Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 08:59 pm GMT

PDB ID	:	4ALM
Title	:	Crystal structure of S. aureus FabI (P43212)
Authors	:	Schiebel, J.; Kisker, C.
Deposited on	:	2012-03-04
Resolution	:	2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

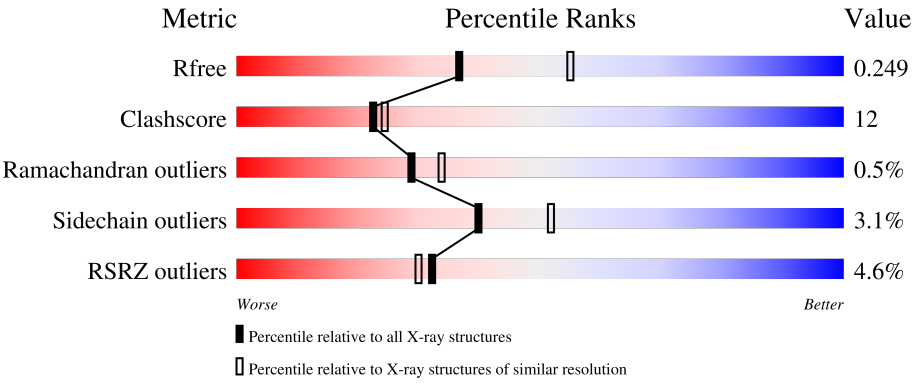
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	282	2% 72% 21% 6%
1	B	282	6% 65% 19% • 14%
1	C	282	5% 62% 16% • 21%
1	D	282	3% 66% 20% • 13%

