



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 02:25 PM BST

PDB ID : 5GPJ
Title : Crystal Structure of Proton-Pumping Pyrophosphatase
Authors : Li, K.M.; Tsai, J.Y.; Sun, Y.J.
Deposited on : 2016-08-03
Resolution : 3.50 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
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) : 2.13

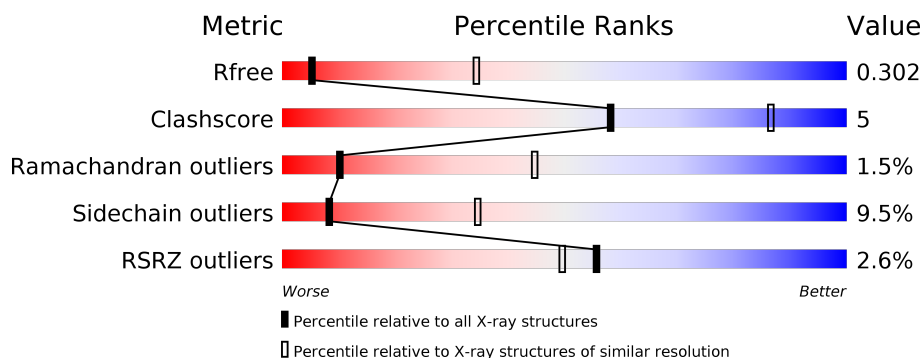
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 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	774	
1	B	774	
1	C	774	
1	D	774	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	1001	-	-	-	X
2	PO4	C	1001	-	-	-	X
2	PO4	D	1001	-	-	-	X
3	MG	C	1002	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21413 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 Pyrophosphate-energized vacuolar membrane proton pump.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			5374	3505	851	989	29			
1	B	726	Total	C	N	O	S	0	0	0
			5324	3474	843	978	29			
1	C	728	Total	C	N	O	S	0	0	0
			5344	3486	846	983	29			
1	D	728	Total	C	N	O	S	0	0	0
			5343	3486	845	983	29			

There are 32 discrepancies between the modelled and reference sequences:

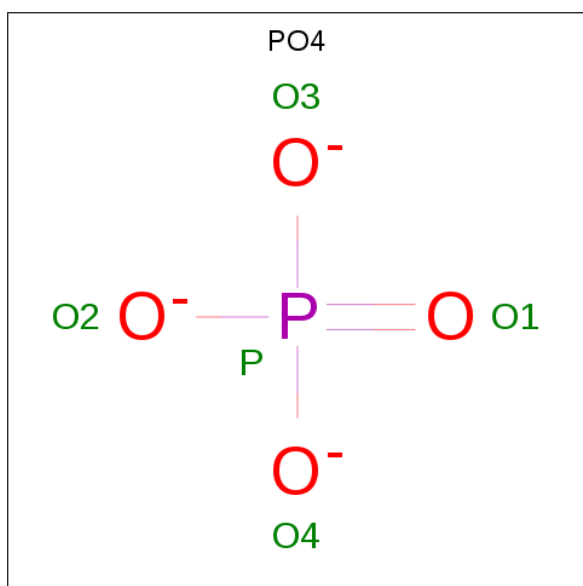
Chain	Residue	Modelled	Actual	Comment	Reference
A	767	SER	-	expression tag	UNP P21616
A	768	SER	-	expression tag	UNP P21616
A	769	HIS	-	expression tag	UNP P21616
A	770	HIS	-	expression tag	UNP P21616
A	771	HIS	-	expression tag	UNP P21616
A	772	HIS	-	expression tag	UNP P21616
A	773	HIS	-	expression tag	UNP P21616
A	774	HIS	-	expression tag	UNP P21616
B	767	SER	-	expression tag	UNP P21616
B	768	SER	-	expression tag	UNP P21616
B	769	HIS	-	expression tag	UNP P21616
B	770	HIS	-	expression tag	UNP P21616
B	771	HIS	-	expression tag	UNP P21616
B	772	HIS	-	expression tag	UNP P21616
B	773	HIS	-	expression tag	UNP P21616
B	774	HIS	-	expression tag	UNP P21616
C	767	SER	-	expression tag	UNP P21616
C	768	SER	-	expression tag	UNP P21616
C	769	HIS	-	expression tag	UNP P21616
C	770	HIS	-	expression tag	UNP P21616
C	771	HIS	-	expression tag	UNP P21616

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Chain	Residue	Modelled	Actual	Comment	Reference
C	772	HIS	-	expression tag	UNP P21616
C	773	HIS	-	expression tag	UNP P21616
C	774	HIS	-	expression tag	UNP P21616
D	767	SER	-	expression tag	UNP P21616
D	768	SER	-	expression tag	UNP P21616
D	769	HIS	-	expression tag	UNP P21616
D	770	HIS	-	expression tag	UNP P21616
D	771	HIS	-	expression tag	UNP P21616
D	772	HIS	-	expression tag	UNP P21616
D	773	HIS	-	expression tag	UNP P21616
D	774	HIS	-	expression tag	UNP P21616

