



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:31 PM UTC

PDB ID : 4LZN / pdb_00004lzn
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

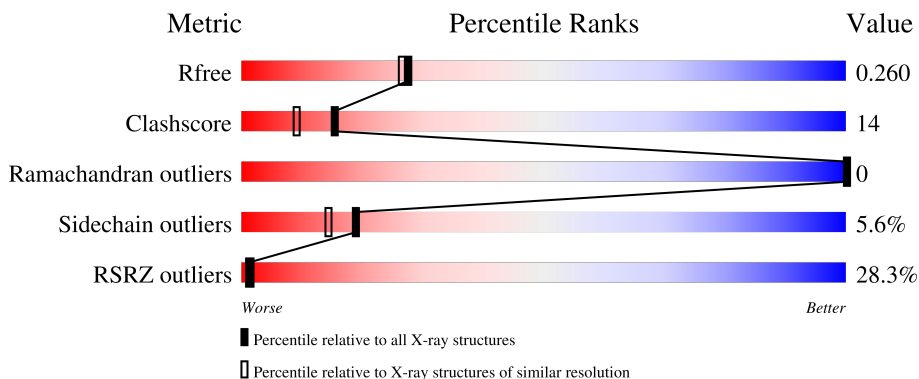
1 Overall quality at a glance

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}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (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	31% 67% 24% 7%
1	B	326	22% 71% 21% 6%

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 (CCD ID: 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		

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 0.221 , 0.260	Depositor DCC
R_{free} test set	1759 reflections (4.77%)	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)	0.32 , 41.8	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	0.48	0/2356	0.80	2/3185 (0.1%)
1	B	0.58	0/2382	0.95	10/3222 (0.3%)
All	All	0.53	0/4738	0.88	12/6407 (0.2%)

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 (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	60	CYS	N-CA-C	-14.81	94.79	113.16
1	B	12	HIS	N-CA-C	-10.82	88.95	107.99
1	B	9	GLY	N-CA-C	-8.56	97.92	112.30
1	B	63	ILE	N-CA-C	8.02	118.78	110.36
1	A	169	SER	CA-C-N	7.09	127.08	119.28
1	A	169	SER	C-N-CA	7.09	127.08	119.28
1	B	59	GLY	N-CA-C	6.74	129.15	113.18
1	B	60	CYS	N-CA-CB	6.63	120.58	110.44
1	B	11	SER	N-CA-C	6.17	123.94	110.80
1	B	311	TYR	N-CA-CB	-5.29	102.12	110.06
1	B	59	GLY	CA-C-N	-5.05	113.24	122.38
1	B	59	GLY	C-N-CA	-5.05	113.24	122.38

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	80	0
1	B	2349	0	2382	64	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	127	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 (127) 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:111:LEU:HG	1:B:115:MET:HE2	1.23	1.10
1:B:63:ILE:HD13	1:A:39:GLU:HG2	1.33	1.06
1:B:112:VAL:HA	1:B:115:MET:HE3	1.49	0.95
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:B:10:SER:C	1:B:58:SER:HG	1.83	0.86
1:A:96:ARG:HD2	1:A:222:MET:SD	2.14	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:A:273:ASN:H	1:A:273:ASN:HD22	1.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:SER:HB3	1:B:69:GLU:CD	2.07	0.77
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: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:A:22:ARG:HH11	1:A:294:MET:HE2	1.51	0.74
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: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:A:22:ARG:NH1	1:A:294:MET:HE2	2.12	0.64
1:B:33:LYS:HG2	1:B:41:CYS:HB3	1.80	0.63
1:A:298:GLU:CD	1:A:301:ARG:HH12	2.07	0.62
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: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:68:MET:HE1	1:A:115:MET:HE1	1.84	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: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: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:A:10:SER:HB3	1:A:69:GLU:CD	2.32	0.54
1:A:112:VAL:HA	1:A:115:MET:HE3	1.89	0.54
1:A:57:GLN:HE22	1:A:90:PRO:HD2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:9:GLY:C	1:B:58:SER:HB2	2.34	0.52
1:A:161:GLU:CD	1:A:243:ARG:HH21	2.17	0.52
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:B:115:MET:HE1	1:A:68:MET:HE1	1.90	0.52
1:B:221:ASP:O	1:B:249:THR:HG23	2.10	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: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:B:97:GLN:HB2	1:B:108:SER:HB2	1.96	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:291:ASP:O	1:B:294:MET:HE1	2.14	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:A:9:GLY:C	1:A:58:SER:HB2	2.41	0.46
1:B:63:ILE:HD12	1:A:39:GLU:N	2.31	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:B:111:LEU:HG	1:B:115:MET:CE	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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: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: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:112:VAL:CA	1:B:115:MET:HE3	2.34	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:294:MET:H	1:B:294:MET:HE3	1.86	0.40
1:B:152:LEU:HD11	1:B:184:ARG:HD2	2.04	0.40
1:A:298:GLU:CD	1:A:301:ARG:NH1	2.76	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%)	242 (94%)	14 (6%)	19	15
1	B	259/278 (93%)	244 (94%)	15 (6%)	18	13
All	All	515/556 (93%)	486 (94%)	29 (6%)	19	14