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	B	1251	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7820 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 ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2042	1287	346	403	6			
1	B	242	Total	C	N	O	S	0	0	0
			1879	1186	323	365	5			
1	C	224	Total	C	N	O	S	0	0	0
			1731	1090	295	342	4			
1	D	246	Total	C	N	O	S	0	0	0
			1889	1190	324	370	5			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	expression tag	UNP Q7A6D8
A	-24	LYS	-	expression tag	UNP Q7A6D8
A	-23	HIS	-	expression tag	UNP Q7A6D8
A	-22	HIS	-	expression tag	UNP Q7A6D8
A	-21	HIS	-	expression tag	UNP Q7A6D8
A	-20	HIS	-	expression tag	UNP Q7A6D8
A	-19	HIS	-	expression tag	UNP Q7A6D8
A	-18	HIS	-	expression tag	UNP Q7A6D8
A	-17	PRO	-	expression tag	UNP Q7A6D8
A	-16	MET	-	expression tag	UNP Q7A6D8
A	-15	SER	-	expression tag	UNP Q7A6D8
A	-14	ASP	-	expression tag	UNP Q7A6D8
A	-13	TYR	-	expression tag	UNP Q7A6D8
A	-12	ASP	-	expression tag	UNP Q7A6D8
A	-11	ILE	-	expression tag	UNP Q7A6D8
A	-10	PRO	-	expression tag	UNP Q7A6D8
A	-9	THR	-	expression tag	UNP Q7A6D8
A	-8	THR	-	expression tag	UNP Q7A6D8
A	-7	GLU	-	expression tag	UNP Q7A6D8
A	-6	ASN	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP Q7A6D8
A	-4	TYR	-	expression tag	UNP Q7A6D8
A	-3	PHE	-	expression tag	UNP Q7A6D8
A	-2	GLN	-	expression tag	UNP Q7A6D8
A	-1	GLY	-	expression tag	UNP Q7A6D8
A	0	ALA	-	expression tag	UNP Q7A6D8
B	-25	MET	-	expression tag	UNP Q7A6D8
B	-24	LYS	-	expression tag	UNP Q7A6D8
B	-23	HIS	-	expression tag	UNP Q7A6D8
B	-22	HIS	-	expression tag	UNP Q7A6D8
B	-21	HIS	-	expression tag	UNP Q7A6D8
B	-20	HIS	-	expression tag	UNP Q7A6D8
B	-19	HIS	-	expression tag	UNP Q7A6D8
B	-18	HIS	-	expression tag	UNP Q7A6D8
B	-17	PRO	-	expression tag	UNP Q7A6D8
B	-16	MET	-	expression tag	UNP Q7A6D8
B	-15	SER	-	expression tag	UNP Q7A6D8
B	-14	ASP	-	expression tag	UNP Q7A6D8
B	-13	TYR	-	expression tag	UNP Q7A6D8
B	-12	ASP	-	expression tag	UNP Q7A6D8
B	-11	ILE	-	expression tag	UNP Q7A6D8
B	-10	PRO	-	expression tag	UNP Q7A6D8
B	-9	THR	-	expression tag	UNP Q7A6D8
B	-8	THR	-	expression tag	UNP Q7A6D8
B	-7	GLU	-	expression tag	UNP Q7A6D8
B	-6	ASN	-	expression tag	UNP Q7A6D8
B	-5	LEU	-	expression tag	UNP Q7A6D8
B	-4	TYR	-	expression tag	UNP Q7A6D8
B	-3	PHE	-	expression tag	UNP Q7A6D8
B	-2	GLN	-	expression tag	UNP Q7A6D8
B	-1	GLY	-	expression tag	UNP Q7A6D8
B	0	ALA	-	expression tag	UNP Q7A6D8
C	-25	MET	-	expression tag	UNP Q7A6D8
C	-24	LYS	-	expression tag	UNP Q7A6D8
C	-23	HIS	-	expression tag	UNP Q7A6D8
C	-22	HIS	-	expression tag	UNP Q7A6D8
C	-21	HIS	-	expression tag	UNP Q7A6D8
C	-20	HIS	-	expression tag	UNP Q7A6D8
C	-19	HIS	-	expression tag	UNP Q7A6D8
C	-18	HIS	-	expression tag	UNP Q7A6D8
C	-17	PRO	-	expression tag	UNP Q7A6D8
C	-16	MET	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	SER	-	expression tag	UNP Q7A6D8
C	-14	ASP	-	expression tag	UNP Q7A6D8
C	-13	TYR	-	expression tag	UNP Q7A6D8
C	-12	ASP	-	expression tag	UNP Q7A6D8
C	-11	ILE	-	expression tag	UNP Q7A6D8
C	-10	PRO	-	expression tag	UNP Q7A6D8
C	-9	THR	-	expression tag	UNP Q7A6D8
C	-8	THR	-	expression tag	UNP Q7A6D8
C	-7	GLU	-	expression tag	UNP Q7A6D8
C	-6	ASN	-	expression tag	UNP Q7A6D8
C	-5	LEU	-	expression tag	UNP Q7A6D8
C	-4	TYR	-	expression tag	UNP Q7A6D8
C	-3	PHE	-	expression tag	UNP Q7A6D8
C	-2	GLN	-	expression tag	UNP Q7A6D8
C	-1	GLY	-	expression tag	UNP Q7A6D8
C	0	ALA	-	expression tag	UNP Q7A6D8
D	-25	MET	-	expression tag	UNP Q7A6D8
D	-24	LYS	-	expression tag	UNP Q7A6D8
D	-23	HIS	-	expression tag	UNP Q7A6D8
D	-22	HIS	-	expression tag	UNP Q7A6D8
D	-21	HIS	-	expression tag	UNP Q7A6D8
D	-20	HIS	-	expression tag	UNP Q7A6D8
D	-19	HIS	-	expression tag	UNP Q7A6D8
D	-18	HIS	-	expression tag	UNP Q7A6D8
D	-17	PRO	-	expression tag	UNP Q7A6D8
D	-16	MET	-	expression tag	UNP Q7A6D8
D	-15	SER	-	expression tag	UNP Q7A6D8
D	-14	ASP	-	expression tag	UNP Q7A6D8
D	-13	TYR	-	expression tag	UNP Q7A6D8
D	-12	ASP	-	expression tag	UNP Q7A6D8
D	-11	ILE	-	expression tag	UNP Q7A6D8
D	-10	PRO	-	expression tag	UNP Q7A6D8
D	-9	THR	-	expression tag	UNP Q7A6D8
D	-8	THR	-	expression tag	UNP Q7A6D8
D	-7	GLU	-	expression tag	UNP Q7A6D8
D	-6	ASN	-	expression tag	UNP Q7A6D8
D	-5	LEU	-	expression tag	UNP Q7A6D8
D	-4	TYR	-	expression tag	UNP Q7A6D8
D	-3	PHE	-	expression tag	UNP Q7A6D8
D	-2	GLN	-	expression tag	UNP Q7A6D8
D	-1	GLY	-	expression tag	UNP Q7A6D8
D	0	ALA	-	expression tag	UNP Q7A6D8

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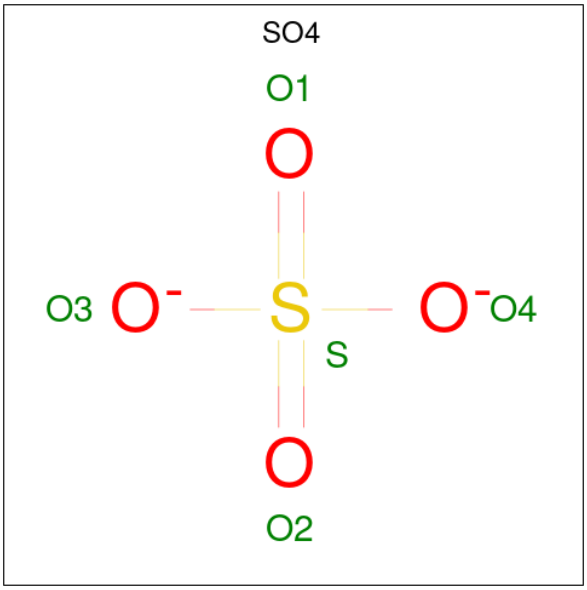
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	engineered mutation	UNP Q7A6D8
B	2	VAL	LEU	engineered mutation	UNP Q7A6D8
C	2	VAL	LEU	engineered mutation	UNP Q7A6D8
D	2	VAL	LEU	engineered mutation	UNP Q7A6D8

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



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

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

- Molecule 3 is water.

