Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 04:34 PM EDT

PDB ID	:	3S5J
Title	:	2.0A Crystal structure of human phosphoribosyl pyrophosphate synthetase 1
Authors	:	Chen, P.; Teng, M.; Li, X.
Deposited on	:	2011-05-23
Resolution	:	2.02 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 (i) 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 (i)) were used in the production of this report:

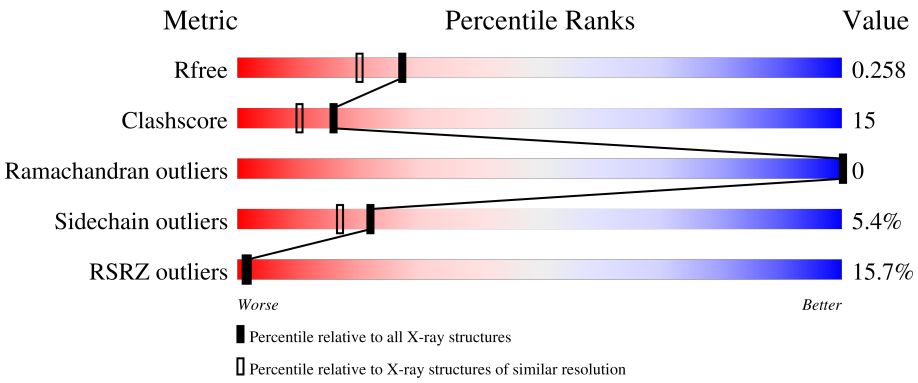
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 >=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 <=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	15% 66% 25% • 7%
1	B	326	14% 75% 17% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4888 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.

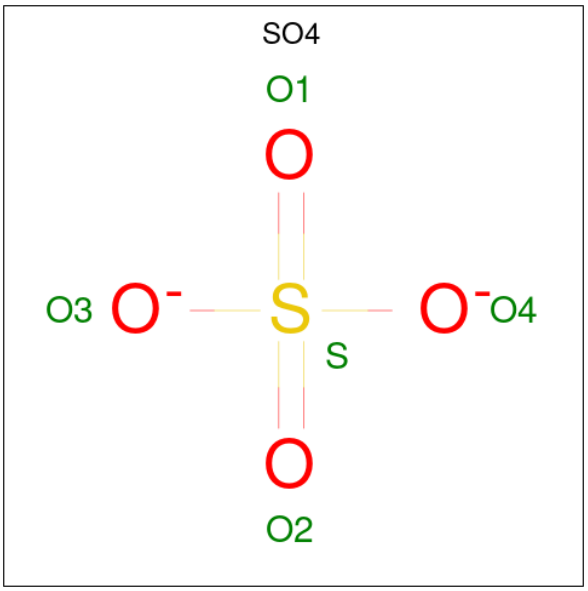
- Molecule 1 is a protein called Ribose-phosphate pyrophosphokinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	308	2355	1477	414	447	17	0	0	0
1	A	304	2325	1458	408	442	17	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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: O_4S).



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

- Molecule 3 is water.

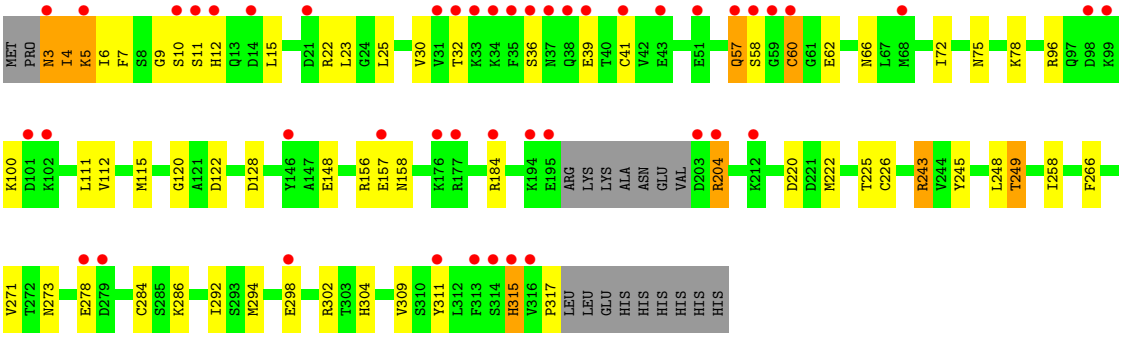
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	106	Total O 106 106	0	0
3	A	72	Total O 72 72	0	0

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.

