



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:23 pm GMT

PDB ID : 3SYN
Title : Crystal structure of FlhF in complex with its activator
Authors : Bange, G.; Kuemmerer, N.; Wild, K.; Sinning, I.
Deposited on : 2011-07-18
Resolution : 3.06 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

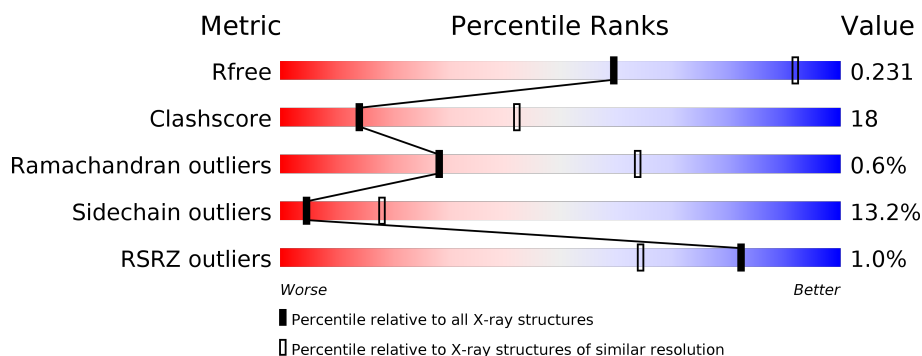
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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}	100719	1348 (3.10-3.02)
Clashscore	112137	1462 (3.10-3.02)
Ramachandran outliers	110173	1410 (3.10-3.02)
Sidechain outliers	110143	1410 (3.10-3.02)
RSRZ outliers	101464	1355 (3.10-3.02)

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. 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	296	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>28%</div> <div>5%</div> <div>13%</div> </div> </div>
1	B	296	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>29%</div> <div>5%</div> <div>13%</div> </div> </div>
1	C	296	<div> <div></div> <div> <div>54%</div> <div>29%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	296	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>27%</div> <div>•</div> <div>13%</div> </div> </div>
2	E	23	<div> <div></div> <div> <div>35%</div> <div>35%</div> <div>30%</div> </div> </div>
2	F	23	<div> <div></div> <div> <div>30%</div> <div>39%</div> <div>30%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	23	
2	H	23	

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
6	SO4	A	10	-	-	X	X
6	SO4	A	13	-	-	X	-
6	SO4	A	3	-	-	-	X
6	SO4	A	5	-	-	X	-
6	SO4	B	1	-	-	X	-
6	SO4	B	14	-	-	X	-
6	SO4	B	8	-	-	X	X
6	SO4	C	4	-	-	X	-
6	SO4	C	9	-	-	X	X
6	SO4	D	6	-	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9010 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 Flagellar biosynthesis protein flhF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			
1	B	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			
1	C	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			
1	D	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	MET	-	EXPRESSION TAG	UNP Q01960
A	72	GLY	-	EXPRESSION TAG	UNP Q01960
A	73	HIS	-	EXPRESSION TAG	UNP Q01960
A	74	HIS	-	EXPRESSION TAG	UNP Q01960
A	75	HIS	-	EXPRESSION TAG	UNP Q01960
A	76	HIS	-	EXPRESSION TAG	UNP Q01960
A	77	HIS	-	EXPRESSION TAG	UNP Q01960
A	78	HIS	-	EXPRESSION TAG	UNP Q01960
B	71	MET	-	EXPRESSION TAG	UNP Q01960
B	72	GLY	-	EXPRESSION TAG	UNP Q01960
B	73	HIS	-	EXPRESSION TAG	UNP Q01960
B	74	HIS	-	EXPRESSION TAG	UNP Q01960
B	75	HIS	-	EXPRESSION TAG	UNP Q01960
B	76	HIS	-	EXPRESSION TAG	UNP Q01960
B	77	HIS	-	EXPRESSION TAG	UNP Q01960
B	78	HIS	-	EXPRESSION TAG	UNP Q01960
C	71	MET	-	EXPRESSION TAG	UNP Q01960
C	72	GLY	-	EXPRESSION TAG	UNP Q01960
C	73	HIS	-	EXPRESSION TAG	UNP Q01960
C	74	HIS	-	EXPRESSION TAG	UNP Q01960
C	75	HIS	-	EXPRESSION TAG	UNP Q01960

Continued on next page...

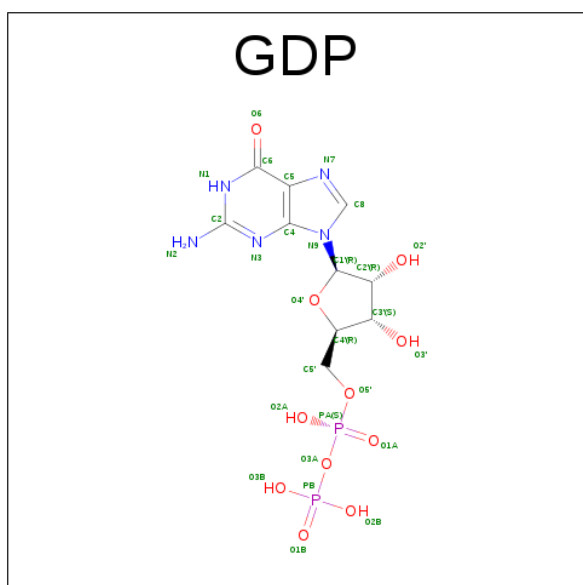
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	76	HIS	-	EXPRESSION TAG	UNP Q01960
C	77	HIS	-	EXPRESSION TAG	UNP Q01960
C	78	HIS	-	EXPRESSION TAG	UNP Q01960
D	71	MET	-	EXPRESSION TAG	UNP Q01960
D	72	GLY	-	EXPRESSION TAG	UNP Q01960
D	73	HIS	-	EXPRESSION TAG	UNP Q01960
D	74	HIS	-	EXPRESSION TAG	UNP Q01960
D	75	HIS	-	EXPRESSION TAG	UNP Q01960
D	76	HIS	-	EXPRESSION TAG	UNP Q01960
D	77	HIS	-	EXPRESSION TAG	UNP Q01960
D	78	HIS	-	EXPRESSION TAG	UNP Q01960

- Molecule 2 is a protein called ATP-binding protein YlxH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	16	Total	C	N	O	S	0	0	0
			136	82	28	25	1			
2	F	16	Total	C	N	O	S	0	0	0
			136	82	28	25	1			
2	G	16	Total	C	N	O	S	0	0	0
			136	82	28	25	1			
2	H	16	Total	C	N	O	S	0	0	0
			136	82	28	25	1			

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

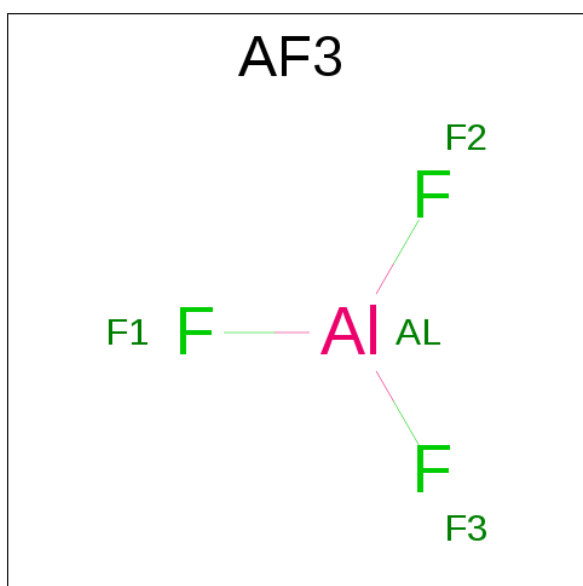


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF₃).



