Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 10:15 am BST

PDB ID	:	1I74
Title	:	STREPTOCOCCUS MUTANS INORGANIC PYROPHOSPHATASE
Authors	:	Merckel, M.C.; Fabrichniy, I.P.; Goldman, A.; Lahti, R.; Salminen, A.
Deposited on	:	2001-03-07
Resolution	:	2.20 Å(reported)

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	:	2.11
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)	:	2.11

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	Percentile Ranks	Value
Rfree		0.256
Clashscore		20
Ramachandran outliers		1.1%
Sidechain outliers		6.0%
RSRZ outliers		7.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
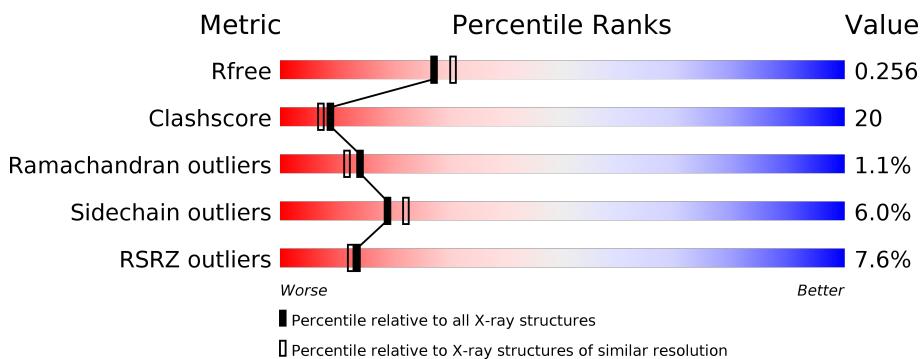
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	309	% 77% 21% •
1	B	309	14% 57% 38% 5%
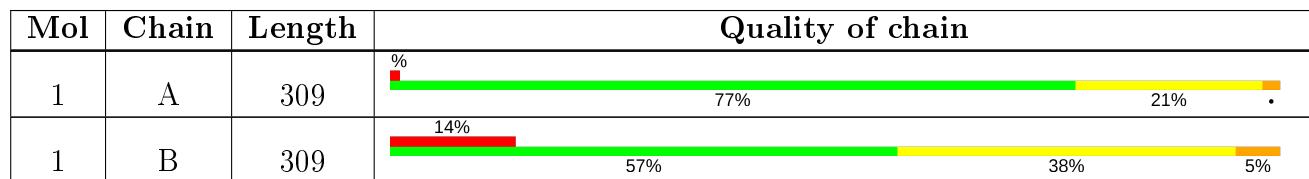
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	404	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5076 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 PROBABLE MANGANESE-DEPENDENT INORGANIC PYROPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total 2343	C 1472	N 398	O 468	Se 5	0	0	0
1	B	309	Total 2343	C 1472	N 398	O 468	Se 5	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MSE	MET	MODIFIED RESIDUE	UNP O68579
A	111	MSE	MET	MODIFIED RESIDUE	UNP O68579
A	142	MSE	MET	MODIFIED RESIDUE	UNP O68579
A	184	MSE	MET	MODIFIED RESIDUE	UNP O68579
A	253	MSE	MET	MODIFIED RESIDUE	UNP O68579
B	20	MSE	MET	MODIFIED RESIDUE	UNP O68579
B	111	MSE	MET	MODIFIED RESIDUE	UNP O68579
B	142	MSE	MET	MODIFIED RESIDUE	UNP O68579
B	184	MSE	MET	MODIFIED RESIDUE	UNP O68579
B	253	MSE	MET	MODIFIED RESIDUE	UNP O68579

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Mn 2	0	0
2	A	2	Total 2	Mn 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0

• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
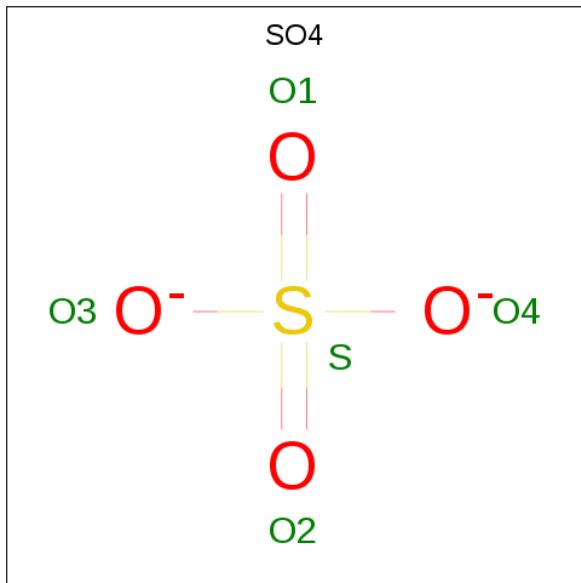
