



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 09:57 PM EDT

PDB ID : 2H06  
Title : Crystal structure of human phosphoribosyl pyrophosphate synthetase 1  
Authors : Li, S.; Peng, B.; Ding, J.  
Deposited on : 2006-05-14  
Resolution : 2.20 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

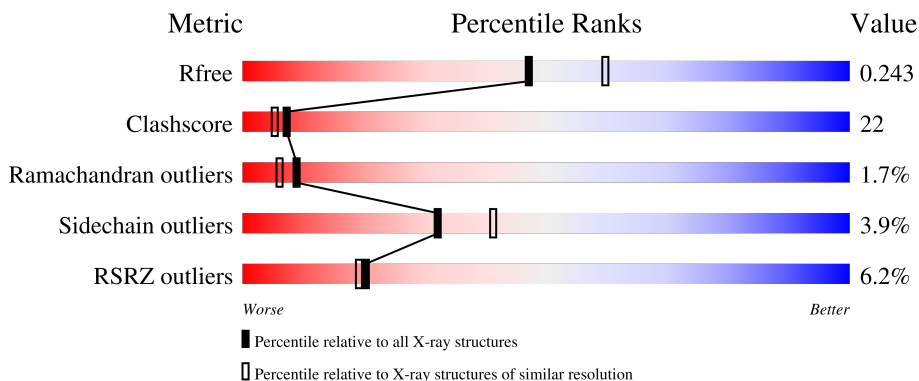
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	 9% 60% 30% • 6%
1	B	326	 2% 66% 27% • 6%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4904 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 I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	305	Total	C	N	O	S	0	0	0
			2336	1464	412	443	17			
1	B	308	Total	C	N	O	S	0	0	0
			2355	1477	414	447	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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		
2	B	1	Total	O	S	0	0
			5	4	1		

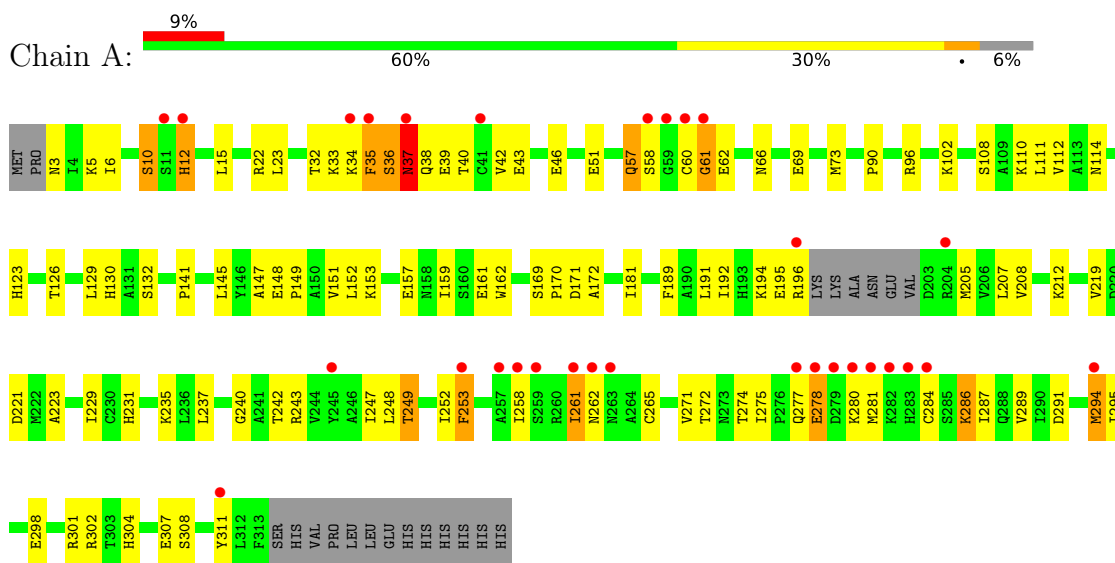
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total	O	0	0
			72	72		
3	B	111	Total	O	0	0
			111	111		

