



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 06:20 AM EDT

PDB ID : 4LYG  
Title : Crystal structure of human PRS1 E43T mutant  
Authors : Chen, P.; Teng, M.; Li, X.  
Deposited on : 2013-07-31  
Resolution : 3.00 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

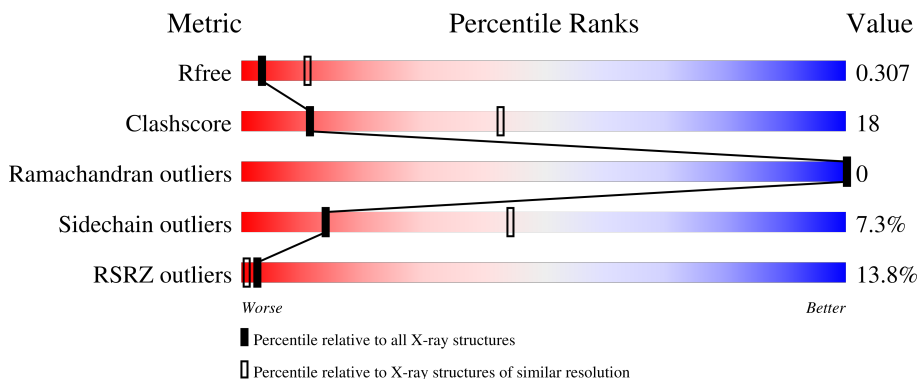
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	
1	B	326	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1002	-	-	X	-
2	SO4	B	403	-	-	X	-

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4719 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
			Total	C	N	O	S			
1	A	304	2321	1457	408	439	17	0	0	0
1	B	310	2373	1488	420	448	17	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	THR	GLU	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
B	43	THR	GLU	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