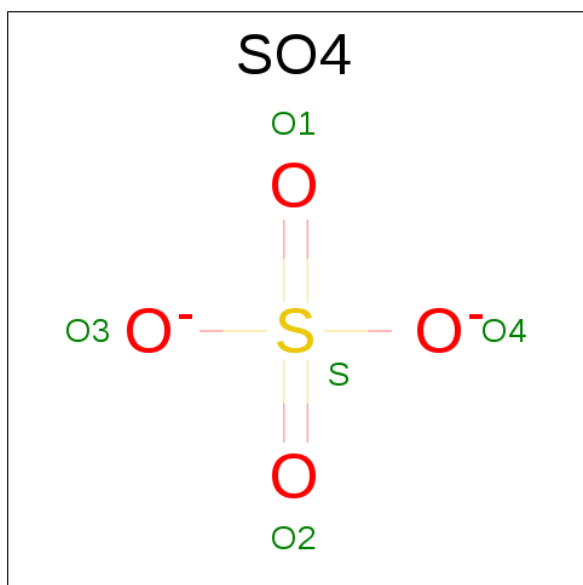
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Al	F	0	0
			4	1	3		
5	B	1	Total	Al	F	0	0
			4	1	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	Al	F	0	0
			4	1	3		
5	D	1	Total	Al	F	0	0
			4	1	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

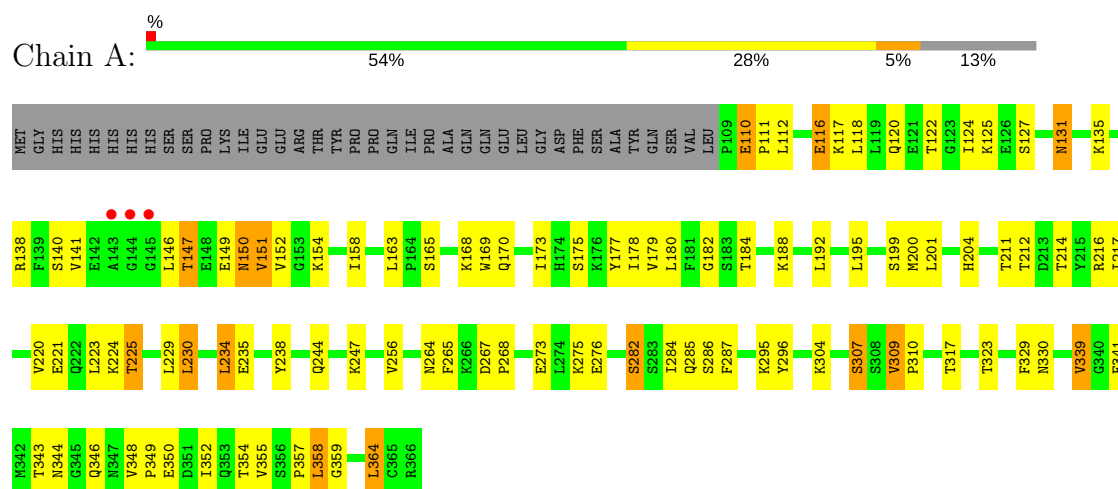
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	20	Total	O	0	0
			20	20		
7	B	21	Total	O	0	0
			21	21		
7	C	20	Total	O	0	0
			20	20		
7	D	26	Total	O	0	0
			26	26		
7	E	2	Total	O	0	0
			2	2		
7	F	1	Total	O	0	0
			1	1		
7	G	1	Total	O	0	0
			1	1		

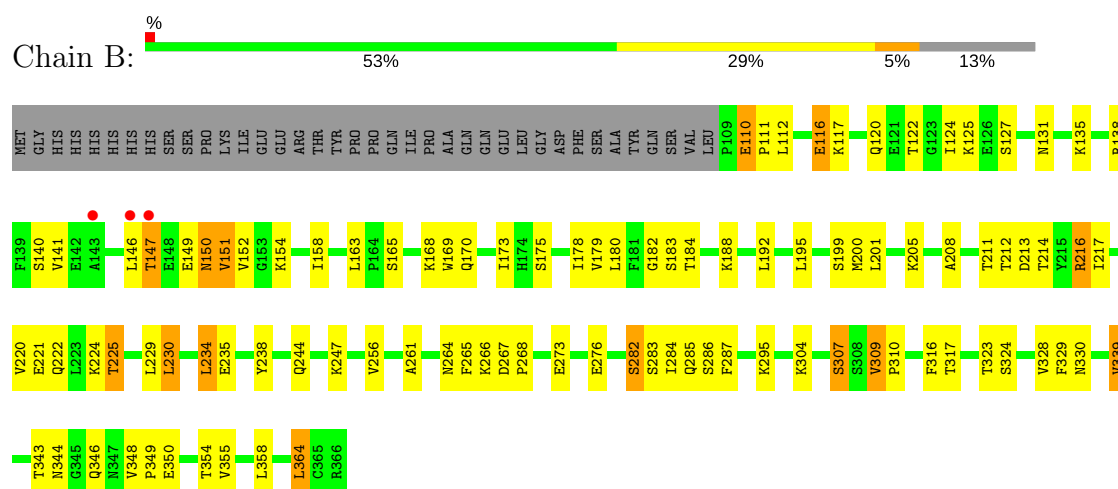
3 Residue-property plots

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.

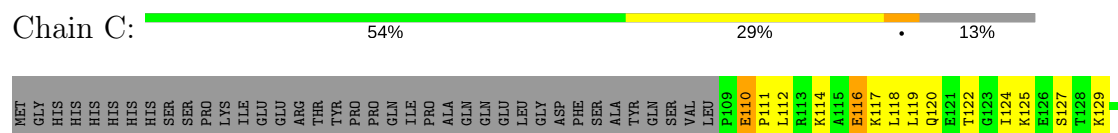
• Molecule 1: Flagellar biosynthesis protein fhfF