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

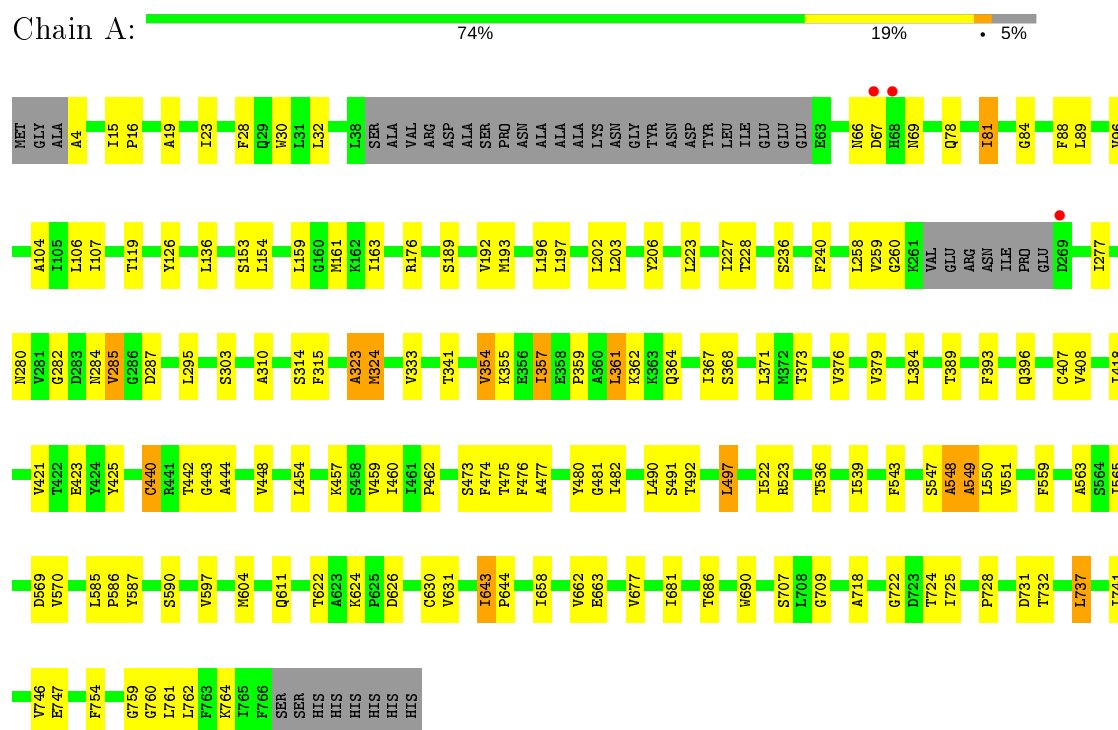
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Mg 2	0	0
3	A	2	Total 2	Mg 2	0	0
3	D	2	Total 2	Mg 2	0	0
3	C	2	Total 2	Mg 2	0	0

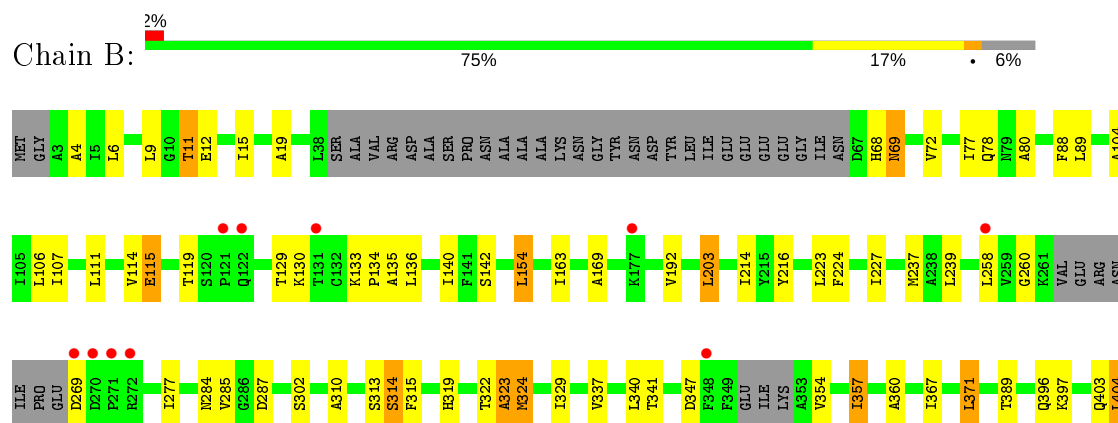
3 Residue-property plots

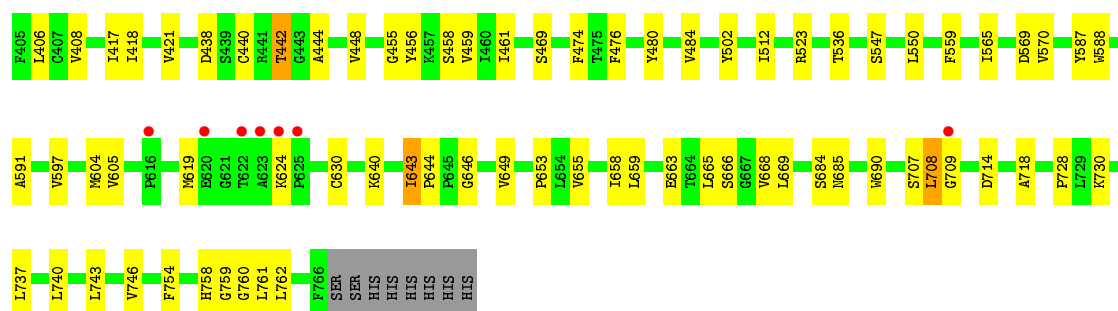
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Pyrophosphate-energized vacuolar membrane proton pump