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

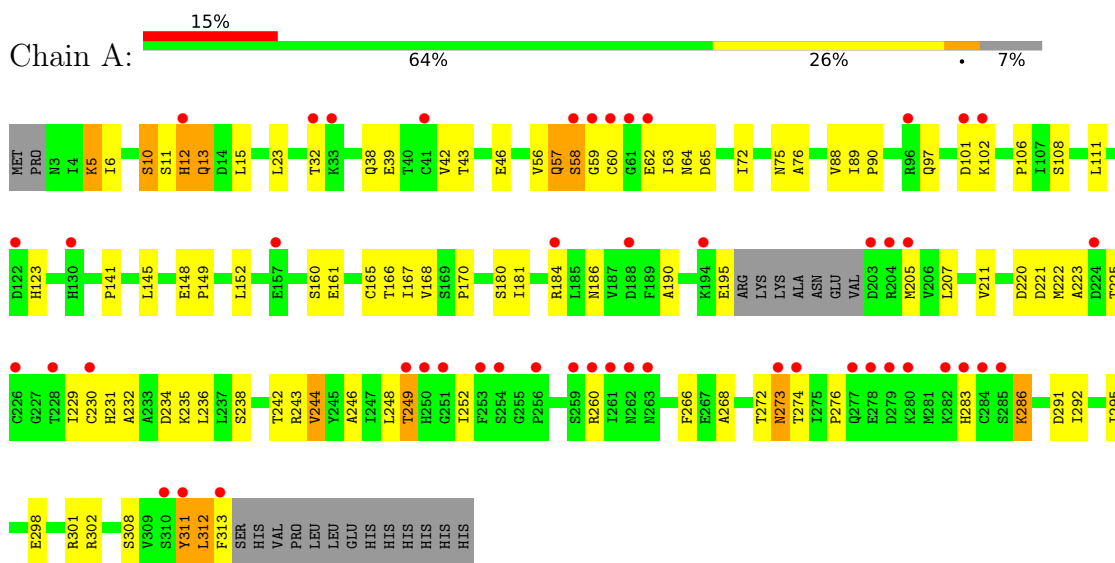


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

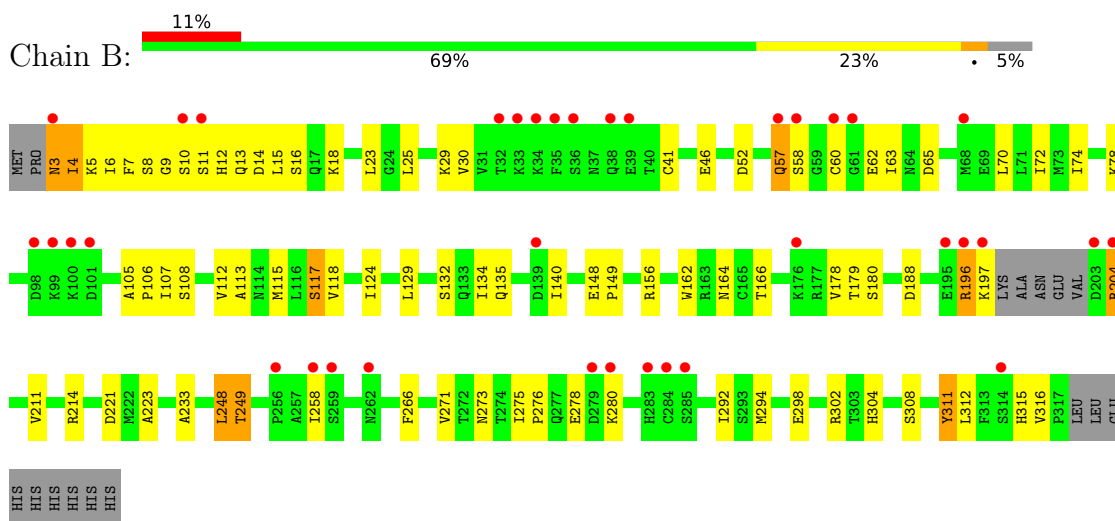
### 3 Residue-property plots i

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 i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.50Å 169.50Å 61.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.93 – 3.00 48.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.93-3.00) 98.5 (48.93-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.253 , 0.298 0.267 , 0.307	Depositor DCC
$R_{free}$ test set	652 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.9	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.914 for H, K, L 0.086 for K, H, -L	Depositor
Outliers	0 of 13109 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	4719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.53	0/2353	0.73	5/3182 (0.2%)
1	B	0.53	0/2407	0.68	0/3254
All	All	0.53	0/4760	0.71	5/6436 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	GLY	N-CA-C	9.81	137.62	113.10
1	A	58	SER	CB-CA-C	-9.22	92.59	110.10
1	A	10	SER	CB-CA-C	-5.27	100.08	110.10
1	A	12	HIS	N-CA-C	-5.25	96.83	111.00
1	A	312	LEU	CB-CA-C	5.04	119.78	110.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2321	0	2355	77	0
1	B	2373	0	2415	91	0
2	A	10	0	0	7	0
2	B	15	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4719	0	4770	162	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 18.