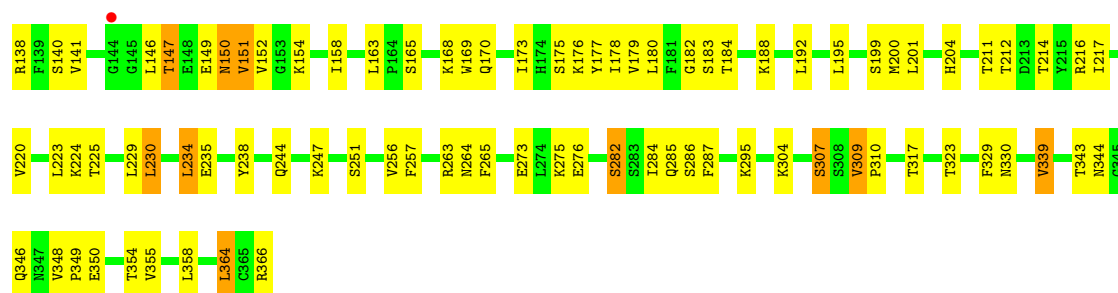


• Molecule 1: Flagellar biosynthesis protein fhfF

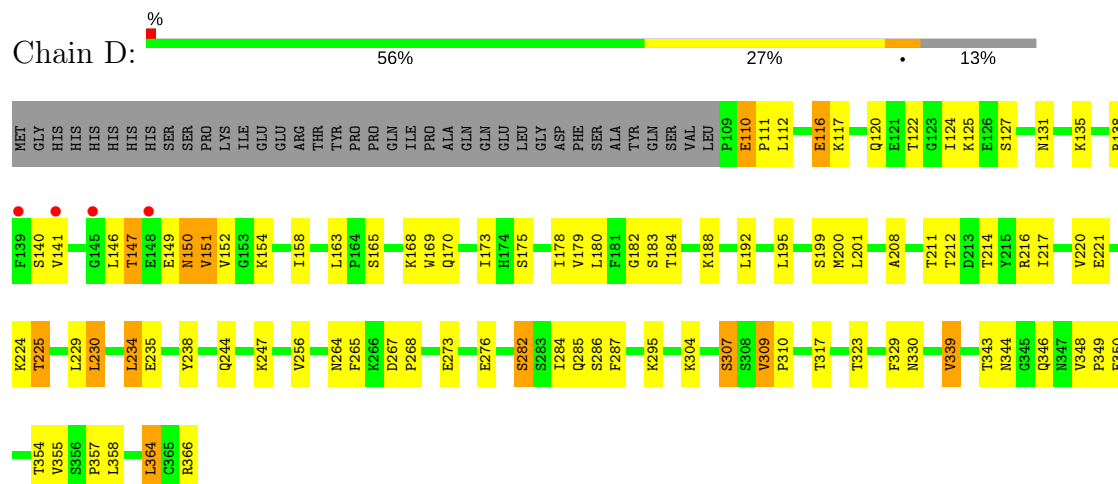


• Molecule 1: Flagellar biosynthesis protein fhfF

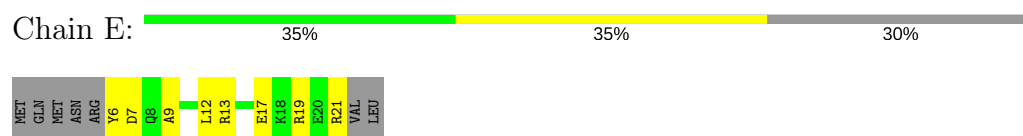




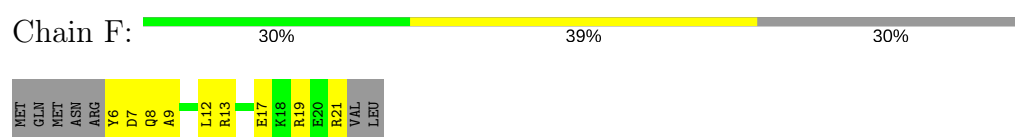
- Molecule 1: Flagellar biosynthesis protein flhF



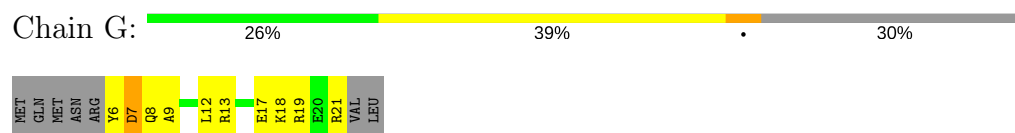
- Molecule 2: ATP-binding protein YlxH



- Molecule 2: ATP-binding protein YlxH



- Molecule 2: ATP-binding protein YlxH



- Molecule 2: ATP-binding protein YlxH



MET	GLN	MET	ASN	ARG	Y6	D7	Q8	A9	L12	R13	E17	K18	R19	E20	R21	VAL	LEU
-----	-----	-----	-----	-----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.79Å 63.36Å 114.50Å 92.26° 100.96° 94.25°	Depositor
Resolution (Å)	63.09 – 3.06 63.09 – 3.06	Depositor EDS
% Data completeness (in resolution range)	92.9 (63.09-3.06) 91.4 (63.09-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.28 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.181 , 0.239 0.173 , 0.231	Depositor DCC
R_{free} test set	1237 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9010	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GDP, MG, SO4, AF3

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	0.48	0/2079	0.59	0/2805
1	B	0.47	0/2079	0.60	0/2805
1	C	0.46	0/2079	0.59	0/2805
1	D	0.47	0/2079	0.60	0/2805
2	E	0.48	0/136	0.63	0/178
2	F	0.44	0/136	0.63	0/178
2	G	0.41	0/136	0.62	0/178
2	H	0.44	0/136	0.61	0/178
All	All	0.47	0/8860	0.60	0/11932

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	2042	0	2079	81	0
1	B	2042	0	2080	80	0
1	C	2042	0	2080	75	0
1	D	2042	0	2080	73	0
2	E	136	0	139	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	136	0	139	10	0
2	G	136	0	139	9	0
2	H	136	0	139	10	0
3	A	28	0	12	0	0
3	B	28	0	12	0	0
3	C	28	0	12	1	0
3	D	28	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	1	0
6	A	25	0	0	9	0
6	B	15	0	0	8	0
6	C	20	0	0	4	0
6	D	15	0	0	3	0
7	A	20	0	0	2	0
7	B	21	0	0	2	0
7	C	20	0	0	1	0
7	D	26	0	0	0	0
7	E	2	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
All	All	9010	0	8923	313	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 18.