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	269	Total 269	O 269	0	0
5	B	95	Total 95	O 95	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: PROBABLE MANGANESE-DEPENDENT INORGANIC PYROPHOSPHATASE
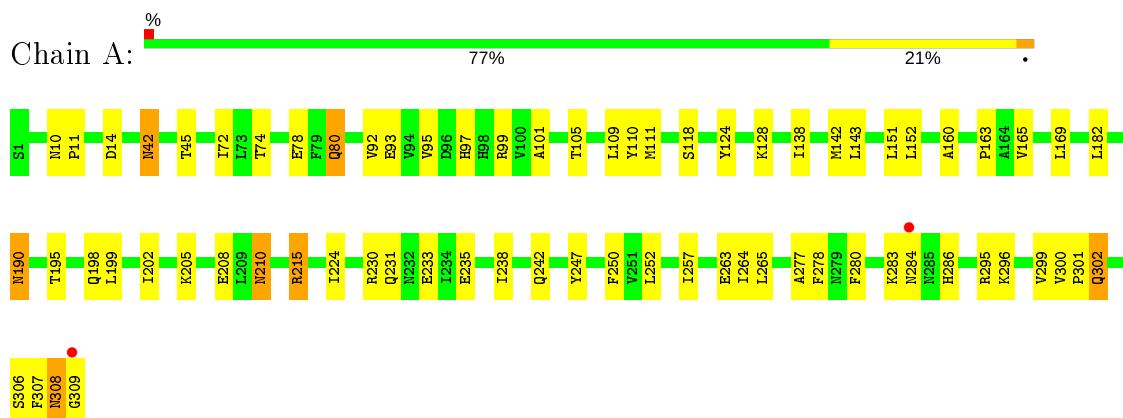
• Molecule 1: PROBABLE MANGANESE-DEPENDENT INORGANIC PYROPHOSPHATASE
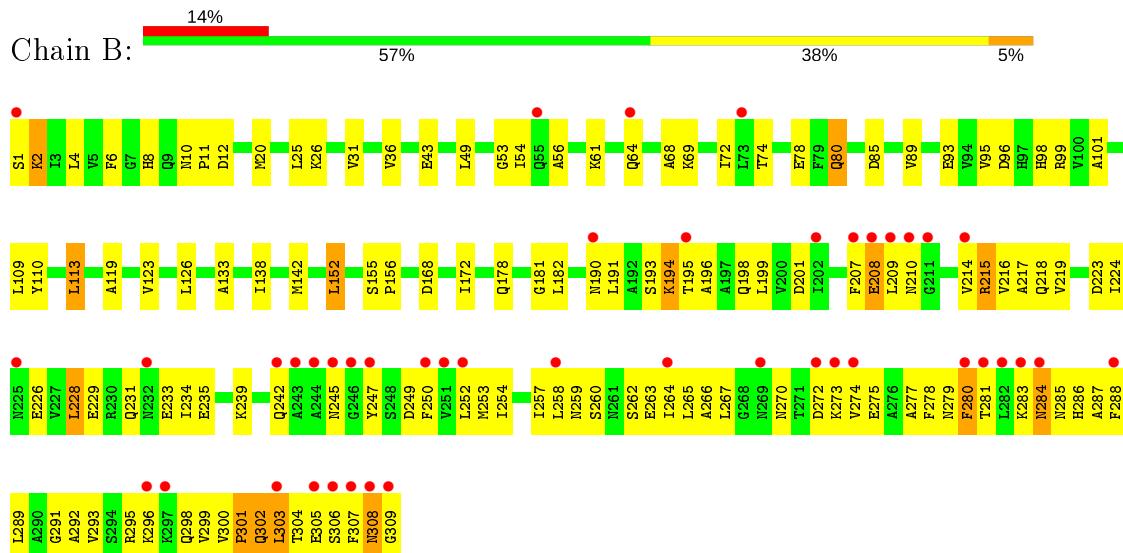
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.60Å 95.30Å 95.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 – 2.20 19.76 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.76-2.20) 91.2 (19.76-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.34 (at 2.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.257 0.208 , 0.256	Depositor DCC
R_{free} test set	3247 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å²)	26.6	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.34 , 42.5	EDS
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.29$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5076	wwPDB-VP
Average B, all atoms (Å²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MG, MN, 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	0.38	0/2372	0.61	0/3212
1	B	0.42	0/2372	0.62	0/3212
All	All	0.40	0/4744	0.62	0/6424

There are no bond length outliers.

There are no bond angle outliers.

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	2343	0	2335	65	0
1	B	2343	0	2335	125	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	2	0
4	B	10	0	0	0	0
5	A	269	0	0	12	0
5	B	95	0	0	2	0
All	All	5076	0	4670	190	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 20.

All (190) 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:296:LYS:HD2	5:A:509:HOH:O	1.47	1.14
1:B:218:GLN:HB2	1:B:253:MSE:HE3	1.32	1.11
4:A:404:SO4:O4	5:A:525:HOH:O	1.71	1.05
1:B:253:MSE:HE1	1:B:295:ARG:HB2	1.49	0.94
1:B:302:GLN:NE2	1:B:302:GLN:H	1.65	0.94
