Full wwPDB X-ray Structure Validation Report (i)

May 24, 2020 – 03:25 am BST

PDB ID	:	5FF5
Title	:	Crystal Structure of SeMet PaaA
Authors	:	Biernat, K.B.; Redinbo, M.R.
Deposited on	:	2015-12-17
Resolution	:	2.93 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 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 (i)

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

The reported resolution of this entry is 2.93 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		0.287
Clashscore		19
Ramachandran outliers		1.0%
Sidechain outliers		2.2%
RSRZ outliers		7.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
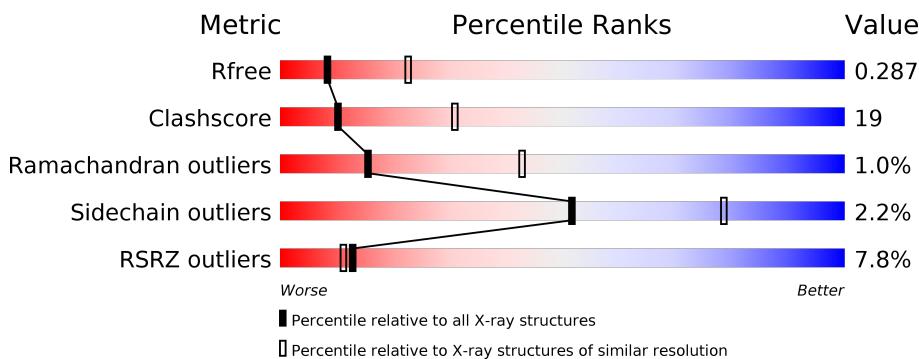
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	381	7% 56% 28% • 15%
1	B	381	6% 53% 25% • 20%
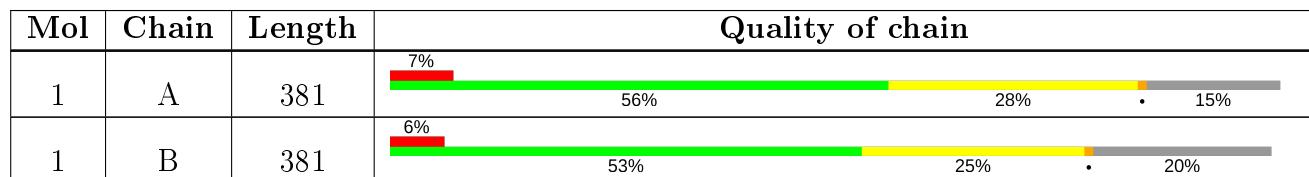
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	402	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4760 atoms, of which 24 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 PaaA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	323	Total 2414	C 1533	N 417	O 458	S 2	Se 4	0	2	0
1	B	303	Total 2271	C 1434	N 394	O 439	S 1	Se 3	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	374	LEU	-	expression tag	UNP Q9ZAR3