All (313) 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:D:179:VAL:HG21	1:D:284:ILE:HD11	1.52	0.93
1:B:179:VAL:HG21	1:B:284:ILE:HD11	1.52	0.92
1:D:110:GLU:HB2	1:D:111:PRO:HD3	1.53	0.90
1:C:110:GLU:HB2	1:C:111:PRO:HD3	1.53	0.90
1:A:110:GLU:HB2	1:A:111:PRO:HD3	1.52	0.89
1:A:179:VAL:HG21	1:A:284:ILE:HD11	1.54	0.89
1:B:110:GLU:HB2	1:B:111:PRO:HD3	1.54	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:VAL:HG21	1:C:284:ILE:HD11	1.54	0.86
1:A:188:LYS:HE2	7:A:9:HOH:O	1.80	0.81
1:B:179:VAL:CG2	1:B:284:ILE:HD11	2.12	0.79
1:D:179:VAL:CG2	1:D:284:ILE:HD11	2.13	0.79
1:C:179:VAL:CG2	1:C:284:ILE:HD11	2.15	0.76
1:A:147:THR:H	1:A:150:ASN:ND2	1.85	0.74
1:A:179:VAL:CG2	1:A:284:ILE:HD11	2.17	0.73
1:C:147:THR:H	1:C:150:ASN:ND2	1.87	0.72
1:B:214:THR:HG21	1:B:238:TYR:CE2	2.26	0.70
1:B:283:SER:HB3	6:B:14:SO4:O1	1.91	0.70
1:A:217:ILE:HD11	2:F:9:ALA:HB2	1.73	0.70
1:B:147:THR:H	1:B:150:ASN:ND2	1.91	0.69
1:D:214:THR:HG21	1:D:238:TYR:CE2	2.28	0.69
1:C:146:LEU:HD13	1:C:151:VAL:HG13	1.74	0.69
1:D:147:THR:H	1:D:150:ASN:ND2	1.92	0.68
1:C:217:ILE:HD11	2:H:9:ALA:HB2	1.74	0.68
1:B:146:LEU:HD13	1:B:151:VAL:HG13	1.75	0.68
1:B:154:LYS:O	1:B:158:ILE:HG13	1.94	0.68
1:D:122:THR:HB	1:D:364:LEU:HD22	1.76	0.68
1:C:214:THR:HG21	1:C:238:TYR:CE2	2.29	0.68
1:D:229:LEU:HD21	2:H:13:ARG:HG3	1.75	0.67
1:A:214:THR:HG21	1:A:238:TYR:CE2	2.30	0.67
1:C:122:THR:HB	1:C:364:LEU:HD22	1.75	0.66
1:A:296:TYR:N	6:A:5:SO4:O1	2.28	0.66
1:B:122:THR:HB	1:B:364:LEU:HD22	1.76	0.66
1:C:229:LEU:HD21	2:G:13:ARG:HG3	1.77	0.66
1:A:146:LEU:HD13	1:A:151:VAL:HG13	1.78	0.65
1:C:110:GLU:CB	1:C:111:PRO:HD3	2.27	0.64
1:D:116:GLU:O	1:D:120:GLN:HG2	1.97	0.64
1:A:110:GLU:CB	1:A:111:PRO:HD3	2.28	0.64
1:A:229:LEU:HD21	2:E:13:ARG:HG3	1.80	0.64
1:B:116:GLU:O	1:B:120:GLN:HG2	1.98	0.63
1:A:214:THR:HB	2:F:6:TYR:HE2	1.64	0.63
1:A:122:THR:HB	1:A:364:LEU:HD22	1.78	0.63
1:B:264:ASN:N	6:B:1:SO4:O1	2.31	0.63
1:C:214:THR:HB	2:H:6:TYR:HE2	1.64	0.63
1:D:234:LEU:HD23	1:D:235:GLU:N	2.14	0.62
1:C:110:GLU:HB2	1:C:111:PRO:CD	2.28	0.62
1:B:229:LEU:HD21	2:F:13:ARG:HG3	1.80	0.62
1:C:116:GLU:O	1:C:120:GLN:HG2	1.99	0.62
1:D:295:LYS:HA	6:D:6:SO4:O1	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ILE:HD11	2:E:9:ALA:HB2	1.82	0.62
1:D:146:LEU:HD13	1:D:151:VAL:HG13	1.80	0.62
1:A:116:GLU:O	1:A:120:GLN:HG2	1.99	0.61
1:C:147:THR:N	1:C:150:ASN:ND2	2.49	0.61
1:A:357:PRO:HD2	6:A:10:SO4:O4	1.99	0.61
1:D:217:ILE:HD11	2:G:9:ALA:HB2	1.82	0.61
1:D:154:LYS:O	1:D:158:ILE:HG13	2.01	0.61
1:D:110:GLU:CB	1:D:111:PRO:HD3	2.27	0.61
1:A:147:THR:N	1:A:150:ASN:ND2	2.49	0.61
1:B:117:LYS:O	1:B:120:GLN:HB2	2.01	0.61
1:C:244:GLN:O	1:C:247:LYS:HB2	2.01	0.61
1:D:117:LYS:O	1:D:120:GLN:HB2	2.01	0.61
1:D:244:GLN:O	1:D:247:LYS:HB2	2.01	0.60
1:C:175:SER:HB2	1:C:285:GLN:HG3	1.83	0.60
1:A:175:SER:HB2	1:A:285:GLN:HG3	1.84	0.60
1:A:244:GLN:O	1:A:247:LYS:HB2	2.02	0.60
1:D:188:LYS:N	3:D:4:GDP:O1B	2.31	0.59
1:A:163:LEU:HD21	1:A:329:PHE:CE2	2.38	0.59
1:D:110:GLU:HB2	1:D:111:PRO:CD	2.30	0.59
1:B:110:GLU:CB	1:B:111:PRO:HD3	2.29	0.59
1:D:264:ASN:N	6:D:2:SO4:O3	2.35	0.59
1:B:110:GLU:HB2	1:B:111:PRO:CD	2.31	0.59
1:B:234:LEU:HD23	1:B:235:GLU:N	2.17	0.59
1:D:163:LEU:HD21	1:D:329:PHE:CE2	2.38	0.59
1:A:217:ILE:HD11	2:F:9:ALA:CB	2.32	0.58
1:C:217:ILE:HD11	2:H:9:ALA:CB	2.33	0.58
1:A:117:LYS:O	1:A:120:GLN:HB2	2.03	0.58
1:B:244:GLN:O	1:B:247:LYS:HB2	2.02	0.58
1:D:230:LEU:HD11	2:H:12:LEU:HD11	1.85	0.58
1:A:110:GLU:HB2	1:A:111:PRO:CD	2.30	0.58
1:B:112:LEU:HD11	1:B:146:LEU:HD21	1.85	0.58
1:B:214:THR:HB	2:E:6:TYR:HE2	1.68	0.58
1:A:154:LYS:O	1:A:158:ILE:HG13	2.03	0.58
1:B:282:SER:HB3	6:B:14:SO4:O3	2.04	0.58
1:C:295:LYS:HA	6:C:9:SO4:O2	2.03	0.58
1:B:147:THR:O	1:B:151:VAL:HG22	2.04	0.58
1:B:147:THR:N	1:B:150:ASN:ND2	2.52	0.58
1:D:112:LEU:HD11	1:D:146:LEU:HD21	1.86	0.58
1:D:317:THR:HA	1:D:343:THR:OG1	2.03	0.58
1:C:234:LEU:HD23	1:C:235:GLU:N	2.19	0.57
6:C:9:SO4:O2	1:D:295:LYS:HG2	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:SER:HB3	6:A:13:SO4:O2	2.04	0.57
1:D:147:THR:N	1:D:150:ASN:ND2	2.52	0.57
1:A:112:LEU:HD11	1:A:146:LEU:HD21	1.86	0.57
1:C:117:LYS:O	1:C:120:GLN:HB2	2.05	0.57
1:C:211:THR:HG21	1:C:220:VAL:HG22	1.87	0.57
1:C:264:ASN:N	6:C:4:SO4:O4	2.37	0.56
6:A:5:SO4:O4	1:B:295:LYS:HG2	2.06	0.56
1:A:234:LEU:HD23	1:A:235:GLU:N	2.21	0.56
1:C:112:LEU:HD11	1:C:146:LEU:HD21	1.88	0.56
1:B:175:SER:HB2	1:B:285:GLN:HG3	1.88	0.56
1:A:125:LYS:HE2	7:A:56:HOH:O	2.06	0.56
1:C:154:LYS:O	1:C:158:ILE:HG13	2.06	0.55
1:D:273:GLU:O	1:D:276:GLU:HG2	2.06	0.55
1:A:317:THR:HA	1:A:343:THR:OG1	2.06	0.55
1:D:211:THR:HG21	1:D:220:VAL:HG22	1.88	0.55
1:D:147:THR:O	1:D:151:VAL:HG22	2.07	0.55
1:B:110:GLU:OE1	1:B:110:GLU:HA	2.07	0.55
1:B:214:THR:HG21	1:B:238:TYR:HE2	1.70	0.55
1:D:110:GLU:OE1	1:D:110:GLU:HA	2.07	0.55
1:D:221:GLU:O	1:D:225:THR:HG23	2.07	0.54
1:A:346:GLN:NE2	6:B:1:SO4:O4	2.41	0.54
1:B:170:GLN:HG2	1:B:354:THR:HB	1.89	0.54