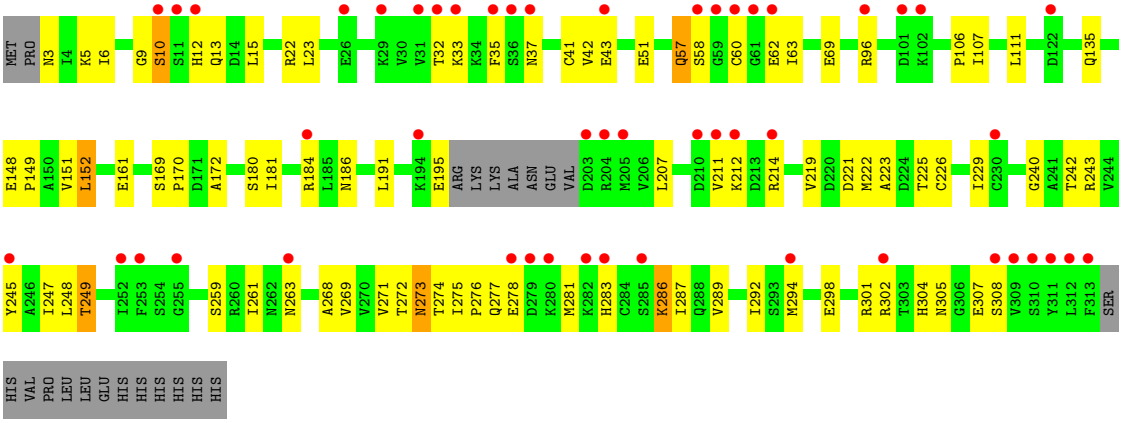
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain B:



• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	170.54Å 170.54Å 61.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.23 – 2.02 49.23 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.23-2.02) 99.8 (49.23-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.215 , 0.256 0.214 , 0.258	Depositor DCC
R_{free} test set	2205 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 29.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.095 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4888	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.34	0/2357	0.58	2/3186 (0.1%)
1	B	0.41	0/2389	0.58	1/3231 (0.0%)
All	All	0.38	0/4746	0.58	3/6417 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	SER	N-CA-C	9.03	135.38	111.00
1	A	10	SER	CB-CA-C	-8.12	94.66	110.10
1	B	243	ARG	NE-CZ-NH1	-5.23	117.68	120.30

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	2325	0	2360	76	0
1	B	2355	0	2388	64	0
2	A	15	0	0	1	0
2	B	15	0	0	0	0
3	A	72	0	0	5	0
3	B	106	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4888	0	4748	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 15.

