Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:30 AM GMT

PDB ID	:	3B07
Title	:	Crystal structure of octameric pore form of gamma-hemolysin from Staphylococcus aureus
Authors	:	Yamashita, K.; Kawai, Y.; Tanaka, Y.; Yao, M.; Tanaka, I.
Deposited on	:	2011-06-06
Resolution	:	2.50 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 (i) symbol.

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

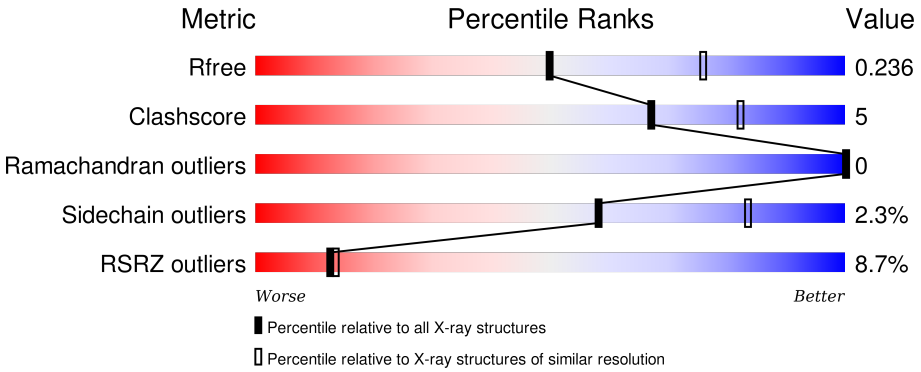
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	7% 78% 14% 8%
1	C	309	8% 79% 13% 8%
1	E	309	9% 78% 14% 8%
1	G	309	8% 78% 13% 8%
2	B	290	8% 80% 12% • 7%

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Mol	Chain	Length	Quality of chain
2	D	290	6% 84% 8% • 7%
2	F	290	8% 81% 10% • 7%
2	H	290	10% 84% 8% 7%

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
3	MPD	A	301	-	-	-	X
3	MPD	C	301	-	-	-	X
3	MPD	E	301	-	-	-	X
3	MPD	G	301	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18377 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 Gamma-hemolysin component B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2292	1450	391	447	4			
1	C	284	Total	C	N	O	S	0	0	0
			2292	1450	391	447	4			
1	E	284	Total	C	N	O	S	0	0	0
			2292	1450	391	447	4			
1	G	284	Total	C	N	O	S	0	0	0
			2292	1450	391	447	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	EXPRESSION TAG	UNP Q931F3
A	-7	GLY	-	EXPRESSION TAG	UNP Q931F3
A	-6	HIS	-	EXPRESSION TAG	UNP Q931F3
A	-5	HIS	-	EXPRESSION TAG	UNP Q931F3
A	-4	HIS	-	EXPRESSION TAG	UNP Q931F3
A	-3	HIS	-	EXPRESSION TAG	UNP Q931F3
A	-2	HIS	-	EXPRESSION TAG	UNP Q931F3
A	-1	HIS	-	EXPRESSION TAG	UNP Q931F3
A	0	ALA	-	EXPRESSION TAG	UNP Q931F3
A	1	MET	-	EXPRESSION TAG	UNP Q931F3
C	-8	MET	-	EXPRESSION TAG	UNP Q931F3
C	-7	GLY	-	EXPRESSION TAG	UNP Q931F3
C	-6	HIS	-	EXPRESSION TAG	UNP Q931F3
C	-5	HIS	-	EXPRESSION TAG	UNP Q931F3
C	-4	HIS	-	EXPRESSION TAG	UNP Q931F3
C	-3	HIS	-	EXPRESSION TAG	UNP Q931F3
C	-2	HIS	-	EXPRESSION TAG	UNP Q931F3
C	-1	HIS	-	EXPRESSION TAG	UNP Q931F3
C	0	ALA	-	EXPRESSION TAG	UNP Q931F3
C	1	MET	-	EXPRESSION TAG	UNP Q931F3
E	-8	MET	-	EXPRESSION TAG	UNP Q931F3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	GLY	-	EXPRESSION TAG	UNP Q931F3
E	-6	HIS	-	EXPRESSION TAG	UNP Q931F3
E	-5	HIS	-	EXPRESSION TAG	UNP Q931F3
E	-4	HIS	-	EXPRESSION TAG	UNP Q931F3
E	-3	HIS	-	EXPRESSION TAG	UNP Q931F3
E	-2	HIS	-	EXPRESSION TAG	UNP Q931F3
E	-1	HIS	-	EXPRESSION TAG	UNP Q931F3
E	0	ALA	-	EXPRESSION TAG	UNP Q931F3
E	1	MET	-	EXPRESSION TAG	UNP Q931F3
G	-8	MET	-	EXPRESSION TAG	UNP Q931F3
G	-7	GLY	-	EXPRESSION TAG	UNP Q931F3
G	-6	HIS	-	EXPRESSION TAG	UNP Q931F3
G	-5	HIS	-	EXPRESSION TAG	UNP Q931F3
G	-4	HIS	-	EXPRESSION TAG	UNP Q931F3
G	-3	HIS	-	EXPRESSION TAG	UNP Q931F3
G	-2	HIS	-	EXPRESSION TAG	UNP Q931F3
G	-1	HIS	-	EXPRESSION TAG	UNP Q931F3
G	0	ALA	-	EXPRESSION TAG	UNP Q931F3
G	1	MET	-	EXPRESSION TAG	UNP Q931F3

- Molecule 2 is a protein called Gamma-hemolysin component A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	270	Total	C	N	O	S	0	0	0
			2182	1389	377	413	3			
2	D	270	Total	C	N	O	S	0	0	0
			2182	1389	377	413	3			
2	F	270	Total	C	N	O	S	0	0	0
			2182	1389	377	413	3			
2	H	270	Total	C	N	O	S	0	0	0
			2182	1389	377	413	3			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	EXPRESSION TAG	UNP P0A071
B	-8	GLY	-	EXPRESSION TAG	UNP P0A071
B	-7	HIS	-	EXPRESSION TAG	UNP P0A071
B	-6	HIS	-	EXPRESSION TAG	UNP P0A071
B	-5	HIS	-	EXPRESSION TAG	UNP P0A071
B	-4	HIS	-	EXPRESSION TAG	UNP P0A071
B	-3	HIS	-	EXPRESSION TAG	UNP P0A071