A	375	GLU	-	expression tag	UNP Q9ZAR3
A	376	HIS	-	expression tag	UNP Q9ZAR3
A	377	HIS	-	expression tag	UNP Q9ZAR3
A	378	HIS	-	expression tag	UNP Q9ZAR3
A	379	HIS	-	expression tag	UNP Q9ZAR3
A	380	HIS	-	expression tag	UNP Q9ZAR3
A	381	HIS	-	expression tag	UNP Q9ZAR3
B	374	LEU	-	expression tag	UNP Q9ZAR3
B	375	GLU	-	expression tag	UNP Q9ZAR3
B	376	HIS	-	expression tag	UNP Q9ZAR3
B	377	HIS	-	expression tag	UNP Q9ZAR3
B	378	HIS	-	expression tag	UNP Q9ZAR3
B	379	HIS	-	expression tag	UNP Q9ZAR3
B	380	HIS	-	expression tag	UNP Q9ZAR3
B	381	HIS	-	expression tag	UNP Q9ZAR3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4
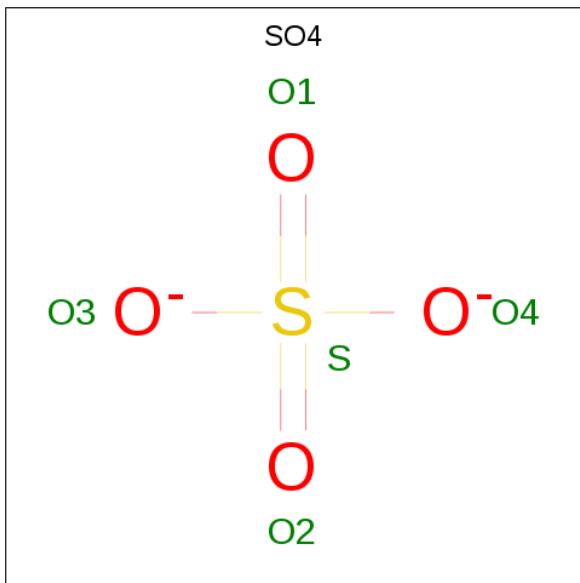
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
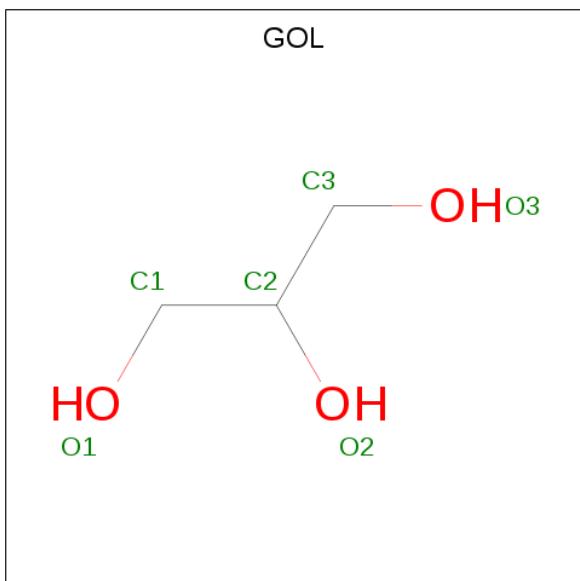
GOL

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ni	0	0
			1	1		

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	3	Total	O	0	0
			3	3		

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 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: PaaA
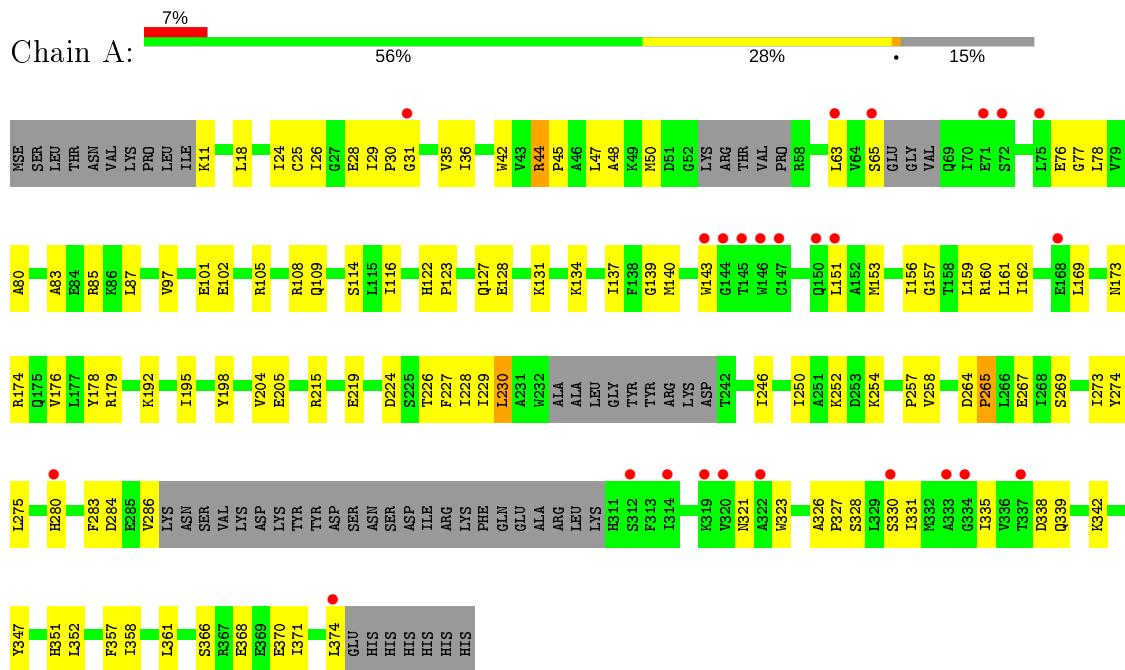
- Molecule 1: PaaA
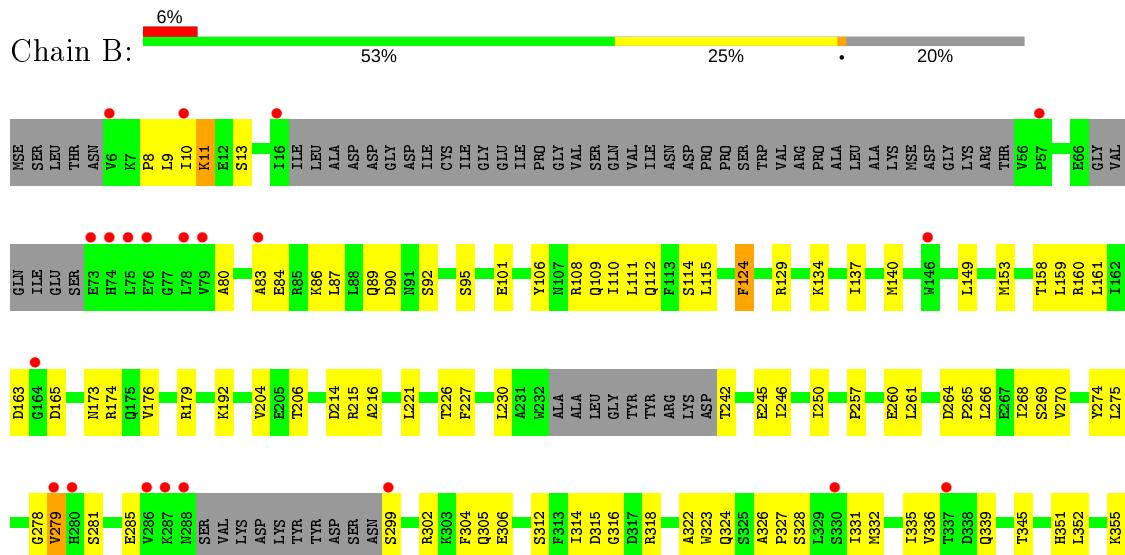
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	68.96Å 170.41Å 64.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 2.93 29.48 – 2.93	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.48-2.93) 98.5 (29.48-2.93)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	5.47 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.210 , 0.289 0.223 , 0.287	Depositor DCC
R_{free} test set	1683 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å^2)	66.3	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 64.5	EDS
L-test for twinning[2]	$<|L|> = 0.45$, $<L^2> = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4760	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: GOL, SO4, NI

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	0.47	0/2450	0.63	0/3318
1	B	0.46	0/2304	0.68	1/3116 (0.0%)
All	All	0.46	0/4754	0.65	1/6434 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	278	GLY	N-CA-C	-5.83	98.54	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	2414	0	2287	100	0
1	B	2271	0	2125	92	0
2	A	10	0	0	0	0
2	B	10	0	0	2	0
3	A	18	24	24	0	0
4	B	1	0	0	0	0
5	A	9	0	0	0	0
5	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4736	24	4436	172	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 19.

