



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:47 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

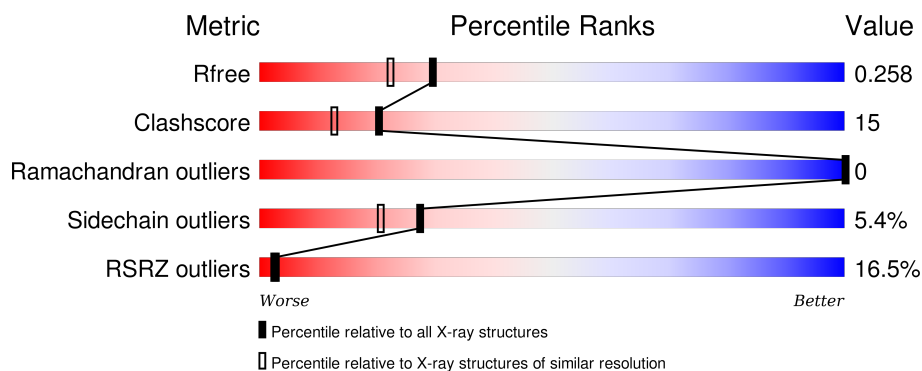
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.02 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))
$R_{free}$	91344	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	

## 2 Entry composition

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
1	B	308	Total	C	N	O	S	0	0	0
			2355	1477	414	447	17			
1	A	304	Total	C	N	O	S	0	0	0
			2325	1458	408	442	17			

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<sub>4</sub>S).



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		

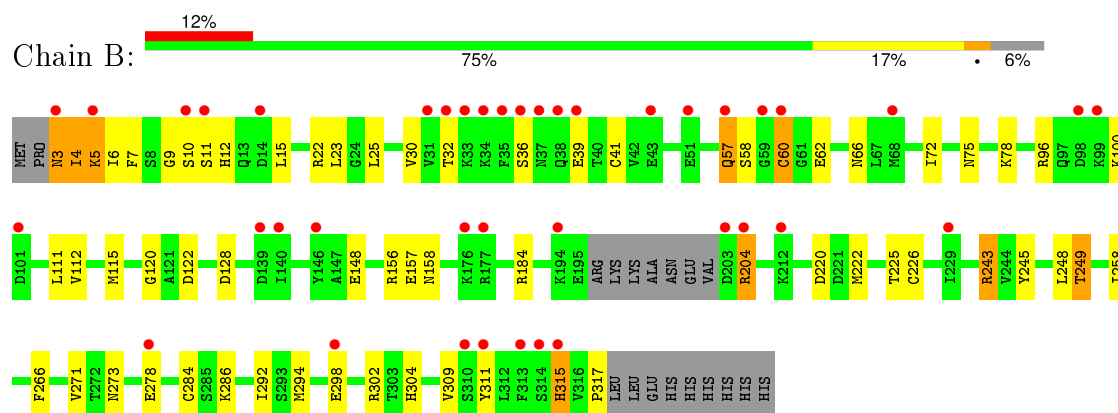
- Molecule 3 is water.