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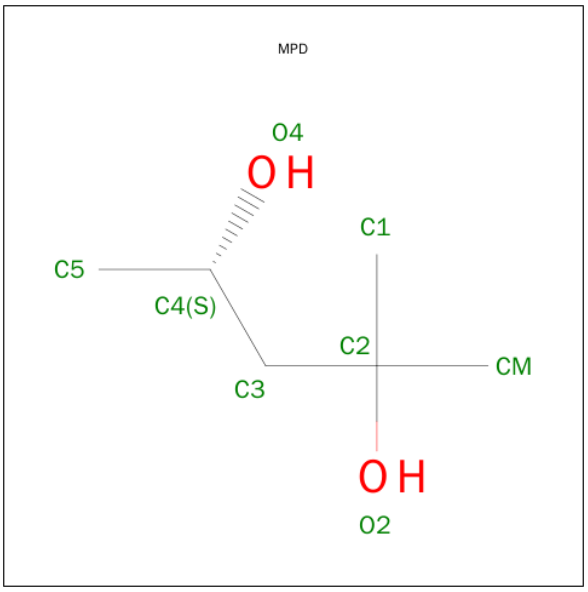
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP P0A071
B	-1	ALA	-	EXPRESSION TAG	UNP P0A071
B	0	MET	-	EXPRESSION TAG	UNP P0A071
D	-9	MET	-	EXPRESSION TAG	UNP P0A071
D	-8	GLY	-	EXPRESSION TAG	UNP P0A071
D	-7	HIS	-	EXPRESSION TAG	UNP P0A071
D	-6	HIS	-	EXPRESSION TAG	UNP P0A071
D	-5	HIS	-	EXPRESSION TAG	UNP P0A071
D	-4	HIS	-	EXPRESSION TAG	UNP P0A071
D	-3	HIS	-	EXPRESSION TAG	UNP P0A071
D	-2	HIS	-	EXPRESSION TAG	UNP P0A071
D	-1	ALA	-	EXPRESSION TAG	UNP P0A071
D	0	MET	-	EXPRESSION TAG	UNP P0A071
F	-9	MET	-	EXPRESSION TAG	UNP P0A071
F	-8	GLY	-	EXPRESSION TAG	UNP P0A071
F	-7	HIS	-	EXPRESSION TAG	UNP P0A071
F	-6	HIS	-	EXPRESSION TAG	UNP P0A071
F	-5	HIS	-	EXPRESSION TAG	UNP P0A071
F	-4	HIS	-	EXPRESSION TAG	UNP P0A071
F	-3	HIS	-	EXPRESSION TAG	UNP P0A071
F	-2	HIS	-	EXPRESSION TAG	UNP P0A071
F	-1	ALA	-	EXPRESSION TAG	UNP P0A071
F	0	MET	-	EXPRESSION TAG	UNP P0A071
H	-9	MET	-	EXPRESSION TAG	UNP P0A071
H	-8	GLY	-	EXPRESSION TAG	UNP P0A071
H	-7	HIS	-	EXPRESSION TAG	UNP P0A071
H	-6	HIS	-	EXPRESSION TAG	UNP P0A071
H	-5	HIS	-	EXPRESSION TAG	UNP P0A071
H	-4	HIS	-	EXPRESSION TAG	UNP P0A071
H	-3	HIS	-	EXPRESSION TAG	UNP P0A071
H	-2	HIS	-	EXPRESSION TAG	UNP P0A071
H	-1	ALA	-	EXPRESSION TAG	UNP P0A071
H	0	MET	-	EXPRESSION TAG	UNP P0A071

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	E	1	Total C O 8 6 2	0	0
3	G	1	Total C O 8 6 2	0	0

- Molecule 4 is water.

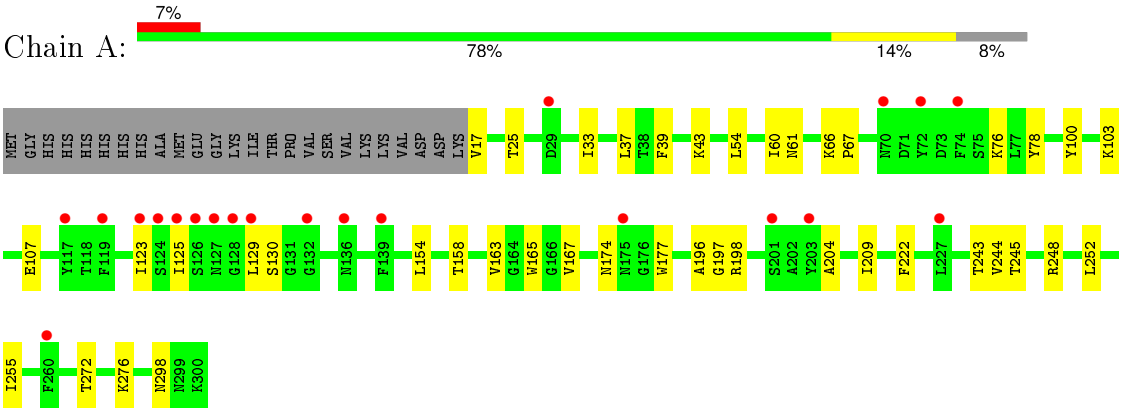
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	69	Total O 69 69	0	0
4	C	61	Total O 61 61	0	0
4	E	53	Total O 53 53	0	0
4	G	59	Total O 59 59	0	0
4	B	49	Total O 49 49	0	0
4	D	60	Total O 60 60	0	0
4	F	48	Total O 48 48	0	0
4	H	50	Total O 50 50	0	0

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 errors 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.