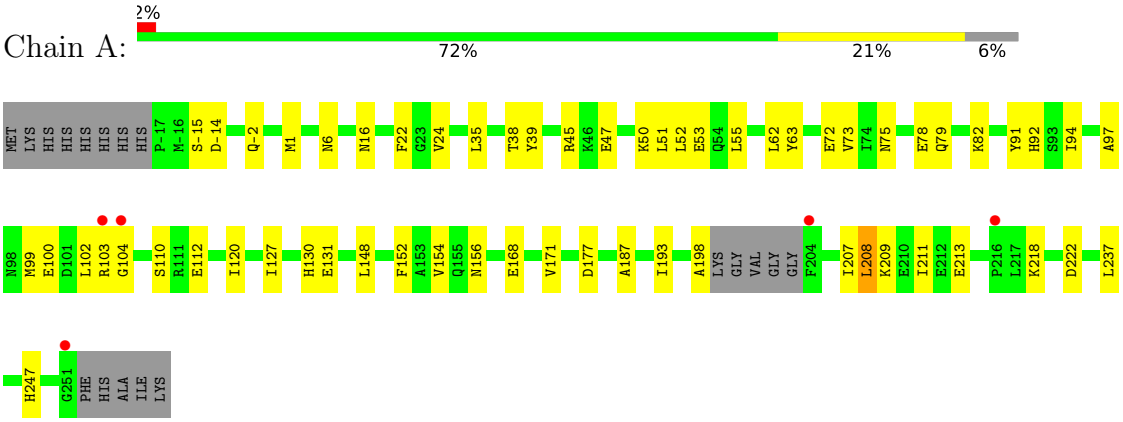
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	65	Total O 65 65	0	0
3	B	46	Total O 46 46	0	0
3	C	49	Total O 49 49	0	0
3	D	54	Total O 54 54	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

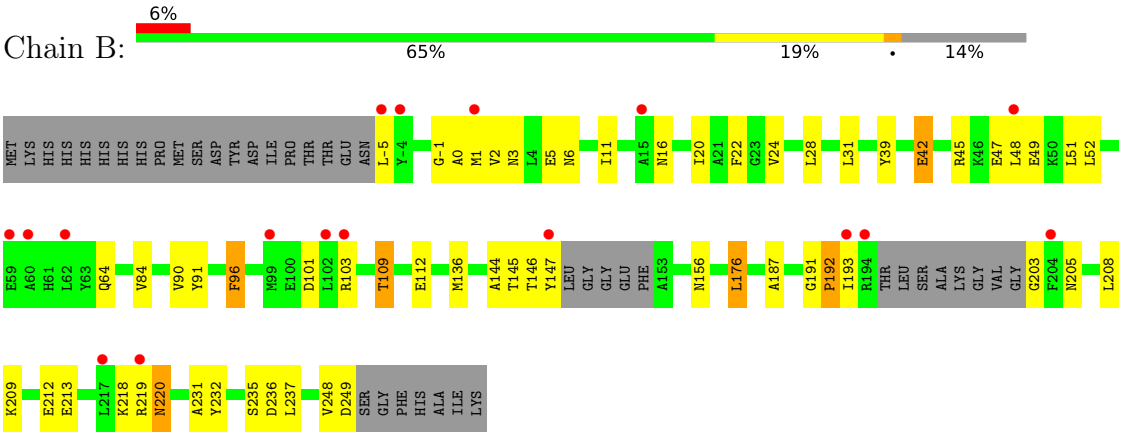
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain A:



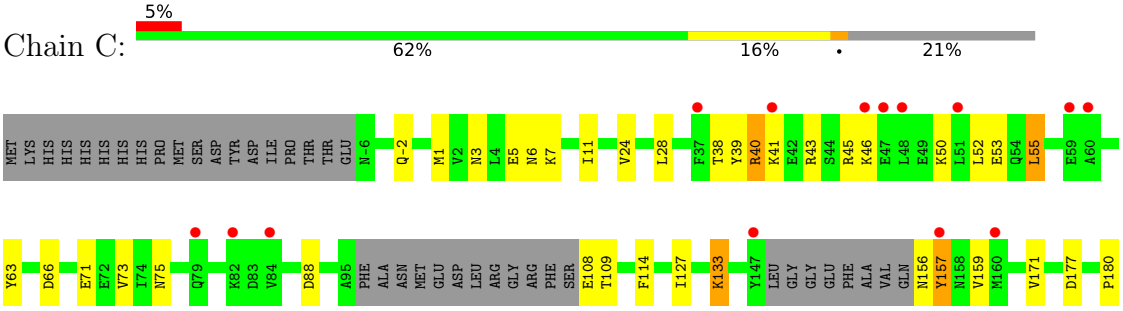
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

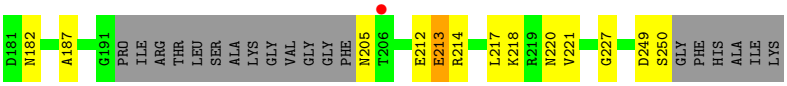
Chain B:



• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

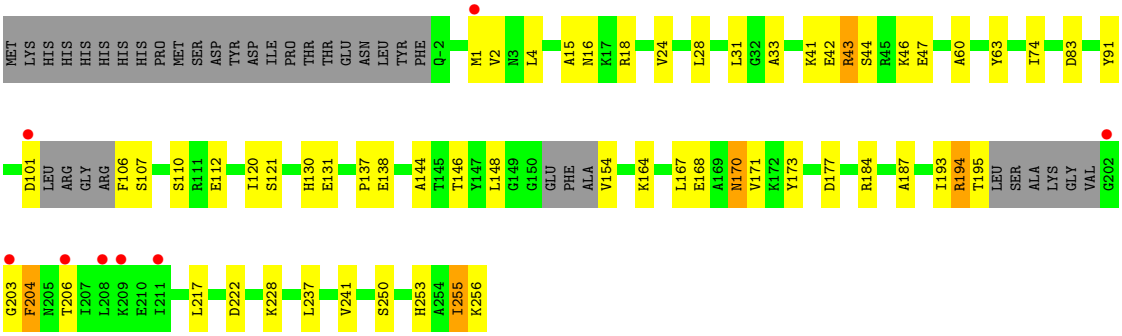
Chain C:





• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	87.49Å 87.49Å 307.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.18 – 2.45 48.18 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.18-2.45) 99.0 (48.18-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4_486)	Depositor
R, R_{free}	0.185 , 0.252 0.182 , 0.249	Depositor DCC
R_{free} test set	2230 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 65.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7820	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.39	0/2071	0.51	0/2796
1	B	0.37	0/1903	0.50	0/2565
1	C	0.37	0/1750	0.49	0/2359
1	D	0.40	0/1912	0.51	0/2575
All	All	0.38	0/7636	0.50	0/10295

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

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	2042	0	2039	44	0
1	B	1879	0	1891	46	0
1	C	1731	0	1743	50	0
1	D	1889	0	1896	60	0
2	A	20	0	0	1	0
2	B	20	0	0	0	0
2	C	5	0	0	0	0
2	D	20	0	0	0	0
3	A	65	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	46	0	0	2	0
3	C	49	0	0	3	0
3	D	54	0	0	3	0
All	All	7820	0	7569	176	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 12.