1:B:93:GLU:HG2	1:B:110:TYR:HB3	1.47	0.93
1:B:61:LYS:HA	1:B:61:LYS:HE2	1.52	0.89
1:B:302:GLN:CD	1:B:302:GLN:H	1.75	0.86
1:A:109:LEU:HD11	1:A:111:MSE:HE2	1.58	0.85
1:B:2:LYS:HA	1:B:2:LYS:HE3	1.59	0.83
1:B:178:GLN:O	1:B:182:LEU:HD13	1.81	0.80
1:B:284:ASN:O	1:B:285:ASN:HB2	1.81	0.78
1:B:96:ASP:OD1	1:B:98:HIS:HD2	1.67	0.78
1:A:215:ARG:HG3	1:A:247:TYR:CE1	2.21	0.75
1:B:257:ILE:HG13	1:B:258:LEU:HD12	1.70	0.74
1:A:42:ASN:ND2	1:A:45:THR:H	1.86	0.73
1:A:109:LEU:HD21	1:A:111:MSE:CE	2.19	0.72
1:B:218:GLN:HB2	1:B:253:MSE:CE	2.17	0.72
1:B:78:GLU:HB3	1:B:80:GLN:HE22	1.54	0.72
1:B:300:VAL:HB	1:B:301:PRO:HD3	1.72	0.71
1:B:196:ALA:HB2	1:B:233:GLU:HG2	1.72	0.71
1:A:302:GLN:NE2	1:A:302:GLN:H	1.89	0.70
1:B:193:SER:C	1:B:194:LYS:HD2	2.11	0.70
1:A:42:ASN:C	1:A:42:ASN:HD22	1.96	0.68
1:B:78:GLU:HG2	1:B:101:ALA:O	1.94	0.68
1:A:210:ASN:HB2	1:A:309:GLY:H	1.59	0.68
1:A:78:GLU:HB3	1:A:80:GLN:HE22	1.58	0.68
1:A:109:LEU:HD21	1:A:111:MSE:HE3	1.75	0.67
1:B:138:ILE:HG22	1:B:142:MSE:HE2	1.75	0.67
1:B:301:PRO:HB2	1:B:302:GLN:NE2	2.09	0.67
1:A:307:PHE:O	1:A:308:ASN:HB2	1.95	0.66
1:A:205:LYS:HD3	5:A:502:HOH:O	1.96	0.65
1:B:275:GLU:HA	1:B:280:PHE:CE2	2.32	0.65
1:B:64:GLN:HG3	1:B:85:ASP:OD2	1.96	0.64
1:B:270:ASN:HB3	1:B:273:LYS:CG	2.28	0.64
1:A:109:LEU:HD11	1:A:111:MSE:CE	2.28	0.63
1:A:302:GLN:H	1:A:302:GLN:CD	2.02	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PHE:CE2	1:A:302:GLN:HG3	2.34	0.63
1:A:93:GLU:HG2	1:A:110:TYR:HB3	1.80	0.62
1:B:49:LEU:HD13	1:B:56:ALA:HB2	1.81	0.62
1:B:193:SER:O	1:B:194:LYS:HD2	1.99	0.62
1:A:230:ARG:HD2	5:A:776:HOH:O	2.00	0.62
1:A:151:LEU:HD11	1:A:257:ILE:HG22	1.82	0.62
1:B:278:PHE:CE2	1:B:302:GLN:HG3	2.34	0.61
1:B:72:ILE:HG12	1:B:93:GLU:HB2	1.81	0.61
1:A:111:MSE:HB2	1:B:113:LEU:HB2	1.82	0.60
1:B:302:GLN:NE2	1:B:302:GLN:N	2.45	0.60
1:B:152:LEU:CD1	1:B:182:LEU:HD12	2.31	0.60
1:B:191:LEU:HD22	1:B:199:LEU:CD2	2.33	0.59