All (172) 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:24:ILE:HD11	1:A:36:ILE:HD12	1.22	1.18
1:A:47:LEU:HA	1:A:50:MSE:HE3	1.41	1.03
1:B:134:LYS:HE3	1:B:158:THR:HG21	1.39	1.03
1:A:176:VAL:HG23	1:B:153:MSE:HE1	1.44	1.00
1:B:134:LYS:HG3	1:B:158:THR:HB	1.41	0.99
1:B:149:LEU:HD11	1:B:153:MSE:HE3	1.49	0.95
1:A:24:ILE:HD11	1:A:36:ILE:CD1	2.04	0.87
1:A:24:ILE:CD1	1:A:36:ILE:HD12	2.07	0.83
1:A:351:HIS:NE2	1:A:368:GLU:OE2	2.10	0.83
1:B:339:GLN:HG3	1:B:352:LEU:HD22	1.59	0.82
1:B:134:LYS:HG3	1:B:158:THR:CB	2.12	0.79
1:A:18:LEU:HD22	1:B:314:ILE:HD11	1.65	0.79
1:B:149:LEU:CD1	1:B:153:MSE:HE3	2.12	0.78
1:A:230:LEU:HD11	1:A:258:VAL:CG1	2.17	0.75
1:A:160:ARG:NH1	1:A:205:GLU:OE1	2.20	0.74
1:A:116:ILE:HD11	1:B:266:LEU:HD21	1.69	0.74
1:A:280:HIS:CD2	1:A:374:LEU:HA	2.23	0.74
1:B:356:LYS:HE2	1:B:358:ILE:HD11	1.71	0.73
1:A:153:MSE:HE1	1:B:176:VAL:HA	1.70	0.72
1:A:161:LEU:C	1:A:162:ILE:HD13	2.10	0.71
1:A:47:LEU:HD23	1:A:50:MSE:HE1	1.72	0.71
1:A:108[B]:ARG:HD3	1:B:322:ALA:O	1.91	0.70
1:A:44:ARG:NH2	1:B:314:ILE:HD12	2.06	0.70
1:A:26:ILE:CG2	1:A:87:LEU:HD23	2.22	0.70
1:B:356:LYS:HE2	1:B:358:ILE:CD1	2.22	0.70
1:B:134:LYS:H	1:B:226:THR:HB	1.58	0.69
1:B:264:ASP:HB2	1:B:265:PRO:HD2	1.74	0.69
1:B:302:ARG:O	1:B:306:GLU:HG2	1.92	0.69
1:A:176:VAL:HG23	1:B:153:MSE:CE	2.21	0.68
1:B:108:ARG:NH2	2:B:402:SO4:O1	2.28	0.67
1:A:24:ILE:CG1	1:A:36:ILE:HB	2.25	0.67
1:A:246:ILE:O	1:A:250:ILE:HG13	1.94	0.67
1:A:230:LEU:HD11	1:A:258:VAL:HG13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ARG:HH11	1:A:174:ARG:HG2	1.59	0.66
1:B:285:GLU:OE1	1:B:285:GLU:N	2.28	0.66
1:B:351:HIS:NE2	1:B:368:GLU:OE2	2.29	0.66
1:A:137:ILE:CG2	1:A:140:MSE:HE1	2.26	0.65
1:A:85:ARG:O	1:A:87:LEU:HD12	1.96	0.65
1:B:137:ILE:HB	1:B:140:MSE:HE1	1.80	0.64
1:B:134:LYS:CE	1:B:158:THR:HG21	2.22	0.64
1:A:24:ILE:HG13	1:A:36:ILE:HB	1.80	0.64
1:A:44:ARG:HH21	1:B:314:ILE:HG23	1.63	0.64
1:A:18:LEU:CD2	1:B:314:ILE:HD11	2.29	0.62
1:A:102:GLU:HA	1:A:105:ARG:HG2	1.82	0.61
1:B:261:LEU:HD22	1:B:336:VAL:HG21	1.82	0.61
1:A:101:GLU:OE2	1:A:105:ARG:HD2	2.01	0.61
1:B:174:ARG:HG2	1:B:174:ARG:HH11	1.65	0.61
