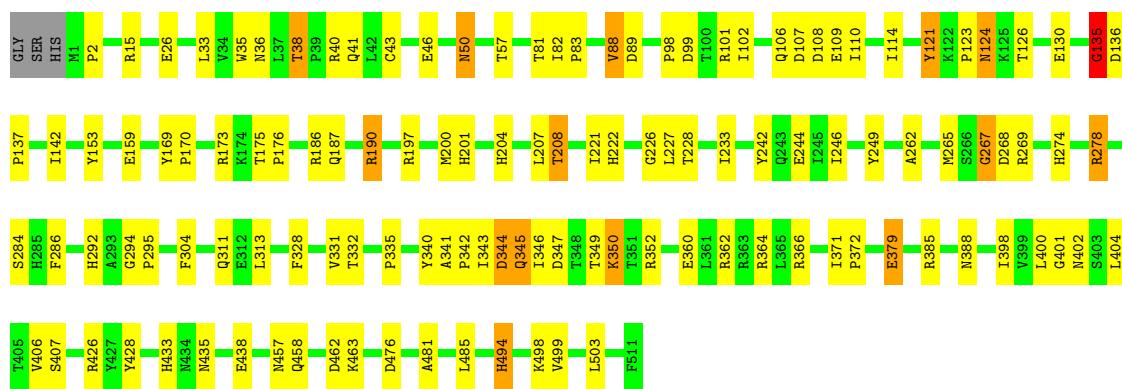
Chain A:

• Molecule 1: ATP SULPHURYLASE

Chain B:

• Molecule 1: ATP SULPHURYLASE

Chain C:

75%   21%

4 Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	230.85Å 230.85Å 69.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.84 – 2.30	Depositor
% Data completeness (in resolution range)	91.8 (29.84-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.73	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.210 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12832	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PO4

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	0.32	0/4190	0.59	0/5693
1	B	0.31	0/4190	0.57	0/5693
1	C	0.38	0/4179	0.63	1/5678 (0.0%)
All	All	0.34	0/12559	0.60	1/17064 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	135	GLY	N-CA-C	5.10	125.86	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4093	0	4054	141	0
1	B	4093	0	4054	157	0
1	C	4083	0	4047	114	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
4	A	157	0	0	1	0
4	B	119	0	0	2	0
4	C	269	0	0	5	0
All	All	12832	0	12155	408	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 17.