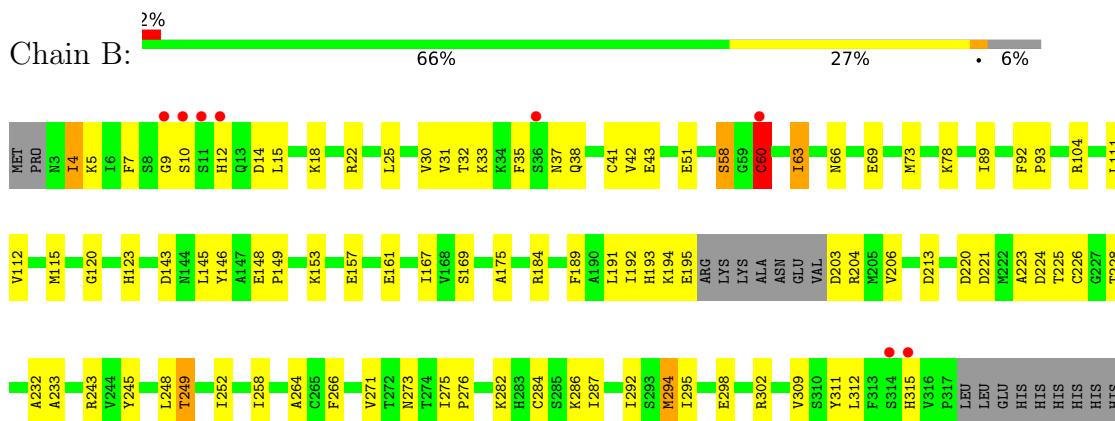
### 3 Residue-property plots

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 I



- Molecule 1: Ribose-phosphate pyrophosphokinase I



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.68Å 169.68Å 61.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.98 – 2.20 48.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.98-2.20) 99.9 (48.98-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.20Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.212 , 0.245 0.208 , 0.243	Depositor DCC
$R_{free}$ test set	1676 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.9	Xtrriage
Anisotropy	0.320	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4904	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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	0.32	0/2368	0.60	1/3200 (0.0%)
1	B	0.35	0/2389	0.61	0/3231
All	All	0.34	0/4757	0.60	1/6431 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	GLY	N-CA-C	5.19	126.08	113.10

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	2336	0	2373	121	0
1	B	2355	0	2388	96	0
2	A	15	0	0	2	0
2	B	15	0	0	1	0
3	A	72	0	0	5	0
3	B	111	0	0	2	0
All	All	4904	0	4761	213	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 22.