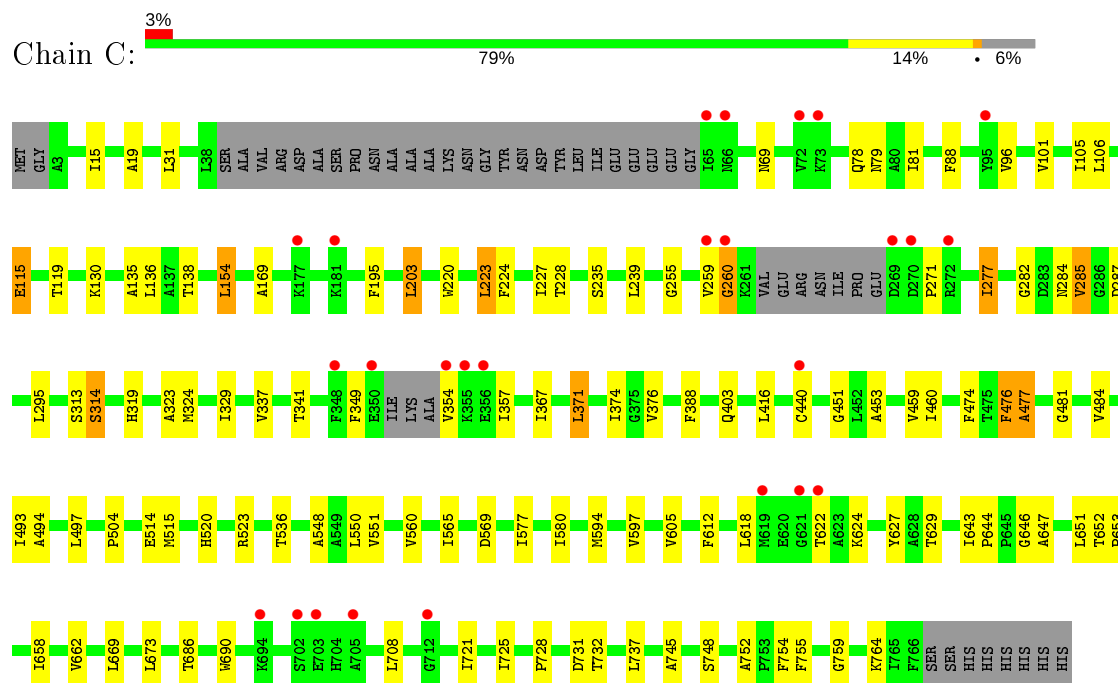


- Molecule 1: Pyrophosphate-energized vacuolar membrane proton pump

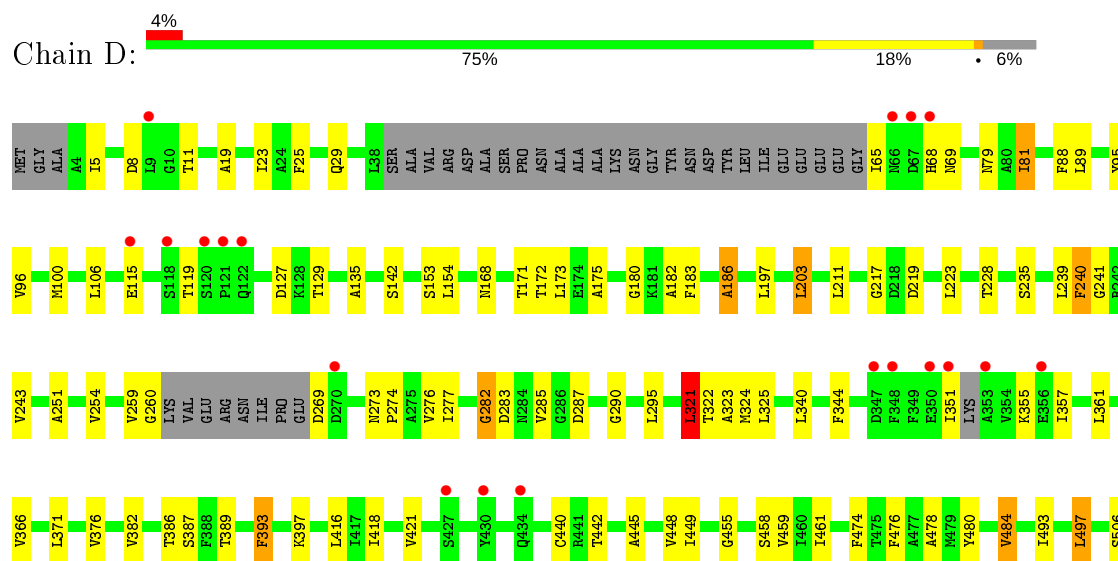


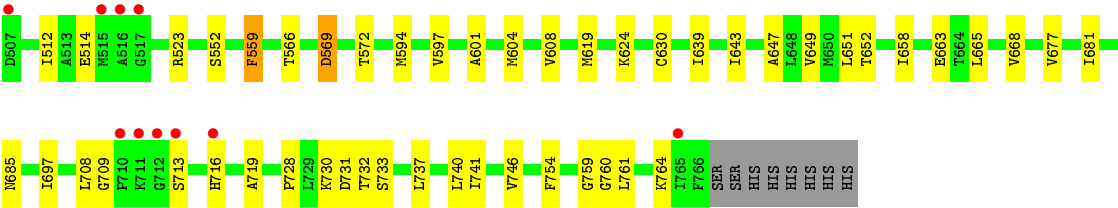


- Molecule 1: Pyrophosphate-energized vacuolar membrane proton pump



- Molecule 1: Pyrophosphate-energized vacuolar membrane proton pump





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.70Å 81.64Å 264.85Å 90.00° 92.87° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50 27.87 – 3.47	Depositor EDS
% Data completeness (in resolution range)	91.1 (30.00-3.50) 91.3 (27.87-3.47)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.226 , 0.304 0.228 , 0.302	Depositor DCC
R_{free} test set	3027 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å ²)	98.7	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 80.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21413	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: PO4, MG

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	0.53	0/5478	0.75	0/7441
1	B	0.49	0/5427	0.69	0/7372
1	C	0.51	0/5447	0.69	0/7399
1	D	0.50	0/5446	0.69	0/7399
All	All	0.51	0/21798	0.70	0/29611

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
1	A	0	2
1	B	0	3
1	C	0	1
1	D	0	2
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	LEU	Peptide
1	A	709	GLY	Peptide
1	B	258	LEU	Peptide
1	B	708	LEU	Peptide
1	B	709	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	C	708	LEU	Peptide
1	D	708	LEU	Peptide
1	D	709	GLY	Peptide

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	5374	0	5516	65	0
1	B	5324	0	5464	56	0
1	C	5344	0	5482	43	0
1	D	5343	0	5480	54	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
All	All	21413	0	21942	209	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 5.