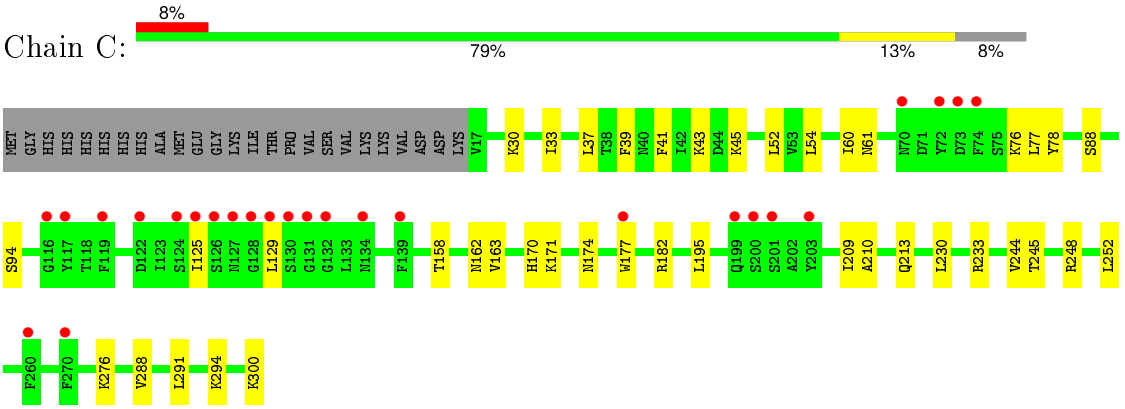
- Molecule 1: Gamma-hemolysin component B

Chain A:



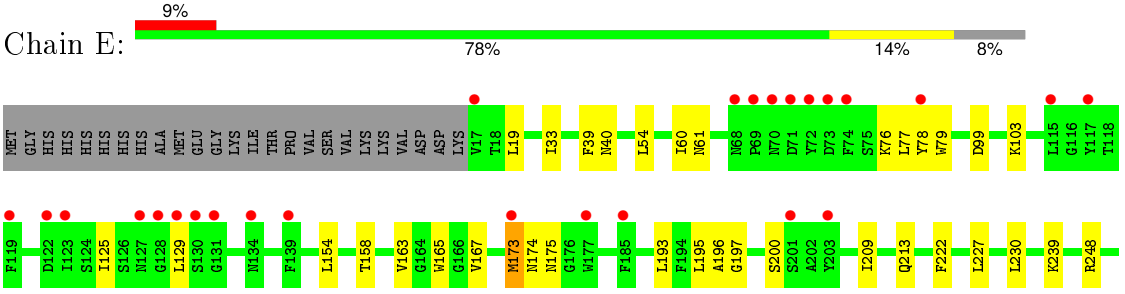
- Molecule 1: Gamma-hemolysin component B

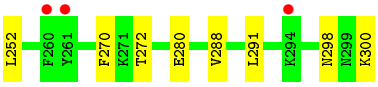
Chain C:



- Molecule 1: Gamma-hemolysin component B

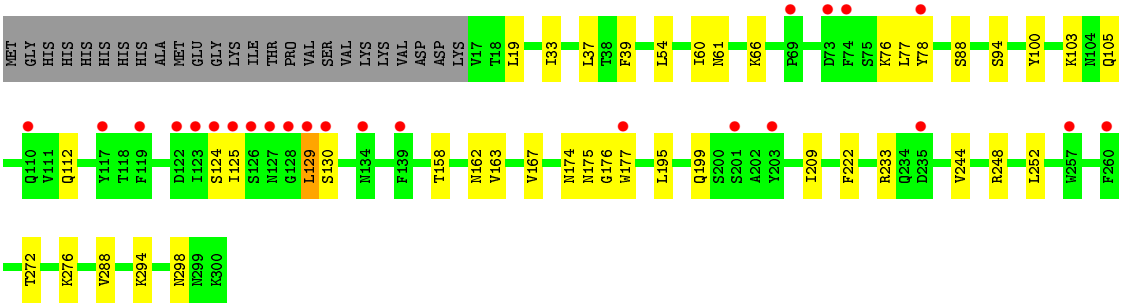
Chain E:





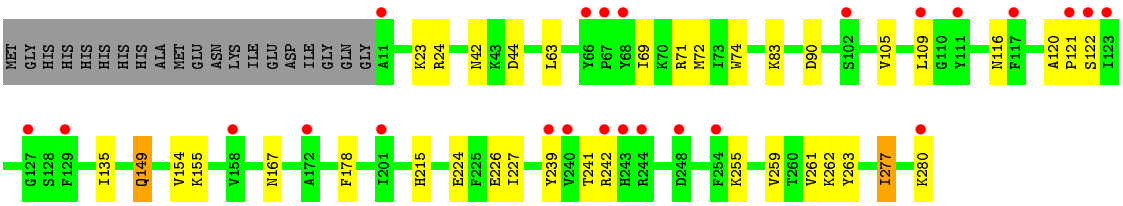
• Molecule 1: Gamma-hemolysin component B

Chain G:



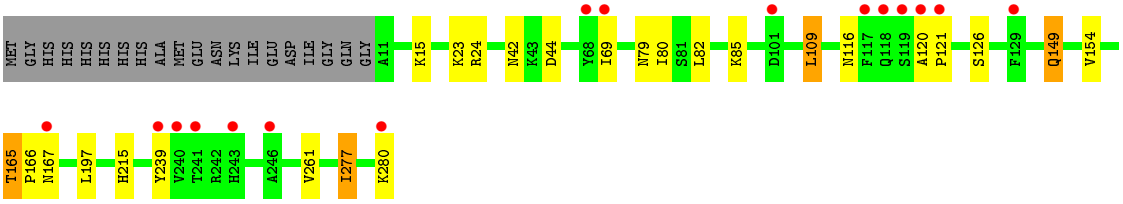
• Molecule 2: Gamma-hemolysin component A

Chain B:



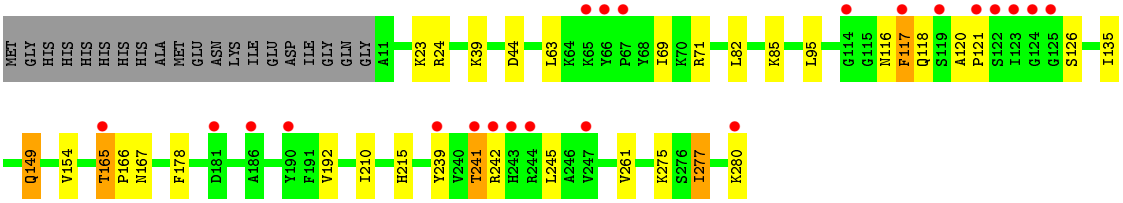
• Molecule 2: Gamma-hemolysin component A

Chain D:



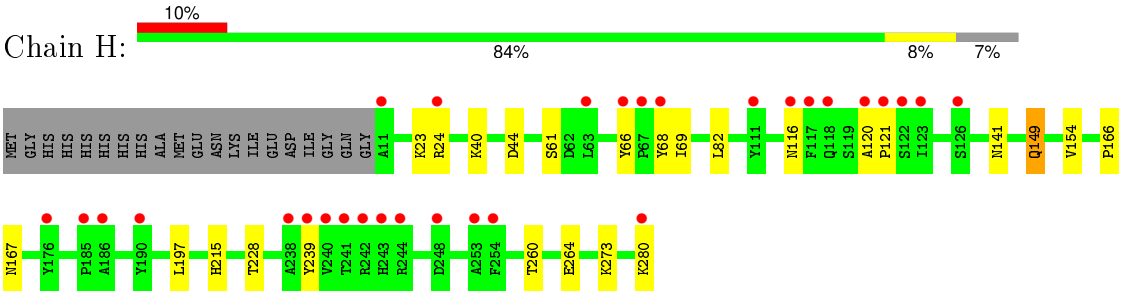
• Molecule 2: Gamma-hemolysin component A

Chain F:



• Molecule 2: Gamma-hemolysin component A

Chain H:


10%
84%
8%
7%
MET GLY HIS HIS HIS HIS HIS ALA MET GLU ASN LYS ILE GLU ASP ILE GLY GLN GLY A11 K23 R24 K40 D44 S61 D62 L63 Y66 P67 Y68 I69 L82 Y111 N116 F117 Q118 S119 A120 P121 S122 I123 S126 N141 Q149 V154 P166
N167 Y176 P185 A186 Y190 L197 H215 T228 A238 Y239 V240 T241 R242 H243 R244 D248 A253 F254 T260 E264 K273 K280

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	206.45Å 206.14Å 190.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.30 – 2.50 43.30 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.9 (43.30-2.50) 98.7 (43.30-2.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_617)	Depositor
R, R_{free}	0.207 , 0.236 0.207 , 0.236	Depositor DCC
R_{free} test set	3956 reflections (2.85%)	DCC
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	1.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 59.1	EDS
Estimated twinning fraction	0.443 for -k,-h,-l 0.436 for -k,-h,-l	Xtriage
Reported twinning fraction	0.443 for -k,-h,-l	Depositor
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	5 of 138828 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	18377	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.07 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.8191e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

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	0.45	0/2349	0.63	0/3177
1	C	0.45	0/2349	0.62	0/3177
1	E	0.46	0/2349	0.63	0/3177
1	G	0.44	0/2349	0.62	0/3177
2	B	0.45	0/2233	0.67	0/3016
2	D	0.45	0/2233	0.65	0/3016
2	F	0.45	0/2233	0.65	0/3016
2	H	0.45	0/2233	0.65	0/3016
All	All	0.45	0/18328	0.64	0/24772

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	2292	0	2183	28	0
1	C	2292	0	2183	24	0
1	E	2292	0	2183	29	0
1	G	2292	0	2183	24	0
2	B	2182	0	2165	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2182	0	2165	13	0
2	F	2182	0	2165	21	0
2	H	2182	0	2165	14	0
3	A	8	0	14	4	0
3	C	8	0	14	2	0
3	E	8	0	14	2	0
3	G	8	0	14	2	0
4	A	69	0	0	2	0
4	B	49	0	0	2	0
4	C	61	0	0	2	0
4	D	60	0	0	1	0
4	E	53	0	0	0	0
4	F	48	0	0	1	0
4	G	59	0	0	0	0
4	H	50	0	0	1	0
All	All	18377	0	17448	168	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 5.