1:B:301:PRO:HD2	1:B:302:GLN:NE2	2.17	0.59
1:A:230:ARG:HD3	5:A:775:HOH:O	2.02	0.58
1:B:210:ASN:N	1:B:210:ASN:HD22	2.01	0.58
1:B:291:GLY:O	1:B:298:GLN:NE2	2.36	0.58
1:A:14:ASP:HB3	5:A:406:HOH:O	2.01	0.58
1:A:277:ALA:HB2	1:A:306:SER:OG	2.03	0.58
1:A:78:GLU:HG2	1:A:101:ALA:O	2.03	0.58
1:A:224:ILE:HD13	1:A:263:GLU:HB2	1.85	0.58
1:B:223:ASP:OD2	1:B:226:GLU:HB2	2.03	0.58
1:B:301:PRO:HB2	1:B:302:GLN:HE22	1.68	0.58
1:B:253:MSE:SE	1:B:299:VAL:HG21	2.54	0.57
1:A:72:ILE:HG12	1:A:93:GLU:HB2	1.85	0.57
1:A:42:ASN:HD21	1:A:45:THR:H	1.52	0.57
1:A:231:GLN:O	1:A:235:GLU:HG3	2.05	0.56
1:B:195:THR:HG23	1:B:198:GLN:OE1	2.06	0.56
1:B:270:ASN:HB3	1:B:273:LYS:HG3	1.87	0.56
1:B:195:THR:N	1:B:198:GLN:OE1	2.27	0.55
1:A:10:ASN:N	1:A:11:PRO:HD3	2.22	0.55
1:B:214:VAL:HG13	1:B:249:ASP:HB2	1.89	0.55
1:B:152:LEU:HD13	1:B:182:LEU:HD12	1.89	0.55
1:B:10:ASN:N	1:B:11:PRO:HD3	2.23	0.54
1:B:283:LYS:O	1:B:284:ASN:HB3	2.08	0.54
1:B:296:LYS:HA	1:B:300:VAL:CG2	2.38	0.54
1:A:300:VAL:HB	1:A:301:PRO:HD3	1.89	0.53
1:B:306:SER:C	1:B:308:ASN:H	2.12	0.53
1:B:78:GLU:HB3	1:B:80:GLN:NE2	2.21	0.53
1:A:264:ILE:O	1:A:286:HIS:HA	2.09	0.53
1:B:168:ASP:O	1:B:172:ILE:HG13	2.09	0.52
1:B:245:ASN:HB2	1:B:247:TYR:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:THR:OG1	1:A:198:GLN:HG3	2.09	0.52
1:B:195:THR:OG1	1:B:198:GLN:HG3	2.10	0.52
1:B:216:VAL:HG12	1:B:295:ARG:HD3	1.91	0.52
1:A:138:ILE:HG22	1:A:142:MSE:HE2	1.91	0.52
1:B:273:LYS:HD2	1:B:307:PHE:HA	1.92	0.52
1:B:20:MSE:HE1	1:B:54:ILE:HD12	1.91	0.52
1:B:26:LYS:HB3	1:B:31:VAL:HB	1.92	0.52
1:B:303:LEU:O	1:B:307:PHE:HD1	1.93	0.52
1:B:301:PRO:HD2	1:B:302:GLN:HE22	1.73	0.52
1:A:80:GLN:HG3	5:A:555:HOH:O	2.11	0.51
1:B:242:GLN:HA	1:B:247:TYR:HB2	1.92	0.51
1:B:253:MSE:CE	1:B:295:ARG:HB2	2.30	0.51
1:A:109:LEU:N	1:A:109:LEU:HD23	2.26	0.51
1:B:262:SER:HB2	1:B:292:ALA:HB3	1.91	0.51
1:B:273:LYS:O	1:B:306:SER:OG	2.27	0.51