All (408) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLN:HE22	1:A:224:VAL:HG23	1.29	0.97
1:C:46:GLU:O	1:C:50:ASN:HB2	1.65	0.97
1:A:46:GLU:O	1:A:50:ASN:HB2	1.64	0.96
1:B:46:GLU:O	1:B:50:ASN:HB2	1.68	0.94
1:A:195:GLN:NE2	1:A:278:ARG:HH22	1.67	0.93
1:C:201:HIS:H	1:C:204:HIS:HD2	1.13	0.93
1:A:195:GLN:HE21	1:A:278:ARG:HH22	1.04	0.91
1:B:201:HIS:H	1:B:204:HIS:HD2	1.21	0.89
1:A:201:HIS:H	1:A:204:HIS:HD2	1.17	0.88
1:A:435:ASN:HD21	1:A:460:GLU:H	1.20	0.87
1:C:402:ASN:H	1:C:458:GLN:HE21	1.26	0.84
1:C:402:ASN:H	1:C:458:GLN:NE2	1.76	0.83
1:B:197:ARG:HB3	1:B:263:MET:HE1	1.60	0.83
1:C:398:ILE:HD11	1:C:503:LEU:HD11	1.61	0.81
1:B:398:ILE:HD11	1:B:503:LEU:HD11	1.63	0.81
1:C:331:VAL:HG11	1:C:340:TYR:HB3	1.64	0.78
1:A:195:GLN:HG2	1:A:278:ARG:NH2	1.97	0.78
1:A:398:ILE:HD11	1:A:503:LEU:HD11	1.65	0.77
1:B:402:ASN:N	1:B:458:GLN:HE21	1.81	0.77
1:B:331:VAL:HG11	1:B:340:TYR:HB3	1.66	0.76
1:A:195:GLN:HE21	1:A:278:ARG:NH2	1.82	0.76
1:A:201:HIS:H	1:A:204:HIS:CD2	2.03	0.76
1:C:433:HIS:HD2	1:C:435:ASN:H	1.34	0.76
1:A:400:LEU:HD12	1:A:456:PRO:HA	1.68	0.76
1:C:36:ASN:ND2	1:C:108:ASP:H	1.84	0.75
1:C:342:PRO:HB2	1:C:344:ASP:HB2	1.68	0.74
1:A:331:VAL:HG11	1:A:340:TYR:HB3	1.67	0.74
1:C:201:HIS:H	1:C:204:HIS:CD2	2.02	0.73
1:B:197:ARG:HD2	1:B:228:THR:HB	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PRO:HG2	1:A:153:TYR:CD2	2.24	0.72
1:A:169:TYR:H	1:B:421:GLN:NE2	1.86	0.72
1:B:402:ASN:H	1:B:458:GLN:HE21	1.37	0.72
1:A:421:GLN:NE2	1:B:169:TYR:H	1.88	0.72
1:C:208:THR:HG21	1:C:249:TYR:OH	1.90	0.72
1:A:385:ARG:HG3	1:A:385:ARG:HH11	1.55	0.72
1:C:433:HIS:CD2	1:C:435:ASN:H	2.07	0.71
1:B:201:HIS:H	1:B:204:HIS:CD2	2.07	0.71
1:A:50:ASN:HD21	1:A:175:THR:HB	1.54	0.71
1:A:390:PRO:HB2	1:A:392:PRO:HD2	1.73	0.71
1:A:435:ASN:HD21	1:A:460:GLU:N	1.90	0.70
1:B:385:ARG:HG3	1:B:385:ARG:HH11	1.57	0.70
1:B:123:PRO:HG2	1:B:153:TYR:CD2	2.26	0.70
1:B:402:ASN:H	1:B:458:GLN:NE2	1.88	0.69
1:C:38:THR:HG22	1:C:41:GLN:H	1.56	0.69
1:B:251:ASN:HD22	1:B:251:ASN:H	1.41	0.69
1:A:364:ARG:NH1	1:A:372:PRO:HD3	2.08	0.68
1:C:190:ARG:HB3	1:C:190:ARG:HH11	1.58	0.68
1:C:402:ASN:N	1:C:458:GLN:HE21	1.91	0.68
1:B:197:ARG:CB	1:B:263:MET:HE1	2.23	0.68
1:A:197:ARG:HB3	1:A:263:MET:CE	2.24	0.68
1:C:385:ARG:HH11	1:C:385:ARG:HG3	1.57	0.67
1:B:311:GLN:HG3	4:B:2476:HOH:O	1.93	0.67
1:B:88:VAL:HG11	1:B:92:PHE:CD2	2.29	0.67
1:A:197:ARG:HB3	1:A:263:MET:HE1	1.77	0.67
1:C:197:ARG:HD2	1:C:228:THR:HB	1.77	0.67
1:B:222:HIS:ND1	1:B:278:ARG:HD2	2.09	0.67
1:A:47:LEU:HD12	1:A:52:GLY:HA3	1.78	0.66
1:C:331:VAL:HG12	1:C:332:THR:N	2.10	0.66
1:C:50:ASN:HD21	1:C:175:THR:HB	1.62	0.65
1:A:402:ASN:H	1:A:458:GLN:HE21	1.42	0.65
1:B:344:ASP:HB2	1:B:345:GLN:NE2	2.11	0.65
1:B:118:GLN:HG3	1:B:156:GLY:HA2	1.79	0.64
1:B:195:GLN:HG3	1:B:278:ARG:NH2	2.12	0.64
1:B:13:ILE:HD13	1:B:160:ALA:HB1	1.80	0.64
1:B:35:TRP:CZ3	1:B:88:VAL:HG13	2.33	0.64
1:C:204:HIS:O	1:C:208:THR:HB	1.98	0.64
1:A:221:ILE:O	1:A:223:PRO:HD3	1.98	0.63
1:C:36:ASN:HD21	1:C:108:ASP:H	1.45	0.63