All (168) 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)
2:D:165:THR:HG22	2:D:167:ASN:H	1.54	0.73
1:A:196:ALA:O	3:A:301:MPD:HM3	1.90	0.72
2:H:120:ALA:N	2:H:121:PRO:HA	2.05	0.72
2:D:120:ALA:N	2:D:121:PRO:HA	2.05	0.71
2:B:120:ALA:N	2:B:121:PRO:HA	2.06	0.71
2:F:165:THR:HG22	2:F:167:ASN:H	1.57	0.70
2:F:120:ALA:N	2:F:121:PRO:HA	2.04	0.70
1:A:107:GLU:HB2	2:H:141:ASN:OD1	1.94	0.68
1:A:37:LEU:HD21	1:A:244:VAL:HG21	1.75	0.68
1:G:177:TRP:NE1	3:G:301:MPD:H53	2.10	0.67
2:D:165:THR:HG23	2:D:166:PRO:HD2	1.77	0.67
1:C:210:ALA:HB3	1:C:213:GLN:HE21	1.59	0.67
1:G:54:LEU:HD23	1:G:54:LEU:C	2.15	0.66
1:G:37:LEU:HD21	1:G:244:VAL:HG21	1.77	0.65
1:E:280:GLU:HB2	1:E:291:LEU:HD13	1.79	0.65
1:G:195:LEU:O	3:G:301:MPD:HM3	1.97	0.64
1:A:17:VAL:N	4:A:331:HOH:O	2.32	0.62
2:H:82:LEU:HD23	2:H:82:LEU:C	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:261:VAL:HG22	2:D:277:ILE:HD12	1.83	0.61
1:E:173:MET:CE	2:F:135:ILE:HD11	2.31	0.61
2:F:261:VAL:HG22	2:F:277:ILE:HD12	1.83	0.61
2:F:165:THR:HG23	2:F:166:PRO:HD2	1.85	0.59
1:A:177:TRP:CD1	3:A:301:MPD:H53	2.38	0.59
2:B:167:ASN:HA	2:D:109:LEU:HD11	1.84	0.59
1:E:195:LEU:O	3:E:301:MPD:HM3	2.02	0.59
1:A:39:PHE:CE1	1:A:54:LEU:HD13	2.38	0.59
1:C:125:ILE:HG12	1:C:129:LEU:HD11	1.84	0.58
2:B:261:VAL:HG22	2:B:277:ILE:HD12	1.85	0.58
1:C:76:LYS:HD2	1:C:252:LEU:HD11	1.85	0.57
1:A:174:ASN:OD1	1:A:209:ILE:HG21	2.05	0.57
1:C:37:LEU:HD21	1:C:244:VAL:HG21	1.85	0.57
2:F:63:LEU:HD12	2:F:69:ILE:HB	1.88	0.56
1:E:174:ASN:OD1	1:E:209:ILE:HG21	2.05	0.56
2:B:226:GLU:HG2	2:B:262:LYS:HG2	1.88	0.56
1:A:25:THR:HG22	2:B:90:ASP:OD2	2.06	0.56
2:B:72:MET:HE3	2:B:178:PHE:HD2	1.72	0.55
2:F:149:GLN:HB3	2:F:154:VAL:HG23	1.89	0.55
1:C:174:ASN:OD1	1:C:209:ILE:HG21	2.07	0.55
1:G:78:TYR:CZ	1:G:252:LEU:HD13	2.41	0.55
1:E:78:TYR:CZ	1:E:252:LEU:HD13	2.42	0.54
1:C:39:PHE:CD1	1:C:54:LEU:HD13	2.42	0.54
1:G:174:ASN:OD1	1:G:209:ILE:HG21	2.08	0.54
1:A:78:TYR:CZ	1:A:252:LEU:HD13	2.43	0.54
1:E:39:PHE:CE1	1:E:54:LEU:HD13	2.42	0.54
1:C:210:ALA:HB3	1:C:213:GLN:NE2	2.22	0.54
1:C:245:THR:HG23	1:C:276:LYS:HG3	1.89	0.53
2:B:109:LEU:HD11	2:H:167:ASN:HA	1.90	0.53
2:D:197:LEU:HD11	4:D:305:HOH:O	2.09	0.52
1:A:154:LEU:HD12	1:A:165:TRP:CD1	2.43	0.52
1:G:129:LEU:HD23	1:G:130:SER:H	1.74	0.52
2:H:228:THR:HG23	2:H:260:THR:HG22	1.92	0.52
1:G:124:SER:C	1:G:125:ILE:HD12	2.30	0.52
1:A:76:LYS:HD2	1:A:252:LEU:HD11	1.91	0.52
1:G:19:LEU:HD23	2:H:40:LYS:HE3	1.91	0.52
2:H:149:GLN:HB3	2:H:154:VAL:HG23	1.92	0.52
1:A:198:ARG:NH2	3:A:301:MPD:H51	2.25	0.51
1:E:125:ILE:HG12	1:E:129:LEU:CD2	2.39	0.51
1:E:61:ASN:O	1:E:248:ARG:HD3	2.10	0.51
1:A:125:ILE:HG22	1:A:129:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:ASN:O	1:G:248:ARG:HD3	2.10	0.51
1:C:61:ASN:O	1:C:248:ARG:HD3	2.10	0.51
1:A:158:THR:HG23	1:A:163:VAL:HA	1.92	0.51
2:F:82:LEU:C	2:F:82:LEU:HD23	2.31	0.51
1:E:39:PHE:CD1	1:E:54:LEU:HD13	2.47	0.50
1:A:61:ASN:O	1:A:248:ARG:HD3	2.11	0.50
2:B:72:MET:HE3	2:B:178:PHE:CD2	2.46	0.50
1:C:39:PHE:CE1	1:C:54:LEU:HD13	2.47	0.50
1:E:76:LYS:HD2	1:E:252:LEU:HD11	1.93	0.50
2:B:149:GLN:HB3	2:B:154:VAL:HG23	1.93	0.50
2:D:149:GLN:HB3	2:D:154:VAL:HG23	1.94	0.50
1:E:270:PHE:HA	1:E:300:LYS:HD2	1.93	0.49
1:E:175:ASN:OD1	1:E:213:GLN:OE1	2.29	0.49
1:G:76:LYS:HD2	1:G:252:LEU:HD11	1.93	0.49
1:A:66:LYS:HG2	1:A:67:PRO:HD2	1.94	0.49
1:A:39:PHE:CD1	1:A:54:LEU:HD13	2.48	0.49
2:B:23:LYS:NZ	4:B:380:HOH:O	2.40	0.48
1:G:39:PHE:CZ	1:G:288:VAL:HG11	2.48	0.48
1:A:197:GLY:HA2	3:A:301:MPD:H13	1.96	0.48
1:C:78:TYR:CZ	1:C:252:LEU:HD13	2.48	0.48
1:G:77:LEU:C	1:G:77:LEU:HD12	2.34	0.48
1:C:39:PHE:CZ	1:C:288:VAL:HG11	2.50	0.47
2:H:166:PRO:O	2:H:167:ASN:OD1	2.32	0.47
1:E:99:ASP:OD1	1:E:103:LYS:NZ	2.40	0.47
2:D:82:LEU:C	2:D:82:LEU:HD23	2.34	0.47
2:D:165:THR:HG23	2:D:166:PRO:CD	2.43	0.47
1:E:154:LEU:HD12	1:E:165:TRP:CD1	2.49	0.47
1:E:167:VAL:HG21	1:E:222:PHE:CZ	2.50	0.47
1:G:94:SER:HB2	1:G:233:ARG:HD3	1.97	0.46
1:E:158:THR:HG23	1:E:163:VAL:HA	1.96	0.46
1:E:197:GLY:HA3	1:E:200:SER:OG	2.16	0.46
1:E:173:MET:HE3	2:F:135:ILE:HD11	1.97	0.46
2:B:72:MET:HE1	2:B:178:PHE:HB2	1.96	0.46
1:E:19:LEU:HD11	1:E:40:ASN:HB3	1.98	0.46