1:B:93:GLU:HA	1:B:110:TYR:O	2.11	0.51
1:B:217:ALA:HB3	1:B:252:LEU:HD23	1.92	0.51
1:B:8:HIS:O	1:B:11:PRO:HG3	2.10	0.51
1:B:96:ASP:OD1	1:B:98:HIS:CD2	2.58	0.50
1:B:2:LYS:HA	1:B:2:LYS:CE	2.38	0.50
1:B:275:GLU:HA	1:B:280:PHE:CD2	2.46	0.50
1:A:205:LYS:HG2	5:A:503:HOH:O	2.11	0.49
1:B:301:PRO:CD	1:B:302:GLN:NE2	2.75	0.49
1:A:105:THR:HG21	1:A:109:LEU:HD13	1.95	0.49
1:A:277:ALA:HB1	1:A:302:GLN:HB2	1.94	0.49
1:B:283:LYS:O	1:B:284:ASN:CB	2.61	0.49
1:B:275:GLU:HA	1:B:280:PHE:HE2	1.76	0.49
1:A:78:GLU:HB3	1:A:80:GLN:NE2	2.26	0.48
1:B:301:PRO:CB	1:B:302:GLN:NE2	2.77	0.48
1:B:215:ARG:HG2	1:B:247:TYR:CE1	2.48	0.48
1:A:198:GLN:O	1:A:202:ILE:HG13	2.14	0.48
1:B:43:GLU:HG3	1:B:190:ASN:HB2	1.96	0.48
1:A:302:GLN:N	1:A:302:GLN:CD	2.66	0.48
1:A:238:ILE:O	1:A:242:GLN:HG3	2.14	0.48
1:B:224:ILE:HG22	1:B:228:LEU:HD22	1.95	0.47
1:B:263:GLU:OE2	1:B:286:HIS:ND1	2.48	0.47
1:B:302:GLN:CD	1:B:302:GLN:N	2.56	0.47
1:B:119:ALA:O	1:B:123:VAL:HG23	2.14	0.47
1:B:109:LEU:N	1:B:109:LEU:HD23	2.29	0.47
1:A:265:LEU:C	1:A:265:LEU:HD23	2.35	0.47
1:B:265:LEU:HD23	1:B:266:ALA:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:HG23	1:A:250:PHE:CG	2.49	0.47
1:B:214:VAL:HG13	1:B:249:ASP:CB	2.45	0.47
1:B:6:PHE:HB3	1:B:36:VAL:HG23	1.96	0.47
1:A:208:GLU:O	1:A:208:GLU:OE2	2.34	0.46
1:B:263:GLU:OE1	1:B:288:PHE:HA	2.15	0.46
1:A:97:HIS:CE1	1:A:118:SER:HA	2.50	0.46
1:A:109:LEU:CD2	1:A:111:MSE:HE3	2.42	0.46
1:A:295:ARG:HB3	4:A:404:SO4:O4	2.16	0.46
1:B:257:ILE:HG13	1:B:258:LEU:CD1	2.43	0.46
1:B:301:PRO:O	1:B:305:GLU:N	2.47	0.46
1:B:273:LYS:O	1:B:306:SER:CB	2.64	0.46
1:B:217:ALA:HB3	1:B:252:LEU:CD2	2.46	0.45
1:B:226:GLU:O	1:B:229:GLU:HB2	2.16	0.45
1:B:74:THR:HA	1:B:95:VAL:O	2.17	0.45
1:A:307:PHE:O	1:A:308:ASN:CB	2.64	0.45
1:B:289:LEU:HG	1:B:292:ALA:HB2	1.99	0.45
1:B:215:ARG:HG2	1:B:247:TYR:CZ	2.52	0.45
1:A:42:ASN:C	1:A:42:ASN:ND2	2.68	0.45
1:B:296:LYS:O	1:B:301:PRO:HD3	2.17	0.44