1:A:195:GLN:NE2	1:A:224:VAL:HG23	2.10	0.63
1:A:169:TYR:H	1:B:421:GLN:HE21	1.44	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:GLN:HG3	1:B:278:ARG:HH22	1.63	0.62
1:B:87:ASP:HB2	1:B:150:GLY:H	1.63	0.62
1:C:124:ASN:HD21	1:C:126:THR:HB	1.64	0.62
1:B:331:VAL:HG12	1:B:332:THR:N	2.15	0.62
1:C:81:THR:HB	1:C:269:ARG:HB3	1.82	0.62
1:A:332:THR:HB	1:A:343:ILE:HD11	1.82	0.61
1:C:433:HIS:HE1	1:C:457:ASN:O	1.83	0.61
1:A:195:GLN:HE22	1:A:224:VAL:CG2	2.08	0.61
1:C:35:TRP:CZ3	1:C:88:VAL:HG22	2.35	0.61
1:B:121:TYR:CD2	1:B:123:PRO:HG3	2.36	0.61
1:B:232:ASP:CG	1:B:233:ILE:H	2.03	0.61
1:A:118:GLN:HG2	1:A:156:GLY:HA2	1.82	0.60
1:A:331:VAL:CG1	1:A:340:TYR:HB3	2.31	0.60
1:A:402:ASN:H	1:A:458:GLN:NE2	1.99	0.60
1:A:208:THR:HG22	1:A:249:TYR:HE2	1.66	0.60
1:B:172:LEU:HD23	1:B:258:LEU:HD11	1.84	0.60
1:C:57:THR:HG22	1:C:57:THR:O	2.00	0.60
1:B:331:VAL:CG1	1:B:340:TYR:HB3	2.31	0.59
1:A:225:VAL:HG11	1:A:258:LEU:HD13	1.84	0.59
1:B:251:ASN:N	1:B:251:ASN:HD22	2.00	0.59
1:A:50:ASN:HD21	1:A:175:THR:CB	2.14	0.59
1:B:88:VAL:HG11	1:B:92:PHE:HD2	1.68	0.59
1:C:50:ASN:ND2	1:C:176:PRO:HD2	2.17	0.59
1:A:251:ASN:H	1:A:251:ASN:HD22	1.51	0.59
1:A:275:ALA:HB1	1:A:323:ILE:CD1	2.33	0.59
1:B:433:HIS:CD2	1:B:435:ASN:H	2.21	0.59
1:A:50:ASN:ND2	1:A:175:THR:HB	2.18	0.58
1:B:207:LEU:HD21	1:B:331:VAL:HG21	1.86	0.58
1:A:406:VAL:HG12	1:A:407:SER:N	2.18	0.58
1:A:35:TRP:CZ3	1:A:88:VAL:HG22	2.38	0.58
1:B:50:ASN:HD21	1:B:175:THR:HB	1.68	0.58
1:C:208:THR:CG2	1:C:249:TYR:HE2	2.16	0.58
1:A:195:GLN:HG3	1:A:274:HIS:ND1	2.19	0.58
1:A:402:ASN:N	1:A:458:GLN:HE21	2.02	0.58
1:B:250:PRO:HB2	1:B:253:ILE:HG13	1.85	0.57
1:B:115:LEU:HD12	1:B:157:SER:O	2.03	0.57
1:B:57:THR:O	1:B:57:THR:HG22	2.04	0.57
1:B:3:ALA:O	1:B:279:LYS:HE2	2.04	0.57
1:C:485:LEU:HD23	1:C:498:LYS:HD3	1.87	0.57
1:B:205:ARG:O	1:B:209:VAL:HG23	2.04	0.57
1:B:385:ARG:NH1	1:B:385:ARG:HG3	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:THR:O	1:A:57:THR:HG22	2.04	0.57
1:B:72:SER:HB3	1:B:81:THR:HG22	1.86	0.57
1:C:362:ARG:NH1	1:C:362:ARG:HB2	2.19	0.57
1:C:244:GLU:HG2	1:C:379:GLU:HB2	1.86	0.57
1:A:407:SER:HB3	1:A:410:GLN:HB2	1.86	0.57
1:B:121:TYR:CE2	1:B:123:PRO:HG3	2.40	0.57
1:C:226:GLY:O	1:C:227:LEU:HD23	2.06	0.56
1:A:42:LEU:HD22	1:A:164:PRO:HB3	1.87	0.56
1:A:208:THR:CG2	1:A:249:TYR:HE2	2.18	0.56
1:C:107:ASP:O	1:C:109:GLU:HG2	2.04	0.56
1:A:274:HIS:O	1:A:278:ARG:HG2	2.06	0.56
1:B:234:ASP:OD2	1:B:236:HIS:HB2	2.06	0.56
1:A:0:HIS:HB2	1:A:189:ASP:OD1	2.06	0.56
1:B:2:PRO:HG2	1:B:284:SER:HA	1.88	0.55
1:B:405:THR:OG1	1:B:489:ASP:HB3	2.07	0.55
1:C:169:TYR:N	1:C:170:PRO:HD3	2.21	0.55
1:C:400:LEU:HB3	1:C:404:LEU:HD12	1.87	0.55
1:C:406:VAL:HG12	1:C:407:SER:N	2.21	0.55
1:C:50:ASN:HD21	1:C:175:THR:CB	2.19	0.55
1:B:169:TYR:N	1:B:170:PRO:HD3	2.22	0.55
1:B:112:ILE:O	1:B:161:ILE:HB	2.06	0.55
1:C:401:GLY:HA2	1:C:458:GLN:HE21	1.71	0.55
1:A:207:LEU:HD21	1:A:331:VAL:HG21	1.87	0.55
1:B:180:ARG:O	1:B:184:GLN:HG3	2.06	0.55
1:B:121:TYR:O	1:B:123:PRO:HD3	2.07	0.54
