



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 05:34 PM EDT

PDB ID : 4LZN
Title : Crystal structure of human PRS1 D65N mutant
Authors : Chen, P.; Teng, M.; Li, X.
Deposited on : 2013-07-31
Resolution : 2.14 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 : 2.37.1
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) : 2.37.1

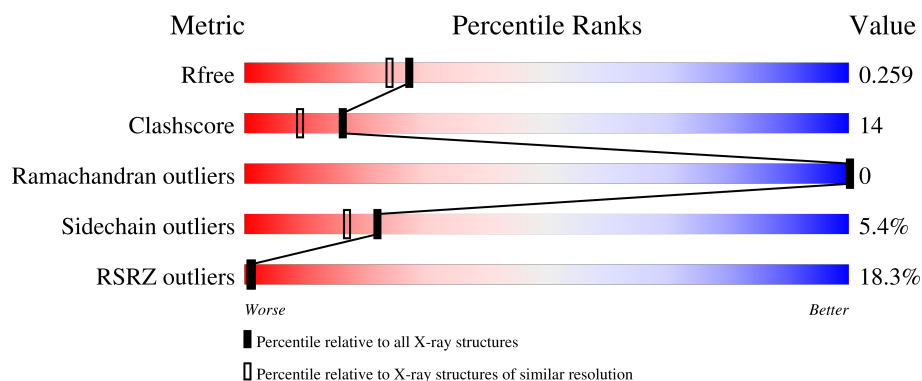
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	326	<div> <div>21%</div> <div>67%</div> <div>25%</div> <div>7%</div> </div>
1	B	326	<div> <div>14%</div> <div>72%</div> <div>21%</div> <div>6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4772 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 Ribose-phosphate pyrophosphokinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	308	Total	C	N	O	S	4	0	0
			2349	1474	413	445	17			
1	A	304	Total	C	N	O	S	0	0	0
			2324	1458	409	440	17			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	65	ASN	ASP	engineered mutation	UNP P60891
B	319	LEU	-	expression tag	UNP P60891
B	320	GLU	-	expression tag	UNP P60891
B	321	HIS	-	expression tag	UNP P60891
B	322	HIS	-	expression tag	UNP P60891
B	323	HIS	-	expression tag	UNP P60891
B	324	HIS	-	expression tag	UNP P60891
B	325	HIS	-	expression tag	UNP P60891
B	326	HIS	-	expression tag	UNP P60891
A	65	ASN	ASP	engineered mutation	UNP P60891
A	319	LEU	-	expression tag	UNP P60891
A	320	GLU	-	expression tag	UNP P60891
A	321	HIS	-	expression tag	UNP P60891
A	322	HIS	-	expression tag	UNP P60891
A	323	HIS	-	expression tag	UNP P60891
A	324	HIS	-	expression tag	UNP P60891
A	325	HIS	-	expression tag	UNP P60891
A	326	HIS	-	expression tag	UNP P60891

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

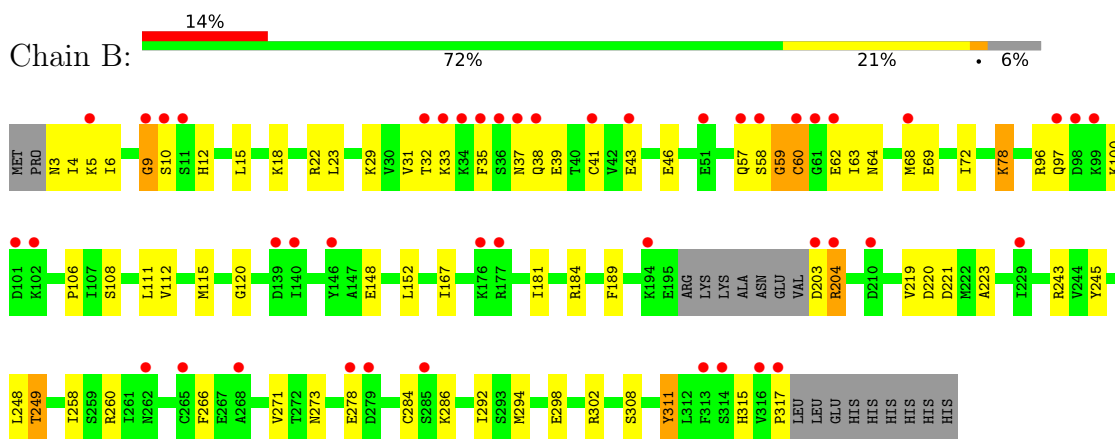
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	36	Total	O	0	0
			36	36		
3	A	33	Total	O	0	0
			33	33		