All (209) 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:D:730:LYS:NZ	2:D:1001:PO4:O2	2.13	0.81
1:A:643:ILE:HG22	1:A:644:PRO:HD3	1.69	0.74
1:A:597:VAL:HG11	1:A:728:PRO:HB3	1.73	0.70
1:C:115:GLU:HB2	1:C:135:ALA:HB3	1.80	0.63
1:B:115:GLU:HB2	1:B:135:ALA:HB3	1.81	0.62
1:C:658:ILE:HD11	1:C:754:PHE:CE2	2.36	0.61
1:C:669:LEU:HD21	1:C:745:ALA:HA	1.82	0.60
1:D:96:VAL:HG22	1:D:240:PHE:CD2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:VAL:HG22	1:B:740:LEU:HD12	1.84	0.60
1:D:115:GLU:HB2	1:D:135:ALA:HB3	1.84	0.59
1:A:310:ALA:HB2	1:A:480:TYR:CE1	2.36	0.59
1:C:453:ALA:HB2	1:D:594:MET:HB3	1.84	0.59
1:C:223:LEU:HD13	1:C:224:PHE:CE1	2.37	0.58
1:B:403:GLN:HB3	1:B:476:PHE:HB3	1.84	0.58
1:B:78:GLN:OE1	1:B:169:ALA:HB3	2.03	0.58
1:A:563:ALA:HB1	1:A:662:VAL:HG21	1.85	0.58
1:B:597:VAL:HG11	1:B:728:PRO:HB3	1.84	0.58
1:C:19:ALA:HB3	1:C:203:LEU:HD23	1.86	0.57
1:A:315:PHE:CD1	1:A:323:ALA:HB1	2.39	0.57
1:A:444:ALA:HA	1:A:718:ALA:HB1	1.85	0.57
1:C:15:ILE:HD11	1:C:329:ILE:HD13	1.87	0.57
1:C:725:ILE:HA	1:D:449:ILE:HD11	1.87	0.57
1:B:88:PHE:HD1	1:B:89:LEU:HD23	1.69	0.56
1:A:333:VAL:HG21	1:A:379:VAL:CG2	2.36	0.56
1:B:11:THR:HB	1:B:322:THR:HG22	1.88	0.55
1:D:19:ALA:HB3	1:D:203:LEU:HD23	1.88	0.55
1:A:161:MET:HE1	1:A:284:ASN:C	2.27	0.55
1:D:597:VAL:HG11	1:D:728:PRO:HB3	1.89	0.55
1:A:459:VAL:HG12	1:A:681:ILE:HB	1.89	0.55
1:B:341:THR:HG22	1:B:367:ILE:HG22	1.88	0.55
1:A:423:GLU:HB2	1:A:539:ILE:HD11	1.89	0.55
1:A:341:THR:HG22	1:A:367:ILE:HG22	1.90	0.54
1:D:658:ILE:HD11	1:D:754:PHE:CE2	2.42	0.54
1:A:658:ILE:HD11	1:A:754:PHE:CE2	2.43	0.53
1:A:354:VAL:O	1:A:357:ILE:HG22	2.07	0.53
1:A:176:ARG:HA	1:A:522:ILE:HD11	1.89	0.53
1:A:96:VAL:HG22	1:A:240:PHE:CD2	2.43	0.53
1:A:724:THR:O	1:A:728:PRO:HD2	2.09	0.53
1:B:389:THR:HA	1:B:397:LYS:O	2.09	0.53
1:C:295:LEU:HD23	1:C:493:ILE:HD11	1.90	0.53
1:A:425:TYR:O	1:A:454:LEU:HD21	2.09	0.52
1:C:195:PHE:CE1	1:C:494:ALA:HB1	2.45	0.52
1:D:88:PHE:HD1	1:D:89:LEU:HD23	1.75	0.52
1:D:559:PHE:CZ	1:D:665:LEU:HD23	2.45	0.52
1:C:612:PHE:HA	1:C:618:LEU:HD23	1.92	0.52
1:B:643:ILE:HG22	1:B:644:PRO:HD3	1.91	0.52
1:C:548:ALA:HA	1:C:551:VAL:HG12	1.92	0.51
1:B:404:LEU:HD11	1:B:480:TYR:HE2	1.73	0.51
1:C:78:GLN:OE1	1:C:169:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:PRO:HG2	1:D:608:VAL:HG22	1.91	0.51
1:B:458:SER:OG	1:B:685:ASN:ND2	2.38	0.51
1:C:282:GLY:HA2	1:C:285:VAL:HG12	1.93	0.51
1:D:389:THR:HA	1:D:397:LYS:O	2.10	0.50
1:A:759:GLY:O	1:A:761:LEU:N	2.44	0.50
1:A:549:ALA:HB2	1:A:677:VAL:HG21	1.93	0.50
1:B:649:VAL:HG12	1:B:743:LEU:HD22	1.92	0.50
1:D:759:GLY:O	1:D:761:LEU:N	2.45	0.50
1:A:324:MET:HE3	1:A:324:MET:HA	1.94	0.50
1:C:341:THR:HG22	1:C:367:ILE:HG22	1.93	0.50
1:A:376:VAL:HG21	1:A:408:VAL:HG21	1.94	0.50
1:B:104:ALA:HA	1:B:107:ILE:HG22	1.94	0.49
1:A:104:ALA:HA	1:A:107:ILE:HG22	1.93	0.49
1:A:341:THR:HG21	1:A:368:SER:HA	1.94	0.49
1:A:490:LEU:HD21	1:A:547:SER:OG	2.13	0.49
1:D:455:GLY:O	1:D:458:SER:HB3	2.13	0.49
1:B:665:LEU:HG	1:B:669:LEU:HD13	1.95	0.49
1:B:448:VAL:HG23	1:B:690:TRP:CZ2	2.48	0.49
1:D:459:VAL:HG12	1:D:681:ILE:HB	1.93	0.49
1:A:15:ILE:HG21	1:A:206:TYR:CD1	2.48	0.49
1:A:84:GLY:CA	1:A:631:VAL:HG21	2.42	0.49