All (176) 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:C:108:GLU:HG3	1:D:130:HIS:CD2	1.97	0.99
1:B:20:ILE:H	1:B:96:PHE:HZ	1.12	0.94
1:C:108:GLU:HG3	1:D:130:HIS:CG	2.03	0.92
1:A:16:ASN:HA	1:A:47:GLU:HG2	1.53	0.90
1:D:43:ARG:H	1:D:43:ARG:HD2	1.38	0.87
1:D:164:LYS:HE2	1:D:168:GLU:OE2	1.82	0.80
1:B:236:ASP:HB2	3:B:2043:HOH:O	1.85	0.77
1:D:41:LYS:HB3	1:D:43:ARG:HD2	1.65	0.77
1:C:11:ILE:HD11	1:C:28:LEU:HD12	1.66	0.77
1:C:218:LYS:NZ	1:C:250:SER:HA	2.00	0.76
1:B:203:GLY:HA2	3:B:2040:HOH:O	1.91	0.71
1:D:43:ARG:H	1:D:43:ARG:CD	2.04	0.70
1:A:198:ALA:HB1	1:B:176:LEU:HD23	1.74	0.69
1:B:16:ASN:HA	1:B:47:GLU:HG2	1.76	0.68
1:A:1:MET:HE3	1:D:2:VAL:HG22	1.77	0.67
1:A:-2:GLN:HA	3:A:2002:HOH:O	1.94	0.67
1:B:191:GLY:O	1:B:249:ASP:HB3	1.94	0.66
1:D:41:LYS:HB3	1:D:43:ARG:CD	2.27	0.65
1:C:40:ARG:NH2	1:C:41:LYS:HE3	2.11	0.64
1:D:2:VAL:HA	3:D:2005:HOH:O	1.96	0.64
1:C:218:LYS:HZ1	1:C:250:SER:HA	1.62	0.63
1:D:255:ILE:O	1:D:255:ILE:HG13	1.99	0.62
1:B:1:MET:O	1:B:1:MET:HG3	1.99	0.62
1:B:205:ASN:O	1:B:209:LYS:HG2	2.00	0.61
1:A:104:GLY:O	1:A:156:ASN:HB2	2.01	0.61
1:D:44:SER:HB3	3:D:2012:HOH:O	2.01	0.60
1:D:171:VAL:HG21	1:D:187:ALA:HB2	1.82	0.60
1:A:218:LYS:HE3	1:A:222:ASP:OD2	2.02	0.60
1:C:3:ASN:OD1	1:C:5:GLU:HG2	2.02	0.60
1:D:24:VAL:HG21	1:D:91:TYR:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HA	1:A:156:ASN:HB3	1.84	0.59
1:B:96:PHE:N	1:B:96:PHE:CD1	2.67	0.59
1:B:145:THR:HG22	1:B:147:TYR:H	1.67	0.58
1:A:130:HIS:HD2	1:A:131:GLU:OE2	1.86	0.58
1:A:112:GLU:H	1:A:112:GLU:CD	2.07	0.58
1:D:193:ILE:O	1:D:195:THR:N	2.37	0.56
1:C:52:LEU:HD23	1:C:52:LEU:O	2.06	0.56
1:C:46:LYS:O	1:C:50:LYS:HD3	2.06	0.56
1:C:109:THR:HB	3:C:2025:HOH:O	2.05	0.56
1:D:18:ARG:HB3	1:D:195:THR:CG2	2.36	0.56
1:D:154:VAL:O	1:D:154:VAL:HG22	2.06	0.55
1:B:248:VAL:O	1:B:249:ASP:HB2	2.07	0.55
1:C:133:LYS:O	1:C:133:LYS:HE2	2.07	0.55
1:B:209:LYS:O	1:B:213:GLU:HG2	2.07	0.54
1:C:157:TYR:HD2	1:D:173:TYR:HB3	1.72	0.54
1:C:40:ARG:HG2	1:C:66:ASP:HA	1.88	0.54
1:C:182:ASN:HB2	3:C:2039:HOH:O	2.07	0.54
1:A:102:LEU:HG	1:A:154:VAL:HG21	1.90	0.54
1:A:168:GLU:HA	1:A:168:GLU:OE1	2.08	0.54
1:B:2:VAL:HG13	1:B:2:VAL:O	2.08	0.54
1:C:171:VAL:HG21	1:C:187:ALA:HB2	1.90	0.54
1:B:145:THR:HG22	1:B:146:THR:N	2.23	0.53
1:C:214:ARG:O	1:C:214:ARG:HG3	2.08	0.53
1:C:108:GLU:CG	1:D:130:HIS:CD2	2.82	0.53
1:B:31:LEU:HD13	1:C:1:MET:HG3	1.91	0.53
1:B:48:LEU:O	1:B:52:LEU:HD23	2.08	0.52
1:A:73:VAL:HG11	1:A:127:ILE:HG13	1.92	0.52
1:B:-1:GLY:O	1:B:0:ALA:HB3	2.10	0.52
1:C:157:TYR:HE2	1:D:170:ASN:ND2	2.08	0.52
1:D:107:SER:HB3	1:D:110:SER:HB3	1.91	0.52
1:A:39:TYR:CZ	1:A:45:ARG:HD2	2.44	0.52
1:C:218:LYS:HZ2	1:C:250:SER:HA	1.74	0.52
1:A:78:GLU:HG3	1:A:82:LYS:HE2	1.92	0.52
1:B:42:GLU:OE2	1:B:45:ARG:HD3	2.09	0.51
