Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 04:30 PM 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 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/ValidationPDFNotes.html

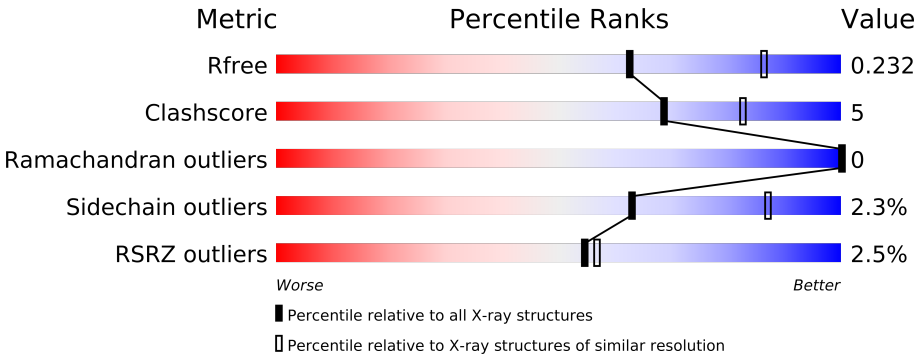
The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	309	
1	C	309	
1	E	309	
1	G	309	
2	B	290	
2	D	290	
2	F	290	
2	H	290	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MPD	A	301	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	MPD	C	301	-	X
3	MPD	E	301	-	X
3	MPD	G	301	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18377 atoms, of which 0 are hydrogen and 0 are deuterium.

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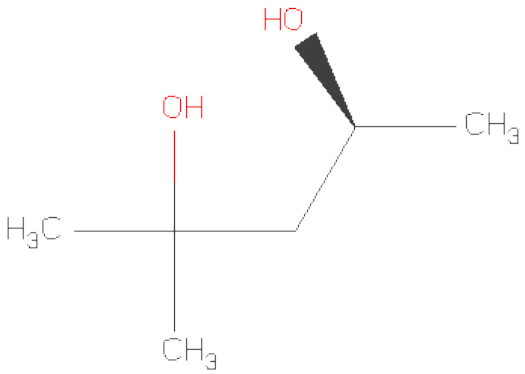
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP P0A071
B	-1	ALA	-	EXPRESSION TAG	UNP P0A071
B	0	MET	-	EXPRESSION TAG	UNP P0A071
D	-9	MET	-	EXPRESSION TAG	UNP P0A071
D	-8	GLY	-	EXPRESSION TAG	UNP P0A071
D	-7	HIS	-	EXPRESSION TAG	UNP P0A071
D	-6	HIS	-	EXPRESSION TAG	UNP P0A071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

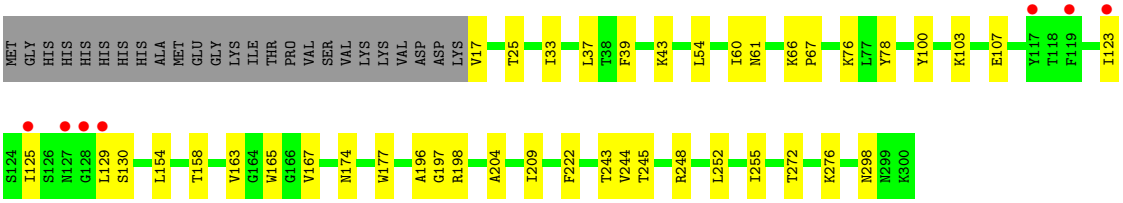
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	69	Total O 69 69	0	0
4	C	61	Total O 61 61	0	0
4	E	53	Total O 53 53	0	0
4	G	59	Total O 59 59	0	0
4	B	49	Total O 49 49	0	0
4	D	60	Total O 60 60	0	0
4	F	48	Total O 48 48	0	0
4	H	50	Total O 50 50	0	0

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.

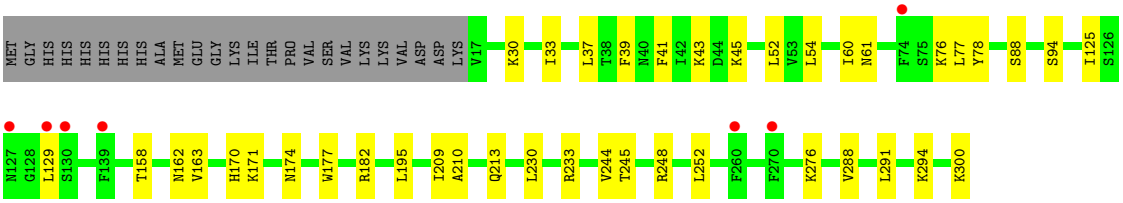
• Molecule 1: Gamma-hemolysin component B

Chain A:



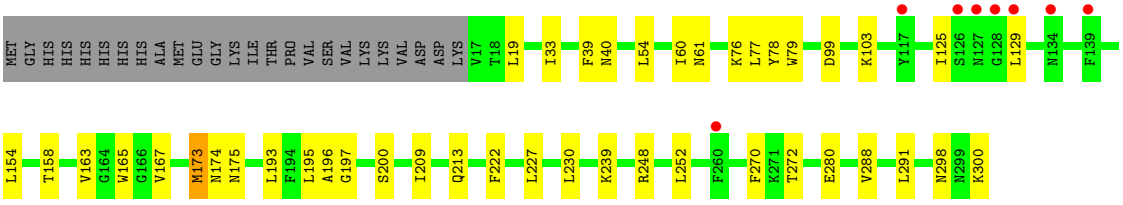
• Molecule 1: Gamma-hemolysin component B

Chain C:



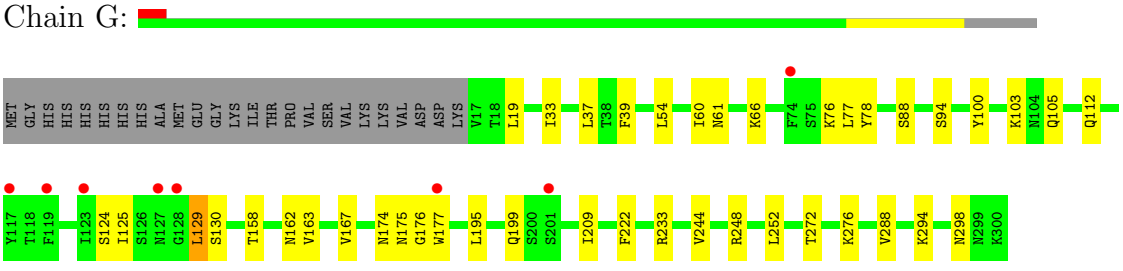
• Molecule 1: Gamma-hemolysin component B

Chain E:



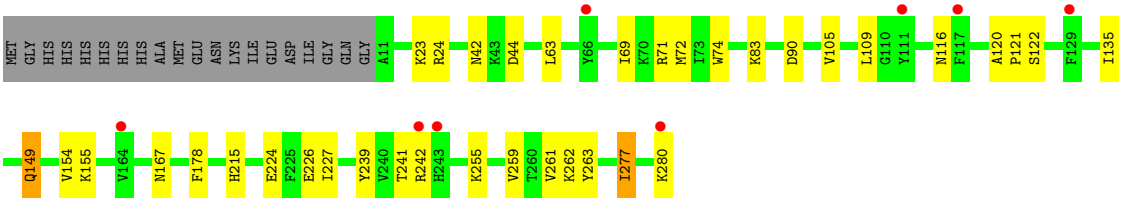
• Molecule 1: Gamma-hemolysin component B

Chain G:



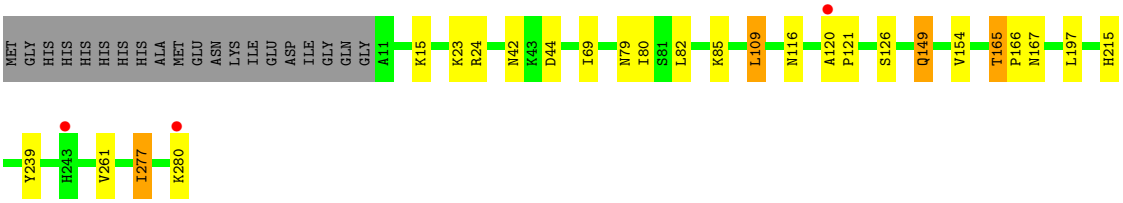
• Molecule 2: Gamma-hemolysin component A

Chain B:



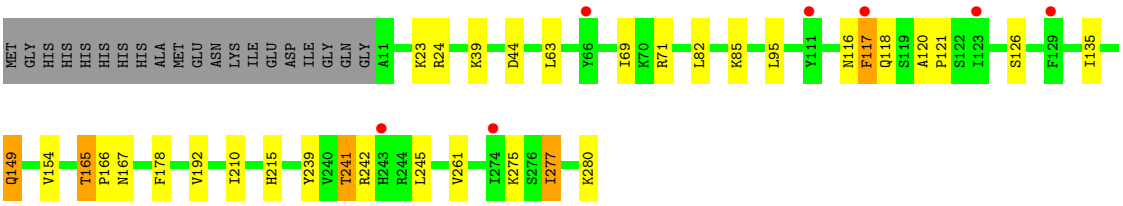
• Molecule 2: Gamma-hemolysin component A

Chain D:



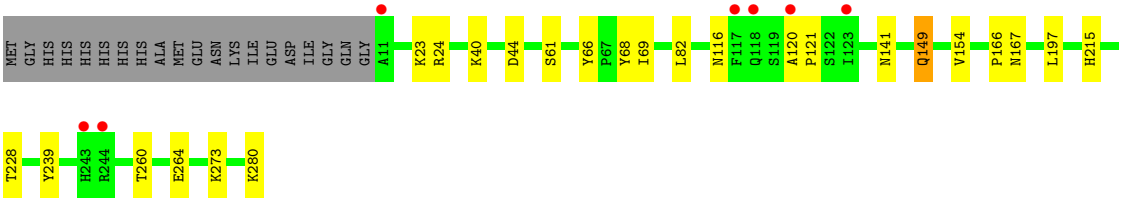
• Molecule 2: Gamma-hemolysin component A