1:B:19:ALA:HB3	1:B:203:LEU:HD23	1.93	0.49
1:C:647:ALA:HB1	1:C:651:LEU:HD12	1.95	0.49
1:A:421:VAL:HG11	1:A:462:PRO:HD3	1.94	0.49
1:A:611:GLN:NE2	1:A:626:ASP:O	2.46	0.48
1:C:560:VAL:HG13	1:C:565:ILE:HB	1.95	0.48
1:D:458:SER:OG	1:D:685:ASN:ND2	2.36	0.48
1:A:548:ALA:O	1:A:549:ALA:C	2.52	0.48
1:C:597:VAL:HG11	1:C:728:PRO:HB3	1.95	0.48
1:B:759:GLY:O	1:B:761:LEU:N	2.46	0.48
1:B:315:PHE:CD1	1:B:323:ALA:HB1	2.49	0.48
1:C:565:ILE:HD11	1:C:662:VAL:HG23	1.95	0.48
1:A:548:ALA:O	1:A:551:VAL:N	2.46	0.48
1:A:587:TYR:HH	1:B:587:TYR:HH	1.56	0.48
1:D:647:ALA:O	1:D:651:LEU:N	2.45	0.47
1:B:216:TYR:CD1	1:B:223:LEU:HA	2.50	0.47
1:C:284:ASN:ND2	1:C:504:PRO:O	2.47	0.47
1:B:559:PHE:CE1	1:B:665:LEU:HD23	2.49	0.47
1:C:403:GLN:HB3	1:C:476:PHE:HB3	1.97	0.47
1:B:11:THR:CB	1:B:322:THR:HG22	2.45	0.47
1:A:448:VAL:HG23	1:A:690:TRP:CZ2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ALA:HB2	1:B:480:TYR:CE1	2.50	0.47
1:D:273:ASN:ND2	1:D:276:VAL:HG23	2.29	0.47
1:D:11:THR:HB	1:D:322:THR:HG22	1.96	0.47
1:D:697:ILE:HG21	1:D:716:HIS:HB2	1.96	0.47
1:C:313:SER:O	1:C:314:SER:C	2.52	0.47
1:B:408:VAL:HG13	1:B:484:VAL:CG1	2.45	0.46
1:B:313:SER:O	1:B:314:SER:C	2.54	0.46
1:C:239:LEU:HD11	1:C:646:GLY:HA2	1.97	0.46
1:A:389:THR:HB	1:A:396:GLN:HB3	1.96	0.46
1:C:259:VAL:HB	1:C:260:GLY:HA2	1.98	0.46
1:A:4:ALA:HB2	1:A:384:LEU:C	2.36	0.46
1:A:477:ALA:HB3	1:A:481:GLY:CA	2.46	0.46
1:B:15:ILE:HD11	1:B:329:ILE:HD13	1.98	0.46
1:C:337:VAL:HG13	1:C:371:LEU:HB3	1.97	0.46
1:C:277:ILE:HG21	1:C:627:TYR:CD1	2.51	0.46
1:A:81:ILE:HD11	1:A:280:ASN:HB3	1.98	0.46
1:B:455:GLY:O	1:B:458:SER:HB3	2.16	0.46
1:D:180:GLY:HA2	1:D:351:ILE:HB	1.97	0.46
1:A:159:LEU:HD13	1:A:196:LEU:HD13	1.98	0.45
1:B:658:ILE:HD11	1:B:754:PHE:CE2	2.51	0.45
1:C:652:THR:HB	1:C:653:PRO:HD3	1.97	0.45
1:B:69:ASN:HA	1:B:72:VAL:HG12	1.96	0.45
1:C:314:SER:CB	1:C:388:PHE:HB2	2.47	0.45
1:D:295:LEU:CD2	1:D:493:ILE:HD11	2.45	0.45
1:D:81:ILE:HG21	1:D:168:ASN:HD21	1.81	0.45
1:A:66:ASN:HA	1:A:67:ASP:HA	1.80	0.45
1:D:393:PHE:HB3	1:D:566:THR:HG22	1.98	0.45
1:B:444:ALA:HA	1:B:718:ALA:HB1	1.98	0.45
1:D:269:ASP:HA	1:D:276:VAL:HG21	1.98	0.45
1:B:154:LEU:HD23	1:B:237:MET:HG3	1.98	0.45
1:D:197:LEU:HD22	1:D:497:LEU:CD1	2.46	0.45
1:D:95:TYR:CD1	1:D:639:ILE:HG21	2.51	0.45
1:B:239:LEU:HD21	1:B:646:GLY:HA2	1.99	0.45
1:B:88:PHE:CE1	1:B:285:VAL:HG21	2.52	0.45
1:D:480:TYR:O	1:D:484:VAL:HB	2.17	0.45
1:D:321:LEU:HD22	1:D:325:LEU:CD1	2.47	0.45
1:D:351:ILE:HD12	1:D:351:ILE:N	2.32	0.45
1:A:28:PHE:CE2	1:A:32:LEU:HD11	2.52	0.45
1:D:239:LEU:O	1:D:243:VAL:HB	2.18	0.44
1:C:577:ILE:HA	1:C:580:ILE:HG22	1.99	0.44
1:D:8:ASP:HA	1:D:322:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:VAL:O	1:C:105:ILE:HD13	2.18	0.44
1:A:548:ALA:O	1:A:550:LEU:N	2.50	0.44
1:A:475:THR:HG22	1:A:476:PHE:N	2.33	0.44
1:D:254:VAL:HG12	1:D:254:VAL:O	2.18	0.44
1:C:96:VAL:HG11	1:C:154:LEU:HD11	2.00	0.44
1:A:19:ALA:HB2	1:A:202:LEU:HD23	1.99	0.44
1:B:421:VAL:HG11	1:B:461:ILE:HB	1.99	0.44
1:B:337:VAL:O	1:B:341:THR:HG23	2.18	0.43
1:D:171:THR:HG23	1:D:186:ALA:HB2	2.00	0.43
1:A:361:LEU:O	1:A:364:GLN:HB2	2.18	0.43
1:A:88:PHE:CE1	1:A:285:VAL:HG21	2.53	0.43
1:A:686:THR:HG22	1:A:690:TRP:CZ3	2.52	0.43