All (162) 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:10:SER:H	1:A:58:SER:CB	1.52	1.22
1:A:311:TYR:C	1:A:311:TYR:CD1	2.09	1.21
1:B:196:ARG:HD2	1:B:196:ARG:C	1.60	1.14
1:B:311:TYR:CZ	1:B:315:HIS:CD2	2.35	1.13
1:A:311:TYR:HD1	1:A:312:LEU:N	1.48	1.12
1:B:196:ARG:HH11	1:B:196:ARG:CG	1.59	1.11
1:B:204:ARG:HH11	1:B:204:ARG:HG3	1.07	1.09
1:B:311:TYR:CZ	1:B:315:HIS:HD2	1.69	1.08
1:B:196:ARG:HD2	1:B:196:ARG:O	1.52	1.07
1:B:196:ARG:HG3	1:B:196:ARG:NH1	1.56	1.06
1:B:311:TYR:CE2	1:B:315:HIS:CD2	2.46	1.04
1:B:12:HIS:CD2	1:B:60:CYS:HA	1.91	1.04
1:B:204:ARG:HH11	1:B:204:ARG:CG	1.72	1.03
1:A:311:TYR:C	1:A:311:TYR:HD1	1.54	0.98
1:A:311:TYR:HD1	1:A:312:LEU:CA	1.79	0.96
1:B:311:TYR:OH	1:B:315:HIS:CD2	2.19	0.95
1:A:311:TYR:CD1	1:A:312:LEU:N	2.35	0.91
1:B:311:TYR:OH	1:B:315:HIS:NE2	2.06	0.88
1:A:10:SER:N	1:A:58:SER:CB	2.36	0.88
1:B:196:ARG:C	1:B:196:ARG:CD	2.34	0.87
1:A:225:THR:N	2:A:1002:SO4:O3	2.08	0.86
1:B:12:HIS:NE2	1:B:60:CYS:HA	1.90	0.85
1:A:311:TYR:CD1	1:A:311:TYR:O	2.30	0.85
1:B:196:ARG:HH11	1:B:196:ARG:HG3	0.73	0.84
1:B:204:ARG:HG3	1:B:204:ARG:NH1	1.89	0.83
1:B:196:ARG:HD3	1:B:197:LYS:C	2.00	0.82
1:A:273:ASN:H	1:A:273:ASN:HD22	1.24	0.82
1:A:311:TYR:CD1	1:A:312:LEU:CA	2.63	0.81
1:A:12:HIS:CD2	1:A:276:PRO:HG3	2.17	0.80
1:A:229:ILE:HD12	1:A:248:LEU:HD21	1.64	0.79
1:A:32:THR:HG22	1:A:42:VAL:HG22	1.65	0.79
1:A:311:TYR:CD1	1:A:312:LEU:HA	2.21	0.76
1:B:10:SER:OG	1:B:11:SER:N	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:TYR:CD2	1:B:311:TYR:O	2.42	0.72
1:B:196:ARG:CG	1:B:196:ARG:NH1	2.29	0.70
1:B:311:TYR:CD2	1:B:311:TYR:C	2.65	0.70
1:B:197:LYS:O	1:B:197:LYS:HG3	1.90	0.69
1:B:278:GLU:H	1:B:278:GLU:CD	1.95	0.69
1:B:223:ALA:HB2	1:B:248:LEU:HG	1.73	0.69
1:A:205:MET:O	1:A:235:LYS:HE3	1.93	0.69
1:B:204:ARG:CG	1:B:204:ARG:NH1	2.42	0.68
1:B:4:ILE:HG23	1:B:25:LEU:HD11	1.77	0.67
1:A:273:ASN:HD21	1:A:292:ILE:H	1.42	0.67
1:A:231:HIS:O	1:A:234:ASP:HB2	1.96	0.65
1:B:221:ASP:O	1:B:249:THR:HG23	1.98	0.64
1:B:12:HIS:CD2	1:B:60:CYS:CA	2.75	0.63
1:B:223:ALA:CB	1:B:248:LEU:HG	2.30	0.62
1:B:298:GLU:HG2	1:B:312:LEU:HD21	1.82	0.61
1:B:204:ARG:NH1	1:B:204:ARG:CB	2.64	0.61
1:B:57:GLN:O	1:B:57:GLN:HG3	2.02	0.60
1:B:311:TYR:C	1:B:311:TYR:HD2	2.06	0.59
1:B:196:ARG:HG2	1:B:197:LYS:N	2.16	0.59
1:B:166:THR:HG21	1:B:211:VAL:HG12	1.84	0.59
1:B:204:ARG:HH11	1:B:204:ARG:CB	2.16	0.59
1:A:72:ILE:HG23	1:B:106:PRO:HG3	1.85	0.59
1:B:196:ARG:CG	1:B:197:LYS:N	2.64	0.59