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

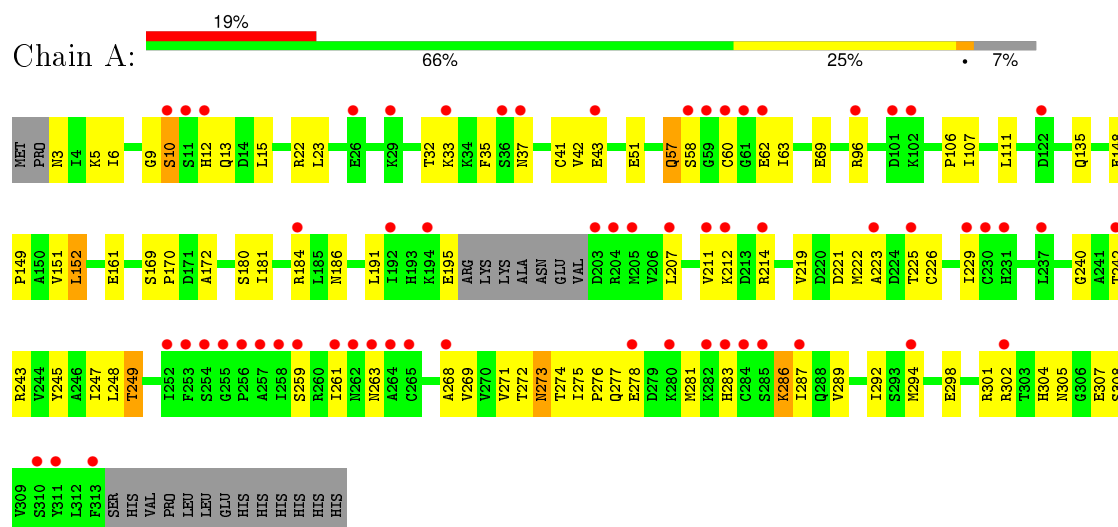
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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, $\alpha$ , $\beta$ , $\gamma$	170.54 Å   170.54 Å   61.78 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.01 Å)	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 (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29   ,   56.1	EDS
Estimated twinning fraction	0.095 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 43878 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4888	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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(°)	Ideal(°)
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:CD	1:B:278:GLU:H	1.96	0.69
1:A:273:ASN:H	1:A:273:ASN:HD22	1.40	0.67
1:A:261:ILE:HG22	1:A:286:LYS:HD2	1.76	0.66
1:A:96:ARG:HD2	1:A:222:MET:SD	2.36	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:CG	1:B:204:ARG:HH11	2.13	0.61
1:A:35:PHE:CE1	1:A:41:CYS:HB2	2.35	0.60
1:B:258:ILE:HG23	1:B:284:CYS:HB2	1.81	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:A:172:ALA:HA	1:A:191:LEU:HD11	1.84	0.58
1:B:39:GLU:HG2	1:A:63:ILE:HD13	1.84	0.58
1:A:273:ASN:N	1:A:273:ASN:HD22	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:248:LEU:O	1:A:271:VAL:HA	2.05	0.56
1:A:6:ILE:HD11	1:A:23:LEU:HD12	1.85	0.56
1:B:184:ARG:HH11	1:B:184:ARG:HG3	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:112:VAL:HA	1:B:115:MET:CE	2.37	0.54
1:B:10:SER:OG	1:B:11:SER:N	2.40	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:273:ASN:ND2	1:A:292:ILE:H	2.00	0.53
1:A:152:LEU:HD11	1:A:181:ILE:HG23	1.91	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:NH1	1:B:204:ARG:CG	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:NH1	1:B:184:ARG:HG3	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:A:271:VAL:O	1:A:289:VAL:HA	2.18	0.43
1:B:22:ARG:CZ	1:B:294:MET:HB3	2.48	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:302:ARG:HG2	1:A:307:GLU:HG2	2.00	0.42
1:A:275:ILE:O	1:A:277:GLN:HG2	2.18	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:A:12:HIS:CD2	1:A:276:PRO:CG	2.89	0.42
1:B:96:ARG:NH2	1:A:37:ASN:HD21	2.17	0.42
1:B:96:ARG:HD3	1:B:222:MET:SD	2.60	0.42
1:A:22:ARG:HH11	1:A:294:MET:CE	2.32	0.42
1:A:207:LEU:HD23	1:A:207:LEU:C	2.39	0.42
1:A:161:GLU:OE1	1:A:243:ARG:NH2	2.53	0.42
1:A:5:LYS:HG3	1:A:51:GLU:OE1	2.20	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 ⓘ

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%)	25	18
1	B	261/278 (94%)	248 (95%)	13 (5%)	30	24
All	All	518/556 (93%)	490 (95%)	28 (5%)	27	21

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

Some 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 ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	0.46	0	6,6,6	0.07	0
2	SO4	A	1004	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	A	1006	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	B	1002	-	4,4,4	0.36	0	6,6,6	0.17	0
2	SO4	B	1003	-	4,4,4	0.13	0	6,6,6	0.16	0
2	SO4	B	1005	-	4,4,4	0.23	0	6,6,6	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1006	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1005	-	-	0/0/0/0	0/0/0/0