1:C:147:THR:O	1:C:151:VAL:HG22	2.07	0.54
1:B:317:THR:HA	1:B:343:THR:OG1	2.08	0.54
1:C:179:VAL:C	1:C:180:LEU:HD23	2.29	0.53
1:A:358:LEU:HB2	6:A:10:SO4:O2	2.08	0.53
1:A:211:THR:HG21	1:A:220:VAL:HG22	1.90	0.53
1:A:224:LYS:HA	1:A:234:LEU:HD12	1.91	0.53
1:D:217:ILE:HD11	2:G:9:ALA:CB	2.37	0.53
1:D:175:SER:HB2	1:D:285:GLN:HG3	1.91	0.53
1:C:147:THR:HB	1:C:149:GLU:H	1.74	0.53
1:B:221:GLU:O	1:B:225:THR:HG23	2.09	0.53
1:C:214:THR:HG21	1:C:238:TYR:HE2	1.74	0.53
1:C:273:GLU:O	1:C:276:GLU:HG2	2.09	0.53
1:C:224:LYS:HA	1:C:234:LEU:HD12	1.92	0.52
1:A:110:GLU:OE1	1:A:110:GLU:HA	2.08	0.52
1:D:214:THR:HG21	1:D:238:TYR:HE2	1.73	0.52
1:C:180:LEU:N	1:C:180:LEU:HD23	2.25	0.52
1:D:147:THR:HB	1:D:149:GLU:H	1.75	0.52
1:A:170:GLN:HG2	1:A:354:THR:HB	1.91	0.52
1:B:273:GLU:O	1:B:276:GLU:HG2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:TRP:CZ3	1:B:339:VAL:HG13	2.44	0.52
1:C:170:GLN:HG2	1:C:354:THR:HB	1.90	0.52
1:A:295:LYS:HG2	6:B:8:SO4:O4	2.10	0.52
1:B:146:LEU:CD1	1:B:151:VAL:HG13	2.39	0.52
1:A:200:MET:HG2	1:A:201:LEU:HD23	1.93	0.51
1:B:295:LYS:HA	6:B:8:SO4:O4	2.10	0.51
1:D:169:TRP:CE3	1:D:339:VAL:HG13	2.46	0.51
1:B:217:ILE:HD11	2:E:9:ALA:CB	2.40	0.51
1:B:180:LEU:HD22	1:B:287:PHE:HB2	1.93	0.51
1:D:140:SER:CB	1:D:146:LEU:HD23	2.41	0.51
1:A:169:TRP:CE3	1:A:339:VAL:HG13	2.46	0.51
1:C:110:GLU:HA	1:C:110:GLU:OE1	2.10	0.51
1:A:179:VAL:C	1:A:180:LEU:HD23	2.31	0.50
1:B:140:SER:CB	1:B:146:LEU:HD23	2.41	0.50
1:B:169:TRP:CE3	1:B:339:VAL:HG13	2.47	0.50
1:C:147:THR:N	1:C:150:ASN:HD21	2.08	0.50
1:D:214:THR:HB	2:G:6:TYR:HE2	1.75	0.50
1:B:179:VAL:C	1:B:180:LEU:HD23	2.31	0.50
1:B:211:THR:HG21	1:B:220:VAL:HG22	1.94	0.50
1:C:230:LEU:HD11	2:G:12:LEU:HD11	1.93	0.50
1:D:180:LEU:HD22	1:D:287:PHE:HB2	1.94	0.50
1:B:182:GLY:N	1:B:188:LYS:HD3	2.26	0.50
1:B:200:MET:HG2	1:B:201:LEU:HD23	1.92	0.50
1:C:163:LEU:HD21	1:C:329:PHE:CE2	2.47	0.50
1:C:140:SER:CB	1:C:146:LEU:HD23	2.41	0.50
1:D:169:TRP:CE2	1:D:357:PRO:HG3	2.47	0.50
1:B:304:LYS:O	1:B:307:SER:HB3	2.12	0.50
1:C:200:MET:HG2	1:C:201:LEU:HD23	1.94	0.49
1:A:147:THR:O	1:A:151:VAL:HG22	2.12	0.49
1:C:182:GLY:O	1:C:265:PHE:HE1	1.95	0.49
1:D:182:GLY:O	1:D:265:PHE:HE1	1.95	0.49
1:A:273:GLU:O	1:A:276:GLU:HG2	2.12	0.49
1:A:140:SER:CB	1:A:146:LEU:HD23	2.42	0.49
1:A:169:TRP:CZ3	1:A:339:VAL:HG13	2.47	0.49
1:D:170:GLN:HG2	1:D:354:THR:HB	1.93	0.49
1:B:230:LEU:HD11	2:F:12:LEU:HD11	1.93	0.49
1:A:304:LYS:O	1:A:307:SER:HB3	2.13	0.49
1:B:182:GLY:O	1:B:265:PHE:HE1	1.96	0.49
1:C:146:LEU:CD1	1:C:151:VAL:HG13	2.41	0.49
1:A:230:LEU:HD11	2:E:12:LEU:HD11	1.95	0.49
1:B:180:LEU:N	1:B:180:LEU:HD23	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:GLY:N	1:D:188:LYS:HD3	2.27	0.49
1:B:147:THR:HB	1:B:149:GLU:H	1.78	0.49
1:D:234:LEU:CD2	1:D:234:LEU:C	2.81	0.49
1:A:147:THR:N	1:A:150:ASN:HD21	2.10	0.49
1:C:169:TRP:CE3	1:C:339:VAL:HG13	2.48	0.49
1:A:125:LYS:HG2	1:A:330:ASN:ND2	2.28	0.48
1:B:224:LYS:HA	1:B:234:LEU:HD12	1.94	0.48
1:D:180:LEU:HG	1:D:192:LEU:HD13	1.95	0.48
1:D:169:TRP:CZ3	1:D:339:VAL:HG13	2.47	0.48
1:B:163:LEU:HD21	1:B:329:PHE:CE2	2.48	0.48
1:D:146:LEU:CD1	1:D:151:VAL:HG13	2.42	0.48
1:C:304:LYS:O	1:C:307:SER:HB3	2.13	0.48
1:C:169:TRP:CZ3	1:C:339:VAL:HG13	2.49	0.48
1:D:304:LYS:O	1:D:307:SER:HB3	2.13	0.48
1:C:180:LEU:HD22	1:C:287:PHE:HB2	1.95	0.47
1:C:124:ILE:CG2	1:C:125:LYS:N	2.77	0.47
1:D:224:LYS:HA	1:D:234:LEU:HD12	1.95	0.47
1:B:266:LYS:HE2	7:B:49:HOH:O	2.15	0.47
1:A:309:VAL:HG23	1:A:310:PRO:HD2	1.95	0.47
1:C:234:LEU:CD2	1:C:234:LEU:C	2.83	0.47
1:C:124:ILE:HG22	1:C:125:LYS:N	2.29	0.47
1:B:234:LEU:C	1:B:234:LEU:CD2	2.83	0.47
1:D:346:GLN:O	2:H:8:GLN:HB2	2.15	0.47
1:B:147:THR:N	1:B:150:ASN:HD21	2.12	0.47
1:D:125:LYS:HG2	1:D:330:ASN:ND2	2.30	0.47
1:C:217:ILE:CD1	2:H:9:ALA:HB2	2.45	0.47
1:B:221:GLU:O	1:B:225:THR:CG2	2.62	0.46
1:C:309:VAL:HG23	1:C:310:PRO:HD2	1.96	0.46
1:B:180:LEU:HG	1:B:192:LEU:HD13	1.98	0.46
1:B:309:VAL:HG23	1:B:310:PRO:HD2	1.98	0.46
1:A:173:ILE:HG23	1:A:178:ILE:HD11	1.98	0.46
1:B:173:ILE:HG23	1:B:178:ILE:HD11	1.97	0.46
1:A:214:THR:HB	2:F:6:TYR:CE2	2.48	0.46
1:B:205:LYS:HE3	7:B:27:HOH:O	2.15	0.46
1:A:180:LEU:HG	1:A:192:LEU:HD13	1.98	0.46
1:A:234:LEU:CD2	1:A:234:LEU:C	2.84	0.46
1:B:124:ILE:HG22	1:B:125:LYS:N	2.30	0.46
1:D:173:ILE:HG23	1:D:178:ILE:HD11	1.97	0.46
1:D:179:VAL:C	1:D:180:LEU:HD23	2.36	0.46
1:A:180:LEU:HD22	1:A:287:PHE:HB2	1.97	0.46
1:A:200:MET:O	1:A:204:HIS:HA	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ILE:CG2	1:B:125:LYS:N	2.79	0.46
1:A:147:THR:HB	1:A:149:GLU:H	1.81	0.45
1:A:182:GLY:N	1:A:188:LYS:HD3	2.31	0.45
1:C:188:LYS:HE2	7:C:373:HOH:O	2.16	0.45
1:C:317:THR:HA	1:C:343:THR:OG1	2.16	0.45
1:C:295:LYS:HG2	6:D:6:SO4:O1	2.16	0.45
1:B:125:LYS:HG2	1:B:330:ASN:ND2	2.31	0.45
1:A:359:GLY:HA3	6:A:7:SO4:O1	2.17	0.45
1:B:346:GLN:O	2:F:8:GLN:HB2	2.17	0.45
1:A:165:SER:OG	1:A:168:LYS:HE3	2.15	0.45
1:A:221:GLU:O	1:A:225:THR:HG23	2.16	0.45
1:D:147:THR:N	1:D:150:ASN:HD21	2.14	0.45