1:G:78:TYR:CE1	1:G:252:LEU:HD13	2.50	0.46
1:A:243:THR:HG21	1:A:276:LYS:HE3	1.97	0.46
1:C:158:THR:HG23	1:C:163:VAL:HA	1.98	0.46
1:C:177:TRP:NE1	3:C:301:MPD:H53	2.31	0.45
2:B:259:VAL:HG21	2:B:277:ILE:HD11	1.99	0.45
1:C:195:LEU:O	3:C:301:MPD:HM3	2.16	0.45
1:A:33:ILE:HG12	1:A:60:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:ILE:HG12	1:G:60:ILE:HG23	1.98	0.45
1:C:94:SER:HB2	1:C:233:ARG:HD3	1.98	0.45
2:H:66:TYR:HB3	2:H:68:TYR:CE2	2.52	0.45
1:G:175:ASN:OD1	1:G:176:GLY:N	2.50	0.45
1:E:230:LEU:HD12	1:E:230:LEU:N	2.32	0.45
1:A:43:LYS:NZ	4:A:432:HOH:O	2.30	0.44
1:C:182:ARG:HG3	4:C:394:HOH:O	2.17	0.44
1:A:167:VAL:HG21	1:A:222:PHE:CZ	2.53	0.44
2:D:69:ILE:HA	2:D:239:TYR:HB3	2.00	0.44
1:A:123:ILE:HD12	1:A:130:SER:O	2.18	0.44
2:D:79:ASN:C	2:D:80:ILE:HD12	2.37	0.44
1:G:88:SER:OG	1:G:162:ASN:OD1	2.31	0.44
1:A:78:TYR:CE1	1:A:252:LEU:HD13	2.53	0.44
1:C:77:LEU:C	1:C:77:LEU:HD12	2.38	0.43
2:B:83:LYS:NZ	4:B:436:HOH:O	2.50	0.43
2:F:69:ILE:HA	2:F:239:TYR:HB3	2.01	0.43
1:A:100:TYR:O	1:A:103:LYS:NZ	2.49	0.43
2:F:24:ARG:HB3	2:F:280:LYS:OXT	2.19	0.43
1:A:272:THR:HB	1:A:298:ASN:HB2	2.00	0.43
1:C:170:HIS:CD2	1:C:171:LYS:HG2	2.54	0.43
1:E:173:MET:CE	2:F:135:ILE:CD1	2.97	0.43
2:D:24:ARG:HB3	2:D:280:LYS:OXT	2.18	0.43
2:H:69:ILE:HA	2:H:239:TYR:HB3	2.00	0.43
2:B:69:ILE:HA	2:B:239:TYR:HB3	2.01	0.43
1:G:100:TYR:O	1:G:103:LYS:NZ	2.52	0.42
2:H:24:ARG:HB3	2:H:280:LYS:OXT	2.18	0.42
2:F:239:TYR:O	2:F:245:LEU:HD12	2.19	0.42
1:E:173:MET:HE1	2:F:135:ILE:HD11	2.01	0.42
2:F:85:LYS:N	4:F:317:HOH:O	2.40	0.42
2:H:264:GLU:HB3	2:H:273:LYS:HG2	2.00	0.42
1:C:41:PHE:CE1	1:C:52:LEU:HD13	2.55	0.42
1:E:196:ALA:O	3:E:301:MPD:HM2	2.18	0.42
2:B:24:ARG:HB3	2:B:280:LYS:OXT	2.19	0.42
2:F:117:PHE:HD1	2:F:118:GLN:N	2.16	0.42
1:G:54:LEU:HD23	1:G:54:LEU:O	2.18	0.42
1:A:245:THR:OG1	1:A:276:LYS:HG3	2.19	0.42
1:C:33:ILE:HG12	1:C:60:ILE:HG23	2.02	0.42
1:E:272:THR:HB	1:E:298:ASN:HB2	2.02	0.42
1:E:78:TYR:CE1	1:E:252:LEU:HD13	2.55	0.41
1:C:291:LEU:HA	1:C:291:LEU:HD12	1.94	0.41
2:B:63:LEU:HD23	2:B:71:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:95:LEU:HB2	2:F:210:ILE:CG2	2.50	0.41
2:F:241:THR:HG23	2:F:242:ARG:HG3	2.01	0.41
1:G:158:THR:HG23	1:G:163:VAL:HA	2.02	0.41
2:D:44:ASP:HB2	2:D:215:HIS:HB3	2.02	0.41
1:E:33:ILE:HG12	1:E:60:ILE:HG23	2.03	0.41
1:G:276:LYS:HD2	1:G:294:LYS:NZ	2.36	0.41
1:G:272:THR:HB	1:G:298:ASN:HB2	2.02	0.41
1:E:79:TRP:CZ2	1:E:193:LEU:HD21	2.56	0.41
1:C:88:SER:OG	1:C:162:ASN:OD1	2.31	0.41
1:A:204:ALA:O	1:A:255:ILE:HD11	2.21	0.41
2:B:227:ILE:HD12	2:B:263:TYR:CE1	2.56	0.41
2:B:226:GLU:OE2	2:B:262:LYS:HE3	2.20	0.41
1:C:45:LYS:NZ	4:C:336:HOH:O	2.54	0.41
1:E:77:LEU:HD12	1:E:77:LEU:C	2.41	0.41
1:G:167:VAL:HG21	1:G:222:PHE:CZ	2.56	0.41
2:B:72:MET:CE	2:B:74:TRP:CD1	3.04	0.41
2:H:197:LEU:HD11	4:H:408:HOH:O	2.20	0.41
2:F:44:ASP:HB2	2:F:215:HIS:HB3	2.02	0.40
2:B:44:ASP:HB2	2:B:215:HIS:HB3	2.02	0.40
2:F:178:PHE:O	2:F:192:VAL:HG13	2.21	0.40
2:F:63:LEU:HD23	2:F:71:ARG:NH1	2.36	0.40
1:E:39:PHE:CZ	1:E:288:VAL:HG11	2.56	0.40
2:H:44:ASP:HB2	2:H:215:HIS:HB3	2.02	0.40
2:B:72:MET:HE2	2:B:74:TRP:CD1	2.57	0.40
2:B:105:VAL:HG22	2:B:135:ILE:HG12	2.03	0.40
2:B:224:GLU:OE2	2:B:262:LYS:HD3	2.22	0.40
2:B:63:LEU:CD2	2:B:71:ARG:NH1	2.85	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	282/309 (91%)	270 (96%)	12 (4%)	0	100	100
1	C	282/309 (91%)	270 (96%)	12 (4%)	0	100	100
1	E	282/309 (91%)	270 (96%)	12 (4%)	0	100	100
1	G	282/309 (91%)	270 (96%)	12 (4%)	0	100	100
2	B	268/290 (92%)	264 (98%)	4 (2%)	0	100	100
2	D	268/290 (92%)	263 (98%)	5 (2%)	0	100	100
2	F	268/290 (92%)	264 (98%)	4 (2%)	0	100	100
2	H	268/290 (92%)	264 (98%)	4 (2%)	0	100	100
All	All	2200/2396 (92%)	2135 (97%)	65 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	249/271 (92%)	249 (100%)	0	100	100
1	C	249/271 (92%)	244 (98%)	5 (2%)	63	86
1	E	249/271 (92%)	246 (99%)	3 (1%)	78	93
1	G	249/271 (92%)	244 (98%)	5 (2%)	63	86
2	B	241/257 (94%)	232 (96%)	9 (4%)	41	68
2	D	241/257 (94%)	231 (96%)	10 (4%)	37	63
2	F	241/257 (94%)	231 (96%)	10 (4%)	37	63
2	H	241/257 (94%)	237 (98%)	4 (2%)	68	89
All	All	1960/2112 (93%)	1914 (98%)	46 (2%)	58	83