1:C:477:ALA:HB3	1:C:481:GLY:CA	2.48	0.43
1:C:748:SER:O	1:C:752:ALA:N	2.51	0.43
1:A:570:VAL:HG23	1:B:570:VAL:CG2	2.48	0.43
1:C:19:ALA:CB	1:C:203:LEU:HD23	2.49	0.43
1:D:119:THR:HG22	1:D:119:THR:O	2.18	0.43
1:D:421:VAL:HG21	1:D:461:ILE:HG21	1.99	0.43
1:D:172:THR:HG21	1:D:512:ILE:HG22	2.00	0.43
1:D:649:VAL:HG22	1:D:740:LEU:HD12	2.00	0.43
1:B:730:LYS:NZ	2:B:1001:PO4:O1	2.52	0.43
1:D:5:ILE:HD13	1:D:382:VAL:HA	1.99	0.43
1:A:460:ILE:HD11	1:B:588:TRP:CG	2.53	0.43
1:B:129:THR:HG23	1:B:130:LYS:N	2.33	0.43
1:C:721:ILE:HG23	1:D:445:ALA:HB2	2.01	0.43
1:D:440:CYS:SG	1:D:719:ALA:HB2	2.58	0.43
1:A:197:LEU:HD22	1:A:497:LEU:CD1	2.48	0.43
1:B:337:VAL:HG13	1:B:371:LEU:HB3	2.01	0.43
1:A:457:LYS:HB2	1:B:591:ALA:HB1	2.01	0.43
1:D:282:GLY:HA2	1:D:285:VAL:HG12	2.01	0.43
1:A:163:ILE:HD13	1:A:192:VAL:HB	2.00	0.42
1:B:653:PRO:HA	1:B:665:LEU:HD11	2.02	0.42
1:D:175:ALA:HA	1:D:182:ALA:HB2	2.01	0.42
1:D:25:PHE:O	1:D:29:GLN:HG2	2.19	0.42
1:A:88:PHE:HD1	1:A:89:LEU:HD23	1.83	0.42
1:B:77:ILE:HG21	1:B:512:ILE:HG12	2.01	0.42
1:D:11:THR:CB	1:D:322:THR:HG22	2.50	0.42
1:A:15:ILE:HB	1:A:16:PRO:HD3	2.01	0.42
1:A:282:GLY:HA2	1:A:285:VAL:HG12	2.00	0.42
1:A:30:TRP:CD2	1:A:163:ILE:HD12	2.55	0.42
1:A:407:CYS:SG	1:A:473:SER:HA	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:GLY:HA2	1:A:725:ILE:HD12	2.02	0.42
1:D:366:VAL:HG22	1:D:416:LEU:HD21	2.02	0.42
1:B:133:LYS:HB3	1:B:134:PRO:CD	2.50	0.42
1:D:96:VAL:HG22	1:D:240:PHE:CE2	2.55	0.42
1:C:271:PRO:HG3	1:C:515:MET:HB3	2.02	0.42
1:B:163:ILE:HD13	1:B:192:VAL:HB	2.02	0.42
1:B:354:VAL:O	1:B:357:ILE:HG22	2.20	0.42
1:C:451:GLY:HA3	1:C:690:TRP:HE1	1.85	0.42
1:B:224:PHE:HE2	1:B:324:MET:SD	2.43	0.41
1:C:725:ILE:CD1	1:D:448:VAL:HG11	2.49	0.41
1:C:755:PHE:O	1:C:759:GLY:N	2.53	0.41
1:A:163:ILE:HD13	1:A:192:VAL:CB	2.50	0.41
1:B:357:ILE:O	1:B:360:ALA:HB3	2.21	0.41
1:C:88:PHE:CD1	1:C:285:VAL:HG21	2.56	0.41
1:A:590:SER:OG	1:A:737:LEU:HD21	2.21	0.41
1:D:65:ILE:HD12	1:D:65:ILE:N	2.35	0.41
1:A:548:ALA:HA	1:A:551:VAL:HG12	2.02	0.41
1:C:459:VAL:O	1:C:460:ILE:C	2.59	0.41
1:C:721:ILE:O	1:C:725:ILE:HG13	2.20	0.41
1:A:359:PRO:O	1:A:362:LYS:N	2.54	0.41
1:A:725:ILE:HG12	1:B:448:VAL:CG1	2.51	0.41
1:D:183:PHE:CD1	1:D:351:ILE:HD13	2.56	0.41
1:D:552:SER:HB3	1:D:741:ILE:HG22	2.03	0.41
1:A:259:VAL:HA	1:A:260:GLY:HA2	1.92	0.40
1:A:585:LEU:N	1:A:586:PRO:HD2	2.36	0.40
1:A:440:CYS:HA	1:A:443:GLY:O	2.21	0.40
1:B:111:LEU:O	1:B:114:VAL:HG22	2.22	0.40
1:B:389:THR:HB	1:B:396:GLN:HB3	2.03	0.40
1:D:259:VAL:HG22	1:D:260:GLY:HA3	2.01	0.40
1:B:655:VAL:O	1:B:659:LEU:HB2	2.22	0.40
1:B:80:ALA:C	1:B:277:ILE:HD11	2.42	0.40
1:B:417:ILE:O	1:B:421:VAL:HG23	2.21	0.40
1:B:456:TYR:O	1:B:459:VAL:HG22	2.21	0.40
1:C:220:TRP:CZ3	1:C:319:HIS:HA	2.56	0.40
1:D:251:ALA:HA	1:D:601:ALA:HB2	2.03	0.40
1:A:686:THR:CG2	1:A:690:TRP:CH2	3.04	0.40
1:D:569:ASP:HB3	1:D:572:THR:HG23	2.04	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	726/774 (94%)	637 (88%)	81 (11%)	8 (1%)	14	52
1	B	718/774 (93%)	649 (90%)	61 (8%)	8 (1%)	14	52
1	C	720/774 (93%)	647 (90%)	64 (9%)	9 (1%)	12	48
1	D	720/774 (93%)	643 (89%)	59 (8%)	18 (2%)	5	34
All	All	2884/3096 (93%)	2576 (89%)	265 (9%)	43 (2%)	10	45