1:C:342:PRO:HD2	1:C:345:GLN:OE1	2.07	0.54
1:A:50:ASN:ND2	1:A:176:PRO:HD2	2.23	0.54
1:A:169:TYR:N	1:A:170:PRO:HD3	2.22	0.54
1:B:124:ASN:HD22	1:B:124:ASN:C	2.11	0.54
1:C:207:LEU:HD21	1:C:331:VAL:HG21	1.88	0.54
1:A:15:ARG:HD2	1:A:16:ASP:OD1	2.08	0.54
1:A:228:THR:HG22	1:A:263:MET:CE	2.38	0.54
1:A:339:ARG:NH1	1:A:341:ALA:HB2	2.23	0.54
1:B:195:GLN:CG	1:B:278:ARG:HH22	2.20	0.54
1:B:87:ASP:HB2	1:B:150:GLY:N	2.22	0.54
1:C:222:HIS:ND1	1:C:278:ARG:HD2	2.22	0.54
1:A:385:ARG:HG3	1:A:385:ARG:NH1	2.21	0.53
1:C:385:ARG:HD3	4:C:2466:HOH:O	2.09	0.53
1:A:121:TYR:O	1:A:123:PRO:HD3	2.08	0.53
1:B:221:ILE:HD12	1:B:246:ILE:HG12	1.90	0.53
1:B:350:LYS:HG2	1:B:350:LYS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:ARG:HG3	1:C:385:ARG:NH1	2.23	0.53
1:A:117:VAL:HG12	1:A:118:GLN:N	2.24	0.53
1:C:349:THR:O	1:C:349:THR:HG22	2.08	0.53
1:B:179:LEU:HD22	1:B:183:PHE:CZ	2.44	0.53
1:C:398:ILE:HD13	1:C:499:VAL:HG11	1.91	0.52
1:B:398:ILE:HD13	1:B:499:VAL:CG1	2.39	0.52
1:B:50:ASN:ND2	1:B:176:PRO:HD2	2.24	0.52
1:C:364:ARG:NH1	1:C:372:PRO:HD3	2.24	0.52
1:B:124:ASN:ND2	1:B:126:THR:H	2.08	0.52
1:B:207:LEU:HB3	1:B:328:PHE:CZ	2.44	0.52
1:C:360:GLU:O	1:C:364:ARG:HG3	2.10	0.52
1:A:234:ASP:OD2	1:A:236:HIS:HB2	2.10	0.52
1:A:359:THR:HA	1:A:362:ARG:NH1	2.24	0.52
1:B:295:PRO:HB2	1:B:304:PHE:CD1	2.45	0.52
1:B:313:LEU:HD22	1:B:317:TYR:CE2	2.45	0.52
1:B:38:THR:HG22	1:B:41:GLN:HB2	1.92	0.52
1:C:345:GLN:O	1:C:346:ILE:HD13	2.08	0.52
1:A:221:ILE:C	1:A:223:PRO:HD3	2.30	0.52
1:C:208:THR:CG2	1:C:249:TYR:CE2	2.93	0.52
1:B:404:LEU:HD21	1:B:485:LEU:HD12	1.92	0.51
1:B:12:LEU:HD12	1:B:49:LEU:HD23	1.93	0.51
1:B:195:GLN:HG2	1:B:278:ARG:HH12	1.75	0.51
1:C:123:PRO:HG3	1:C:153:TYR:CE2	2.45	0.51
1:A:115:LEU:HD11	1:A:156:GLY:HA3	1.92	0.51
1:A:49:LEU:HD22	1:A:160:ALA:HB2	1.91	0.51
1:B:201:HIS:N	1:B:204:HIS:HD2	2.00	0.51
1:B:197:ARG:HB2	1:B:228:THR:CG2	2.40	0.51
1:B:298:ASN:HD21	1:B:302:VAL:HB	1.76	0.51
1:B:400:LEU:HD12	1:B:456:PRO:HA	1.93	0.51
1:B:4:PRO:HG2	1:B:9:LEU:HB2	1.93	0.51
1:C:332:THR:HB	1:C:343:ILE:CD1	2.41	0.51
1:C:35:TRP:CH2	1:C:88:VAL:HG22	2.46	0.51
1:A:421:GLN:HE21	1:B:169:TYR:H	1.57	0.51
1:C:362:ARG:CZ	1:C:362:ARG:HB2	2.41	0.51
1:B:188:TRP:CE2	1:B:218:LYS:HG3	2.46	0.51
1:C:101:ARG:NH2	1:C:159:GLU:OE1	2.43	0.51
1:C:33:LEU:HD23	1:C:102:ILE:HD12	1.92	0.51
1:B:232:ASP:CG	1:B:233:ILE:N	2.64	0.50
1:C:438:GLU:H	1:C:438:GLU:CD	2.14	0.50
1:B:433:HIS:CD2	1:B:440:LEU:HD21	2.46	0.50
1:B:273:TRP:O	1:B:277:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ARG:HH11	1:C:173:ARG:HG3	1.76	0.50
1:C:476:ASP:HB3	1:C:481:ALA:HB2	1.93	0.50
1:A:270:GLU:HG2	1:A:293:ALA:CB	2.42	0.50
1:C:331:VAL:HG12	1:C:332:THR:H	1.75	0.50
1:A:239:VAL:O	1:A:243:GLN:HG3	2.12	0.50
1:A:402:ASN:HD21	1:A:458:GLN:HB2	1.77	0.49
1:B:124:ASN:HD22	1:B:126:THR:H	1.59	0.49
1:B:342:PRO:HD2	1:B:345:GLN:OE1	2.12	0.49
1:B:124:ASN:HD21	1:B:126:THR:HB	1.76	0.49
1:B:345:GLN:NE2	1:B:345:GLN:H	2.10	0.49
1:C:433:HIS:HD2	1:C:435:ASN:N	2.06	0.49
1:B:50:ASN:HD21	1:B:175:THR:CB	2.25	0.49