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	30	LYS
1	C	43	LYS

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Mol	Chain	Res	Type
1	C	230	LEU
1	C	294	LYS
1	C	300	LYS
1	E	173	MET
1	E	227	LEU
1	E	239	LYS
1	G	66	LYS
1	G	105	GLN
1	G	112	GLN
1	G	129	LEU
1	G	199	GLN
2	B	42	ASN
2	B	116	ASN
2	B	122	SER
2	B	149	GLN
2	B	155	LYS
2	B	241	THR
2	B	242	ARG
2	B	255	LYS
2	B	277	ILE
2	D	15	LYS
2	D	23	LYS
2	D	42	ASN
2	D	85	LYS
2	D	109	LEU
2	D	116	ASN
2	D	126	SER
2	D	149	GLN
2	D	165	THR
2	D	277	ILE
2	F	23	LYS
2	F	39	LYS
2	F	116	ASN
2	F	117	PHE
2	F	126	SER
2	F	149	GLN
2	F	165	THR
2	F	241	THR
2	F	275	LYS
2	F	277	ILE
2	H	23	LYS
2	H	61	SER

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Mol	Chain	Res	Type
2	H	116	ASN
2	H	149	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	298	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 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	$\#\|Z\| > 2$
3	MPD	A	301	-	6,7,7	0.21	0	7,10,10	0.34	0
3	MPD	C	301	-	6,7,7	0.27	0	7,10,10	0.32	0
3	MPD	E	301	-	6,7,7	0.27	0	7,10,10	0.35	0
3	MPD	G	301	-	6,7,7	0.26	0	7,10,10	0.33	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	MPD	A	301	-	-	0/5/5/5	0/0/0/0
3	MPD	C	301	-	-	0/5/5/5	0/0/0/0
3	MPD	E	301	-	-	0/5/5/5	0/0/0/0
3	MPD	G	301	-	-	0/5/5/5	0/0/0/0

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.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	MPD	4	0
3	C	301	MPD	2	0
3	E	301	MPD	2	0
3	G	301	MPD	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