1:A:-14:ASP:HA	1:D:60:ALA:O	2.10	0.51
1:A:92:HIS:CE1	1:A:94:ILE:HD13	2.45	0.51
1:D:217:LEU:HB2	1:D:250:SER:HB3	1.93	0.51
1:A:1:MET:HG3	1:D:31:LEU:HD13	1.93	0.51
1:D:193:ILE:HG23	1:D:222:ASP:HA	1.93	0.51
1:C:213:GLU:HA	1:C:218:LYS:HG2	1.91	0.50
1:A:193:ILE:HD11	1:A:211:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ILE:O	1:A:211:ILE:HG12	2.12	0.50
1:D:18:ARG:NH2	3:D:2014:HOH:O	2.42	0.50
1:C:5:GLU:O	1:C:6:ASN:HB2	2.12	0.50
1:D:194:ARG:O	1:D:194:ARG:HG2	2.11	0.50
1:B:112:GLU:CD	1:B:112:GLU:H	2.15	0.50
1:A:16:ASN:HA	1:A:47:GLU:CG	2.36	0.49
1:B:235:SER:OG	1:B:237:LEU:HB2	2.13	0.49
1:C:156:ASN:HB3	1:D:177:ASP:OD2	2.12	0.49
1:C:157:TYR:CE2	1:D:170:ASN:ND2	2.80	0.49
1:A:24:VAL:HG21	1:A:91:TYR:CZ	2.47	0.49
1:A:100:GLU:N	1:A:100:GLU:OE1	2.45	0.49
1:B:5:GLU:O	1:B:6:ASN:HB2	2.13	0.49
1:D:24:VAL:HG21	1:D:91:TYR:CE1	2.48	0.49
1:B:146:THR:O	1:B:147:TYR:CB	2.61	0.48
1:A:97:ALA:HB2	1:A:120:ILE:HD13	1.96	0.48
1:C:39:TYR:CZ	1:C:45:ARG:HB2	2.49	0.48
1:A:177:ASP:OD1	1:B:156:ASN:HB3	2.14	0.47
1:C:38:THR:HA	1:C:63:TYR:O	2.14	0.47
1:A:1:MET:CE	1:D:2:VAL:HG22	2.44	0.47
1:B:231:ALA:O	1:B:235:SER:HB3	2.14	0.47
1:D:101:ASP:O	1:D:106:PHE:CZ	2.67	0.47
1:B:3:ASN:HD21	1:C:-2:GLN:NE2	2.12	0.47
1:B:11:ILE:HD11	1:B:28:LEU:HD12	1.96	0.47
1:C:46:LYS:HE3	1:C:50:LYS:NZ	2.29	0.47
1:C:53:GLU:C	1:C:55:LEU:H	2.18	0.47
1:A:99:MET:HG2	1:A:102:LEU:HD13	1.97	0.47
1:D:63:TYR:OH	1:D:83:ASP:HB2	2.14	0.47
1:B:208:LEU:O	1:B:212:GLU:HG3	2.14	0.47
1:D:146:THR:HG23	1:D:167:LEU:CD2	2.45	0.47
1:B:101:ASP:C	1:B:103:ARG:H	2.18	0.46
1:D:253:HIS:O	1:D:256:LYS:HE3	2.15	0.46
1:A:50:LYS:O	1:A:53:GLU:HG2	2.16	0.46
1:D:256:LYS:HE2	1:D:256:LYS:HB3	1.70	0.46
1:A:110:SER:HB2	1:A:112:GLU:OE1	2.15	0.46
1:A:171:VAL:HG21	1:A:187:ALA:HB2	1.97	0.46
1:B:90:VAL:HG23	1:B:136:MET:HE1	1.97	0.46
1:B:144:ALA:O	1:B:187:ALA:HA	2.16	0.46
1:C:73:VAL:HG11	1:C:127:ILE:HG12	1.99	0.45
1:C:46:LYS:HE3	1:C:50:LYS:HE3	1.99	0.45
1:D:112:GLU:H	1:D:112:GLU:CD	2.20	0.45
1:C:212:GLU:C	1:C:214:ARG:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:O	1:A:78:GLU:HB3	2.16	0.45
1:B:45:ARG:NH2	1:B:49:GLU:OE2	2.50	0.45
1:D:217:LEU:HD12	1:D:250:SER:HA	1.98	0.44
1:A:237:LEU:HD12	1:D:228:LYS:HG2	1.99	0.44
1:C:177:ASP:O	1:C:180:PRO:HD2	2.17	0.44
1:C:249:ASP:O	1:C:250:SER:HB2	2.17	0.44
1:C:157:TYR:CD2	1:D:173:TYR:HB3	2.52	0.44
1:D:203:GLY:HA2	1:D:206:THR:HG23	1.98	0.44
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.85	0.44
1:B:22:PHE:CE1	1:B:51:LEU:HB3	2.53	0.44
1:B:84:VAL:HG12	1:B:84:VAL:O	2.17	0.44
1:C:41:LYS:HD3	1:C:43:ARG:HH21	1.82	0.43
1:B:237:LEU:HD12	1:C:1:MET:HE2	2.00	0.43
1:C:24:VAL:O	1:C:28:LEU:HG	2.18	0.43
1:C:71:GLU:HG2	1:C:75:ASN:ND2	2.33	0.43
1:D:144:ALA:O	1:D:187:ALA:HA	2.18	0.43