1:A:301:PRO:HD2	1:A:302:GLN:NE2	2.33	0.44
1:B:235:GLU:HB3	1:B:267:LEU:HD11	2.00	0.44
1:B:274:VAL:O	1:B:277:ALA:HB3	2.18	0.44
1:B:278:PHE:HB2	1:B:280:PHE:CZ	2.53	0.44
1:A:124:TYR:CE1	1:A:128:LYS:HE2	2.53	0.44
1:A:143:LEU:HB2	1:A:169:LEU:HB3	2.00	0.44
1:B:259:ASN:O	1:B:260:SER:HB2	2.17	0.44
1:B:196:ALA:HB2	1:B:233:GLU:CG	2.44	0.43
1:B:1:SER:O	1:B:2:LYS:HB3	2.18	0.43
1:A:160:ALA:O	1:A:163:PRO:HD2	2.18	0.43
1:A:230:ARG:NH1	5:A:857:HOH:O	2.21	0.43
1:B:152:LEU:HD11	1:B:181:GLY:HA3	1.99	0.43
1:B:209:LEU:HD12	1:B:214:VAL:HG21	2.00	0.43
1:B:235:GLU:O	1:B:239:LYS:HG3	2.18	0.43
1:B:280:PHE:CD1	1:B:287:ALA:HB3	2.54	0.43
1:B:4:LEU:HD13	1:B:68:ALA:CB	2.49	0.43
1:A:165:VAL:HG12	1:A:169:LEU:HD23	1.99	0.43
1:B:133:ALA:HB3	5:B:812:HOH:O	2.18	0.43
1:A:299:VAL:O	1:A:302:GLN:HG2	2.18	0.43
1:B:231:GLN:O	1:B:234:ILE:HB	2.18	0.43
1:B:277:ALA:HB1	1:B:302:GLN:HB2	2.00	0.43
1:B:80:GLN:NE2	1:B:80:GLN:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ILE:O	1:B:286:HIS:HA	2.18	0.43
1:B:301:PRO:O	1:B:304:THR:HB	2.18	0.43
1:A:199:LEU:C	1:A:199:LEU:HD23	2.39	0.43
1:B:273:LYS:O	1:B:277:ALA:HB2	2.18	0.43
1:B:69:LYS:O	1:B:89:VAL:HB	2.19	0.42
1:B:199:LEU:C	1:B:201:ASP:H	2.22	0.42
1:B:208:GLU:OE1	1:B:210:ASN:N	2.52	0.42
1:B:228:LEU:HA	1:B:228:LEU:HD12	1.83	0.42
1:B:306:SER:C	1:B:308:ASN:N	2.72	0.42
1:A:190:ASN:ND2	1:A:190:ASN:C	2.72	0.42
1:B:1:SER:O	1:B:2:LYS:CB	2.68	0.42
1:A:92:VAL:O	1:A:109:LEU:HB2	2.19	0.42
1:A:278:PHE:CE2	1:A:302:GLN:CG	3.01	0.42
1:B:295:ARG:O	1:B:299:VAL:HB	2.19	0.42
1:B:301:PRO:CD	1:B:302:GLN:HE22	2.31	0.42
1:B:219:VAL:O	1:B:219:VAL:HG23	2.20	0.42
1:B:258:LEU:HD12	1:B:258:LEU:N	2.35	0.42
1:B:219:VAL:CG2	1:B:254:ILE:HA	2.49	0.41
1:B:278:PHE:CE1	1:B:303:LEU:HD13	2.54	0.41
1:B:155:SER:OG	1:B:156:PRO:HD2	2.20	0.41
1:B:207:PHE:CD1	1:B:207:PHE:N	2.88	0.41
1:B:215:ARG:HD2	5:B:623:HOH:O	2.20	0.41
1:B:308:ASN:O	1:B:309:GLY:OXT	2.39	0.41