All (29) 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	42	VAL
1	B	57	GLN
1	B	60	CYS
1	B	62	GLU
1	B	104	ARG
1	B	203	ASP
1	B	204	ARG
1	B	248	LEU
1	B	249	THR
1	B	260	ARG
1	B	316	VAL

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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 (19) 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	158	ASN
1	A	193	HIS
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 oligosaccharides 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	B	401	-	4,4,4	0.23	0	6,6,6	0.28	0
2	SO4	B	403	-	4,4,4	0.23	0	6,6,6	0.18	0
2	SO4	A	1001	-	4,4,4	0.21	0	6,6,6	0.20	0
2	SO4	A	1003	-	4,4,4	0.25	0	6,6,6	0.15	0
2	SO4	B	402	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	A	1002	-	4,4,4	0.24	0	6,6,6	0.10	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%)	1.90	100 (32%)  	1, 55, 96, 117	44 (14%)
1	B	307/326 (94%)	1.75	73 (23%)  	1, 45, 72, 107	51 (16%)
All	All	611/652 (93%)	1.83	173 (28%)  	1, 48, 89, 117	95 (15%)

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	CYS	35.9
1	A	12	HIS	35.8
1	B	61	GLY	30.3
1	A	62	GLU	18.2
1	B	98	ASP	14.1
1	A	101	ASP	13.5
1	A	33	LYS	12.6
1	B	33	LYS	12.1
1	B	62	GLU	11.8
1	A	61	GLY	10.9
1	B	278	GLU	9.5
1	B	32	THR	9.0
1	A	36	SER	9.0
1	B	57	GLN	9.0
1	A	230	CYS	8.8
1	B	204	ARG	8.6
1	B	99	LYS	8.5
1	B	176	LYS	8.4
1	B	11	SER	8.3
1	A	60	CYS	7.5
1	B	317	PRO	7.4
1	A	204	ARG	7.1
1	A	278	GLU	6.7
1	B	35	PHE	6.3