1:A:38:THR:HA	1:A:63:TYR:O	2.18	0.43
1:B:192:PRO:HD2	1:B:193:ILE:H	1.84	0.43
1:B:146:THR:O	1:B:147:TYR:CG	2.72	0.43
1:B:16:ASN:HA	1:B:47:GLU:CG	2.47	0.43
1:B:146:THR:O	1:B:147:TYR:HB2	2.18	0.43
1:D:2:VAL:HG21	1:D:237:LEU:HG	2.01	0.43
1:D:15:ALA:O	1:D:47:GLU:HG2	2.19	0.43
1:A:208:LEU:HD22	1:A:208:LEU:HA	1.89	0.42
1:B:22:PHE:CZ	1:B:51:LEU:HD22	2.54	0.42
1:C:24:VAL:HG22	1:C:227:GLY:HA2	2.01	0.42
1:C:7:LYS:HA	1:C:88:ASP:OD2	2.19	0.42
1:C:114:PHE:CD1	1:C:114:PHE:C	2.93	0.42
1:D:204:PHE:HD1	1:D:204:PHE:HA	1.73	0.42
1:C:217:LEU:O	1:C:221:VAL:HG23	2.18	0.42
1:A:209:LYS:O	1:A:213:GLU:HG3	2.20	0.42
1:D:42:GLU:O	1:D:46:LYS:HG3	2.20	0.42
1:A:22:PHE:CE1	1:A:51:LEU:HB3	2.55	0.42
1:C:212:GLU:O	1:C:214:ARG:N	2.53	0.42
1:A:148:LEU:HA	1:A:152:PHE:CE1	2.55	0.42
1:B:39:TYR:O	1:B:64:GLN:HA	2.20	0.42
1:B:22:PHE:CE2	1:B:51:LEU:HD22	2.55	0.42
1:D:2:VAL:O	1:D:2:VAL:HG13	2.20	0.42
1:A:52:LEU:HD23	1:A:55:LEU:HD12	2.02	0.41
1:B:24:VAL:HG21	1:B:91:TYR:CZ	2.56	0.41
1:D:74:ILE:HG12	1:D:131:GLU:CD	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ILE:CG2	1:D:121:SER:N	2.83	0.41
1:A:22:PHE:CZ	1:A:51:LEU:HD22	2.56	0.41
1:A:177:ASP:OD2	2:A:1255:SO4:O3	2.38	0.41
1:A:247:HIS:HB3	3:A:2051:HOH:O	2.19	0.41
1:B:220:ASN:ND2	1:B:249:ASP:OD1	2.54	0.41
1:C:157:TYR:HB3	1:D:177:ASP:HB2	2.03	0.41
1:D:16:ASN:HA	1:D:47:GLU:HG2	2.03	0.41
1:C:133:LYS:HE2	1:C:133:LYS:C	2.41	0.41
1:A:1:MET:HG3	1:D:31:LEU:CD1	2.50	0.41
1:A:193:ILE:HD13	1:A:207:ILE:HG23	2.03	0.41
1:D:1:MET:SD	1:D:2:VAL:N	2.94	0.41
1:D:24:VAL:O	1:D:28:LEU:HG	2.21	0.41
1:D:146:THR:HG23	1:D:167:LEU:HD22	2.03	0.41
1:B:232:TYR:HA	1:C:1:MET:CE	2.51	0.40
1:C:157:TYR:HD2	1:D:173:TYR:CB	2.33	0.40
1:D:184:ARG:HD2	1:D:241:VAL:O	2.21	0.40
1:B:145:THR:HG22	1:B:146:THR:H	1.83	0.40
1:C:205:ASN:ND2	3:C:2043:HOH:O	2.38	0.40
1:A:130:HIS:CE1	1:B:109:THR:HG21	2.56	0.40
1:C:108:GLU:HG3	1:D:130:HIS:CB	2.47	0.40
1:D:4:LEU:HB3	1:D:33:ALA:HB2	2.04	0.40
1:D:18:ARG:HB3	1:D:195:THR:HG21	2.03	0.40
1:D:137:PRO:HD2	1:D:138:GLU:OE1	2.22	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	260/282 (92%)	251 (96%)	9 (4%)	0	100 100
1	B	236/282 (84%)	223 (94%)	12 (5%)	1 (0%)	34 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	216/282 (77%)	210 (97%)	5 (2%)	1 (0%)	29 34
1	D	238/282 (84%)	220 (92%)	15 (6%)	3 (1%)	12 11
All	All	950/1128 (84%)	904 (95%)	41 (4%)	5 (0%)	29 34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	192	PRO
1	D	194	ARG
1	C	213	GLU
1	D	148	LEU
1	D	255	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	220/234 (94%)	212 (96%)	8 (4%)	35 46
1	B	201/234 (86%)	193 (96%)	8 (4%)	31 41
1	C	187/234 (80%)	181 (97%)	6 (3%)	39 50
1	D	202/234 (86%)	199 (98%)	3 (2%)	65 76
All	All	810/936 (86%)	785 (97%)	25 (3%)	40 52