1:A:221:GLU:O	1:A:225:THR:CG2	2.64	0.45
1:A:247:LYS:NZ	1:A:282:SER:HB3	2.32	0.45
1:B:267:ASP:OD1	1:B:268:PRO:N	2.50	0.45
1:B:348:VAL:HA	1:B:349:PRO:HA	1.68	0.45
1:C:348:VAL:HA	1:C:349:PRO:HA	1.69	0.45
1:C:177:TYR:CD1	1:C:256:VAL:HB	2.52	0.44
1:D:221:GLU:O	1:D:225:THR:CG2	2.64	0.44
1:A:146:LEU:CD1	1:A:151:VAL:HG13	2.45	0.44
1:B:208:ALA:O	1:B:256:VAL:HA	2.17	0.44
1:B:264:ASN:HB2	6:B:1:SO4:O1	2.18	0.44
1:D:200:MET:HG2	1:D:201:LEU:HD23	1.98	0.44
1:A:264:ASN:N	6:A:3:SO4:O3	2.49	0.44
1:D:180:LEU:HD23	1:D:180:LEU:N	2.32	0.44
3:D:4:GDP:O3B	5:D:368:AF3:F2	2.26	0.44
1:A:182:GLY:O	1:A:265:PHE:HE1	2.01	0.44
1:A:180:LEU:N	1:A:180:LEU:HD23	2.33	0.44
1:A:348:VAL:HA	1:A:349:PRO:HA	1.69	0.44
1:C:346:GLN:O	2:G:8:GLN:HB2	2.17	0.44
1:C:188:LYS:N	3:C:3:GDP:O1B	2.48	0.44
1:A:131:ASN:O	1:A:135:LYS:HG3	2.18	0.43
1:B:267:ASP:C	1:B:267:ASP:OD1	2.56	0.43
1:D:124:ILE:HG22	1:D:125:LYS:N	2.33	0.43
1:D:163:LEU:HD21	1:D:329:PHE:CD2	2.52	0.43
1:A:124:ILE:HG22	1:A:125:LYS:N	2.33	0.43
1:D:309:VAL:HG23	1:D:310:PRO:HD2	2.00	0.43
1:D:124:ILE:CG2	1:D:125:LYS:N	2.81	0.43
1:A:282:SER:CB	6:A:13:SO4:O2	2.67	0.43
1:B:165:SER:OG	1:B:168:LYS:HE3	2.18	0.43
1:C:125:LYS:HG2	1:C:330:ASN:ND2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:MET:O	1:C:204:HIS:HA	2.19	0.43
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.83	0.43
1:D:267:ASP:OD1	1:D:268:PRO:CD	2.66	0.43
1:C:140:SER:HB2	1:C:146:LEU:HD23	2.01	0.43
1:B:214:THR:HG22	1:B:214:THR:O	2.19	0.43
1:C:119:LEU:HB3	1:C:129:LYS:CG	2.49	0.43
1:C:173:ILE:HG23	1:C:178:ILE:HD11	2.00	0.43
1:D:230:LEU:CD1	2:H:12:LEU:HD11	2.47	0.43
1:C:366:ARG:N	1:C:366:ARG:HD3	2.34	0.42
1:D:234:LEU:C	1:D:234:LEU:HD23	2.40	0.42
1:D:247:LYS:NZ	1:D:282:SER:HB3	2.34	0.42
2:G:18:LYS:HB2	2:G:18:LYS:HE3	1.84	0.42
1:A:124:ILE:CG2	1:A:125:LYS:N	2.82	0.42
1:A:267:ASP:HA	1:A:268:PRO:HD3	1.86	0.42
1:A:217:ILE:O	1:B:222:GLN:HG3	2.20	0.42
1:C:247:LYS:NZ	1:C:282:SER:HB3	2.34	0.42
1:D:348:VAL:HA	1:D:349:PRO:HA	1.67	0.42
1:A:358:LEU:N	6:A:10:SO4:O2	2.48	0.42
1:D:366:ARG:HD3	1:D:366:ARG:N	2.35	0.42
2:H:18:LYS:HE3	2:H:18:LYS:HB2	1.86	0.42
1:B:247:LYS:NZ	1:B:282:SER:HB3	2.35	0.42
1:C:223:LEU:HA	1:C:223:LEU:HD12	1.86	0.42
1:A:163:LEU:HD21	1:A:329:PHE:CD2	2.53	0.42
1:C:180:LEU:HG	1:C:192:LEU:HD13	2.01	0.42
1:D:267:ASP:HA	1:D:268:PRO:HD3	1.88	0.42
2:F:7:ASP:C	2:F:9:ALA:N	2.73	0.42
1:D:131:ASN:O	1:D:135:LYS:HG3	2.20	0.42
1:A:140:SER:HB2	1:A:146:LEU:HD23	2.02	0.42
1:B:316:PHE:CZ	1:B:328:VAL:HG13	2.55	0.42
1:A:267:ASP:OD1	1:A:268:PRO:CD	2.67	0.42
1:C:118:LEU:HD23	1:C:118:LEU:HA	1.80	0.42
1:D:165:SER:OG	1:D:168:LYS:HE3	2.20	0.42
2:G:7:ASP:C	2:G:9:ALA:N	2.73	0.42
1:A:341:PHE:CD1	1:A:352:ILE:HD11	2.55	0.41
1:B:213:ASP:HA	1:B:261:ALA:HB2	2.00	0.41
1:B:234:LEU:C	1:B:234:LEU:HD23	2.41	0.41
1:B:230:LEU:CD1	2:F:12:LEU:HD11	2.50	0.41
1:B:264:ASN:CB	6:B:1:SO4:O1	2.68	0.41
1:C:182:GLY:N	1:C:188:LYS:HD3	2.35	0.41
1:D:140:SER:HB2	1:D:146:LEU:HD23	2.02	0.41
1:D:217:ILE:CD1	2:G:9:ALA:HB2	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ARG:O	1:B:216:ARG:HG3	2.15	0.41
1:B:267:ASP:OD1	1:B:268:PRO:CD	2.68	0.41
1:A:177:TYR:CD1	1:A:256:VAL:HB	2.56	0.41
1:B:131:ASN:O	1:B:135:LYS:HG3	2.21	0.41
1:A:217:ILE:CD1	2:F:9:ALA:HB2	2.45	0.41
1:A:214:THR:HG21	1:A:238:TYR:HE2	1.80	0.41
1:C:214:THR:HB	2:H:6:TYR:CE2	2.51	0.41
1:C:192:LEU:HD11	1:C:257:PHE:HB3	2.02	0.41
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.86	0.41
1:D:208:ALA:O	1:D:256:VAL:HA	2.21	0.41
1:B:267:ASP:HA	1:B:268:PRO:HD3	1.90	0.40
1:C:176:LYS:NZ	1:C:251:SER:HA	2.36	0.40
1:C:165:SER:OG	1:C:168:LYS:HE3	2.20	0.40
1:C:110:GLU:CB	1:C:111:PRO:CD	2.93	0.40
1:C:111:PRO:O	1:C:114:LYS:HB3	2.22	0.40
1:C:263:ARG:HA	6:C:4:SO4:O4	2.21	0.40
1:D:267:ASP:OD1	1:D:268:PRO:N	2.54	0.40
1:B:140:SER:HB2	1:B:146:LEU:HD23	2.04	0.40
1:C:214:THR:HG22	1:C:214:THR:O	2.20	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	256/296 (86%)	238 (93%)	17 (7%)	1 (0%)	38	72
1	B	256/296 (86%)	238 (93%)	17 (7%)	1 (0%)	38	72
1	C	256/296 (86%)	235 (92%)	20 (8%)	1 (0%)	38	72
1	D	256/296 (86%)	237 (93%)	18 (7%)	1 (0%)	38	72
2	E	14/23 (61%)	12 (86%)	1 (7%)	1 (7%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	14/23 (61%)	12 (86%)	2 (14%)	0	100	100
2	G	14/23 (61%)	12 (86%)	1 (7%)	1 (7%)	1	6
2	H	14/23 (61%)	12 (86%)	2 (14%)	0	100	100
All	All	1080/1276 (85%)	996 (92%)	78 (7%)	6 (1%)	28	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	GLU
1	B	110	GLU
1	C	110	GLU
1	D	110	GLU
2	E	7	ASP
2	G	7	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	228/262 (87%)	199 (87%)	29 (13%)	5	19
1	B	228/262 (87%)	199 (87%)	29 (13%)	5	19
1	C	228/262 (87%)	199 (87%)	29 (13%)	5	19
1	D	228/262 (87%)	200 (88%)	28 (12%)	5	20
2	E	13/20 (65%)	10 (77%)	3 (23%)	1	3
2	F	13/20 (65%)	10 (77%)	3 (23%)	1	3
2	G	13/20 (65%)	10 (77%)	3 (23%)	1	3
2	H	13/20 (65%)	10 (77%)	3 (23%)	1	3
All	All	964/1128 (86%)	837 (87%)	127 (13%)	5	18