Chain F:



• Molecule 2: Gamma-hemolysin component A

Chain H:



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) 98.4 (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 0.204 , 0.232	Depositor DCC
R_{free} test set	3954 reflections (2.94%)	DCC
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	1.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 25.9	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	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	5 of 138828 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.94	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2182	0	2165	24	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (168) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
2:D:261:VAL:HG22	2:D:277:ILE:HD12	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

5.3.1 Protein backbone

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	68	89
1	E	249/271 (92%)	246 (99%)	3 (1%)	82	95
1	G	249/271 (92%)	244 (98%)	5 (2%)	68	89
2	B	241/257 (94%)	232 (96%)	9 (4%)	45	72
2	D	241/257 (94%)	231 (96%)	10 (4%)	41	67
2	F	241/257 (94%)	231 (96%)	10 (4%)	41	67
2	H	241/257 (94%)	237 (98%)	4 (2%)	73	92
All	All	1960/2112 (93%)	1914 (98%)	46 (2%)	63	87

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

Mol	Chain	Res	Type
1	C	30	LYS
1	C	43	LYS
1	C	230	LEU
1	C	294	LYS
1	C	300	LYS
1	E	173	MET
1	E	227	LEU
1	E	239	LYS

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Mol	Chain	Res	Type
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
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 chains 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	-	7,7,7	0.23	0	10,10,10	0.29	0
3	MPD	C	301	-	7,7,7	0.25	0	10,10,10	0.28	0
3	MPD	E	301	-	7,7,7	0.26	0	10,10,10	0.32	0
3	MPD	G	301	-	7,7,7	0.26	0	10,10,10	0.29	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.35	7 (2%)	54	57	23, 37, 73, 124	0
1	C	284/309 (91%)	0.18	7 (2%)	54	57	24, 37, 76, 90	0
1	E	284/309 (91%)	0.31	8 (2%)	50	53	22, 38, 76, 120	0
1	G	284/309 (91%)	0.27	8 (2%)	50	53	25, 41, 73, 89	0
2	B	270/290 (93%)	0.34	8 (2%)	48	50	20, 40, 81, 100	0
2	D	270/290 (93%)	0.28	3 (1%)	77	79	24, 40, 80, 108	0
2	F	270/290 (93%)	0.31	7 (2%)	53	55	25, 38, 79, 102	0
2	H	270/290 (93%)	0.36	7 (2%)	53	55	28, 41, 78, 119	0
All	All	2216/2396 (92%)	0.30	55 (2%)	54	57	20, 39, 78, 124	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	127	ASN	9.8
1	A	127	ASN	9.1
1	E	129	LEU	8.2
1	A	129	LEU	6.4
1	E	128	GLY	5.5
2	H	243	HIS	4.5
1	C	127	ASN	4.5
1	G	127	ASN	4.3
1	C	129	LEU	4.3
1	A	128	GLY	4.3
2	B	117	PHE	4.1
2	H	120	ALA	4.0
2	D	280	LYS	3.6
1	G	74	PHE	3.5
1	G	177	TRP	3.5
2	H	123	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	243	HIS	3.2
1	G	201	SER	3.1
1	E	117	TYR	3.1
2	B	243	HIS	3.1
1	E	260	PHE	3.0
1	G	117	TYR	2.9
2	B	111	TYR	2.9
1	G	128	GLY	2.8
2	D	243	HIS	2.7
2	B	164	VAL	2.6
1	G	123	ILE	2.6
2	B	280	LYS	2.6
2	H	118	GLN	2.6
2	H	244	ARG	2.6
2	B	66	TYR	2.6
2	F	66	TYR	2.6
1	C	74	PHE	2.5
2	F	274	ILE	2.5
1	A	125	ILE	2.5
1	A	117	TYR	2.4
1	E	139	PHE	2.2
1	C	130	SER	2.2
2	H	11	ALA	2.2
1	G	119	PHE	2.2
1	A	119	PHE	2.2
2	F	129	PHE	2.2
1	E	134	ASN	2.2
2	F	123	ILE	2.2
1	C	260	PHE	2.2
2	F	117	PHE	2.2
1	A	123	ILE	2.2
1	C	139	PHE	2.1
1	C	270	PHE	2.1
2	D	120	ALA	2.1
2	F	111	TYR	2.1
2	B	242	ARG	2.0
2	H	117	PHE	2.0
1	E	126	SER	2.0
2	B	129	PHE	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	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MPD	E	301	8/8	0.42	11.71	62,74,80,84	0
3	MPD	C	301	8/8	0.64	9.69	62,73,81,82	0
3	MPD	A	301	8/8	0.35	6.73	58,63,64,72	0
3	MPD	G	301	8/8	0.36	2.98	56,64,73,75	0

6.5 Other polymers (i)

There are no such residues in this entry.