All (213) 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:294:MET:HE3	1:B:295:ILE:H	1.36	0.91
1:A:253:PHE:HB3	1:A:280:LYS:NZ	1.88	0.89
1:B:35:PHE:HE1	1:B:41:CYS:HG	0.88	0.88
1:B:223:ALA:HB2	1:B:248:LEU:HG	1.59	0.84
1:A:258:ILE:HG12	1:A:280:LYS:HE3	1.58	0.83
1:A:242:THR:HG22	1:A:243:ARG:HG3	1.60	0.83
1:A:57:GLN:HG3	3:A:1075:HOH:O	1.81	0.81
1:A:253:PHE:HB3	1:A:280:LYS:HZ3	1.44	0.81
1:A:258:ILE:HA	1:A:280:LYS:HZ1	1.47	0.80
1:A:172:ALA:HA	1:A:191:LEU:HD11	1.64	0.79
1:B:78:LYS:HE3	1:B:120:GLY:O	1.82	0.79
1:A:223:ALA:HB3	1:A:248:LEU:HD13	1.64	0.79
1:B:298:GLU:O	1:B:302:ARG:HG2	1.82	0.77
1:A:34:LYS:HZ3	1:A:40:THR:HG23	1.51	0.76
1:A:194:LYS:HG2	1:A:205:MET:HG2	1.68	0.75
1:B:111:LEU:HG	1:B:115:MET:CE	2.17	0.75
1:A:258:ILE:HG12	1:A:280:LYS:CE	2.16	0.75
1:B:194:LYS:NZ	1:B:203:ASP:HA	2.02	0.75
1:B:35:PHE:HE1	1:B:41:CYS:SG	2.07	0.75
1:B:33:LYS:HB2	1:B:41:CYS:SG	2.27	0.74
1:A:34:LYS:NZ	1:A:40:THR:HG23	2.03	0.73
1:A:253:PHE:HB2	1:A:280:LYS:HD3	1.70	0.72
1:A:261:ILE:HD13	1:A:262:ASN:H	1.56	0.71
1:B:294:MET:HE3	1:B:295:ILE:N	2.06	0.70
1:A:126:THR:HG21	1:A:129:LEU:HD21	1.76	0.68
1:A:301:ARG:HB3	1:A:301:ARG:HH11	1.58	0.68
1:A:34:LYS:HA	1:A:34:LYS:HE2	1.75	0.67
1:B:294:MET:CE	1:B:295:ILE:HG13	2.25	0.66
1:B:31:VAL:HB	1:B:43:GLU:HB3	1.78	0.66
1:B:111:LEU:HG	1:B:115:MET:HE2	1.78	0.65
1:B:294:MET:HE3	1:B:295:ILE:HG13	1.79	0.64
1:A:37:ASN:N	1:A:37:ASN:HD22	1.93	0.64
1:B:292:ILE:HA	1:B:294:MET:CE	2.28	0.64
1:B:10:SER:N	1:B:58:SER:OG	2.31	0.64
1:A:102:LYS:HG2	1:B:146:TYR:CZ	2.33	0.63
1:A:284:CYS:SG	1:A:287:ILE:HG13	2.38	0.63
1:A:34:LYS:HZ3	1:A:40:THR:CG2	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:PHE:HB2	1:A:280:LYS:CD	2.28	0.63
1:B:60:CYS:HB3	1:B:66:ASN:OD1	2.00	0.62
1:B:9:GLY:HA2	1:B:73:MET:CE	2.29	0.62
1:B:264:ALA:O	1:B:286:LYS:NZ	2.32	0.62
1:B:18:LYS:HE3	3:B:1103:HOH:O	1.99	0.61
1:B:12:HIS:NE2	1:B:60:CYS:HA	2.16	0.60
1:B:32:THR:O	1:B:33:LYS:HD3	2.00	0.60
1:A:229:ILE:HD12	1:A:248:LEU:HD21	1.83	0.60
1:A:57:GLN:NE2	1:A:90:PRO:HD2	2.16	0.60
1:B:220:ASP:HB3	1:B:248:LEU:HD12	1.83	0.60
1:B:248:LEU:O	1:B:271:VAL:HA	2.02	0.60
1:A:37:ASN:N	1:A:37:ASN:ND2	2.50	0.59
1:A:205:MET:HE1	1:A:231:HIS:O	2.03	0.59
1:B:252:ILE:HD13	1:B:275:ILE:CD1	2.32	0.59
1:B:148:GLU:HB3	1:B:149:PRO:HD3	1.85	0.59
1:B:111:LEU:HG	1:B:115:MET:HE1	1.84	0.58