1:B:156:ARG:HA	1:B:162:TRP:CD1	2.38	0.58
1:B:135:GLN:NE2	2:B:403:SO4:O1	2.35	0.58
1:A:221:ASP:HA	1:A:249:THR:HG23	1.85	0.58
1:A:225:THR:CB	2:A:1002:SO4:O3	2.51	0.58
1:B:196:ARG:CD	1:B:197:LYS:C	2.71	0.58
1:A:225:THR:OG1	2:A:1002:SO4:O3	2.20	0.58
1:A:232:ALA:O	1:A:236:LEU:HG	2.05	0.56
1:A:223:ALA:HB2	1:A:248:LEU:HD22	1.87	0.56
1:A:273:ASN:HD22	1:A:273:ASN:N	1.98	0.56
1:A:273:ASN:ND2	1:A:291:ASP:HA	2.20	0.56
1:A:97:GLN:HB2	1:A:108:SER:HB2	1.87	0.56
1:B:6:ILE:HD11	1:B:23:LEU:CD1	2.36	0.55
1:B:204:ARG:NH1	1:B:204:ARG:HB3	2.21	0.55
1:B:196:ARG:CD	1:B:197:LYS:N	2.69	0.55
1:B:7:PHE:HD2	1:B:30:VAL:CG2	2.21	0.54
1:A:242:THR:HG22	1:A:243:ARG:HG3	1.89	0.54
1:B:258:ILE:HD11	1:B:280:LYS:HB3	1.89	0.54
1:A:57:GLN:O	1:A:57:GLN:NE2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASN:HD21	1:A:291:ASP:HA	1.73	0.52
1:B:273:ASN:OD1	1:B:292:ILE:HG13	2.09	0.52
1:B:311:TYR:CE2	1:B:315:HIS:HD2	1.98	0.52
1:A:161:GLU:OE1	1:A:243:ARG:NH2	2.43	0.52
1:A:39:GLU:HG2	1:B:63:ILE:HD13	1.92	0.52
1:B:4:ILE:CG2	1:B:25:LEU:HD11	2.40	0.52
1:A:62:GLU:HB3	1:A:65:ASP:HB2	1.92	0.51
1:B:52:ASP:OD2	1:B:304:HIS:ND1	2.37	0.51
1:B:311:TYR:HH	1:B:315:HIS:CD2	2.18	0.51
1:A:230:CYS:SG	1:A:260:ARG:HB3	2.51	0.51
1:B:113:ALA:O	1:B:117:SER:OG	2.29	0.51
1:A:170:PRO:HG2	1:A:220:ASP:HB2	1.93	0.51
1:A:225:THR:HG23	2:A:1002:SO4:O3	2.11	0.50
1:A:311:TYR:CE1	1:A:312:LEU:HA	2.46	0.50
1:A:11:SER:O	1:A:12:HIS:C	2.47	0.50
1:B:148:GLU:HB3	1:B:149:PRO:HD3	1.94	0.50
1:A:64:ASN:HD22	1:B:65:ASP:HA	1.77	0.49
1:B:8:SER:HB2	1:B:16:SER:HB3	1.95	0.49
1:A:220:ASP:HB3	1:A:248:LEU:HD23	1.93	0.49
1:B:108:SER:O	1:B:112:VAL:HG23	2.13	0.49
1:A:5:LYS:HE3	1:A:46:GLU:OE1	2.13	0.49
1:A:148:GLU:HB3	1:A:149:PRO:HD3	1.94	0.49
1:B:129:LEU:HD13	1:B:134:ILE:HB	1.95	0.49
1:B:8:SER:HB2	1:B:16:SER:CB	2.43	0.49
1:A:168:VAL:HG22	1:A:190:ALA:HB3	1.94	0.48
1:A:63:ILE:HG23	1:A:64:ASN:N	2.28	0.48
1:B:9:GLY:O	1:B:58:SER:HB2	2.14	0.48
1:A:123:HIS:HD2	1:A:141:PRO:HB2	1.78	0.48
1:A:145:LEU:HD13	1:A:295:ILE:HG22	1.94	0.48
1:B:188:ASP:OD2	1:B:214:ARG:NH2	2.47	0.48
1:A:302:ARG:HD3	1:A:308:SER:O	2.14	0.48
1:B:3:ASN:HB3	1:B:304:HIS:CE1	2.49	0.48
1:A:11:SER:O	1:A:13:GLN:N	2.47	0.47
1:B:70:LEU:O	1:B:74:ILE:HG13	2.14	0.47
1:B:6:ILE:HD11	1:B:23:LEU:HD12	1.95	0.47
1:A:89:ILE:O	1:A:90:PRO:C	2.53	0.47
1:A:6:ILE:HD11	1:A:23:LEU:HD12	1.97	0.47
1:A:207:LEU:C	1:A:207:LEU:HD23	2.35	0.46
1:A:244:VAL:O	1:A:266:PHE:HA	2.15	0.46
1:B:204:ARG:HB3	1:B:204:ARG:CZ	2.46	0.46