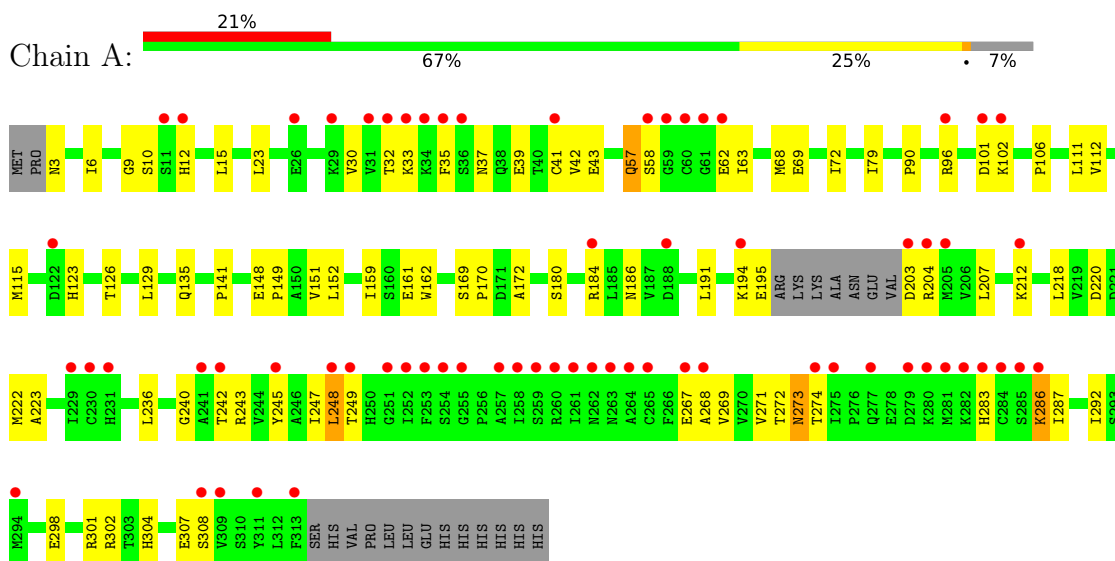
3 Residue-property plots [i](#)

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: Ribose-phosphate pyrophosphokinase 1



• Molecule 1: Ribose-phosphate pyrophosphokinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	170.78Å 170.78Å 61.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.30 – 2.14 49.30 – 2.14	Depositor EDS
% Data completeness (in resolution range)	95.3 (49.30-2.14) 95.3 (49.30-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.224 , 0.263 0.222 , 0.259	Depositor DCC
R_{free} test set	1759 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4772	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/2356	0.50	0/3185
1	B	0.41	0/2382	0.64	5/3222 (0.2%)
All	All	0.38	0/4738	0.58	5/6407 (0.1%)

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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	12	HIS	N-CA-C	-8.17	88.95	111.00
1	B	59	GLY	N-CA-C	6.42	129.15	113.10
1	B	9	GLY	N-CA-C	-6.07	97.92	113.10
1	B	60	CYS	N-CA-C	-6.00	94.79	111.00
1	B	60	CYS	N-CA-CB	5.54	120.58	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	59	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	2324	0	2359	77	0
1	B	2349	0	2382	73	0
2	A	15	0	0	1	0
2	B	15	0	0	0	0
3	A	33	0	0	0	0
3	B	36	0	0	0	0
All	All	4772	0	4741	135	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 14.