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	GLU
1	A	127	SER
1	A	131	ASN
1	A	138	ARG
1	A	141	VAL
1	A	147	THR
1	A	150	ASN
1	A	151	VAL
1	A	152	VAL
1	A	184	THR
1	A	195	LEU
1	A	199	SER
1	A	212	THR
1	A	216	ARG
1	A	225	THR
1	A	230	LEU
1	A	234	LEU
1	A	275	LYS
1	A	282	SER
1	A	286	SER
1	A	307	SER
1	A	309	VAL
1	A	323	THR
1	A	339	VAL
1	A	344	ASN
1	A	350	GLU
1	A	355	VAL
1	A	358	LEU
1	A	364	LEU
1	B	116	GLU
1	B	127	SER
1	B	138	ARG
1	B	141	VAL
1	B	147	THR
1	B	150	ASN
1	B	151	VAL
1	B	152	VAL
1	B	183	SER
1	B	184	THR
1	B	195	LEU
1	B	199	SER
1	B	212	THR
1	B	216	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	225	THR
1	B	230	LEU
1	B	234	LEU
1	B	282	SER
1	B	286	SER
1	B	307	SER
1	B	309	VAL
1	B	323	THR
1	B	324	SER
1	B	339	VAL
1	B	344	ASN
1	B	350	GLU
1	B	355	VAL
1	B	358	LEU
1	B	364	LEU
1	C	116	GLU
1	C	127	SER
1	C	138	ARG
1	C	141	VAL
1	C	147	THR
1	C	150	ASN
1	C	151	VAL
1	C	152	VAL
1	C	183	SER
1	C	184	THR
1	C	195	LEU
1	C	199	SER
1	C	212	THR
1	C	216	ARG
1	C	225	THR
1	C	230	LEU
1	C	234	LEU
1	C	275	LYS
1	C	282	SER
1	C	286	SER
1	C	307	SER
1	C	309	VAL
1	C	323	THR
1	C	339	VAL
1	C	344	ASN
1	C	350	GLU
1	C	355	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	358	LEU
1	C	364	LEU
1	D	116	GLU
1	D	127	SER
1	D	138	ARG
1	D	141	VAL
1	D	147	THR
1	D	150	ASN
1	D	151	VAL
1	D	152	VAL
1	D	183	SER
1	D	184	THR
1	D	195	LEU
1	D	199	SER
1	D	212	THR
1	D	216	ARG
1	D	225	THR
1	D	230	LEU
1	D	234	LEU
1	D	282	SER
1	D	286	SER
1	D	307	SER
1	D	309	VAL
1	D	323	THR
1	D	339	VAL
1	D	344	ASN
1	D	350	GLU
1	D	355	VAL
1	D	358	LEU
1	D	364	LEU
2	E	17	GLU
2	E	19	ARG
2	E	21	ARG
2	F	17	GLU
2	F	19	ARG
2	F	21	ARG
2	G	17	GLU
2	G	19	ARG
2	G	21	ARG
2	H	17	GLU
2	H	19	ARG
2	H	21	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	231	GLN
1	A	269	GLN
1	B	150	ASN
1	B	231	GLN
1	B	244	GLN
1	B	269	GLN
1	C	150	ASN
1	C	174	HIS
1	C	231	GLN
1	C	244	GLN
1	C	269	GLN
1	C	301	HIS
1	C	330	ASN
1	D	150	ASN
1	D	231	GLN
1	D	269	GLN
1	D	301	HIS
1	D	330	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 4 are monoatomic - leaving 23 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	GDP	A	1	4	25,30,30	1.11	3 (12%)	26,47,47	2.09	6 (23%)
6	SO4	A	10	-	4,4,4	0.20	0	6,6,6	0.21	0
6	SO4	A	13	-	4,4,4	0.18	0	6,6,6	0.28	0
6	SO4	A	3	-	4,4,4	0.18	0	6,6,6	0.20	0
5	AF3	A	368	-	0,3,3	0.00	-	0,3,3	0.00	-
6	SO4	A	5	-	4,4,4	0.19	0	6,6,6	0.18	0
6	SO4	A	7	-	4,4,4	0.22	0	6,6,6	0.16	0
6	SO4	B	1	-	4,4,4	0.07	0	6,6,6	0.42	0
6	SO4	B	14	-	4,4,4	0.14	0	6,6,6	0.20	0
3	GDP	B	2	4	25,30,30	1.11	2 (8%)	26,47,47	2.08	7 (26%)
5	AF3	B	368	-	0,3,3	0.00	-	0,3,3	0.00	-
6	SO4	B	8	-	4,4,4	0.20	0	6,6,6	0.34	0
6	SO4	C	11	-	4,4,4	0.19	0	6,6,6	0.39	0
6	SO4	C	15	-	4,4,4	0.15	0	6,6,6	0.31	0
3	GDP	C	3	4	25,30,30	1.23	4 (16%)	26,47,47	2.11	7 (26%)
5	AF3	C	368	-	0,3,3	0.00	-	0,3,3	0.00	-
6	SO4	C	4	-	4,4,4	0.11	0	6,6,6	0.21	0
6	SO4	C	9	-	4,4,4	0.23	0	6,6,6	0.24	0
6	SO4	D	12	-	4,4,4	0.18	0	6,6,6	0.27	0
6	SO4	D	2	-	4,4,4	0.15	0	6,6,6	0.32	0
5	AF3	D	368	-	0,3,3	0.00	-	0,3,3	0.00	-
3	GDP	D	4	4	25,30,30	1.04	2 (8%)	26,47,47	1.85	6 (23%)
6	SO4	D	6	-	4,4,4	0.15	0	6,6,6	0.22	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	GDP	A	1	4	-	0/12/32/32	0/3/3/3
6	SO4	A	10	-	-	0/0/0/0	0/0/0/0
6	SO4	A	13	-	-	0/0/0/0	0/0/0/0
6	SO4	A	3	-	-	0/0/0/0	0/0/0/0
5	AF3	A	368	-	-	0/0/0/0	0/0/0/0
6	SO4	A	5	-	-	0/0/0/0	0/0/0/0
6	SO4	A	7	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	B	1	-	-	0/0/0/0	0/0/0/0
6	SO4	B	14	-	-	0/0/0/0	0/0/0/0
3	GDP	B	2	4	-	0/12/32/32	0/3/3/3
5	AF3	B	368	-	-	0/0/0/0	0/0/0/0
6	SO4	B	8	-	-	0/0/0/0	0/0/0/0
6	SO4	C	11	-	-	0/0/0/0	0/0/0/0
6	SO4	C	15	-	-	0/0/0/0	0/0/0/0
3	GDP	C	3	4	-	0/12/32/32	0/3/3/3
5	AF3	C	368	-	-	0/0/0/0	0/0/0/0
6	SO4	C	4	-	-	0/0/0/0	0/0/0/0
6	SO4	C	9	-	-	0/0/0/0	0/0/0/0
6	SO4	D	12	-	-	0/0/0/0	0/0/0/0
6	SO4	D	2	-	-	0/0/0/0	0/0/0/0
5	AF3	D	368	-	-	0/0/0/0	0/0/0/0
3	GDP	D	4	4	-	0/12/32/32	0/3/3/3
6	SO4	D	6	-	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	GDP	PB-O3A	2.24	1.63	1.60
3	C	3	GDP	PB-O3A	2.42	1.64	1.60
3	C	3	GDP	O4'-C1'	2.49	1.44	1.41
3	A	1	GDP	C5-C4	2.58	1.46	1.40
3	D	4	GDP	C5-C4	2.59	1.46	1.40
3	C	3	GDP	C5-C4	2.74	1.46	1.40
3	B	2	GDP	C5-C4	2.77	1.46	1.40
3	A	1	GDP	C6-C5	2.94	1.46	1.41
3	D	4	GDP	C6-C5	3.16	1.47	1.41
3	C	3	GDP	C6-C5	3.27	1.47	1.41
3	B	2	GDP	C6-C5	3.63	1.48	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	GDP	C6-C5-C4	-4.06	116.80	120.84
3	A	1	GDP	C5-C6-N1	-3.93	117.89	123.48
3	C	3	GDP	C5-C6-N1	-3.83	118.03	123.48
3	A	1	GDP	N3-C2-N1	-3.72	122.02	127.46
3	C	3	GDP	N3-C2-N1	-3.66	122.12	127.46
3	B	2	GDP	N3-C2-N1	-3.60	122.20	127.46
3	D	4	GDP	C5-C6-N1	-3.50	118.49	123.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	GDP	C5-C6-N1	-3.47	118.54	123.48
3	D	4	GDP	C6-C5-C4	-3.39	117.47	120.84
3	D	4	GDP	N3-C2-N1	-3.23	122.75	127.46
3	C	3	GDP	C6-C5-C4	-3.13	117.73	120.84
3	A	1	GDP	C6-C5-C4	-3.06	117.80	120.84
3	A	1	GDP	C4-C5-N7	-2.87	106.64	109.41
3	B	2	GDP	C4-C5-N7	-2.79	106.71	109.41
3	D	4	GDP	C4-C5-N7	-2.77	106.73	109.41
3	C	3	GDP	C4-C5-N7	-2.31	107.18	109.41
3	C	3	GDP	O3'-C3'-C2'	-2.23	104.69	111.83
3	B	2	GDP	O3'-C3'-C2'	-2.18	104.84	111.83
3	D	4	GDP	C6-N1-C2	4.08	121.94	116.06
3	B	2	GDP	C6-N1-C2	4.17	122.06	116.06
3	C	3	GDP	C6-N1-C2	4.43	122.43	116.06
3	A	1	GDP	C6-N1-C2	4.75	122.89	116.06
3	D	4	GDP	C2-N3-C4	4.86	120.83	115.16
3	A	1	GDP	C2-N3-C4	5.50	121.58	115.16
3	B	2	GDP	C2-N3-C4	5.54	121.63	115.16
3	C	3	GDP	C2-N3-C4	5.86	122.00	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	10	SO4	3	0
6	A	13	SO4	2	0
6	A	3	SO4	1	0
6	A	5	SO4	2	0
6	A	7	SO4	1	0
6	B	1	SO4	4	0
6	B	14	SO4	2	0
6	B	8	SO4	2	0
3	C	3	GDP	1	0
6	C	4	SO4	2	0
6	C	9	SO4	2	0
6	D	2	SO4	1	0
5	D	368	AF3	1	0
3	D	4	GDP	2	0
6	D	6	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	258/296 (87%)	-0.42	3 (1%) 79 59	7, 22, 74, 103	0
1	B	258/296 (87%)	-0.37	3 (1%) 79 59	7, 22, 76, 99	0
1	C	258/296 (87%)	-0.48	1 (0%) 92 81	7, 22, 74, 97	0
1	D	258/296 (87%)	-0.32	4 (1%) 72 49	8, 22, 75, 101	0
2	E	16/23 (69%)	-0.40	0 100 100	12, 20, 90, 98	0
2	F	16/23 (69%)	-0.31	0 100 100	13, 21, 90, 103	0
2	G	16/23 (69%)	-0.44	0 100 100	13, 21, 93, 100	0
2	H	16/23 (69%)	-0.35	0 100 100	13, 21, 90, 104	0
All	All	1096/1276 (85%)	-0.40	11 (1%) 82 64	7, 22, 78, 104	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	145	GLY	9.2
1	B	143	ALA	4.1
1	A	145	GLY	3.1
1	C	144	GLY	3.1
1	B	146	LEU	2.8
1	D	148	GLU	2.5
1	A	144	GLY	2.4
1	A	143	ALA	2.3
1	D	141	VAL	2.1
1	B	147	THR	2.1
1	D	139	PHE	2.1