1:B:9:LEU:HB3	1:B:89:GLN:HB3	1.83	0.61
1:A:338:ASP:OD2	1:A:342:LYS:HE2	2.01	0.60
1:B:149:LEU:CG	1:B:153:MSE:HE3	2.31	0.60
1:A:230:LEU:CD1	1:A:258:VAL:HG13	2.32	0.60
1:A:331:ILE:O	1:A:335:ILE:HG13	2.01	0.59
1:B:106:TYR:O	1:B:110:ILE:HG13	2.01	0.59
1:A:137:ILE:HG21	1:A:140:MSE:HE1	1.83	0.59
1:A:47:LEU:HD23	1:A:50:MSE:CE	2.32	0.59
1:B:80:ALA:O	1:B:83:ALA:HB3	2.04	0.58
1:A:76:GLU:O	1:A:80:ALA:N	2.30	0.58
1:A:18:LEU:HD22	1:B:314:ILE:CD1	2.34	0.57
1:A:48:ALA:O	1:B:316:GLY:HA3	2.04	0.57
1:B:192:LYS:HG3	1:B:204:VAL:HB	1.87	0.56
1:A:139:GLY:O	1:A:140:MSE:HE2	2.05	0.56
1:A:42:TRP:O	1:A:45:PRO:HD2	2.06	0.56
1:A:140:MSE:SE	1:A:161:LEU:HD22	2.55	0.56
1:B:356:LYS:HG2	1:B:358:ILE:HD11	1.89	0.55
1:A:134:LYS:NZ	1:A:224:ASP:OD1	2.38	0.54
1:A:339:GLN:HG3	1:A:352:LEU:HD22	1.90	0.54
1:B:11:LYS:HE2	1:B:114:SER:OG	2.07	0.54
1:B:84:GLU:C	1:B:86:LYS:H	2.10	0.54
1:A:215:ARG:NE	1:A:219:GLU:OE2	2.24	0.54
1:A:228:ILE:HG22	1:A:230:LEU:HD12	1.90	0.53
1:A:250:ILE:O	1:A:254:LYS:HG3	2.08	0.53
1:B:192:LYS:HE3	1:B:204:VAL:HB	1.89	0.53
1:A:370:GLU:O	1:A:371:ILE:HD13	2.08	0.53
1:A:342:LYS:HG2	1:A:347:TYR:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:PRO:HA	1:B:274:TYR:O	2.10	0.52
1:B:174:ARG:NE	2:B:401:SO4:O4	2.42	0.52
1:A:25:CYS:HB3	1:B:304:PHE:CD1	2.45	0.52
1:A:77:GLY:HA2	1:A:80:ALA:HB3	1.92	0.52
1:B:315:ASP:OD1	1:B:318:ARG:NH2	2.42	0.52
1:A:226:THR:O	1:A:257:PRO:HD2	2.10	0.51
1:A:269:SER:HA	1:A:357:PHE:O	2.11	0.51
1:A:159:LEU:HD12	1:A:195:ILE:HD13	1.94	0.50
1:A:264:ASP:HB2	1:A:265:PRO:HD2	1.93	0.50
1:A:280:HIS:NE2	1:A:374:LEU:HG	2.26	0.50
1:A:179[B]:ARG:CZ	1:B:179:ARG:HH11	2.24	0.50
1:A:101:GLU:O	1:A:101:GLU:HG2	2.10	0.50
1:A:140:MSE:HB3	1:A:178:TYR:OH	2.12	0.50
1:A:143:TRP:HZ3	1:A:229:ILE:HG22	1.76	0.50
1:A:323:TRP:CZ3	1:B:115:LEU:HD13	2.47	0.49
1:B:269:SER:HB2	1:B:358:ILE:CD1	2.43	0.49
1:A:26:ILE:HG22	1:A:87:LEU:HD23	1.91	0.49
1:A:122:HIS:ND1	1:A:123:PRO:HD2	2.28	0.49
1:A:169:LEU:HD21	1:B:101:GLU:HG2	1.94	0.49
1:A:192:LYS:HG3	1:A:204:VAL:HB	1.95	0.48
1:A:26:ILE:HG21	1:A:87:LEU:HD23	1.94	0.48
1:B:140:MSE:HB2	1:B:163:ASP:HB2	1.96	0.48