1:A:253:PHE:CB	1:A:280:LYS:HZ3	2.16	0.58
1:A:205:MET:HE1	1:A:231:HIS:C	2.23	0.58
1:A:248:LEU:O	1:A:271:VAL:HA	2.03	0.57
1:B:9:GLY:HA2	1:B:73:MET:HE3	1.84	0.57
1:B:292:ILE:HA	1:B:294:MET:HE2	1.87	0.57
1:A:3:ASN:ND2	1:A:304:HIS:HE1	2.03	0.57
1:B:298:GLU:HG2	1:B:312:LEU:HD21	1.87	0.57
1:A:36:SER:C	1:A:38:GLN:H	2.08	0.56
1:A:57:GLN:NE2	1:A:57:GLN:O	2.38	0.56
1:A:253:PHE:HB3	1:A:280:LYS:HZ2	1.70	0.56
1:A:32:THR:HG22	1:A:34:LYS:HE3	1.86	0.56
1:B:302:ARG:HB2	1:B:309:VAL:HG22	1.88	0.56
1:A:34:LYS:HE2	1:A:34:LYS:CA	2.36	0.55
1:A:294:MET:SD	1:A:294:MET:N	2.78	0.55
1:B:12:HIS:CD2	1:B:60:CYS:HA	2.41	0.55
1:A:229:ILE:CD1	1:A:248:LEU:HD21	2.37	0.55
1:A:6:ILE:HD11	1:A:23:LEU:HD12	1.87	0.55
1:A:294:MET:CE	1:A:295:ILE:HG13	2.37	0.55
1:B:243:ARG:NH1	1:B:245:TYR:OH	2.32	0.55
1:B:5:LYS:HD3	1:B:51:GLU:OE2	2.08	0.54
1:B:112:VAL:HA	1:B:115:MET:CE	2.37	0.54
1:A:278:GLU:HA	1:A:281:MET:HE3	1.90	0.54
1:A:130:HIS:HD2	1:A:221:ASP:OD1	1.90	0.54
1:B:4:ILE:HD13	1:B:5:LYS:N	2.23	0.54
1:A:261:ILE:HD13	1:A:262:ASN:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:HE3	1:A:46:GLU:OE1	2.08	0.53
1:A:37:ASN:ND2	1:A:37:ASN:H	2.06	0.53
1:A:294:MET:HE2	1:A:295:ILE:HG13	1.91	0.53
1:A:35:PHE:HB2	1:A:39:GLU:HB3	1.90	0.52
1:A:145:LEU:HD13	1:A:295:ILE:HG22	1.91	0.52
1:B:194:LYS:CE	1:B:203:ASP:HA	2.39	0.52
1:A:12:HIS:ND1	1:A:12:HIS:C	2.63	0.52
1:B:258:ILE:HG23	1:B:284:CYS:HB2	1.92	0.52
1:B:69:GLU:HG2	1:B:73:MET:CE	2.40	0.51
1:A:205:MET:O	1:A:235:LYS:HE3	2.10	0.51
1:B:22:ARG:HG3	1:B:22:ARG:HH11	1.75	0.51
1:A:271:VAL:O	1:A:289:VAL:HA	2.11	0.51
1:B:194:LYS:HZ3	1:B:203:ASP:HA	1.73	0.51
1:B:38:GLN:HA	1:B:38:GLN:OE1	2.11	0.50
1:B:298:GLU:CD	1:B:302:ARG:HE	2.14	0.50
1:B:273:ASN:OD1	1:B:292:ILE:HG13	2.11	0.50
1:A:102:LYS:HG2	1:B:146:TYR:OH	2.11	0.50
1:A:22:ARG:NH2	1:A:294:MET:HG3	2.27	0.50
1:A:58:SER:HB3	1:A:66:ASN:ND2	2.27	0.50
1:A:161:GLU:N	1:A:161:GLU:OE1	2.44	0.49
1:A:237:LEU:HD11	1:A:265:CYS:SG	2.52	0.49
1:A:57:GLN:HG2	1:A:58:SER:O	2.13	0.49
1:A:148:GLU:HB3	1:A:149:PRO:HD3	1.93	0.49
1:A:130:HIS:HE1	3:A:1059:HOH:O	1.95	0.49
1:B:153:LYS:O	1:B:157:GLU:HG3	2.12	0.49
1:A:258:ILE:O	1:A:261:ILE:CD1	2.61	0.49
1:A:3:ASN:HD22	1:A:304:HIS:CE1	2.31	0.49
1:A:6:ILE:CD1	1:A:23:LEU:HD12	2.43	0.49
1:B:63:ILE:HD11	1:B:93:PRO:HB3	1.94	0.49
1:B:221:ASP:O	1:B:249:THR:HG23	2.13	0.49