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:A:32:THR:HG22	1:A:42:VAL:HG22	1.47	0.97
1:A:3:ASN:HD22	1:A:304:HIS:HE1	1.03	0.96
1:A:12:HIS:CD2	1:A:276:PRO:HG3	2.00	0.95
1:A:3:ASN:HD22	1:A:304:HIS:CE1	1.87	0.93
1:A:273:ASN:HD21	1:A:292:ILE:H	1.23	0.84
1:A:3:ASN:ND2	1:A:304:HIS:HE1	1.78	0.82
1:A:35:PHE:CZ	1:A:41:CYS:HB2	2.16	0.79
1:A:242:THR:HG22	1:A:243:ARG:HG3	1.64	0.79
1:B:3:ASN:HB3	1:B:304:HIS:HE1	1.50	0.76
1:B:204:ARG:HH11	1:B:204:ARG:HG3	1.50	0.76
1:B:6:ILE:HD11	1:B:23:LEU:HD12	1.69	0.75
1:A:12:HIS:HD2	1:A:276:PRO:HG3	1.51	0.73
1:B:111:LEU:HG	1:B:115:MET:CE	2.19	0.72
1:B:12:HIS:CD2	1:B:60:CYS:HA	2.25	0.71
1:A:298:GLU:CD	1:A:301:ARG:HH12	1.94	0.71
1:B:243:ARG:NH1	1:B:245:TYR:OH	2.23	0.69
1:B:278:GLU:H	1:B:278:GLU:CD	1.96	0.69
1:A:273:ASN:H	1:A:273:ASN:HD22	1.40	0.67
1:A:96:ARG:HD2	1:A:222:MET:SD	2.36	0.66
1:A:261:ILE:HG22	1:A:286:LYS:HD2	1.76	0.66
1:A:248:LEU:HB2	1:A:271:VAL:HG12	1.78	0.66
1:B:298:GLU:O	1:B:302:ARG:HG2	1.98	0.64
1:B:111:LEU:HG	1:B:115:MET:HE1	1.80	0.63
1:A:57:GLN:C	1:A:57:GLN:HE21	2.00	0.63
1:A:148:GLU:HB3	1:A:149:PRO:HD3	1.82	0.61
1:A:221:ASP:O	1:A:249:THR:HG23	2.00	0.61
1:A:229:ILE:HD13	1:A:248:LEU:HD21	1.82	0.61
1:B:204:ARG:HH11	1:B:204:ARG:CG	2.13	0.61
1:B:258:ILE:HG23	1:B:284:CYS:HB2	1.81	0.60
1:A:35:PHE:CE1	1:A:41:CYS:HB2	2.35	0.60
1:A:10:SER:N	1:A:69:GLU:OE1	2.31	0.60
1:B:6:ILE:HD11	1:B:23:LEU:CD1	2.33	0.58
1:A:302:ARG:HD3	1:A:308:SER:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLU:HG2	1:A:63:ILE:HD13	1.84	0.58
1:A:172:ALA:HA	1:A:191:LEU:HD11	1.84	0.58
1:A:273:ASN:HD22	1:A:273:ASN:N	2.00	0.58
1:B:78:LYS:HE2	1:B:120:GLY:O	2.03	0.58
1:B:3:ASN:HB3	1:B:304:HIS:CE1	2.33	0.58
1:B:39:GLU:HG2	1:A:63:ILE:CD1	2.33	0.57
1:B:111:LEU:HG	1:B:115:MET:HE2	1.86	0.57
1:A:298:GLU:OE1	1:A:301:ARG:NH1	2.37	0.57
1:A:261:ILE:CG2	1:A:286:LYS:HD2	2.35	0.57
1:A:278:GLU:CD	1:A:278:GLU:H	2.08	0.57
1:A:58:SER:HA	3:A:3078:HOH:O	2.05	0.57
1:A:307:GLU:HG3	1:A:308:SER:N	2.20	0.56
1:A:6:ILE:HD11	1:A:23:LEU:HD12	1.85	0.56
1:A:248:LEU:O	1:A:271:VAL:HA	2.05	0.56
1:B:184:ARG:HG3	1:B:184:ARG:HH11	1.71	0.56
1:A:211:VAL:O	1:A:214:ARG:HG2	2.06	0.56