1:A:42:ASN:HB2	5:A:660:HOH:O	2.20	0.41
1:B:305:GLU:O	1:B:308:ASN:HA	2.20	0.41
1:A:74:THR:HA	1:A:95:VAL:O	2.21	0.41
1:A:283:LYS:HB2	5:A:617:HOH:O	2.20	0.41
1:A:233:GLU:HG3	5:A:673:HOH:O	2.21	0.40
1:A:109:LEU:HD21	1:A:111:MSE:HE1	1.98	0.40
1:B:265:LEU:HD23	1:B:265:LEU:C	2.41	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	307/309 (99%)	295 (96%)	11 (4%)	1 (0%)	41	46
1	B	307/309 (99%)	274 (89%)	27 (9%)	6 (2%)	7	4
All	All	614/618 (99%)	569 (93%)	38 (6%)	7 (1%)	14	12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	ASN
1	B	284	ASN
1	B	308	ASN
1	B	279	ASN
1	B	301	PRO
1	B	53	GLY
1	B	293	VAL

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	252/247 (102%)	240 (95%)	12 (5%)	25	32
1	B	252/247 (102%)	234 (93%)	18 (7%)	14	16
All	All	504/494 (102%)	474 (94%)	30 (6%)	19	22

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	80	GLN
1	A	99	ARG
1	A	152	LEU
1	A	182	LEU
1	A	190	ASN

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Mol	Chain	Res	Type
1	A	210	ASN
1	A	215	ARG
1	A	252	LEU
1	A	280	PHE
1	A	284	ASN
1	A	302	GLN
1	B	2	LYS
1	B	12	ASP
1	B	25	LEU
1	B	80	GLN
1	B	99	ARG
1	B	113	LEU
1	B	126	LEU
1	B	152	LEU
1	B	194	LYS
1	B	208	GLU
1	B	215	ARG
1	B	228	LEU
1	B	250	PHE
1	B	272	ASP
1	B	280	PHE
1	B	281	THR
1	B	302	GLN
1	B	303	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	28	GLN
1	A	34	GLN
1	A	42	ASN
1	A	70	GLN
1	A	80	GLN
1	A	190	ASN
1	A	210	ASN
1	A	218	GLN
1	A	302	GLN
1	A	308	ASN
1	B	34	GLN
1	B	55	GLN
1	B	70	GLN

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Mol	Chain	Res	Type
1	B	80	GLN
1	B	98	HIS
1	B	178	GLN
1	B	210	ASN
1	B	245	ASN
1	B	269	ASN
1	B	284	ASN
1	B	302	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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	$\#|Z| > 2$
4	SO4	A	404	3	4,4,4	0.36	0	6,6,6	0.14	0
4	SO4	B	1404	-	4,4,4	0.43	0	6,6,6	0.09	0