1:A:174:ARG:NH1	1:A:174:ARG:HG2	2.26	0.48
1:A:97:VAL:HB	1:A:128:GLU:HG2	1.96	0.48
1:B:174:ARG:HG2	1:B:174:ARG:NH1	2.29	0.48
1:B:270:VAL:HG13	1:B:336:VAL:HG22	1.95	0.48
1:B:134:LYS:HG3	1:B:158:THR:CG2	2.44	0.48
1:B:242:THR:O	1:B:245:GLU:N	2.46	0.48
1:A:257:PRO:HA	1:A:274:TYR:O	2.15	0.47
1:A:286:VAL:HG11	1:A:371:ILE:HG22	1.97	0.47
1:B:109:GLN:O	1:B:112:GLN:HB3	2.15	0.47
1:A:162:ILE:N	1:A:162:ILE:HD13	2.29	0.47
1:A:151:LEU:HD22	1:A:156:ILE:HD13	1.97	0.46
1:B:149:LEU:HG	1:B:153:MSE:HE3	1.97	0.46
1:A:252:LYS:NZ	1:A:284:ASP:HB2	2.31	0.46
1:B:268:ILE:HD12	1:B:332:MSE:HB3	1.98	0.46
1:B:302:ARG:O	1:B:305:GLN:HB3	2.15	0.46
1:A:173:ASN:OD1	1:A:174:ARG:HG2	2.15	0.46
1:A:161:LEU:O	1:A:162:ILE:HD13	2.16	0.46
1:B:356:LYS:CE	1:B:358:ILE:HD11	2.42	0.46
1:A:230:LEU:HD13	1:A:230:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ALA:N	1:A:327:PRO:CD	2.79	0.46
1:B:204:VAL:HG12	1:B:206:THR:HG23	1.97	0.46
1:A:283:PHE:O	1:A:286:VAL:HG22	2.16	0.45
1:A:321:ASN:HB2	1:B:111:LEU:HD11	1.98	0.45
1:B:173:ASN:OD1	1:B:174:ARG:HG2	2.15	0.45
1:B:160:ARG:HD3	1:B:221:LEU:O	2.16	0.45
1:A:137:ILE:CG2	1:A:140:MSE:CE	2.94	0.45
1:A:267:GLU:O	1:A:267:GLU:HG3	2.15	0.45
1:B:230:LEU:O	1:B:260:GLU:HA	2.17	0.45
1:B:227:PHE:CE1	1:B:257:PRO:HB2	2.51	0.45
1:B:355:LYS:HA	1:B:369:GLU:O	2.17	0.45
1:A:35:VAL:HG11	1:B:299:SER:CB	2.47	0.44
1:A:179[B]:ARG:HH11	1:A:179[B]:ARG:HG3	1.82	0.44
1:B:285:GLU:N	1:B:285:GLU:CD	2.71	0.44
1:B:260:GLU:O	1:B:261:LEU:HB3	2.18	0.44
1:A:169:LEU:HD21	1:B:101:GLU:CG	2.47	0.44
1:B:265:PRO:HD3	1:B:324:GLN:OE1	2.17	0.44
1:A:42:TRP:HH2	1:A:78:LEU:HB2	1.82	0.44
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.53	0.44
1:B:215:ARG:HG3	1:B:215:ARG:O	2.18	0.43
1:B:281:SER:OG	1:B:372:PHE:HB2	2.18	0.43
1:A:80:ALA:O	1:A:83:ALA:HB3	2.18	0.43
1:B:163:ASP:OD2	1:B:165:ASP:HB2	2.19	0.43
1:B:264:ASP:HB2	1:B:265:PRO:CD	2.46	0.43
1:A:28:GLU:CD	1:B:323:TRP:HE1	2.22	0.43
1:B:87:LEU:HD23	1:B:87:LEU:HA	1.81	0.43
1:A:109:GLN:NE2	1:A:127:GLN:OE1	2.46	0.43
1:A:29:ILE:O	1:A:31:GLY:HA3	2.17	0.43
1:A:358:ILE:O	1:A:366:SER:HA	2.19	0.43