1:A:6:ILE:HD11	1:A:23:LEU:CD1	2.36	0.55
1:A:259:SER:O	1:A:263:ASN:HB2	2.06	0.55
1:A:57:GLN:HG3	3:A:3037:HOH:O	2.05	0.55
1:B:157:GLU:HG3	1:B:158:ASN:ND2	2.22	0.54
1:A:272:THR:OG1	1:A:274:THR:HG23	2.05	0.54
1:B:57:GLN:O	1:B:57:GLN:HG3	2.06	0.54
1:A:243:ARG:NH1	1:A:245:TYR:OH	2.36	0.54
1:B:10:SER:OG	1:B:11:SER:N	2.40	0.54
1:B:112:VAL:HA	1:B:115:MET:CE	2.37	0.54
1:B:156:ARG:HD2	3:B:3048:HOH:O	2.08	0.54
1:A:181:ILE:HD12	1:A:219:VAL:HG11	1.90	0.54
1:B:4:ILE:HG23	1:B:25:LEU:HD11	1.89	0.53
1:A:152:LEU:HD11	1:A:181:ILE:HG23	1.91	0.53
1:A:273:ASN:ND2	1:A:292:ILE:H	2.00	0.53
1:A:180:SER:O	1:A:184:ARG:HD3	2.09	0.53
1:A:3:ASN:N	3:A:3165:HOH:O	2.42	0.52
1:B:4:ILE:HD13	1:B:5:LYS:N	2.25	0.52
1:B:6:ILE:CD1	1:B:23:LEU:HD12	2.38	0.52
1:A:225:THR:O	1:A:226:CYS:HB2	2.10	0.52
1:A:223:ALA:HB3	1:A:248:LEU:HD13	1.90	0.51
1:B:220:ASP:HB3	1:B:248:LEU:HD12	1.93	0.51
1:B:111:LEU:C	1:B:115:MET:HE2	2.31	0.51
1:B:294:MET:HG2	1:B:317:PRO:HG2	1.93	0.50
1:B:78:LYS:NZ	1:B:122:ASP:OD2	2.35	0.50
1:A:151:VAL:HG13	1:A:247:ILE:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ARG:CG	1:B:204:ARG:NH1	2.74	0.50
1:A:9:GLY:HA3	1:A:58:SER:HB2	1.94	0.50
1:B:4:ILE:CG2	1:B:25:LEU:HD11	2.41	0.49
1:A:278:GLU:HA	1:A:281:MET:CE	2.41	0.49
1:A:161:GLU:CD	1:A:243:ARG:HH21	2.15	0.49
1:B:60:CYS:HB3	1:B:66:ASN:HD21	1.77	0.49
1:A:57:GLN:HG2	1:A:58:SER:N	2.26	0.49
1:B:273:ASN:OD1	1:B:292:ILE:HG13	2.13	0.49
1:A:301:ARG:HG2	1:A:305:ASN:ND2	2.28	0.49
1:B:204:ARG:HB3	1:B:204:ARG:CZ	2.42	0.48
1:A:212:LYS:HD2	1:A:240:GLY:HA3	1.95	0.48
1:A:6:ILE:CD1	1:A:23:LEU:HD12	2.44	0.48
1:A:273:ASN:H	1:A:273:ASN:ND2	2.09	0.48
1:B:12:HIS:NE2	1:B:60:CYS:HA	2.28	0.47
1:B:184:ARG:HG3	1:B:184:ARG:NH1	2.29	0.47
1:B:7:PHE:CD2	1:B:30:VAL:CG2	2.97	0.47
1:A:268:ALA:HA	1:A:286:LYS:HB2	1.96	0.46
1:A:223:ALA:HB2	1:A:248:LEU:HD22	1.97	0.46
1:B:100:LYS:NZ	3:B:3175:HOH:O	2.47	0.46
1:B:128:ASP:OD2	1:B:249:THR:HG21	2.16	0.46
1:A:135:GLN:NE2	2:A:1006:SO4:O4	2.48	0.46
1:A:278:GLU:HA	1:A:281:MET:HE3	1.98	0.46
1:A:10:SER:HB3	1:A:69:GLU:OE2	2.16	0.45
1:B:112:VAL:HA	1:B:115:MET:HE2	1.98	0.45
1:A:169:SER:HA	1:A:170:PRO:HD3	1.79	0.45
1:B:5:LYS:HE2	3:B:3012:HOH:O	2.15	0.45