4	SO4	A	405	3,2	4,4,4	0.24	0	6,6,6	0.14	0
4	SO4	B	1405	3,2	4,4,4	0.54	0	6,6,6	0.13	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	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 (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	304/309 (98%)	-0.36	2 (0%)	87	86	16, 24, 37, 51	0
1	B	304/309 (98%)	0.56	44 (14%)	2	2	18, 40, 70, 78	0
All	All	608/618 (98%)	0.10	46 (7%)	13	12	16, 29, 65, 78	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	GLY	6.8
1	B	269	ASN	5.5
1	B	308	ASN	5.4
1	B	251	VAL	5.2
1	B	210	ASN	5.1
1	B	281	THR	5.0
1	B	307	PHE	4.9
1	A	309	GLY	4.7
1	B	244	ALA	4.6
1	B	288	PHE	4.4
1	B	243	ALA	4.0
1	B	246	GLY	3.9
1	B	280	PHE	3.9
1	B	306	SER	3.8
1	B	225	ASN	3.7
1	B	252	LEU	3.5
1	B	64	GLN	3.1
1	B	211	GLY	3.1
1	B	284	ASN	3.1
1	B	273	LYS	3.0
1	B	209	LEU	3.0
1	B	282	LEU	3.0
1	B	283	LYS	3.0
1	B	250	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	305	GLU	2.9
1	B	247	TYR	2.7
1	B	55	GLN	2.7
1	B	208	GLU	2.5
1	B	195	THR	2.4
1	B	242	GLN	2.4
1	B	264	ILE	2.4
1	B	296	LYS	2.4
1	B	207	PHE	2.4
1	B	232	ASN	2.4
1	B	214	VAL	2.3
1	B	297	LYS	2.3
1	B	258	LEU	2.2
1	B	272	ASP	2.2
1	B	245	ASN	2.2
1	B	202	ILE	2.2
1	B	190	ASN	2.1
1	B	303	LEU	2.1
1	B	1	SER	2.1
1	A	284	ASN	2.1
1	B	73	LEU	2.0
1	B	274	VAL	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 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. 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
3	MG	B	1403	1/1	0.65	0.35	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
4	SO4	B	1405	5/5	0.91	0.18	51,51,53,54	0
3	MG	A	403	1/1	0.94	0.06	26,26,26,26	0
4	SO4	B	1404	5/5	0.95	0.20	61,61,61,62	0
4	SO4	A	404	5/5	0.96	0.11	34,35,36,38	0
2	MN	B	401	1/1	0.97	0.04	38,38,38,38	0
4	SO4	A	405	5/5	0.99	0.06	20,22,24,25	0
2	MN	A	402	1/1	0.99	0.06	24,24,24,24	0
2	MN	A	401	1/1	0.99	0.04	29,29,29,29	0
2	MN	B	402	1/1	0.99	0.06	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.