1:B:282:LYS:NZ	1:B:282:LYS:HB3	2.28	0.49
1:A:278:GLU:OE1	1:A:278:GLU:N	2.46	0.49
1:B:146:TYR:OH	2:B:1005:SO4:O3	2.31	0.49
1:A:151:VAL:HG13	1:A:247:ILE:HG21	1.95	0.48
1:B:89:ILE:HG21	1:B:93:PRO:HD3	1.95	0.48
1:A:302:ARG:NH1	1:A:307:GLU:HG3	2.28	0.48
1:B:123:HIS:CE1	1:B:143:ASP:OD2	2.67	0.48
1:A:42:VAL:HG11	1:A:73:MET:HG2	1.95	0.48
1:A:102:LYS:NZ	1:B:184:ARG:NH2	2.61	0.48
1:A:262:ASN:HA	1:A:286:LYS:HE2	1.96	0.48
1:A:5:LYS:HD3	3:A:1021:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:HG3	1:A:51:GLU:OE1	2.14	0.48
1:B:228:THR:HB	3:B:1113:HOH:O	2.13	0.47
1:A:194:LYS:CG	1:A:205:MET:HG2	2.42	0.47
1:A:132:SER:HB3	2:A:1006:SO4:O3	2.14	0.47
1:B:112:VAL:HA	1:B:115:MET:HE3	1.97	0.47
1:B:78:LYS:HG3	1:B:120:GLY:HA3	1.96	0.47
1:A:249:THR:HA	1:A:272:THR:HG23	1.95	0.47
1:B:42:VAL:CG1	1:B:43:GLU:N	2.78	0.47
1:A:36:SER:O	1:A:38:GLN:N	2.44	0.47
1:B:284:CYS:HB3	1:B:287:ILE:HD12	1.97	0.47
1:A:38:GLN:O	1:A:38:GLN:HG3	2.15	0.47
1:B:69:GLU:HG2	1:B:73:MET:HE2	1.96	0.47
1:B:161:GLU:OE1	1:B:243:ARG:NH2	2.48	0.46
1:A:208:VAL:O	1:A:208:VAL:HG23	2.14	0.46
1:B:22:ARG:HD3	1:B:294:MET:HA	1.97	0.46
1:A:37:ASN:HD21	1:A:39:GLU:HB2	1.81	0.46
1:A:261:ILE:O	1:A:286:LYS:HE3	2.16	0.46
1:B:33:LYS:O	1:B:41:CYS:SG	2.73	0.46
1:A:189:PHE:HE2	1:B:206:VAL:HG21	1.81	0.46
1:A:57:GLN:NE2	1:A:90:PRO:CD	2.79	0.46
1:A:302:ARG:NH1	1:A:308:SER:O	2.48	0.45
1:A:22:ARG:CD	1:A:294:MET:HA	2.46	0.45
1:A:60:CYS:O	1:A:62:GLU:N	2.49	0.45
1:A:108:SER:O	1:A:112:VAL:HG23	2.16	0.45
1:A:191:LEU:C	1:A:191:LEU:HD23	2.36	0.45
1:A:291:ASP:O	1:A:294:MET:SD	2.75	0.45
1:B:92:PHE:HA	1:B:93:PRO:HD3	1.78	0.45
1:A:153:LYS:O	1:A:157:GLU:HG3	2.16	0.45
1:B:9:GLY:O	1:B:73:MET:HE1	2.16	0.45
1:B:223:ALA:CB	1:B:248:LEU:HG	2.39	0.45
1:B:112:VAL:HA	1:B:115:MET:HE2	1.98	0.45
1:B:175:ALA:HA	1:B:191:LEU:HD21	1.97	0.45
1:A:10:SER:N	1:A:69:GLU:OE1	2.49	0.45
1:A:37:ASN:O	1:A:38:GLN:HB3	2.17	0.45
1:A:110:LYS:HZ2	1:A:114:ASN:HD21	1.65	0.45
1:A:258:ILE:HG12	1:A:280:LYS:NZ	2.30	0.45
1:B:224:ASP:HA	1:B:252:ILE:HB	1.97	0.45
1:B:243:ARG:NH1	1:B:245:TYR:CE1	2.85	0.45
1:A:34:LYS:NZ	1:A:40:THR:CG2	2.76	0.45
1:B:4:ILE:HD12	1:B:25:LEU:CD1	2.47	0.45
1:A:181:ILE:HD12	1:A:219:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLU:CD	1:A:278:GLU:H	2.20	0.45
1:A:42:VAL:CG1	1:A:43:GLU:N	2.79	0.44
1:A:35:PHE:HB3	1:A:36:SER:H	1.52	0.44
