Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:34 AM GMT

PDB ID	:	3F65
Title	:	The F4 fimbrial chaperone FaeE does not self-cap its interactive surfaces
Authors	:	Van Molle, I.; Moonens, K.; Buts, L.; Garcia-Pino, A.; Wyns, L.; De Greve, H.; Bouckaert, J.
Deposited on	:	2008-11-05
Resolution	:	2.29 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 ①) were used in the production of this report:

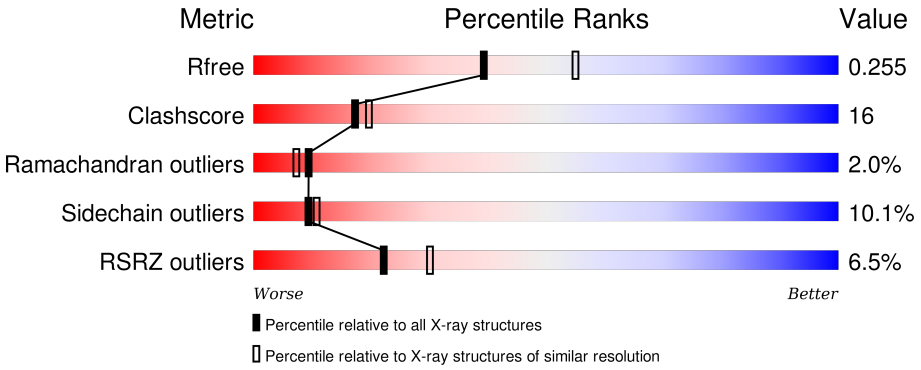
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.29 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	224	67% 22% 8%
1	B	224	68% 20% 8%
1	C	224	70% 17% 8%
1	D	224	3% 51% 15% 5% 28%
1	E	224	12% 58% 25% 13%

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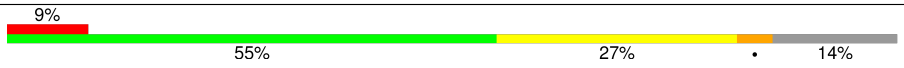
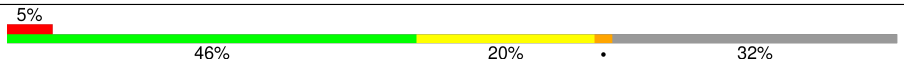
Mol	Chain	Length	Quality of chain
1	F	224	
1	G	224	
1	H	224	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	A	225	-	-	X	-
2	MPD	C	225	X	-	-	X
2	MPD	G	225	X	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11425 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.

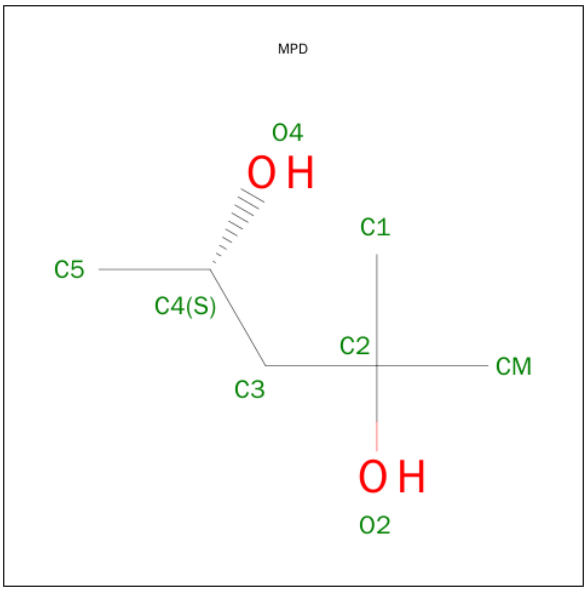
- Molecule 1 is a protein called Chaperone protein faeE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1587	1006	272	305	4			
1	B	205	Total	C	N	O	S	0	0	0
			1567	993	269	301	4			
1	C	206	Total	C	N	O	S	0	0	0
			1569	996	271	298	4			
1	D	161	Total	C	N	O	S	0	0	0
			1215	778	202	232	3			
1	E	194	Total	C	N	O	S	0	0	0
			1418	895	242	277	4			
1	F	166	Total	C	N	O	S	0	0	0
			1232	790	205	233	4			
1	G	193	Total	C	N	O	S	0	0	0
			1371	865	234	268	4			
1	H	153	Total	C	N	O	S	0	0	0
			1138	726	193	216	3			