1:A:124:ASN:OD1	1:A:127:ILE:HG13	2.13	0.49
1:B:332:THR:HA	1:B:355:ASN:OD1	2.13	0.49
1:A:331:VAL:HG12	1:A:332:THR:N	2.28	0.49
1:A:360:GLU:O	1:A:364:ARG:HG3	2.13	0.48
1:B:88:VAL:HG12	1:B:89:ASP:N	2.27	0.48
1:C:190:ARG:CB	1:C:190:ARG:HH11	2.25	0.48
1:C:331:VAL:CG1	1:C:332:THR:N	2.76	0.48
1:A:246:ILE:HD13	1:A:246:ILE:O	2.13	0.48
1:B:228:THR:HA	1:B:263:MET:CE	2.43	0.48
1:A:81:THR:HB	1:A:269:ARG:HB3	1.93	0.48
1:C:342:PRO:C	1:C:344:ASP:N	2.63	0.48
1:B:372:PRO:HB3	1:B:374:TRP:NE1	2.29	0.48
1:C:2:PRO:CG	1:C:284:SER:HA	2.44	0.48
1:A:415:LEU:HB2	1:A:454:ILE:HD13	1.96	0.48
1:C:435:ASN:O	1:C:463:LYS:HE3	2.14	0.48
1:B:179:LEU:HD22	1:B:183:PHE:CE2	2.49	0.48
1:C:124:ASN:C	1:C:124:ASN:HD22	2.16	0.48
1:C:136:ASP:O	1:C:142:ILE:HD12	2.14	0.48
1:A:398:ILE:HD13	1:A:499:VAL:HG11	1.95	0.47
1:B:192:VAL:HA	1:B:285:HIS:HB2	1.95	0.47
1:B:81:THR:HB	1:B:269:ARG:HB3	1.95	0.47
1:B:364:ARG:HD3	1:B:370:GLU:O	2.14	0.47
1:A:2:PRO:HG2	1:A:284:SER:HA	1.96	0.47
1:C:207:LEU:HB3	1:C:328:PHE:CZ	2.50	0.47
1:A:115:LEU:HD12	1:A:157:SER:O	2.15	0.47
1:A:284:SER:OG	1:A:285:HIS:HD2	1.97	0.47
1:A:331:VAL:CG1	1:A:332:THR:N	2.77	0.47
1:C:101:ARG:NH1	1:C:114:ILE:HG21	2.29	0.47
1:B:190:ARG:HD3	1:B:216:ASN:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASN:ND2	1:A:126:THR:H	2.11	0.47
1:A:336:ASP:OD2	1:A:352:ARG:HD3	2.14	0.47
1:B:406:VAL:HG12	1:B:407:SER:N	2.29	0.47
1:B:438:GLU:H	1:B:438:GLU:CD	2.18	0.47
1:A:123:PRO:HG2	1:A:153:TYR:CG	2.50	0.47
1:B:2:PRO:HG3	4:B:2538:HOH:O	2.15	0.47
1:B:504:GLU:HG3	1:B:511:PHE:HE1	1.80	0.47
1:B:88:VAL:CG1	1:B:92:PHE:HB3	2.44	0.47
1:B:426:ARG:HG3	1:B:450:GLY:O	2.14	0.46
1:B:225:VAL:HG11	1:B:258:LEU:HD13	1.97	0.46
1:A:275:ALA:HB1	1:A:323:ILE:HD13	1.96	0.46
1:A:98:PRO:O	1:A:99:ASP:HB2	2.16	0.46
1:C:130:GLU:HA	1:C:135:GLY:N	2.31	0.46
1:C:50:ASN:ND2	1:C:175:THR:HB	2.29	0.46
1:C:347:ASP:HB3	1:C:350:LYS:HE3	1.97	0.46
1:A:29:SER:O	1:A:32:ILE:HG22	2.16	0.46
1:B:101:ARG:NH2	1:B:159:GLU:OE1	2.48	0.46
1:B:15:ARG:NH1	1:B:16:ASP:OD2	2.48	0.46
1:B:364:ARG:NH1	1:B:372:PRO:HD3	2.31	0.46
1:C:124:ASN:ND2	1:C:126:THR:HB	2.30	0.46
1:C:331:VAL:HG13	1:C:341:ALA:O	2.16	0.46
1:C:26:GLU:OE1	1:C:101:ARG:NH1	2.49	0.46
1:C:426:ARG:HD2	1:C:428:TYR:CZ	2.51	0.46
1:B:379:GLU:H	1:B:379:GLU:CD	2.19	0.46
1:A:124:ASN:HD21	1:A:126:THR:HB	1.81	0.46
1:A:274:HIS:HB3	1:A:286:PHE:CZ	2.51	0.46
1:C:244:GLU:CG	1:C:379:GLU:HB2	2.46	0.46
1:A:267:GLY:HA2	1:A:292:HIS:O	2.16	0.45
1:B:433:HIS:HE1	1:B:457:ASN:O	1.97	0.45
1:B:228:THR:HA	1:B:263:MET:HE2	1.98	0.45
1:B:38:THR:HG22	1:B:41:GLN:CG	2.47	0.45
1:C:331:VAL:HG13	1:C:341:ALA:C	2.36	0.45
1:A:313:LEU:HD22	1:A:317:TYR:CE2	2.52	0.45
1:B:133:PHE:O	1:B:134:ARG:HB2	2.17	0.45
1:B:38:THR:HG22	1:B:41:GLN:CB	2.46	0.45
1:A:400:LEU:HB2	1:A:456:PRO:O	2.16	0.45
1:B:15:ARG:HH11	1:B:16:ASP:CG	2.19	0.45
1:B:50:ASN:ND2	1:B:175:THR:HB	2.32	0.45
1:A:398:ILE:HD13	1:A:499:VAL:CG1	2.47	0.45
1:B:195:GLN:CG	1:B:278:ARG:NH2	2.77	0.45