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
6	SO4	A	10	5/5	0.97	0.36	3.87	25,45,65,97	0
6	SO4	A	3	5/5	0.99	0.22	3.02	14,15,31,53	0
6	SO4	B	8	5/5	0.96	0.34	2.76	35,38,56,61	0
6	SO4	D	6	5/5	0.98	0.39	2.53	23,44,54,55	0
6	SO4	C	9	5/5	0.98	0.38	2.19	11,28,51,75	0
6	SO4	C	4	5/5	0.99	0.19	1.76	17,19,40,46	0
6	SO4	A	5	5/5	0.98	0.29	1.33	28,36,46,54	0
6	SO4	B	1	5/5	0.99	0.17	1.26	13,24,30,33	0
6	SO4	D	2	5/5	0.99	0.17	0.26	21,25,35,50	0
6	SO4	D	12	5/5	0.87	0.19	0.00	30,46,99,107	0
3	GDP	D	4	28/28	0.99	0.16	-0.01	5,13,17,19	0
6	SO4	A	7	5/5	0.97	0.17	-0.05	37,46,51,61	0
6	SO4	C	11	5/5	0.92	0.18	-0.22	31,35,79,97	0
5	AF3	C	368	4/4	0.99	0.16	-0.26	15,16,27,41	0
5	AF3	D	368	4/4	0.99	0.14	-0.33	13,15,23,31	0
3	GDP	B	2	28/28	0.99	0.15	-0.53	6,12,19,20	0
5	AF3	B	368	4/4	0.98	0.14	-0.62	7,19,24,31	0
5	AF3	A	368	4/4	0.98	0.14	-0.66	10,15,18,34	0
3	GDP	A	1	28/28	0.99	0.14	-0.69	6,10,15,19	0
3	GDP	C	3	28/28	0.99	0.14	-0.79	6,12,18,21	0
4	MG	C	367	1/1	0.92	0.09	-1.92	23,23,23,23	0
4	MG	D	367	1/1	0.97	0.10	-2.04	4,4,4,4	0
4	MG	A	367	1/1	0.96	0.10	-3.55	14,14,14,14	0
4	MG	B	367	1/1	0.98	0.07	-5.43	10,10,10,10	0
6	SO4	A	13	5/5	0.91	0.18	-	47,60,92,107	0
6	SO4	C	15	5/5	0.92	0.16	-	42,68,92,109	0
6	SO4	B	14	5/5	0.93	0.26	-	66,72,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.