1:A:194:LYS:O	1:A:196:ARG:HG3	2.17	0.44
1:A:301:ARG:HH11	1:A:301:ARG:CB	2.29	0.44
1:A:6:ILE:HD11	1:A:23:LEU:CD1	2.48	0.44
1:B:35:PHE:CE1	1:B:41:CYS:SG	2.96	0.44
1:B:195:GLU:OE1	1:B:204:ARG:NH2	2.50	0.44
1:A:207:LEU:HD23	1:A:208:VAL:N	2.32	0.44
1:A:298:GLU:OE2	1:A:301:ARG:NH1	2.50	0.44
1:B:9:GLY:HA2	1:B:73:MET:HE1	2.00	0.44
1:A:237:LEU:HD23	1:A:237:LEU:HA	1.89	0.44
1:B:292:ILE:HA	1:B:294:MET:HE1	1.98	0.44
1:B:311:TYR:O	1:B:315:HIS:HB3	2.18	0.44
1:A:147:ALA:O	1:A:151:VAL:HG23	2.18	0.43
1:A:212:LYS:HD2	1:A:240:GLY:HA3	2.00	0.43
1:A:258:ILE:HA	1:A:280:LYS:NZ	2.26	0.43
1:B:4:ILE:HD13	1:B:4:ILE:C	2.38	0.43
1:B:161:GLU:CD	1:B:243:ARG:HH21	2.21	0.43
1:A:307:GLU:HG3	1:A:308:SER:N	2.34	0.43
1:B:194:LYS:HE2	1:B:203:ASP:HA	2.00	0.43
1:A:33:LYS:C	1:A:34:LYS:HE2	2.39	0.43
1:B:193:HIS:O	1:B:206:VAL:HG22	2.18	0.43
1:A:249:THR:HG22	3:A:1049:HOH:O	2.18	0.43
1:B:275:ILE:HG23	1:B:276:PRO:HD2	2.01	0.43
1:A:248:LEU:HB2	1:A:271:VAL:HG12	2.00	0.43
1:B:192:ILE:HD12	1:B:232:ALA:HB1	2.01	0.42
1:B:233:ALA:HB2	1:B:266:PHE:CE2	2.54	0.42
2:A:1004:SO4:O2	1:B:104:ARG:HD3	2.19	0.42
1:B:7:PHE:HD2	1:B:30:VAL:CG2	2.32	0.42
1:B:169:SER:HB3	1:B:191:LEU:HD23	2.02	0.42
1:A:169:SER:HA	1:A:170:PRO:HD3	1.86	0.42
1:A:272:THR:OG1	1:A:274:THR:HG23	2.19	0.42
1:A:159:ILE:O	1:A:162:TRP:HD1	2.02	0.42
1:B:37:ASN:OD1	1:B:37:ASN:N	2.53	0.42
1:B:169:SER:HB3	1:B:191:LEU:CD2	2.50	0.42
1:A:253:PHE:CB	1:A:280:LYS:NZ	2.72	0.42
1:B:148:GLU:OE2	1:B:184:ARG:HD2	2.20	0.42
1:B:167:ILE:O	1:B:189:PHE:HA	2.20	0.42
1:B:225:THR:O	1:B:226:CYS:HB2	2.20	0.42
1:A:22:ARG:HH11	1:A:22:ARG:HG2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASP:HA	1:A:192:ILE:O	2.21	0.41
1:B:145:LEU:HD13	1:B:295:ILE:HG22	2.02	0.41
1:B:292:ILE:CA	1:B:294:MET:HE2	2.50	0.41
1:A:37:ASN:ND2	1:A:39:GLU:HB2	2.36	0.41
1:A:123:HIS:HD2	1:A:141:PRO:O	2.04	0.41
1:A:221:ASP:HA	1:A:249:THR:HG23	2.02	0.41
1:A:207:LEU:HD23	1:A:207:LEU:C	2.42	0.41
1:A:275:ILE:O	1:A:277:GLN:HG2	2.21	0.40
1:B:248:LEU:N	1:B:248:LEU:HD22	2.36	0.40
1:A:223:ALA:HB2	1:A:248:LEU:HD22	2.03	0.40
1:A:96:ARG:HG3	3:A:1057:HOH:O	2.21	0.40
1:B:294:MET:H	1:B:294:MET:HG3	1.55	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	301/326 (92%)	277 (92%)	17 (6%)	7 (2%)	6	3
1	B	304/326 (93%)	287 (94%)	14 (5%)	3 (1%)	15	14
All	All	605/652 (93%)	564 (93%)	31 (5%)	10 (2%)	9	6