All (135) 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:B:10:SER:O	1:B:58:SER:OG	1.59	1.20
1:B:63:ILE:CD1	1:A:39:GLU:HG2	1.74	1.17
1:B:63:ILE:HD13	1:A:39:GLU:HG2	1.33	1.06
1:B:204:ARG:HH11	1:B:204:ARG:HG3	1.17	1.02
1:A:3:ASN:ND2	1:A:304:HIS:HE1	1.68	0.92
1:A:273:ASN:HD21	1:A:292:ILE:H	1.21	0.89
1:A:194:LYS:HE2	1:A:203:ASP:HB2	1.55	0.88
1:A:96:ARG:HD2	1:A:222:MET:SD	2.14	0.86
1:B:204:ARG:HH11	1:B:204:ARG:CG	1.89	0.86
1:A:57:GLN:NE2	1:A:90:PRO:HD2	1.91	0.85
1:A:3:ASN:HD22	1:A:304:HIS:CE1	1.96	0.84
1:B:63:ILE:CD1	1:A:39:GLU:CG	2.55	0.83
1:A:32:THR:HG22	1:A:42:VAL:HG22	1.59	0.82
1:B:10:SER:C	1:B:58:SER:HG	1.83	0.81
1:A:273:ASN:H	1:A:273:ASN:HD22	1.29	0.81
1:B:10:SER:HB3	1:B:69:GLU:OE1	1.84	0.77
1:B:10:SER:HB3	1:B:69:GLU:OE2	1.84	0.77
1:B:111:LEU:HG	1:B:115:MET:CE	2.17	0.75
1:B:6:ILE:HD11	1:B:23:LEU:HD12	1.67	0.75
1:B:35:PHE:CZ	1:B:41:CYS:HB2	2.22	0.74
1:B:10:SER:HB3	1:B:69:GLU:CD	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ILE:HD12	1:A:39:GLU:HG2	1.72	0.72
1:A:10:SER:O	1:A:58:SER:OG	2.09	0.71
1:A:3:ASN:HD22	1:A:304:HIS:HE1	1.29	0.70
1:A:57:GLN:NE2	1:A:57:GLN:O	2.25	0.70
1:A:3:ASN:ND2	1:A:304:HIS:CE1	2.53	0.69
1:B:6:ILE:HD11	1:B:23:LEU:CD1	2.22	0.68
1:B:243:ARG:NH1	1:B:245:TYR:OH	2.26	0.68
1:B:111:LEU:HG	1:B:115:MET:HE1	1.75	0.67
1:B:6:ILE:CD1	1:B:23:LEU:HD12	2.27	0.65
1:B:294:MET:HG2	1:B:317:PRO:HG2	1.78	0.65
1:A:273:ASN:HD22	1:A:273:ASN:N	1.95	0.64
1:B:33:LYS:HG2	1:B:41:CYS:HB3	1.80	0.63
1:B:35:PHE:CE1	1:B:41:CYS:HB2	2.34	0.62
1:B:39:GLU:HG2	1:A:63:ILE:HD13	1.82	0.61
1:B:204:ARG:HG3	1:B:204:ARG:NH1	1.99	0.61
1:A:9:GLY:HA3	1:A:58:SER:HB2	1.81	0.61
1:A:180:SER:O	1:A:184:ARG:HD3	2.01	0.60
1:B:106:PRO:HG3	1:A:72:ILE:HG23	1.82	0.60
1:B:96:ARG:NH2	1:A:37:ASN:HD21	1.99	0.60
1:B:148:GLU:OE2	1:B:184:ARG:NH1	2.35	0.59
1:A:212:LYS:HD2	1:A:240:GLY:HA3	1.85	0.59
1:B:184:ARG:HG3	1:B:184:ARG:HH11	1.68	0.59
1:B:111:LEU:HG	1:B:115:MET:HE2	1.85	0.58
1:A:30:VAL:HG22	1:A:32:THR:HG23	1.84	0.58
1:A:172:ALA:HA	1:A:191:LEU:HD11	1.85	0.58
1:A:10:SER:HB3	1:A:69:GLU:OE2	2.03	0.58