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	760	GLY
1	D	760	GLY
1	A	323	ALA
1	A	543	PHE
1	B	442	THR
1	B	619	MET
1	B	760	GLY
1	C	69	ASN
1	C	255	GLY
1	C	314	SER
1	C	323	ALA
1	C	622	THR
1	D	186	ALA
1	D	217	GLY
1	D	240	PHE
1	D	241	GLY
1	D	321	LEU
1	D	713	SER
1	A	548	ALA
1	A	549	ALA
1	B	4	ALA
1	B	323	ALA

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Mol	Chain	Res	Type
1	D	219	ASP
1	D	283	ASP
1	D	386	THR
1	D	442	THR
1	A	69	ASN
1	B	314	SER
1	D	344	PHE
1	D	619	MET
1	A	126	TYR
1	A	314	SER
1	B	319	HIS
1	C	476	PHE
1	C	477	ALA
1	D	323	ALA
1	D	476	PHE
1	D	478	ALA
1	C	644	PRO
1	C	260	GLY
1	B	260	GLY
1	D	282	GLY
1	D	290	GLY

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	562/596 (94%)	506 (90%)	56 (10%)	7	32
1	B	556/596 (93%)	499 (90%)	57 (10%)	7	32
1	C	559/596 (94%)	512 (92%)	47 (8%)	11	40
1	D	559/596 (94%)	506 (90%)	53 (10%)	8	34
All	All	2236/2384 (94%)	2023 (90%)	213 (10%)	8	34

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	78	GLN
1	A	81	ILE
1	A	106	LEU
1	A	119	THR
1	A	136	LEU
1	A	153	SER
1	A	154	LEU
1	A	189	SER
1	A	193	MET
1	A	203	LEU
1	A	223	LEU
1	A	227	ILE
1	A	228	THR
1	A	236	SER
1	A	277	ILE
1	A	285	VAL
1	A	287	ASP
1	A	295	LEU
1	A	303	SER
1	A	324	MET
1	A	354	VAL
1	A	355	LYS
1	A	357	ILE
1	A	361	LEU
1	A	371	LEU
1	A	373	THR
1	A	393	PHE
1	A	418	ILE
1	A	440	CYS
1	A	442	THR
1	A	474	PHE
1	A	482	ILE
1	A	491	SER
1	A	492	THR
1	A	497	LEU
1	A	523	ARG
1	A	536	THR
1	A	559	PHE
1	A	565	ILE
1	A	569	ASP
1	A	604	MET
1	A	622	THR

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Mol	Chain	Res	Type
1	A	624	LYS
1	A	630	CYS
1	A	643	ILE
1	A	663	GLU
1	A	707	SER
1	A	731	ASP
1	A	732	THR
1	A	737	LEU
1	A	741	ILE
1	A	746	VAL
1	A	747	GLU
1	A	762	LEU
1	A	764	LYS
1	B	6	LEU
1	B	9	LEU
1	B	11	THR
1	B	12	GLU
1	B	68	HIS
1	B	69	ASN
1	B	106	LEU
1	B	115	GLU
1	B	119	THR
1	B	136	LEU
1	B	140	ILE
1	B	142	SER
1	B	154	LEU
1	B	203	LEU
1	B	214	ILE
1	B	227	ILE
1	B	269	ASP
1	B	284	ASN
1	B	287	ASP
1	B	302	SER
1	B	324	MET
1	B	340	LEU
1	B	347	ASP
1	B	357	ILE
1	B	371	LEU
1	B	404	LEU
1	B	406	LEU
1	B	418	ILE
1	B	438	ASP

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Mol	Chain	Res	Type
1	B	440	CYS
1	B	442	THR
1	B	469	SER
1	B	474	PHE
1	B	502	TYR
1	B	523	ARG
1	B	536	THR
1	B	547	SER
1	B	550	LEU
1	B	565	ILE
1	B	569	ASP
1	B	604	MET
1	B	605	VAL
1	B	624	LYS
1	B	630	CYS
1	B	640	LYS
1	B	643	ILE
1	B	663	GLU
1	B	666	SER
1	B	668	VAL
1	B	684	SER
1	B	707	SER
1	B	708	LEU
1	B	714	ASP
1	B	737	LEU
1	B	746	VAL
1	B	758	HIS
1	B	762	LEU
1	C	31	LEU
1	C	79	ASN
1	C	81	ILE
1	C	106	LEU
1	C	115	GLU
1	C	119	THR
1	C	130	LYS
1	C	136	LEU
1	C	138	THR
1	C	154	LEU
1	C	203	LEU
1	C	223	LEU
1	C	227	ILE
1	C	228	THR

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Mol	Chain	Res	Type
1	C	235	SER
1	C	277	ILE
1	C	285	VAL
1	C	287	ASP
1	C	324	MET
1	C	349	PHE
1	C	354	VAL
1	C	357	ILE
1	C	371	LEU
1	C	374	ILE
1	C	376	VAL
1	C	416	LEU
1	C	440	CYS
1	C	474	PHE
1	C	484	VAL
1	C	497	LEU
1	C	514	GLU
1	C	520	HIS
1	C	523	ARG
1	C	536	THR
1	C	550	LEU
1	C	569	ASP
1	C	594	MET
1	C	605	VAL
1	C	624	LYS
1	C	629	THR
1	C	643	ILE
1	C	673	LEU
1	C	686	THR
1	C	731	ASP
1	C	732	THR
1	C	737	LEU
1	C	764	LYS
1	D	23	ILE
1	D	68	HIS
1	D	69	ASN
1	D	79	ASN
1	D	81	ILE
1	D	100	MET
1	D	106	LEU
1	D	127	ASP
1	D	129	THR