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-15	SER
1	A	6	ASN
1	A	35	LEU
1	A	62	LEU
1	A	72	GLU
1	A	79	GLN
1	A	103	ARG

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Mol	Chain	Res	Type
1	A	208	LEU
1	B	-5	LEU
1	B	42	GLU
1	B	96	PHE
1	B	109	THR
1	B	176	LEU
1	B	218	LYS
1	B	219	ARG
1	B	220	ASN
1	C	40	ARG
1	C	55	LEU
1	C	133	LYS
1	C	157	TYR
1	C	159	VAL
1	C	220	ASN
1	D	43	ARG
1	D	170	ASN
1	D	204	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-6	ASN
1	A	92	HIS
1	A	130	HIS
1	C	-2	GLN
1	C	75	ASN
1	C	158	ASN
1	D	68	GLN
1	D	130	HIS
1	D	170	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	D	1259	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	B	1253	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	D	1260	-	4,4,4	0.14	0	6,6,6	0.18	0
2	SO4	A	1255	-	4,4,4	0.14	0	6,6,6	0.27	0
2	SO4	D	1257	-	4,4,4	0.12	0	6,6,6	0.16	0
2	SO4	C	1251	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	B	1252	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	1253	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	1250	-	4,4,4	0.16	0	6,6,6	0.15	0
2	SO4	D	1258	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	B	1251	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	A	1252	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	A	1254	-	4,4,4	0.14	0	6,6,6	0.14	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	1255	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^{th} 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	264/282 (93%)	-0.00	5 (1%)	66	64	31, 52, 91, 112	0
1	B	242/282 (85%)	0.30	17 (7%)	16	13	29, 55, 110, 137	0
1	C	224/282 (79%)	0.33	15 (6%)	17	14	33, 60, 100, 125	0
1	D	246/282 (87%)	0.11	8 (3%)	46	43	32, 55, 111, 155	0
All	All	976/1128 (86%)	0.18	45 (4%)	32	30	29, 55, 105, 155	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	ILE	5.6
1	B	194	ARG	5.2
1	D	1	MET	4.5
1	B	103	ARG	4.4
1	B	48	LEU	4.3
1	B	60	ALA	4.0
1	C	60	ALA	4.0
1	B	1	MET	3.6
1	C	157	TYR	3.6
1	A	103	ARG	3.2
1	B	-5	LEU	3.2
1	C	46	LYS	3.1
1	B	217	LEU	3.0
1	B	147	TYR	3.0
1	D	202	GLY	3.0
1	B	99	MET	2.9
1	C	37	PHE	2.8
1	A	251	GLY	2.8
1	D	211	ILE	2.7
1	C	84	VAL	2.6
1	D	208	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	47	GLU	2.6
1	B	59	GLU	2.5
1	D	101	ASP	2.5
1	C	48	LEU	2.5
1	B	204	PHE	2.5
1	D	209	LYS	2.4
1	B	62	LEU	2.4
1	C	41	LYS	2.4
1	C	79	GLN	2.4
1	C	160	MET	2.3
1	D	206	THR	2.3
1	A	204	PHE	2.3
1	B	219	ARG	2.2
1	C	82	LYS	2.1
1	B	15	ALA	2.1
1	C	51	LEU	2.1
1	A	216	PRO	2.1
1	B	102	LEU	2.1
1	B	-4	TYR	2.1
1	C	206	THR	2.0
1	A	104	GLY	2.0
1	D	203	GLY	2.0
1	C	147	TYR	2.0
1	C	59	GLU	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^{th} 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	B	1251	5/5	0.67	0.52	142,144,145,149	0
2	SO4	C	1251	5/5	0.80	0.45	153,154,156,157	0
2	SO4	D	1258	5/5	0.81	0.28	151,154,155,155	0
2	SO4	B	1253	5/5	0.91	0.20	127,129,130,132	0
2	SO4	D	1259	5/5	0.91	0.16	137,137,139,142	0
2	SO4	A	1255	5/5	0.93	0.31	87,93,104,106	0
2	SO4	B	1252	5/5	0.94	0.29	139,141,141,142	0
2	SO4	D	1257	5/5	0.94	0.15	103,104,109,110	0
2	SO4	A	1252	5/5	0.95	0.15	87,94,98,100	0
2	SO4	D	1260	5/5	0.95	0.13	111,111,112,116	0
2	SO4	A	1253	5/5	0.96	0.20	94,96,100,104	0
2	SO4	A	1254	5/5	0.98	0.10	62,63,65,68	0
2	SO4	B	1250	5/5	0.98	0.11	63,71,74,76	0

6.5 Other polymers (i)

There are no such residues in this entry.