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Mol	Chain	Res	Type	RSRZ
1	B	229	ILE	6.2
1	B	230	CYS	5.9
1	B	38	GLN	5.8
1	B	101	ASP	5.8
1	B	43	GLU	5.6
1	A	310	SER	5.6
1	A	96	ARG	5.3
1	A	203	ASP	5.2
1	A	309	VAL	4.9
1	B	36	SER	4.9
1	B	259	SER	4.7
1	A	32	THR	4.7
1	B	268	ALA	4.6
1	A	59	GLY	4.6
1	A	287	ILE	4.4
1	B	248	LEU	4.4
1	A	58	SER	4.2
1	A	102	LYS	4.2
1	A	29	LYS	4.1
1	A	43	GLU	4.1
1	A	311	TYR	4.1
1	A	261	ILE	4.1
1	B	311	TYR	4.1
1	B	9	GLY	4.0
1	A	194	LYS	4.0
1	A	11	SER	4.0
1	B	152	LEU	4.0
1	B	103	SER	4.0
1	B	314	SER	4.0
1	B	5	LYS	4.0
1	A	229	ILE	3.8
1	A	95	ALA	3.8
1	A	267	GLU	3.8
1	A	41	CYS	3.8
1	A	245	TYR	3.7
1	A	253	PHE	3.7
1	B	265	CYS	3.7
1	A	31	VAL	3.7
1	B	315	HIS	3.6
1	A	252	ILE	3.6
1	B	37	ASN	3.6
1	A	250	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	313	PHE	3.6
1	A	262	ASN	3.6
1	A	26	GLU	3.6
1	A	219	VAL	3.6
1	A	248	LEU	3.6
1	B	146	TYR	3.6
1	A	251	GLY	3.5
1	A	162	TRP	3.5
1	A	149	PRO	3.5
1	A	255	GLY	3.5
1	A	308	SER	3.5
1	A	35	PHE	3.4
1	A	239	ALA	3.4
1	A	257	ALA	3.4
1	A	307	GLU	3.4
1	A	188	ASP	3.4
1	B	262	ASN	3.3
1	B	58	SER	3.3
1	B	194	LYS	3.3
1	A	212	LYS	3.3
1	B	51	GLU	3.2
1	B	3	ASN	3.2
1	A	241	ALA	3.2
1	A	259	SER	3.2
1	A	205	MET	3.2
1	A	249	THR	3.2
1	B	203	ASP	3.1
1	B	157	GLU	3.1
1	B	282	LYS	3.1
1	B	41	CYS	3.1
1	A	240	GLY	3.0
1	B	231	HIS	3.0
1	A	282	LYS	3.0
1	A	268	ALA	3.0
1	A	97	GLN	3.0
1	B	68	MET	3.0
1	A	153	LYS	3.0
1	B	206	VAL	3.0
1	B	207	LEU	3.0
1	A	42	VAL	2.9
1	A	290	ILE	2.9
1	A	283	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	166	THR	2.9
1	B	90	PRO	2.9
1	B	316	VAL	2.9
1	B	83	SER	2.9
1	B	14	ASP	2.8
1	B	39	GLU	2.8
1	B	294	MET	2.8
1	A	294	MET	2.8
1	B	139	ASP	2.8
1	B	263	ASN	2.7
1	A	134	ILE	2.7
1	A	264	ALA	2.7
1	A	182	ALA	2.6
1	A	187	VAL	2.6
1	A	233	ALA	2.6
1	A	234	ASP	2.6
1	B	177	ARG	2.6
1	A	258	ILE	2.6
1	A	232	ALA	2.6
1	A	213	ASP	2.6
1	B	191	LEU	2.5
1	A	293	SER	2.5
1	B	162	TRP	2.5
1	B	34	LYS	2.5
1	B	187	VAL	2.5
1	B	254	SER	2.5
1	B	53	VAL	2.4
1	A	215	VAL	2.4
1	B	279	ASP	2.4
1	A	265	CYS	2.4
1	A	178	VAL	2.4
1	B	257	ALA	2.4
1	A	223	ALA	2.4
1	B	6	ILE	2.4
1	A	146	TYR	2.3
1	B	72	ILE	2.3
1	A	274	THR	2.3
1	B	264	ALA	2.3
1	A	210	ASP	2.3
1	A	45	GLY	2.3
1	A	254	SER	2.2
1	A	313	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	192	ILE	2.2
1	A	218	LEU	2.2
1	A	244	VAL	2.2
1	A	209	GLY	2.2
1	A	237	LEU	2.2
1	A	286	LYS	2.2
1	A	279	ASP	2.2
1	A	289	VAL	2.1
1	B	12	HIS	2.1
1	A	184	ARG	2.1
1	B	95	ALA	2.1
1	A	132	SER	2.1
1	A	177	ARG	2.1
1	B	10	SER	2.1
1	A	130	HIS	2.1
1	A	9	GLY	2.1
1	B	147	ALA	2.0
1	A	175	ALA	2.0
1	A	186	ASN	2.0
1	B	213	ASP	2.0
1	A	243	ARG	2.0
1	A	284	CYS	2.0
1	B	255	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 oligosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1003	5/5	0.68	0.14	63,64,65,65	5
2	SO4	B	403	5/5	0.75	0.14	65,65,66,66	5
2	SO4	A	1002	5/5	0.76	0.14	101,101,101,101	5
2	SO4	B	402	5/5	0.87	0.10	78,79,80,80	0
2	SO4	A	1001	5/5	0.96	0.09	53,53,54,54	0
2	SO4	B	401	5/5	0.97	0.07	48,49,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.