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	284/309 (91%)	0.53	21 (7%)	17	19	23, 37, 73, 124	0
1	C	284/309 (91%)	0.57	26 (9%)	11	12	24, 37, 76, 90	0
1	E	284/309 (91%)	0.67	29 (10%)	9	9	22, 38, 76, 120	0
1	G	284/309 (91%)	0.66	24 (8%)	13	14	25, 41, 73, 89	0
2	B	270/290 (93%)	0.67	24 (8%)	12	13	20, 40, 81, 100	0
2	D	270/290 (93%)	0.57	16 (5%)	26	29	24, 40, 80, 108	0
2	F	270/290 (93%)	0.66	22 (8%)	15	16	25, 38, 79, 102	0
2	H	270/290 (93%)	0.78	30 (11%)	7	7	28, 41, 78, 119	0
All	All	2216/2396 (92%)	0.64	192 (8%)	13	13	20, 39, 78, 124	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	129	LEU	11.4
1	A	127	ASN	10.2
2	H	243	HIS	8.1
1	G	127	ASN	7.8
1	E	128	GLY	6.7
1	E	127	ASN	6.3
1	C	129	LEU	6.2
2	H	123	ILE	6.0
2	H	120	ALA	5.8
1	A	126	SER	5.1
1	C	260	PHE	5.1
1	E	130	SER	5.1
1	G	260	PHE	5.0
1	A	129	LEU	5.0
2	B	280	LYS	4.9
1	C	134	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
2	F	243	HIS	4.6
2	H	244	ARG	4.6
2	F	123	ILE	4.5
1	A	128	GLY	4.5
2	D	118	GLN	4.4
2	B	117	PHE	4.4
2	H	118	GLN	4.3
2	B	243	HIS	4.3
1	A	139	PHE	4.3
1	C	125	ILE	4.3
1	G	126	SER	4.2
1	A	201	SER	4.0
2	F	124	GLY	4.0
2	H	66	TYR	3.9
1	C	127	ASN	3.9
2	H	122	SER	3.9
2	H	242	ARG	3.9
1	A	74	PHE	3.9
1	E	260	PHE	3.9
2	B	66	TYR	3.8
2	F	242	ARG	3.8
1	A	125	ILE	3.8
1	C	201	SER	3.8
1	C	74	PHE	3.8
1	E	117	TYR	3.7
1	C	117	TYR	3.7
2	F	190	TYR	3.7
1	C	132	GLY	3.7
2	D	117	PHE	3.6
1	E	119	PHE	3.6
2	F	117	PHE	3.6
2	B	121	PRO	3.6
2	H	117	PHE	3.6
2	B	123	ILE	3.6
1	G	74	PHE	3.5
1	A	227	LEU	3.5
2	B	11	ALA	3.5
1	C	70	ASN	3.5
2	B	68	TYR	3.5
2	H	67	PRO	3.4
1	E	177	TRP	3.4
1	G	128	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	242	ARG	3.3
1	G	201	SER	3.3
2	B	248	ASP	3.3
1	E	134	ASN	3.3
1	C	177	TRP	3.3
1	A	124	SER	3.2
2	H	280	LYS	3.2
1	C	124	SER	3.2
1	C	72	TYR	3.2
1	E	78	TYR	3.2
1	G	177	TRP	3.2
1	G	129	LEU	3.1
1	G	119	PHE	3.1
2	H	238	ALA	3.1
1	A	260	PHE	3.0
1	G	235	ASP	3.0
2	H	248	ASP	3.0
2	F	241	THR	3.0
1	E	69	PRO	3.0
2	F	119	SER	3.0
1	G	125	ILE	3.0
1	C	130	SER	2.9
1	G	203	TYR	2.9
2	F	66	TYR	2.9
2	F	121	PRO	2.9
1	E	122	ASP	2.9
1	E	74	PHE	2.9
1	C	119	PHE	2.8
1	G	110	GLN	2.8
2	B	122	SER	2.8
2	B	111	TYR	2.8
2	B	239	TYR	2.8
2	F	65	LYS	2.8
2	F	125	GLY	2.8
2	D	243	HIS	2.8
2	H	68	TYR	2.8
1	G	134	ASN	2.8
2	H	11	ALA	2.8
2	F	280	LYS	2.8
1	A	72	TYR	2.8
2	H	190	TYR	2.8
2	H	116	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	123	ILE	2.7
1	C	203	TYR	2.7
1	E	203	TYR	2.7
2	B	254	PHE	2.7
1	G	123	ILE	2.7
1	C	270	PHE	2.7
1	G	139	PHE	2.7
2	D	120	ALA	2.7
2	D	280	LYS	2.6
2	H	186	ALA	2.6
1	A	175	ASN	2.6
1	A	203	TYR	2.6
1	G	117	TYR	2.6
2	D	239	TYR	2.6
2	D	167	ASN	2.6
1	G	122	ASP	2.6
2	D	119	SER	2.6
1	A	70	ASN	2.6
1	A	29	ASP	2.5
2	H	121	PRO	2.5
2	F	186	ALA	2.5
1	E	68	ASN	2.5
2	B	201	ILE	2.5
2	H	126	SER	2.5
2	B	67	PRO	2.5
1	E	72	TYR	2.5
1	C	200	SER	2.5
1	E	73	ASP	2.4
2	D	68	TYR	2.4
2	D	69	ILE	2.4
2	F	239	TYR	2.4
2	F	247	VAL	2.4
1	G	130	SER	2.4
1	E	185	PHE	2.4
2	D	121	PRO	2.4
2	F	122	SER	2.4
1	C	128	GLY	2.4
2	B	127	GLY	2.3
2	D	240	VAL	2.3
2	H	253	ALA	2.3
2	H	24	ARG	2.3
2	H	111	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	241	THR	2.3
2	H	63	LEU	2.3
1	A	123	ILE	2.3
1	G	69	PRO	2.3
1	A	119	PHE	2.3
1	E	261	TYR	2.3
2	F	67	PRO	2.3
1	A	117	TYR	2.3
1	A	136	ASN	2.3
2	H	239	TYR	2.3
1	C	122	ASP	2.3
2	B	240	VAL	2.3
2	B	244	ARG	2.3
2	D	101	ASP	2.2
1	C	116	GLY	2.2
2	B	109	LEU	2.2
1	E	17	VAL	2.2
1	E	294	LYS	2.2
2	H	240	VAL	2.2
2	F	244	ARG	2.2
1	A	132	GLY	2.2
1	G	73	ASP	2.2
2	F	165	THR	2.2
1	C	131	GLY	2.1
1	G	124	SER	2.1
1	C	199	GLN	2.1
1	E	115	LEU	2.1
2	H	241	THR	2.1
1	G	78	TYR	2.1
2	B	129	PHE	2.1
2	H	185	PRO	2.1
1	E	131	GLY	2.1
1	C	126	SER	2.1
2	B	102	SER	2.1
2	B	172	ALA	2.1
1	E	139	PHE	2.1
1	G	257	TRP	2.1
1	E	70	ASN	2.1
1	C	139	PHE	2.1
2	F	114	GLY	2.1
2	H	254	PHE	2.1
1	E	201	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	158	VAL	2.0
2	H	176	TYR	2.0
2	D	129	PHE	2.0
1	E	173	MET	2.0
1	C	73	ASP	2.0
2	D	246	ALA	2.0
1	E	71	ASP	2.0
2	F	181	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no 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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	MPD	A	301	8/8	0.76	0.47	12.02	58,63,64,72	0
3	MPD	C	301	8/8	0.71	0.67	9.47	62,73,81,82	0
3	MPD	E	301	8/8	0.82	0.51	5.48	62,74,80,84	0
3	MPD	G	301	8/8	0.78	0.42	4.00	56,64,73,75	0

6.5 Other polymers (i)

There are no such residues in this entry.