1:B:95:SER:HB2	1:B:124:PHE:CG	2.54	0.43
1:B:314:ILE:HG22	1:B:314:ILE:O	2.19	0.43
1:B:358:ILE:O	1:B:366:SER:HA	2.19	0.43
1:B:246:ILE:O	1:B:250:ILE:HG13	2.18	0.42
1:A:63:LEU:C	1:A:65:SER:H	2.23	0.42
1:A:374:LEU:N	1:A:374:LEU:HD12	2.34	0.42
1:B:214:ASP:OD1	1:B:216:ALA:N	2.52	0.42
1:B:270:VAL:HG21	1:B:335:ILE:HB	2.01	0.42
1:A:323:TRP:CE3	1:B:115:LEU:HD13	2.55	0.42
1:A:11:LYS:HE2	1:A:114:SER:OG	2.19	0.41
1:B:140:MSE:HE3	1:B:161:LEU:HB3	2.02	0.41
1:B:356:LYS:HG2	1:B:358:ILE:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:THR:O	1:B:257:PRO:HD2	2.20	0.41
1:B:129:ARG:NH1	1:B:345:THR:O	2.49	0.41
1:A:134:LYS:HB3	1:A:134:LYS:HE2	1.74	0.41
1:A:361:LEU:HA	1:A:361:LEU:HD23	1.61	0.41
1:A:176:VAL:HG22	1:A:176:VAL:O	2.19	0.41
1:B:279:VAL:HG22	1:B:279:VAL:O	2.21	0.41
1:A:42:TRP:C	1:A:45:PRO:HD2	2.42	0.41
1:A:227:PHE:CE1	1:A:257:PRO:HB2	2.55	0.41
1:B:281:SER:HB2	1:B:372:PHE:CD1	2.56	0.40
1:A:131:LYS:O	1:A:157:GLY:HA3	2.22	0.40
1:A:273:ILE:HD11	1:A:339:GLN:HB3	2.03	0.40
1:B:326:ALA:N	1:B:327:PRO:CD	2.85	0.40
1:B:331:ILE:O	1:B:335:ILE:HG13	2.21	0.40
1:B:90:ASP:C	1:B:92:SER:H	2.25	0.40
1:A:105:ARG:NH1	1:A:198:TYR:O	2.54	0.40
1:B:230:LEU:C	1:B:230:LEU:HD12	2.42	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	315/381 (83%)	295 (94%)	18 (6%)	2 (1%)	25	56
1	B	293/381 (77%)	273 (93%)	16 (6%)	4 (1%)	11	34
All	All	608/762 (80%)	568 (93%)	34 (6%)	6 (1%)	15	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	11	LYS
1	A	30	PRO

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Mol	Chain	Res	Type
1	B	8	PRO
1	B	10	ILE
1	B	279	VAL
1	A	265	PRO

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	240/325 (74%)	235 (98%)	5 (2%)	53	79
1	B	226/325 (70%)	221 (98%)	5 (2%)	52	78
All	All	466/650 (72%)	456 (98%)	10 (2%)	52	79

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	230	LEU
1	A	275	LEU
1	A	328	SER
1	A	330	SER
1	B	13	SER
1	B	124	PHE
1	B	275	LEU
1	B	312	SER
1	B	328	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\#|Z| > 2$
3	GOL	A	404	-	5,5,5	0.40	0	5,5,5	0.13	0
2	SO4	A	402	-	4,4,4	0.19	0	6,6,6	0.32	0
3	GOL	A	405	-	5,5,5	0.34	0	5,5,5	0.41	0