1:B:266:PHE:O	1:B:286:LYS:HE2	2.16	0.45
1:B:7:PHE:HD2	1:B:30:VAL:CG2	2.29	0.45
1:B:148:GLU:OE2	1:B:184:ARG:NH1	2.50	0.45
1:B:72:ILE:CG2	1:A:106:PRO:HG3	2.47	0.44
1:B:9:GLY:O	1:B:58:SER:HB2	2.17	0.44
1:B:248:LEU:O	1:B:271:VAL:HA	2.17	0.44
1:A:57:GLN:O	1:A:57:GLN:NE2	2.37	0.44
1:B:22:ARG:CZ	1:B:294:MET:HB3	2.48	0.43
1:A:271:VAL:O	1:A:289:VAL:HA	2.18	0.43
1:B:4:ILE:HD13	1:B:4:ILE:C	2.38	0.43
1:B:112:VAL:HA	1:B:115:MET:HE3	2.00	0.43
1:B:7:PHE:HD2	1:B:30:VAL:HG23	1.83	0.43
1:B:311:TYR:CE1	1:B:315:HIS:HD2	2.36	0.43
1:A:275:ILE:O	1:A:277:GLN:HG2	2.18	0.42
1:A:302:ARG:HG2	1:A:307:GLU:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:NZ	3:A:3119:HOH:O	2.52	0.42
1:A:161:GLU:OE1	1:A:161:GLU:N	2.40	0.42
1:A:222:MET:HE2	3:A:3073:HOH:O	2.19	0.42
1:B:75:ASN:HD21	1:A:107:ILE:H	1.67	0.42
1:B:96:ARG:HD3	1:B:222:MET:SD	2.60	0.42
1:B:96:ARG:NH2	1:A:37:ASN:HD21	2.17	0.42
1:A:12:HIS:CD2	1:A:276:PRO:CG	2.89	0.42
1:A:22:ARG:HH11	1:A:294:MET:CE	2.32	0.42
1:A:207:LEU:C	1:A:207:LEU:HD23	2.39	0.42
1:A:5:LYS:HG3	1:A:51:GLU:OE1	2.20	0.42
1:A:161:GLU:OE1	1:A:243:ARG:NH2	2.53	0.42
1:B:6:ILE:HD12	1:B:25:LEU:HD12	2.01	0.41
1:A:269:VAL:O	1:A:287:ILE:HA	2.21	0.41
1:B:278:GLU:CD	1:B:278:GLU:N	2.68	0.41
1:B:302:ARG:HB2	1:B:309:VAL:HG22	2.03	0.41
1:B:225:THR:O	1:B:226:CYS:HB2	2.20	0.41
1:B:111:LEU:O	1:B:115:MET:HE2	2.21	0.40
1:B:6:ILE:CD1	1:B:25:LEU:HD12	2.51	0.40
1:B:58:SER:HA	3:B:3161:HOH:O	2.21	0.40
1:B:311:TYR:CE1	1:B:315:HIS:CD2	3.09	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%)	285 (95%)	15 (5%)	0	100	100
1	B	304/326 (93%)	290 (95%)	14 (5%)	0	100	100
All	All	604/652 (93%)	575 (95%)	29 (5%)	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	257/278 (92%)	242 (94%)	15 (6%)	20	15
1	B	261/278 (94%)	248 (95%)	13 (5%)	24	19
All	All	518/556 (93%)	490 (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	32	THR
1	B	36	SER
1	B	41	CYS
1	B	57	GLN
1	B	60	CYS
1	B	62	GLU
1	B	204	ARG
1	B	249	THR
1	B	315	HIS
1	A	13	GLN
1	A	15	LEU
1	A	33	LYS
1	A	43	GLU
1	A	57	GLN
1	A	60	CYS
1	A	62	GLU
1	A	111	LEU
1	A	152	LEU
1	A	186	ASN
1	A	195	GLU
1	A	249	THR
1	A	273	ASN
1	A	283	HIS