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	1.71	61 (20%) 1 1	17, 39, 59, 68	45 (14%)
1	B	308/326 (94%)	1.16	40 (12%) 5 5	15, 31, 46, 58	48 (15%)
All	All	612/652 (93%)	1.43	101 (16%) 2 3	15, 34, 54, 68	93 (15%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	ASP	63.1
1	A	61	GLY	33.1
1	B	99	LYS	29.9
1	A	59	GLY	28.0
1	A	204	ARG	23.2
1	B	98	ASP	21.6
1	A	101	ASP	21.6
1	B	36	SER	21.3
1	B	203	ASP	21.0
1	B	35	PHE	20.7
1	A	311	TYR	20.2
1	A	33	LYS	19.4
1	A	36	SER	19.3
1	B	38	GLN	18.9
1	A	60	CYS	17.2
1	A	58	SER	17.1
1	A	102	LYS	16.4
1	B	68	MET	16.4
1	A	310	SER	16.1
1	B	60	CYS	15.9
1	A	62	GLU	14.6
1	B	101	ASP	14.1
1	B	176	LYS	14.0
1	B	37	ASN	13.8

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Mol	Chain	Res	Type	RSRZ
1	B	33	LYS	13.2
1	B	10	SER	13.2
1	A	96	ARG	12.0
1	B	57	GLN	10.3
1	B	59	GLY	10.0
1	B	11	SER	9.4
1	B	3	ASN	8.5
1	A	313	PHE	8.2
1	B	194	LYS	7.6
1	A	194	LYS	6.6
1	B	204	ARG	6.6
1	B	278	GLU	6.1
1	A	184	ARG	5.8
1	A	282	LYS	5.8
1	A	280	LYS	5.6
1	A	253	PHE	4.9
1	A	122	ASP	4.8
1	B	139	ASP	4.7
1	A	12	HIS	4.7
1	A	214	ARG	4.5
1	A	230	CYS	4.3
1	B	5	LYS	4.2
1	B	39	GLU	4.2
1	A	278	GLU	4.2
1	A	257	ALA	4.1
1	A	263	ASN	4.1
1	A	264	ALA	4.1
1	A	258	ILE	4.1
1	B	146	TYR	3.9
1	A	255	GLY	3.8
1	A	10	SER	3.7
1	B	51	GLU	3.7
1	A	43	GLU	3.7
1	B	43	GLU	3.6
1	A	205	MET	3.6
1	B	315	HIS	3.6
1	A	212	LYS	3.5
1	A	252	ILE	3.5
1	A	285	SER	3.4
1	A	256	PRO	3.4
1	A	259	SER	3.3
1	A	262	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	212	LYS	3.3
1	B	311	TYR	3.3
1	B	14	ASP	3.2
1	B	32	THR	3.1
1	A	261	ILE	3.1
1	A	11	SER	3.1
1	A	229	ILE	3.1
1	B	177	ARG	3.0
1	A	29	LYS	3.0
1	A	284	CYS	3.0
1	A	283	HIS	2.9
1	B	298	GLU	2.9
1	A	254	SER	2.8
1	A	231	HIS	2.8
1	A	37	ASN	2.8
1	B	314	SER	2.8
1	A	211	VAL	2.7
1	A	294	MET	2.7
1	B	34	LYS	2.7
1	A	26	GLU	2.5
1	A	237	LEU	2.4
1	B	313	PHE	2.4
1	A	265	CYS	2.4
1	A	225	THR	2.3
1	A	268	ALA	2.3
1	B	229	ILE	2.2
1	A	223	ALA	2.1
1	B	31	VAL	2.1
1	A	302	ARG	2.1
1	A	242	THR	2.1
1	A	207	LEU	2.1
1	B	310	SER	2.1
1	A	192	ILE	2.0
1	A	287	ILE	2.0
1	B	140	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	1006	5/5	0.87	0.32	-0.23	33,42,49,50	5
2	SO4	A	1004	5/5	0.91	0.23	-0.29	51,54,57,58	5
2	SO4	B	1005	5/5	0.86	0.18	-0.46	30,38,42,43	5
2	SO4	A	1001	5/5	0.99	0.09	-0.55	37,38,40,44	0
2	SO4	B	1003	5/5	0.97	0.08	-0.91	34,41,50,52	0
2	SO4	B	1002	5/5	0.99	0.09	-1.31	32,33,34,39	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.