1:B:345:GLN:NE2	1:B:345:GLN:N	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ASN:HD22	1:C:126:THR:H	1.65	0.45
1:C:201:HIS:HA	4:C:2659:HOH:O	2.15	0.45
1:A:332:THR:HB	1:A:343:ILE:CD1	2.47	0.45
1:B:331:VAL:CG1	1:B:332:THR:N	2.79	0.45
1:B:387:SER:C	1:B:389:PRO:HD3	2.37	0.45
1:B:98:PRO:O	1:B:99:ASP:HB2	2.17	0.45
1:C:101:ARG:HG3	4:C:2681:HOH:O	2.15	0.45
1:C:342:PRO:C	1:C:344:ASP:H	2.19	0.45
1:C:366:ARG:HG3	4:C:2507:HOH:O	2.17	0.45
1:C:88:VAL:HG13	1:C:89:ASP:N	2.32	0.45
1:A:491:PRO:O	1:A:494:HIS:HB3	2.17	0.45
1:A:15:ARG:HG3	1:A:16:ASP:N	2.32	0.45
1:A:197:ARG:HB3	1:A:263:MET:HE3	1.98	0.45
1:A:244:GLU:HG2	1:A:379:GLU:HB2	1.99	0.45
1:C:267:GLY:HA2	1:C:292:HIS:O	2.17	0.45
1:C:371:ILE:HA	1:C:372:PRO:HD3	1.85	0.45
1:A:406:VAL:HG12	1:A:407:SER:H	1.83	0.44
1:C:197:ARG:HB2	1:C:228:THR:HG21	1.99	0.44
1:C:265:MET:HB3	1:C:295:PRO:HG3	1.98	0.44
1:C:331:VAL:CG1	1:C:340:TYR:HB3	2.39	0.44
1:A:359:THR:HA	1:A:362:ARG:HH12	1.80	0.44
1:B:195:GLN:NE2	1:B:196:THR:N	2.66	0.44
1:C:121:TYR:N	1:C:121:TYR:CD1	2.84	0.44
1:B:221:ILE:C	1:B:223:PRO:HD3	2.38	0.44
1:B:467:VAL:HG12	1:B:468:GLY:N	2.32	0.44
1:A:201:HIS:N	1:A:204:HIS:HD2	1.99	0.44
1:A:372:PRO:HB3	1:A:374:TRP:NE1	2.33	0.44
1:A:32:ILE:HD13	1:A:103:ALA:HB2	2.00	0.44
1:A:333:TYR:OH	1:A:338:ASP:OD1	2.30	0.44
1:A:88:VAL:HG13	1:A:89:ASP:N	2.33	0.44
1:B:181:LEU:HD23	1:B:184:GLN:NE2	2.31	0.44
1:B:331:VAL:HG12	1:B:332:THR:H	1.81	0.44
1:C:173:ARG:NH1	1:C:173:ARG:HG3	2.33	0.44
1:C:433:HIS:CE1	1:C:457:ASN:O	2.67	0.44
1:A:239:VAL:HA	1:A:242:TYR:HD2	1.83	0.44
1:B:43:CYS:HB2	1:B:262:ALA:HB2	2.00	0.44
1:C:43:CYS:HB2	1:C:262:ALA:HB2	1.99	0.44
1:A:379:GLU:H	1:A:379:GLU:CD	2.20	0.44
1:A:401:GLY:HA3	1:A:476:ASP:OD1	2.18	0.44
1:A:188:TRP:CD2	1:A:218:LYS:HG3	2.53	0.44
1:B:476:ASP:HB3	1:B:481:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ILE:HD13	1:B:499:VAL:HG11	2.00	0.43
1:B:406:VAL:CG1	1:B:407:SER:N	2.81	0.43
1:A:124:ASN:HD22	1:A:124:ASN:C	2.21	0.43
1:A:57:THR:CG2	1:A:57:THR:O	2.66	0.43
1:B:2:PRO:HD3	1:B:284:SER:HB3	1.99	0.43
1:B:334:LEU:CD2	1:B:353:THR:HG22	2.49	0.43
1:A:173:ARG:HH11	1:A:173:ARG:HG3	1.83	0.43
1:A:267:GLY:HA2	1:A:293:ALA:HB3	2.01	0.43
1:C:335:PRO:HB2	1:C:352:ARG:NH2	2.34	0.43
1:B:49:LEU:HD22	1:B:160:ALA:HB2	1.99	0.43
1:B:332:THR:HB	1:B:343:ILE:CD1	2.49	0.43
1:A:387:SER:C	1:A:389:PRO:HD3	2.39	0.43
1:A:426:ARG:HG3	1:A:450:GLY:O	2.19	0.43
1:A:435:ASN:ND2	1:A:460:GLU:H	2.01	0.43
1:A:121:TYR:N	1:A:121:TYR:CD1	2.87	0.43
1:B:299:SER:C	1:B:301:GLY:H	2.22	0.43
1:B:201:HIS:HB3	1:B:375:PHE:O	2.19	0.43
1:A:265:MET:HB3	1:A:295:PRO:HG3	2.00	0.43
1:A:467:VAL:HG12	1:A:468:GLY:N	2.33	0.43
1:B:235:HIS:O	1:B:239:VAL:HG23	2.19	0.43
1:C:344:ASP:HB3	1:C:345:GLN:NE2	2.34	0.43
1:A:239:VAL:HA	1:A:242:TYR:CD2	2.54	0.43
1:A:2:PRO:CG	1:A:284:SER:HA	2.49	0.43
1:B:265:MET:HB3	1:B:295:PRO:HG3	2.01	0.43
1:C:401:GLY:CA	1:C:458:GLN:HE21	2.32	0.43
1:C:98:PRO:O	1:C:99:ASP:HB2	2.19	0.43
1:C:38:THR:HB	1:C:41:GLN:OE1	2.19	0.42
1:A:222:HIS:HB3	1:A:278:ARG:HH11	1.84	0.42
1:A:389:PRO:HA	1:A:390:PRO:HD3	1.90	0.42