2	SO4	B	402	-	4,4,4	0.15	0	6,6,6	0.10	0
3	GOL	A	403	-	5,5,5	0.35	0	5,5,5	0.31	0
2	SO4	B	401	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	A	401	-	4,4,4	0.13	0	6,6,6	0.37	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
3	GOL	A	404	-	-	3/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	A	405	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	GOL	O1-C1-C2-C3
3	A	403	GOL	O1-C1-C2-O2
3	A	404	GOL	O2-C2-C3-O3
3	A	404	GOL	O1-C1-C2-O2
3	A	404	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	SO4	1	0
2	B	401	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(Å²)	Q<0.9
1	A	319/381 (83%)	0.27	25 (7%)	13	11	42, 55, 76, 85	0
1	B	300/381 (78%)	0.35	23 (7%)	13	11	43, 56, 80, 88	0
All	All	619/762 (81%)	0.31	48 (7%)	13	11	42, 56, 78, 88	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299	SER	7.2
1	A	63	LEU	5.4
1	B	83	ALA	5.2
1	A	322	ALA	4.5
1	B	286	VAL	4.4
1	A	71	GLU	4.3
1	A	314	ILE	3.9
1	B	79	VAL	3.5
1	A	312	SER	3.4
1	B	16	ILE	3.3
1	A	146	TRP	3.2
1	A	144	GLY	3.2
1	A	330	SER	3.1
1	B	6	VAL	3.1
1	B	279	VAL	3.0
1	B	288	ASN	2.9
1	A	147	CYS	2.8
1	B	57	PRO	2.8
1	A	319	LYS	2.7
1	A	31	GLY	2.7
1	B	10	ILE	2.7
1	A	151	LEU	2.7
1	A	337	THR	2.6
1	A	374	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	75	LEU	2.6
1	B	73	GLU	2.5
1	B	372	PHE	2.5
1	A	168	GLU	2.4
1	B	74	HIS	2.4
1	A	320	VAL	2.4
1	B	164	GLY	2.3
1	B	280	HIS	2.3
1	A	334	GLY	2.3
1	B	337	THR	2.3
1	A	333	ALA	2.3
1	A	65	SER	2.2
1	A	72	SER	2.2
1	A	150	GLN	2.2
1	B	371	ILE	2.1
1	A	280	HIS	2.1
1	B	330	SER	2.1
1	A	145	THR	2.1
1	A	75	LEU	2.1
1	B	76	GLU	2.1
1	A	143	TRP	2.1
1	B	146	TRP	2.1
1	B	78	LEU	2.0
1	B	287	LYS	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
2	SO4	A	402	5/5	0.76	0.43	66,67,78,102	5
4	NI	B	403	1/1	0.77	0.27	126,126,126,126	0
3	GOL	A	403	6/6	0.78	0.31	56,70,84,92	0
3	GOL	A	404	6/6	0.83	0.27	60,77,86,92	0
3	GOL	A	405	6/6	0.92	0.50	65,82,97,106	0
2	SO4	B	402	5/5	0.94	0.19	68,71,83,88	5
2	SO4	B	401	5/5	0.95	0.18	54,56,66,72	5
2	SO4	A	401	5/5	0.98	0.17	62,68,76,82	0

6.5 Other polymers (i)

There are no such residues in this entry.