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	PHE
1	A	61	GLY
1	A	253	PHE
1	B	14	ASP
1	A	10	SER
1	A	36	SER

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Mol	Chain	Res	Type
1	A	37	ASN
1	B	58	SER
1	B	60	CYS
1	A	252	ILE

### 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	258/278 (93%)	245 (95%)	13 (5%)	24	30
1	B	261/278 (94%)	254 (97%)	7 (3%)	44	57
All	All	519/556 (93%)	499 (96%)	20 (4%)	32	41

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	15	LEU
1	A	37	ASN
1	A	57	GLN
1	A	111	LEU
1	A	152	LEU
1	A	195	GLU
1	A	249	THR
1	A	261	ILE
1	A	278	GLU
1	A	286	LYS
1	A	294	MET
1	A	311	TYR
1	B	4	ILE
1	B	15	LEU
1	B	60	CYS
1	B	63	ILE
1	B	213	ASP
1	B	249	THR

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Mol	Chain	Res	Type
1	B	294	MET

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

Mol	Chain	Res	Type
1	A	3	ASN
1	A	13	GLN
1	A	37	ASN
1	A	57	GLN
1	A	66	ASN
1	A	130	HIS
1	A	277	GLN
1	B	64	ASN
1	B	123	HIS
1	B	186	ASN
1	B	263	ASN
1	B	277	GLN
1	B	288	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](#)

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	1003	-	4,4,4	0.18	0	6,6,6	0.10	0
2	SO4	A	1006	-	4,4,4	0.26	0	6,6,6	0.14	0
2	SO4	A	1004	-	4,4,4	0.20	0	6,6,6	0.07	0
2	SO4	B	1005	-	4,4,4	0.26	0	6,6,6	0.17	0
2	SO4	A	1002	-	4,4,4	0.26	0	6,6,6	0.04	0
2	SO4	B	1001	-	4,4,4	0.28	0	6,6,6	0.07	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1006	SO4	1	0
2	A	1004	SO4	1	0
2	B	1005	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, 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	305/326 (93%)	0.37	30 (9%) <b>7</b> <b>6</b>	22, 45, 81, 90	0
1	B	308/326 (94%)	-0.06	8 (2%) 56 53	20, 36, 68, 89	0
All	All	613/652 (94%)	0.15	38 (6%) <b>20</b> <b>19</b>	20, 39, 78, 90	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	HIS	5.0
1	B	36	SER	4.8
1	B	60	CYS	4.8
1	B	11	SER	4.8
1	A	60	CYS	4.7
1	A	284	CYS	4.5
1	A	258	ILE	4.4
1	A	282	LYS	4.4
1	A	61	GLY	4.3
1	A	261	ILE	4.2
1	A	253	PHE	3.8
1	A	262	ASN	3.4
1	A	11	SER	3.2
1	A	311	TYR	3.2
1	B	9	GLY	3.2
1	A	263	ASN	3.1
1	A	59	GLY	3.0
1	A	196	ARG	3.0
1	A	58	SER	2.8
1	A	12	HIS	2.8
1	A	294	MET	2.7
1	A	257	ALA	2.7
1	A	277	GLN	2.7
1	A	280	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	35	PHE	2.6
1	A	281	MET	2.5
1	A	278	GLU	2.5
1	B	314	SER	2.4
1	A	259	SER	2.4
1	B	12	HIS	2.3
1	A	37	ASN	2.3
1	A	34	LYS	2.2
1	A	41	CYS	2.2
1	B	10	SER	2.2
1	B	315	HIS	2.1
1	A	245	TYR	2.1
1	A	204	ARG	2.1
1	A	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, 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	1002	5/5	0.93	0.14	79,79,79,79	0
2	SO4	A	1006	5/5	0.97	0.12	65,65,66,68	0
2	SO4	B	1001	5/5	0.97	0.09	59,62,63,63	0
2	SO4	A	1004	5/5	0.99	0.12	33,34,38,38	0
2	SO4	B	1003	5/5	0.99	0.13	30,31,33,34	0
2	SO4	B	1005	5/5	0.99	0.11	38,39,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.