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Mol	Chain	Res	Type
1	A	286	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	64	ASN
1	B	75	ASN
1	B	263	ASN
1	B	277	GLN
1	B	315	HIS
1	A	3	ASN
1	A	12	HIS
1	A	13	GLN
1	A	57	GLN
1	A	273	ASN
1	A	277	GLN
1	A	304	HIS
1	A	305	ASN

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)

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	0.19	0	6,6,6	0.07	0
2	SO4	A	1006	-	4,4,4	0.12	0	6,6,6	0.20	0
2	SO4	B	1005	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	B	1002	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	B	1003	-	4,4,4	0.18	0	6,6,6	0.14	0
2	SO4	A	1004	-	4,4,4	0.15	0	6,6,6	0.16	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	1006	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	1.20	50 (16%)	1	1	17, 39, 59, 68	45 (14%)
1	B	308/326 (94%)	0.84	46 (14%)	2	2	15, 31, 46, 58	48 (15%)
All	All	612/652 (93%)	1.02	96 (15%)	2	1	15, 34, 54, 68	93 (15%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	ASP	31.3
1	A	61	GLY	25.2
1	A	58	SER	20.6
1	A	59	GLY	19.2
1	A	33	LYS	17.5
1	B	60	CYS	17.0
1	B	10	SER	16.3
1	B	99	LYS	16.2
1	B	35	PHE	16.2
1	A	36	SER	16.1
1	A	310	SER	16.0
1	B	68	MET	15.3
1	B	38	GLN	14.6
1	A	204	ARG	14.1
1	A	62	GLU	14.1
1	B	98	ASP	13.9
1	A	280	LYS	13.7
1	B	11	SER	12.9
1	B	176	LYS	12.4
1	B	203	ASP	11.9
1	B	59	GLY	11.6
1	A	311	TYR	11.6
1	A	101	ASP	10.8
1	B	36	SER	10.4

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Mol	Chain	Res	Type	RSRZ
1	A	102	LYS	10.1
1	B	57	GLN	9.2
1	B	278	GLU	9.0
1	B	33	LYS	8.0
1	B	37	ASN	8.0
1	B	101	ASP	7.8
1	A	278	GLU	7.5
1	A	96	ARG	7.4
1	B	194	LYS	7.0
1	A	313	PHE	6.9
1	A	194	LYS	6.8
1	A	283	HIS	6.6
1	A	282	LYS	6.5
1	A	60	CYS	6.2
1	B	3	ASN	5.3
1	A	184	ARG	5.2
1	B	314	SER	5.0
1	B	43	GLU	5.0
1	B	204	ARG	5.0
1	B	5	LYS	4.8
1	B	34	LYS	4.6
1	B	311	TYR	4.6
1	A	29	LYS	4.5
1	B	146	TYR	4.4
1	A	10	SER	4.4
1	A	212	LYS	4.0
1	A	214	ARG	4.0
1	A	26	GLU	3.9
1	B	212	LYS	3.8
1	A	312	LEU	3.7
1	A	12	HIS	3.7
1	B	14	ASP	3.6
1	B	315	HIS	3.6
1	A	11	SER	3.6
1	A	294	MET	3.6
1	B	51	GLU	3.5
1	B	39	GLU	3.5
1	A	245	TYR	3.4
1	A	43	GLU	3.1
1	A	263	ASN	3.1
1	B	32	THR	3.1
1	A	279	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	313	PHE	2.9
1	B	31	VAL	2.9
1	B	12	HIS	2.9
1	B	58	SER	2.8
1	A	255	GLY	2.8
1	A	211	VAL	2.8
1	A	205	MET	2.8
1	B	316	VAL	2.8
1	A	309	VAL	2.8
1	B	298	GLU	2.7
1	B	21	ASP	2.7
1	A	253	PHE	2.6
1	A	31	VAL	2.5
1	B	41	CYS	2.5
1	A	302	ARG	2.4
1	A	285	SER	2.3
1	A	308	SER	2.3
1	A	210	ASP	2.3
1	A	122	ASP	2.2
1	B	157	GLU	2.2
1	B	184	ARG	2.2
1	A	252	ILE	2.2
1	B	195	GLU	2.2
1	A	230	CYS	2.2
1	A	32	THR	2.2
1	A	37	ASN	2.1
1	B	102	LYS	2.1
1	A	35	PHE	2.0
1	B	177	ARG	2.0
1	B	279	ASP	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(Å^2)	Q<0.9
2	SO4	A	1004	5/5	0.72	0.27	51,54,57,58	5
2	SO4	B	1005	5/5	0.84	0.22	30,38,42,43	5
2	SO4	A	1006	5/5	0.84	0.38	33,42,49,50	5
2	SO4	B	1003	5/5	0.96	0.12	34,41,50,52	0
2	SO4	B	1002	5/5	0.98	0.08	32,33,34,39	0
2	SO4	A	1001	5/5	0.99	0.05	37,38,40,44	0

6.5 Other polymers (i)

There are no such residues in this entry.