1:B:105:ALA:HB1	1:B:106:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ALA:HB2	1:B:266:PHE:CE2	2.51	0.46
1:A:13:GLN:HE21	1:A:13:GLN:HB3	1.52	0.46
1:B:132:SER:HB3	2:B:403:SO4:O4	2.15	0.45
1:B:178:VAL:HG23	1:B:179:THR:N	2.31	0.45
1:A:225:THR:CA	2:A:1002:SO4:O3	2.63	0.45
1:A:268:ALA:HA	1:A:286:LYS:HB2	1.99	0.44
1:A:308:SER:OG	2:A:1001:SO4:O3	2.21	0.44
1:B:298:GLU:O	1:B:302:ARG:HG2	2.18	0.44
1:A:6:ILE:HD11	1:A:23:LEU:CD1	2.47	0.44
1:B:302:ARG:HD2	1:B:308:SER:O	2.18	0.44
1:A:221:ASP:HA	1:A:249:THR:CG2	2.46	0.44
1:A:166:THR:HG21	1:A:211:VAL:HG12	2.00	0.44
1:A:56:VAL:HA	1:A:88:VAL:HB	1.99	0.44
1:A:101:ASP:O	1:A:102:LYS:HB2	2.18	0.44
1:B:248:LEU:HB2	1:B:271:VAL:HG12	2.00	0.43
1:A:298:GLU:CD	1:A:301:ARG:HH12	2.21	0.43
1:B:29:LYS:HG3	1:B:46:GLU:OE2	2.18	0.43
1:A:75:ASN:O	1:A:76:ALA:C	2.57	0.43
1:B:3:ASN:HB3	1:B:304:HIS:HE1	1.82	0.43
1:B:6:ILE:CD1	1:B:23:LEU:HD12	2.49	0.43
1:A:273:ASN:H	1:A:273:ASN:ND2	2.03	0.43
1:B:8:SER:OG	1:B:13:GLN:HG2	2.18	0.43
1:B:311:TYR:O	1:B:315:HIS:HB3	2.19	0.43
1:B:166:THR:OG1	1:B:214:ARG:HD3	2.19	0.43
1:A:106:PRO:HG3	1:B:72:ILE:HG23	2.01	0.43
1:B:107:ILE:HG22	1:B:107:ILE:O	2.19	0.42
1:B:196:ARG:NH1	1:B:196:ARG:CB	2.81	0.42
1:A:10:SER:C	1:A:12:HIS:N	2.71	0.42
1:A:272:THR:OG1	1:A:274:THR:HG23	2.19	0.42
1:A:42:VAL:CG1	1:A:43:THR:N	2.82	0.42
1:A:167:ILE:HG13	1:A:181:ILE:HG22	2.02	0.42
1:B:7:PHE:HD2	1:B:30:VAL:HG23	1.85	0.42
1:A:64:ASN:ND2	1:B:65:ASP:HA	2.35	0.42
1:A:313:PHE:N	1:A:313:PHE:CD2	2.88	0.41
1:A:57:GLN:HE21	1:A:57:GLN:C	2.16	0.41
1:B:112:VAL:HA	1:B:115:MET:HE2	2.02	0.41
1:A:180:SER:O	1:A:184:ARG:HD3	2.22	0.41
1:B:14:ASP:OD2	1:B:18:LYS:HE3	2.21	0.41
1:B:124:ILE:HG12	1:B:140:ILE:HD11	2.03	0.40
1:B:164:ASN:O	1:B:214:ARG:NH1	2.55	0.40
1:A:38:GLN:HB2	1:B:63:ILE:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:VAL:HG11	1:A:236:LEU:HD21	2.04	0.40
1:A:229:ILE:HD11	1:A:246:ALA:HB1	2.04	0.40
1:B:311:TYR:O	1:B:311:TYR:HD2	1.94	0.40
1:A:225:THR:CG2	2:A:1002:SO4:O3	2.69	0.40
1:B:57:GLN:HE21	1:B:57:GLN:HB2	1.61	0.40
1:B:275:ILE:HG23	1:B:276:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/326 (92%)	280 (93%)	20 (7%)	0	100	100
1	B	306/326 (94%)	283 (92%)	23 (8%)	0	100	100
All	All	606/652 (93%)	563 (93%)	43 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	255/278 (92%)	235 (92%)	20 (8%)	12	42
1	B	263/278 (95%)	245 (93%)	18 (7%)	16	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	518/556 (93%)	480 (93%)	38 (7%)	14 44