1:B:78:LYS:HE2	1:B:120:GLY:O	2.04	0.57
1:A:298:GLU:CD	1:A:301:ARG:HH12	2.07	0.57
1:A:35:PHE:CE1	1:A:41:CYS:HB2	2.41	0.56
1:A:248:LEU:O	1:A:271:VAL:HA	2.05	0.56
1:A:298:GLU:HG3	1:A:302:ARG:HD2	1.87	0.56
1:B:72:ILE:HG23	1:A:106:PRO:HG3	1.88	0.55
1:B:258:ILE:HG23	1:B:284:CYS:HB2	1.87	0.55
1:B:37:ASN:OD1	1:B:39:GLU:HG3	2.07	0.54
1:A:57:GLN:HE22	1:A:90:PRO:HD2	1.73	0.53
1:A:268:ALA:HA	1:A:286:LYS:HB2	1.90	0.53
1:A:307:GLU:HG3	1:A:308:SER:N	2.24	0.53
1:A:6:ILE:HD11	1:A:23:LEU:CD1	2.39	0.52
1:A:159:ILE:O	1:A:162:TRP:HD1	1.93	0.52
1:A:33:LYS:HG3	1:A:41:CYS:HB3	1.92	0.52
1:B:221:ASP:O	1:B:249:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:GLU:H	1:B:278:GLU:CD	2.13	0.51
1:A:135:GLN:NE2	2:A:1003:SO4:O4	2.44	0.51
1:A:220:ASP:O	1:A:248:LEU:HA	2.10	0.51
1:B:72:ILE:CG2	1:A:106:PRO:HG3	2.40	0.51
1:A:6:ILE:HD11	1:A:23:LEU:HD12	1.93	0.50
1:B:184:ARG:NH1	1:B:184:ARG:HG3	2.26	0.50
1:B:204:ARG:CG	1:B:204:ARG:NH1	2.56	0.50
1:A:10:SER:HB3	1:A:69:GLU:CD	2.32	0.50
1:A:35:PHE:CZ	1:A:41:CYS:HB2	2.47	0.49
1:B:223:ALA:HB2	1:B:248:LEU:HG	1.95	0.49
1:B:298:GLU:O	1:B:302:ARG:HG2	2.11	0.49
1:A:273:ASN:H	1:A:273:ASN:ND2	2.04	0.49
1:B:18:LYS:O	1:B:22:ARG:HG3	2.13	0.49
1:B:31:VAL:HB	1:B:43:GLU:HB3	1.94	0.49
1:B:63:ILE:HD13	1:A:39:GLU:CG	2.23	0.49
1:B:311:TYR:CE2	1:B:315:HIS:CD2	3.01	0.49
1:B:248:LEU:HB2	1:B:271:VAL:HG12	1.94	0.48
1:A:161:GLU:CD	1:A:243:ARG:HH21	2.17	0.48
1:B:9:GLY:C	1:B:58:SER:HB2	2.34	0.48
1:B:68:MET:HB3	1:B:68:MET:HE2	1.80	0.48
1:B:97:GLN:HB2	1:B:108:SER:HB2	1.96	0.48
1:A:101:ASP:O	1:A:102:LYS:HB2	2.12	0.48
1:A:90:PRO:HB2	1:A:274:THR:HB	1.96	0.47
1:B:311:TYR:CZ	1:B:315:HIS:HD2	2.32	0.47
1:A:273:ASN:ND2	1:A:292:ILE:HG13	2.29	0.47
1:A:161:GLU:OE1	1:A:243:ARG:NH2	2.48	0.47
1:B:112:VAL:HA	1:B:115:MET:CE	2.44	0.47
1:B:96:ARG:HH22	1:A:37:ASN:HD21	1.60	0.47
1:B:220:ASP:HB3	1:B:248:LEU:HD12	1.97	0.47
1:A:242:THR:HG22	1:A:243:ARG:HG3	1.96	0.47
1:B:100:LYS:HE2	1:A:79:ILE:HD12	1.97	0.46
1:B:273:ASN:OD1	1:B:292:ILE:HG13	2.15	0.46
1:B:63:ILE:HD12	1:A:39:GLU:N	2.31	0.45