1:B:82:ILE:HA	1:B:83:PRO:HD3	1.76	0.42
1:B:333:TYR:HB3	1:B:354:LEU:O	2.19	0.42
1:C:406:VAL:CG1	1:C:407:SER:N	2.82	0.42
1:B:195:GLN:HG2	1:B:278:ARG:NH1	2.35	0.42
1:B:197:ARG:HB2	1:B:228:THR:HG21	2.02	0.42
1:B:259:LEU:HA	1:B:260:PRO:HD3	1.88	0.42
1:C:200:MET:HE2	1:C:221:ILE:HG21	2.01	0.42
1:A:136:ASP:O	1:A:142:ILE:HD12	2.20	0.42
1:A:433:HIS:CD2	1:A:435:ASN:H	2.37	0.42
1:B:207:LEU:HB3	1:B:328:PHE:CE2	2.55	0.42
1:A:205:ARG:HD3	1:A:205:ARG:C	2.39	0.42
1:B:270:GLU:HG3	1:B:273:TRP:HE3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:THR:CG2	1:A:249:TYR:CE2	3.02	0.42
1:A:192:VAL:HA	1:A:285:HIS:HB2	2.02	0.42
1:A:266:SER:O	1:A:267:GLY:C	2.57	0.42
1:A:59:PHE:CG	1:A:86:LEU:HB2	2.55	0.42
1:B:461:ASP:HA	1:B:464:ASP:OD2	2.20	0.42
1:B:459:TRP:CE2	1:B:467:VAL:HG21	2.55	0.42
1:C:494:HIS:C	1:C:494:HIS:CD2	2.93	0.42
1:C:274:HIS:HB3	1:C:286:PHE:CZ	2.55	0.41
1:C:398:ILE:HD13	1:C:499:VAL:CG1	2.50	0.41
1:B:188:TRP:CD1	1:B:218:LYS:HG3	2.56	0.41
1:C:200:MET:HE3	1:C:242:TYR:HD1	1.85	0.41
1:A:345:GLN:O	1:A:346:ILE:HD13	2.21	0.41
1:B:221:ILE:O	1:B:223:PRO:HD3	2.20	0.41
1:B:202:ARG:HD3	1:B:374:TRP:O	2.20	0.41
1:B:437:THR:HG23	1:B:466:VAL:HG11	2.03	0.41
1:B:267:GLY:HA2	1:B:292:HIS:O	2.20	0.41
1:B:34:VAL:HG13	1:B:105:PHE:CD1	2.55	0.41
1:A:259:LEU:HA	1:A:260:PRO:HD3	1.85	0.41
1:B:200:MET:HA	1:B:204:HIS:CD2	2.56	0.41
1:B:228:THR:HG22	1:B:263:MET:HE2	2.03	0.41
1:C:106:GLN:HB3	1:C:110:ILE:HB	2.02	0.41
1:C:200:MET:HE1	1:C:221:ILE:HD13	2.03	0.41
1:A:188:TRP:CG	1:A:218:LYS:HG3	2.55	0.41
1:A:401:GLY:HA2	1:A:458:GLN:HE21	1.85	0.41
1:A:406:VAL:HG11	1:A:492:ILE:HG12	2.02	0.41
1:B:331:VAL:HG13	1:B:341:ALA:O	2.20	0.41
1:B:35:TRP:CH2	1:B:88:VAL:HG13	2.55	0.41
1:C:43:CYS:CB	1:C:262:ALA:HB2	2.50	0.41
1:A:123:PRO:HG2	1:A:153:TYR:CE2	2.55	0.41
1:A:335:PRO:CG	1:A:354:LEU:HG	2.51	0.41
1:A:43:CYS:HB2	1:A:262:ALA:HB2	2.03	0.41
1:A:455:ILE:HA	1:A:456:PRO:HD3	1.79	0.41
1:B:121:TYR:N	1:B:121:TYR:CD1	2.89	0.41
1:B:251:ASN:N	1:B:251:ASN:ND2	2.67	0.41
1:A:362:ARG:CZ	1:A:362:ARG:HB2	2.50	0.41
1:A:205:ARG:O	1:A:205:ARG:HD3	2.22	0.40
1:B:266:SER:O	1:B:267:GLY:C	2.59	0.40
1:C:57:THR:CG2	1:C:57:THR:O	2.66	0.40
1:B:17:ALA:C	1:B:19:LYS:H	2.24	0.40
1:B:335:PRO:HG3	1:B:354:LEU:HD12	2.02	0.40
1:A:270:GLU:OE2	1:A:274:HIS:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ALA:HA	1:B:161:ILE:HG13	2.03	0.40
1:C:186:ARG:O	1:C:187:GLN:HB2	2.22	0.40
1:C:311:GLN:HG3	4:C:2453:HOH:O	2.21	0.40
1:C:82:ILE:HA	1:C:83:PRO:HD3	1.81	0.40
1:A:117:VAL:CG1	1:A:118:GLN:N	2.84	0.40
1:A:461:ASP:C	1:A:463:LYS:H	2.25	0.40
1:C:136:ASP:HA	1:C:137:PRO:HD3	1.92	0.40
1:C:294:GLY:HA2	1:C:295:PRO:HD3	1.90	0.40
1:A:228:THR:HB	4:A:2471:HOH:O	2.22	0.40
1:C:295:PRO:HB2	1:C:304:PHE:CD1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	510/514 (99%)	480 (94%)	25 (5%)	5 (1%)	18	20
1	B	510/514 (99%)	471 (92%)	35 (7%)	4 (1%)	22	26
1	C	509/514 (99%)	482 (95%)	22 (4%)	5 (1%)	18	20
All	All	1529/1542 (99%)	1433 (94%)	82 (5%)	14 (1%)	20	23