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Mol	Chain	Res	Type
1	D	142	SER
1	D	153	SER
1	D	154	LEU
1	D	173	LEU
1	D	203	LEU
1	D	211	LEU
1	D	223	LEU
1	D	228	THR
1	D	235	SER
1	D	277	ILE
1	D	287	ASP
1	D	321	LEU
1	D	324	MET
1	D	340	LEU
1	D	355	LYS
1	D	357	ILE
1	D	361	LEU
1	D	371	LEU
1	D	376	VAL
1	D	387	SER
1	D	393	PHE
1	D	418	ILE
1	D	474	PHE
1	D	484	VAL
1	D	497	LEU
1	D	506	SER
1	D	514	GLU
1	D	523	ARG
1	D	559	PHE
1	D	569	ASP
1	D	604	MET
1	D	624	LYS
1	D	630	CYS
1	D	643	ILE
1	D	652	THR
1	D	663	GLU
1	D	668	VAL
1	D	677	VAL
1	D	731	ASP
1	D	732	THR
1	D	733	SER
1	D	737	LEU

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Mol	Chain	Res	Type
1	D	746	VAL
1	D	764	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	66	ASN
1	A	79	ASN
1	A	210	ASN
1	A	280	ASN
1	B	69	ASN
1	B	210	ASN
1	B	284	ASN
1	C	29	GLN
1	C	79	ASN
1	C	210	ASN
1	D	29	GLN
1	D	68	HIS
1	D	364	GLN
1	D	434	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](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	C	1001	3	4,4,4	1.05	0	6,6,6	0.56	0
2	PO4	D	1001	3	4,4,4	0.64	0	6,6,6	1.11	0
2	PO4	A	1001	3	4,4,4	1.53	1 (25%)	6,6,6	1.03	0
2	PO4	B	1001	3	4,4,4	0.87	0	6,6,6	0.49	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	PO4	P-O1	2.89	1.57	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001	PO4	1	0
2	B	1001	PO4	1	0

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

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	732/774 (94%)	-0.56	3 (0%) 92 90	59, 87, 121, 190	0
1	B	726/774 (93%)	-0.35	17 (2%) 60 54	58, 112, 161, 224	0
1	C	728/774 (94%)	-0.23	26 (3%) 42 38	83, 134, 184, 225	0
1	D	728/774 (94%)	-0.24	29 (3%) 38 33	79, 128, 178, 225	0
All	All	2914/3096 (94%)	-0.35	75 (2%) 56 49	58, 115, 173, 225	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	66	ASN	5.4
1	C	622	THR	5.1
1	D	710	PRO	5.1
1	C	355	LYS	5.0
1	D	711	LYS	4.9
1	D	353	ALA	4.8
1	B	271	PRO	4.8
1	B	272	ARG	4.4
1	C	694	LYS	3.9
1	C	65	ILE	3.9
1	D	122	GLN	3.8
1	D	356	GLU	3.8
1	D	517	GLY	3.7
1	B	122	GLN	3.7
1	D	712	GLY	3.7
1	D	66	ASN	3.6
1	B	625	PRO	3.6
1	C	73	LYS	3.6
1	B	270	ASP	3.5
1	C	269	ASP	3.5
1	A	67	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	121	PRO	3.4
1	D	270	ASP	3.3
1	D	516	ALA	3.2
1	D	716	HIS	3.2
1	C	348	PHE	3.2
1	C	621	GLY	3.2
1	B	121	PRO	3.2
1	B	623	ALA	3.1
1	C	440	CYS	3.1
1	D	350	GLU	3.0
1	B	348	PHE	3.0
1	C	619	MET	2.9
1	B	622	THR	2.9
1	D	115	GLU	2.9
1	D	120	SER	2.8
1	B	269	ASP	2.8
1	C	350	GLU	2.7
1	C	712	GLY	2.7
1	C	181	LYS	2.7
1	C	95	TYR	2.7
1	D	9	LEU	2.7
1	C	356	GLU	2.7
1	D	430	TYR	2.6
1	C	270	ASP	2.5
1	C	272	ARG	2.5
1	B	131	THR	2.5
1	D	351	ILE	2.4
1	D	347	ASP	2.4
1	C	260	GLY	2.4
1	B	624	LYS	2.4
1	B	709	GLY	2.4
1	B	258	LEU	2.4
1	C	705	ALA	2.3
1	D	118	SER	2.3
1	D	68	HIS	2.3
1	B	616	PRO	2.3
1	D	515	MET	2.3
1	D	765	ILE	2.3
1	C	259	VAL	2.3
1	A	68	HIS	2.3
1	B	620	GLU	2.3
1	D	348	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	177	LYS	2.2
1	C	354	VAL	2.2
1	D	507	ASP	2.2
1	C	702	SER	2.2
1	A	269	ASP	2.1
1	B	177	LYS	2.1
1	C	72	VAL	2.1
1	C	703	GLU	2.0
1	D	427	SER	2.0
1	D	67	ASP	2.0
1	D	434	GLN	2.0
1	D	713	SER	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
2	PO4	D	1001	5/5	0.70	0.50	166,183,190,192	0
2	PO4	C	1001	5/5	0.73	0.53	141,166,174,175	0
3	MG	C	1003	1/1	0.73	0.35	108,108,108,108	0
2	PO4	B	1001	5/5	0.76	0.71	156,157,172,174	0
3	MG	C	1002	1/1	0.79	0.85	81,81,81,81	0
3	MG	D	1002	1/1	0.82	0.30	130,130,130,130	0
3	MG	A	1003	1/1	0.89	0.40	107,107,107,107	0
2	PO4	A	1001	5/5	0.91	0.47	103,114,133,136	0
3	MG	B	1003	1/1	0.94	0.45	102,102,102,102	0
3	MG	D	1003	1/1	0.94	0.21	161,161,161,161	0
3	MG	A	1002	1/1	0.95	0.41	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	1002	1/1	0.96	0.58	120,120,120,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.