1:A:112:VAL:HA	1:A:115:MET:HE2	1.97	0.45
1:A:273:ASN:ND2	1:A:292:ILE:H	2.02	0.45
1:B:311:TYR:CZ	1:B:315:HIS:CD2	3.04	0.45
1:A:272:THR:OG1	1:A:274:THR:HG23	2.16	0.45
1:A:6:ILE:CD1	1:A:23:LEU:HD12	2.47	0.45
1:A:10:SER:HB3	1:A:69:GLU:OE1	2.17	0.44
1:A:9:GLY:CA	1:A:58:SER:HB2	2.46	0.44
1:A:302:ARG:HG2	1:A:307:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:THR:HG23	1:B:32:THR:O	2.16	0.44
1:B:181:ILE:HD12	1:B:219:VAL:HG11	1.99	0.44
1:B:106:PRO:HG3	1:A:72:ILE:CG2	2.47	0.44
1:B:167:ILE:O	1:B:189:PHE:HA	2.18	0.44
1:A:223:ALA:HB2	1:A:248:LEU:HD22	1.99	0.44
1:A:269:VAL:O	1:A:287:ILE:HA	2.17	0.44
1:B:37:ASN:ND2	1:B:39:GLU:HG3	2.33	0.43
1:A:223:ALA:HB3	1:A:248:LEU:HD13	2.01	0.43
1:A:243:ARG:NH1	1:A:245:TYR:OH	2.47	0.43
1:A:151:VAL:HG13	1:A:247:ILE:HG21	1.99	0.43
1:A:170:PRO:HG3	1:A:218:LEU:HD22	2.00	0.43
1:B:37:ASN:CG	1:B:39:GLU:HG3	2.39	0.43
1:B:112:VAL:HA	1:B:115:MET:HE3	2.01	0.42
1:A:245:TYR:CZ	1:A:267:GLU:HG2	2.54	0.42
1:B:298:GLU:O	1:B:302:ARG:CG	2.67	0.42
1:A:112:VAL:HA	1:A:115:MET:CE	2.50	0.42
1:B:111:LEU:C	1:B:115:MET:HE2	2.39	0.42
1:B:29:LYS:HG3	1:B:46:GLU:OE2	2.20	0.42
1:A:207:LEU:HD11	1:A:236:LEU:HD23	2.02	0.42
1:B:302:ARG:HD2	1:B:308:SER:O	2.19	0.42
1:A:9:GLY:C	1:A:58:SER:HB2	2.41	0.41
1:A:126:THR:HG21	1:A:129:LEU:HD21	2.01	0.41
1:A:148:GLU:HB3	1:A:149:PRO:HD3	2.01	0.41
1:B:37:ASN:O	1:B:38:GLN:CB	2.69	0.41
1:B:64:ASN:ND2	1:A:68:MET:HG3	2.36	0.41
1:A:169:SER:HA	1:A:170:PRO:HD3	1.84	0.41
1:B:248:LEU:O	1:B:271:VAL:HA	2.20	0.41
1:B:266:PHE:O	1:B:286:LYS:HE2	2.21	0.41
1:A:123:HIS:HD2	1:A:141:PRO:HB2	1.85	0.41
1:B:33:LYS:HG2	1:B:41:CYS:CB	2.48	0.40
1:B:33:LYS:HE2	1:B:41:CYS:SG	2.62	0.40
1:B:152:LEU:HD11	1:B:184:ARG:HD2	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	300/326 (92%)	287 (96%)	13 (4%)	0	100	100
1	B	304/326 (93%)	290 (95%)	14 (5%)	0	100	100
All	All	604/652 (93%)	577 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	256/278 (92%)	241 (94%)	15 (6%)	19	14
1	B	259/278 (93%)	246 (95%)	13 (5%)	24	20
All	All	515/556 (93%)	487 (95%)	28 (5%)	22	17