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	267	GLY
1	A	135	GLY
1	A	267	GLY
1	A	268	ASP
1	C	267	GLY
1	B	268	ASP
1	C	135	GLY

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Mol	Chain	Res	Type
1	C	233	ILE
1	B	18	LEU
1	A	109	GLU
1	C	350	LYS
1	C	268	ASP
1	A	467	VAL
1	B	467	VAL

5.3.2 Protein sidechains ⓘ

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	447/448 (100%)	432 (97%)	15 (3%)	42	57
1	B	447/448 (100%)	434 (97%)	13 (3%)	48	64
1	C	446/448 (100%)	428 (96%)	18 (4%)	36	50
All	All	1340/1344 (100%)	1294 (97%)	46 (3%)	42	57

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	36	ASN
1	A	40	ARG
1	A	50	ASN
1	A	124	ASN
1	A	179	LEU
1	A	195	GLN
1	A	197	ARG
1	A	208	THR
1	A	232	ASP
1	A	246	ILE
1	A	268	ASP
1	A	270	GLU
1	A	313	LEU
1	A	388	ASN

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Mol	Chain	Res	Type
1	B	15	ARG
1	B	50	ASN
1	B	124	ASN
1	B	179	LEU
1	B	195	GLN
1	B	246	ILE
1	B	251	ASN
1	B	278	ARG
1	B	313	LEU
1	B	345	GLN
1	B	373	GLU
1	B	388	ASN
1	B	462	ASP
1	C	15	ARG
1	C	38	THR
1	C	40	ARG
1	C	50	ASN
1	C	88	VAL
1	C	121	TYR
1	C	124	ASN
1	C	190	ARG
1	C	208	THR
1	C	246	ILE
1	C	278	ARG
1	C	313	LEU
1	C	344	ASP
1	C	345	GLN
1	C	379	GLU
1	C	388	ASN
1	C	462	ASP
1	C	494	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	50	ASN
1	A	124	ASN
1	A	184	GLN
1	A	195	GLN
1	A	204	HIS
1	A	251	ASN

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Mol	Chain	Res	Type
1	A	285	HIS
1	A	388	ASN
1	A	402	ASN
1	A	421	GLN
1	A	435	ASN
1	A	458	GLN
1	A	484	GLN
1	B	0	HIS
1	B	36	ASN
1	B	50	ASN
1	B	124	ASN
1	B	184	GLN
1	B	195	GLN
1	B	204	HIS
1	B	251	ASN
1	B	345	GLN
1	B	388	ASN
1	B	402	ASN
1	B	421	GLN
1	B	433	HIS
1	B	458	GLN
1	C	36	ASN
1	C	50	ASN
1	C	95	GLN
1	C	118	GLN
1	C	124	ASN
1	C	162	GLN
1	C	184	GLN
1	C	204	HIS
1	C	251	ASN
1	C	345	GLN
1	C	355	ASN
1	C	388	ASN
1	C	402	ASN
1	C	433	HIS
1	C	458	GLN
1	C	484	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	PO4	A	2445	-	4,4,4	0.92	0	6,6,6	0.38	0
2	PO4	B	2444	-	4,4,4	0.81	0	6,6,6	0.39	0
2	PO4	C	2443	-	4,4,4	1.00	0	6,6,6	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	2445	-	-	0/0/0/0	0/0/0/0
2	PO4	B	2444	-	-	0/0/0/0	0/0/0/0
2	PO4	C	2443	-	-	0/0/0/0	0/0/0/0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.