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	13	GLN
1	A	15	LEU
1	A	57	GLN
1	A	60	CYS
1	A	111	LEU
1	A	152	LEU
1	A	160	SER
1	A	165	CYS
1	A	186	ASN
1	A	195	GLU
1	A	222	MET
1	A	238	SER
1	A	244	VAL
1	A	249	THR
1	A	252	ILE
1	A	273	ASN
1	A	283	HIS
1	A	286	LYS
1	A	311	TYR
1	B	3	ASN
1	B	4	ILE
1	B	5	LYS
1	B	15	LEU
1	B	41	CYS
1	B	57	GLN
1	B	62	GLU
1	B	78	LYS
1	B	117	SER
1	B	118	VAL
1	B	180	SER
1	B	196	ARG
1	B	204	ARG
1	B	248	LEU
1	B	249	THR
1	B	294	MET
1	B	311	TYR

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Mol	Chain	Res	Type
1	B	316	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	13	GLN
1	A	158	ASN
1	A	273	ASN
1	B	57	GLN
1	B	64	ASN
1	B	66	ASN
1	B	186	ASN
1	B	263	ASN
1	B	277	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](#)

5 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	402	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	A	1002	-	4,4,4	0.27	0	6,6,6	0.28	0
2	SO4	A	1001	-	4,4,4	0.18	0	6,6,6	0.34	0
2	SO4	B	401	-	4,4,4	0.16	0	6,6,6	0.61	0
2	SO4	B	403	-	4,4,4	0.16	0	6,6,6	0.26	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.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	SO4	6	0
2	A	1001	SO4	1	0
2	B	403	SO4	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	304/326 (93%)	0.67	49 (16%) <b>1</b> <b>0</b>	22, 44, 59, 65	51 (16%)
1	B	310/326 (95%)	0.51	36 (11%) <b>4</b> <b>1</b>	19, 39, 56, 62	54 (17%)
All	All	614/652 (94%)	0.59	85 (13%) <b>2</b> <b>1</b>	19, 41, 57, 65	105 (17%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	ARG	16.6
1	A	279	ASP	13.8
1	B	197	LYS	12.0
1	A	203	ASP	10.5
1	A	61	GLY	8.9
1	A	311	TYR	8.7
1	A	204	ARG	8.6
1	B	38	GLN	7.3
1	A	283	HIS	7.2
1	B	33	LYS	7.0
1	B	98	ASP	6.6
1	A	310	SER	6.2
1	B	57	GLN	6.2
1	B	61	GLY	5.5
1	A	278	GLU	5.2
1	B	11	SER	5.1
1	B	99	LYS	5.1
1	A	284	CYS	5.0
1	B	101	ASP	4.6
1	A	41	CYS	4.5
1	A	60	CYS	4.4
1	B	100	LYS	4.3
1	A	12	HIS	4.2
1	B	10	SER	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	250	HIS	4.1
1	B	34	LYS	4.1
1	A	259	SER	4.0
1	B	36	SER	3.9
1	A	62	GLU	3.9
1	B	262	ASN	3.8
1	B	3	ASN	3.8
1	B	68	MET	3.8
1	A	263	ASN	3.8
1	A	249	THR	3.7
1	B	139	ASP	3.6
1	B	259	SER	3.5
1	B	279	ASP	3.5
1	B	58	SER	3.5
1	A	101	ASP	3.5
1	A	285	SER	3.4
1	B	203	ASP	3.4
1	A	33	LYS	3.4
1	B	204	ARG	3.4
1	A	277	GLN	3.4
1	A	261	ILE	3.3
1	A	96	ARG	3.3
1	B	285	SER	3.2
1	A	256	PRO	3.2
1	A	251	GLY	3.1
1	A	130	HIS	3.1
1	A	262	ASN	3.1
1	A	205	MET	3.0
1	B	280	LYS	3.0
1	A	313	PHE	2.9
1	A	282	LYS	2.9
1	A	254	SER	2.8
1	B	60	CYS	2.8
1	B	39	GLU	2.8
1	B	195	GLU	2.7
1	B	283	HIS	2.7
1	A	260	ARG	2.6
1	A	280	LYS	2.6
1	A	253	PHE	2.6
1	B	35	PHE	2.6
1	A	102	LYS	2.5
1	A	122	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	32	THR	2.4
1	B	256	PRO	2.4
1	B	32	THR	2.4
1	A	228	THR	2.4
1	A	188	ASP	2.3
1	A	58	SER	2.3
1	A	230	CYS	2.3
1	A	157	GLU	2.3
1	A	273	ASN	2.2
1	A	194	LYS	2.1
1	B	314	SER	2.1
1	A	224	ASP	2.1
1	A	226	CYS	2.1
1	B	176	LYS	2.1
1	A	59	GLY	2.1
1	B	258	ILE	2.0
1	B	284	CYS	2.0
1	A	274	THR	2.0
1	A	184	ARG	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	B	403	5/5	0.73	0.39	54,54,55,56	5
2	SO4	B	402	5/5	0.81	0.20	90,90,90,91	0
2	SO4	A	1002	5/5	0.82	0.21	87,87,87,87	5
2	SO4	B	401	5/5	0.97	0.17	27,29,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	1001	5/5	0.98	0.11	27,29,29,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.