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	ASN
1	B	4	ILE
1	B	5	LYS
1	B	15	LEU
1	B	57	GLN
1	B	60	CYS
1	B	62	GLU
1	B	78	LYS
1	B	203	ASP
1	B	204	ARG
1	B	249	THR
1	B	260	ARG
1	B	311	TYR
1	A	12	HIS

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Mol	Chain	Res	Type
1	A	15	LEU
1	A	43	GLU
1	A	57	GLN
1	A	62	GLU
1	A	111	LEU
1	A	152	LEU
1	A	186	ASN
1	A	195	GLU
1	A	204	ARG
1	A	248	LEU
1	A	249	THR
1	A	273	ASN
1	A	283	HIS
1	A	286	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	57	GLN
1	B	64	ASN
1	B	123	HIS
1	B	135	GLN
1	B	158	ASN
1	B	263	ASN
1	B	277	GLN
1	B	315	HIS
1	A	3	ASN
1	A	13	GLN
1	A	37	ASN
1	A	57	GLN
1	A	65	ASN
1	A	135	GLN
1	A	273	ASN
1	A	277	GLN
1	A	304	HIS

5.3.3 RNA ⓘ

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](#)

6 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	$\# Z > 2$
2	SO4	A	1001	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	B	402	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	A	1002	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	B	401	-	4,4,4	0.15	0	6,6,6	0.26	0
2	SO4	B	403	-	4,4,4	0.13	0	6,6,6	0.16	0
2	SO4	A	1003	-	4,4,4	0.14	0	6,6,6	0.15	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1003	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	304/326 (93%)	1.18	67 (22%) 0 0	22, 58, 96, 117	44 (14%)
1	B	307/326 (94%)	1.06	45 (14%) 2 3	25, 47, 78, 107	51 (16%)
All	All	611/652 (93%)	1.12	112 (18%) 1 1	22, 51, 90, 117	95 (15%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	SER	34.3
1	B	61	GLY	19.9
1	B	98	ASP	17.4
1	A	60	CYS	14.8
1	B	35	PHE	10.1
1	B	33	LYS	9.9
1	A	61	GLY	9.3
1	B	99	LYS	9.2
1	A	33	LYS	9.0
1	B	37	ASN	8.7
1	A	12	HIS	8.5
1	A	36	SER	8.3
1	B	204	ARG	7.9
1	A	62	GLU	7.8
1	A	59	GLY	6.9
1	B	38	GLN	6.8
1	B	203	ASP	6.6
1	A	283	HIS	6.5
1	B	60	CYS	6.4
1	B	62	GLU	6.4
1	B	57	GLN	6.3
1	A	282	LYS	6.2
1	B	32	THR	6.1
1	B	101	ASP	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	101	ASP	6.0
1	B	176	LYS	5.7
1	A	261	ILE	5.5
1	A	284	CYS	5.4
1	B	34	LYS	5.1
1	A	253	PHE	5.1
1	A	311	TYR	5.0
1	A	96	ARG	4.8
1	A	262	ASN	4.8
1	B	316	VAL	4.7
1	B	278	GLU	4.6
1	A	264	ALA	4.1
1	A	263	ASN	4.1
1	A	259	SER	4.0
1	A	194	LYS	4.0
1	B	229	ILE	3.9
1	B	139	ASP	3.9
1	A	229	ILE	3.8
1	A	265	CYS	3.8
1	A	35	PHE	3.7
1	B	58	SER	3.7
1	B	194	LYS	3.6
1	B	43	GLU	3.6
1	A	260	ARG	3.5
1	B	314	SER	3.4
1	A	58	SER	3.3
1	B	11	SER	3.3
1	A	308	SER	3.2
1	B	262	ASN	3.2
1	B	68	MET	3.2
1	A	34	LYS	3.1
1	A	274	THR	3.1
1	A	204	ARG	3.0
1	A	205	MET	3.0
1	A	41	CYS	3.0
1	A	31	VAL	3.0
1	A	277	GLN	3.0
1	B	317	PRO	2.9
1	A	252	ILE	2.9
1	B	10	SER	2.9
1	A	29	LYS	2.9
1	A	184	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	294	MET	2.8
1	A	285	SER	2.8
1	A	313	PHE	2.8
1	A	255	GLY	2.7
1	A	275	ILE	2.7
1	B	313	PHE	2.6
1	A	254	SER	2.6
1	A	188	ASP	2.6
1	B	51	GLU	2.6
1	B	41	CYS	2.6
1	A	248	LEU	2.6
1	A	212	LYS	2.5
1	A	279	ASP	2.5
1	A	231	HIS	2.5
1	A	258	ILE	2.5
1	B	102	LYS	2.5
1	A	122	ASP	2.5
1	A	268	ALA	2.5
1	A	203	ASP	2.5
1	A	32	THR	2.4
1	B	9	GLY	2.4
1	A	242	THR	2.4
1	A	280	LYS	2.4
1	B	146	TYR	2.4
1	A	286	LYS	2.4
1	B	210	ASP	2.3
1	A	267	GLU	2.3
1	A	251	GLY	2.3
1	B	5	LYS	2.3
1	A	241	ALA	2.3
1	B	279	ASP	2.3
1	A	230	CYS	2.3
1	A	281	MET	2.2
1	A	309	VAL	2.2
1	B	140	ILE	2.2
1	B	268	ALA	2.1
1	A	257	ALA	2.1
1	B	177	ARG	2.1
1	B	285	SER	2.1
1	A	245	TYR	2.1
1	A	102	LYS	2.1
1	B	265	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	11	SER	2.0
1	A	249	THR	2.0
1	A	26	GLU	2.0
1	B	97	GLN	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
2	SO4	A	1003	5/5	0.76	0.29	63,64,65,65	5
2	SO4	A	1002	5/5	0.89	0.14	101,101,101,101	5
2	SO4	B	403	5/5	0.92	0.16	65,65,66,66	5
2	SO4	B	402	5/5	0.95	0.07	78,79,80,80	0
2	SO4	B	401	5/5	0.98	0.10	48,49,49,50	0
2	SO4	A	1001	5/5	0.99	0.08	53,53,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.