There are 8 discrepancies between the modelled and reference sequences:

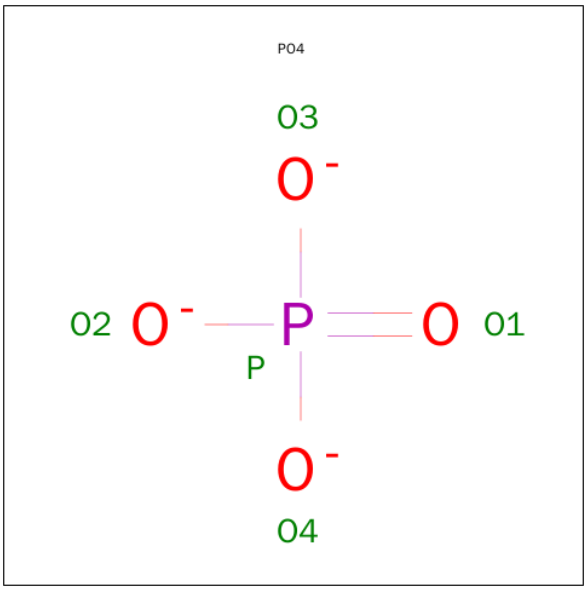
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLU	LYS	ENGINEERED	UNP P25401
B	15	GLU	LYS	ENGINEERED	UNP P25401
C	15	GLU	LYS	ENGINEERED	UNP P25401
D	15	GLU	LYS	ENGINEERED	UNP P25401
E	15	GLU	LYS	ENGINEERED	UNP P25401
F	15	GLU	LYS	ENGINEERED	UNP P25401
G	15	GLU	LYS	ENGINEERED	UNP P25401
H	15	GLU	LYS	ENGINEERED	UNP P25401

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



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

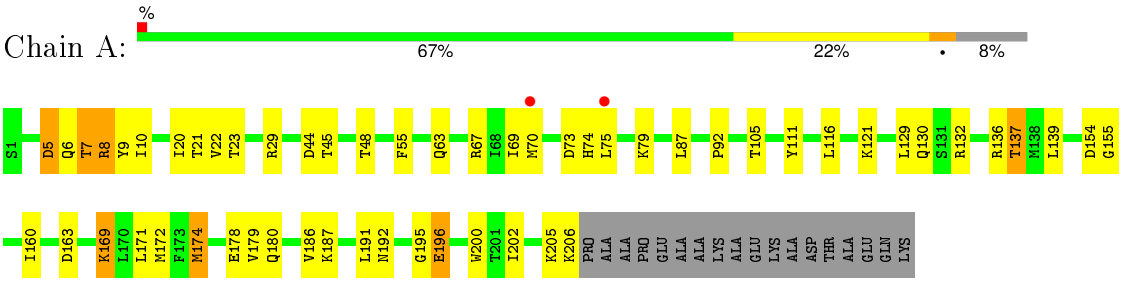
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	89	Total O 89 89	0	0
4	B	58	Total O 58 58	0	0
4	C	85	Total O 85 85	0	0
4	D	32	Total O 32 32	0	0
4	E	18	Total O 18 18	0	0
4	F	5	Total O 5 5	0	0
4	G	1	Total O 1 1	0	0
4	H	11	Total O 11 11	0	0

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.

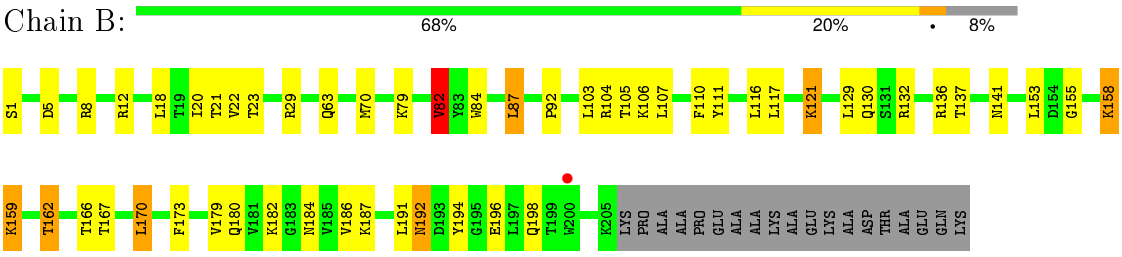
- Molecule 1: Chaperone protein faeE

Chain A:



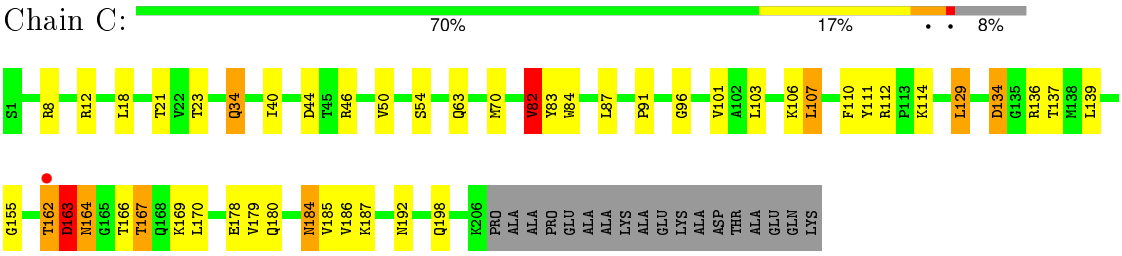
- Molecule 1: Chaperone protein faeE

Chain B:



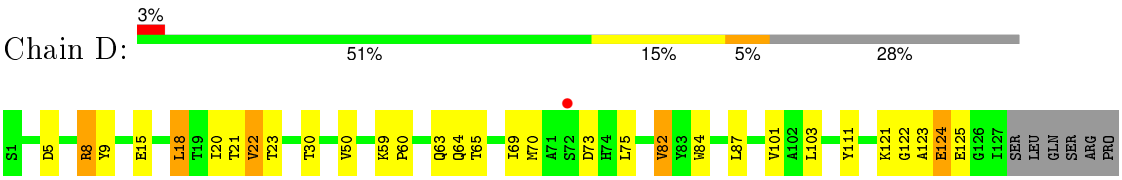
- Molecule 1: Chaperone protein faeE

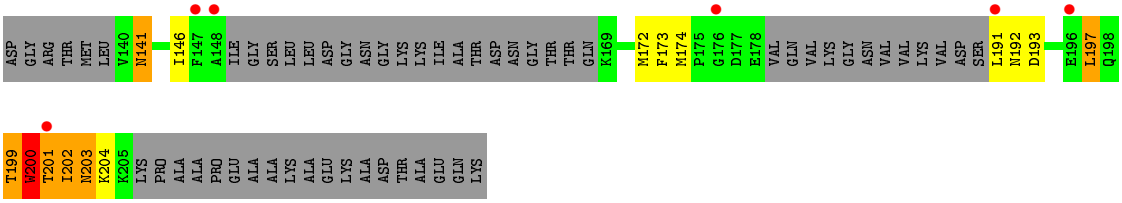
Chain C:



- Molecule 1: Chaperone protein faeE

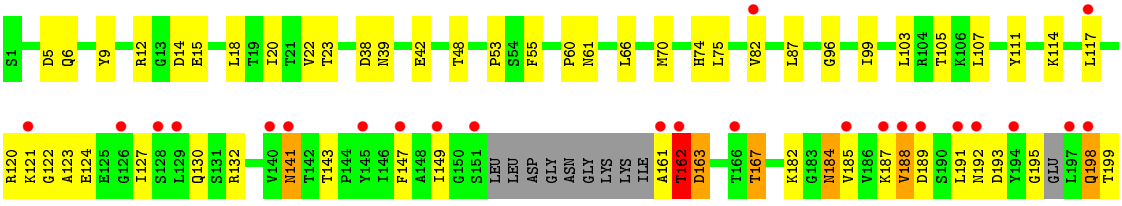
Chain D:

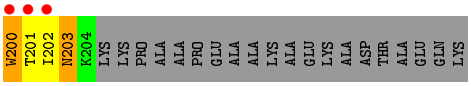




• Molecule 1: Chaperone protein faeE

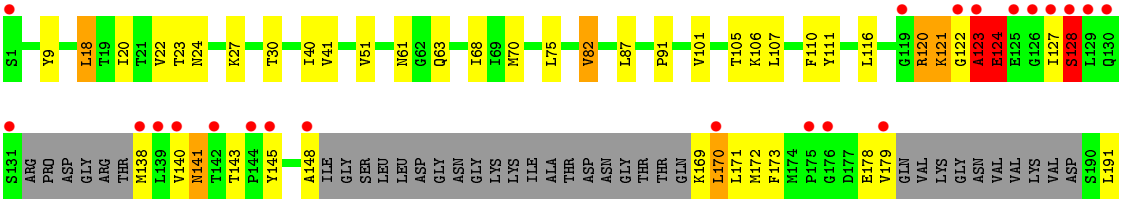
Chain E:

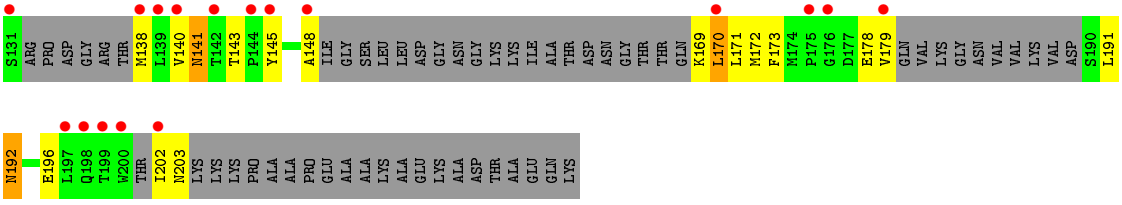




• Molecule 1: Chaperone protein faeE

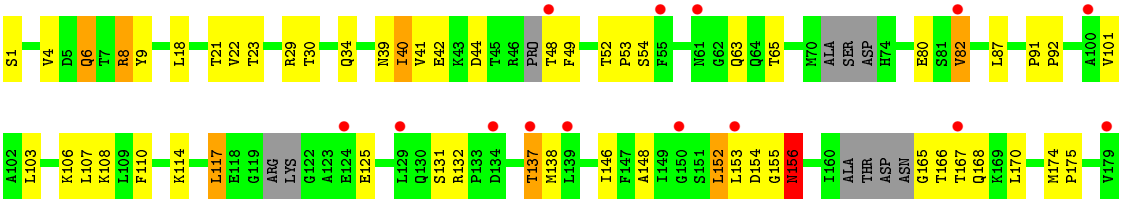
Chain F:

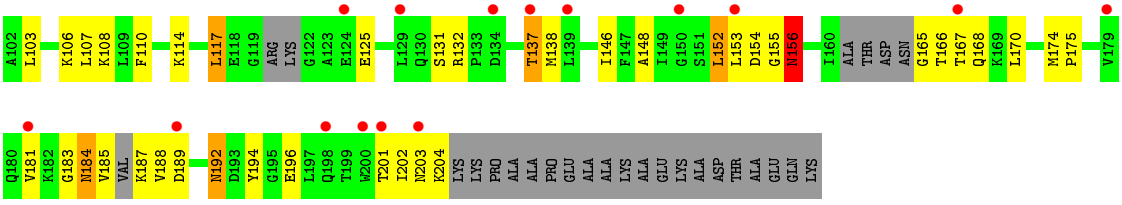




• Molecule 1: Chaperone protein faeE

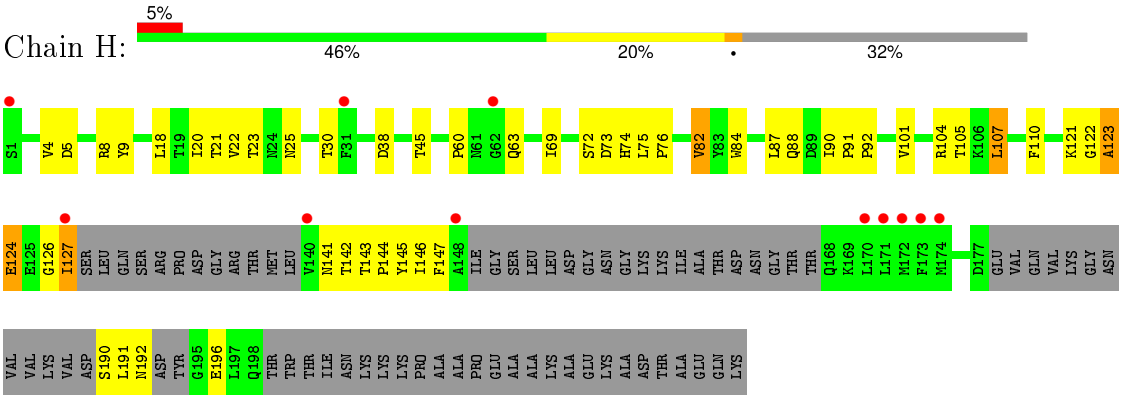
Chain G:





• Molecule 1: Chaperone protein faeE

Chain H:


5%
46%
20%
32%
S1 V4 D5 R8 Y9 L18 T19 I20 T21 V22 T23 N24 N25 T30 P31 D38 T45 P60 N61 G62 Q63 I69 S72 D73 H74 L75 P76 V82 Y83 W84 L87 Q88 D89 I90 P91 P92 V101 R104 T105 K106 L107 F110 K121 G122 A123
E124 E125 G126 I127 SER LEU GLN SER ARG PRO ASP GLY ARG THR MET LEU V140 N141 T142 T143 P144 Y145 I146 F147 A148 ILE GLY SER LEU LEU ASP GLY ASN GLY LYS LYS ILE ALA THR ASP ASN GLY THR THR Q168 K169 L170 L171 M172 F173 M174 D177 GLU VAL GLN VAL LYS GLY ASN
VAL VAL LYS VAL ASP S190 L191 N192 ASP TYR G195 E196 L197 Q198 THR TRP THR ILE ASN LYS LYS LYS PRO ALA ALA ALA PRO GLU ALA ALA LYS ALA GLU LYS ALA ASP THR ALA ALA GLU GLN LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	195.69Å 78.49Å 184.57Å 90.00° 102.15° 90.00°	Depositor
Resolution (Å)	49.85 – 2.29 49.85 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.85-2.29) 99.3 (49.85-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.29Å)	Xtriage
Refinement program	Phenix.refine	Depositor
R, R_{free}	0.224 , 0.260 0.216 , 0.255	Depositor DCC
R_{free} test set	6153 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	50.4	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 51.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 122609 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11425	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: PO4, 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	0/1616	0.62	0/2195
1	B	0.35	0/1595	0.57	1/2168 (0.0%)
1	C	0.41	0/1598	0.64	1/2174 (0.0%)
1	D	0.34	0/1240	0.57	0/1691
1	E	0.29	0/1442	0.52	0/1970
1	F	0.30	0/1255	0.54	2/1714 (0.1%)
1	G	0.24	0/1391	0.51	0/1899
1	H	0.28	0/1159	0.51	0/1579
All	All	0.34	0/11296	0.57	4/15390 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	82	VAL	CB-CA-C	-6.60	98.86	111.40
1	B	82	VAL	CB-CA-C	-6.31	99.41	111.40
1	F	123	ALA	N-CA-C	5.06	124.65	111.00
1	F	128	SER	C-N-CA	5.01	134.24	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	123	ALA	Peptide

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	1587	0	1576	41	0
1	B	1567	0	1552	42	0
1	C	1569	0	1548	40	0
1	D	1215	0	1123	43	0
1	E	1418	0	1327	54	0
1	F	1232	0	1146	54	0
1	G	1371	0	1234	58	0
1	H	1138	0	1060	28	0
2	A	8	0	14	6	0
2	C	8	0	14	3	0
2	G	8	0	14	3	0
3	A	5	0	0	0	0
4	A	89	0	0	3	0
4	B	58	0	0	2	0
4	C	85	0	0	7	0
4	D	32	0	0	0	0
4	E	18	0	0	0	0
4	F	5	0	0	0	0
4	G	1	0	0	0	0
4	H	11	0	0	0	0
All	All	11425	0	10608	349	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 16.

All (349) 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:F:123:ALA:N	1:F:124:GLU:HB2	1.11	1.41
1:F:123:ALA:N	1:F:124:GLU:CB	1.99	1.25
1:F:123:ALA:CA	1:F:124:GLU:HB2	1.85	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:THR:O	1:D:200:TRP:HB2	1.47	1.05
1:D:121:LYS:CB	1:D:122:GLY:HA3	1.92	1.00
1:D:8:ARG:HG2	1:D:8:ARG:HH11	1.27	0.96
1:H:30:THR:HG22	1:H:60:PRO:HD3	1.44	0.96
1:F:124:GLU:HA	1:F:124:GLU:OE2	1.61	0.96
1:G:40:ILE:H	1:G:40:ILE:HD13	1.32	0.94
1:E:200:TRP:HA	1:E:201:THR:HB	1.50	0.94
1:H:123:ALA:HB3	1:H:124:GLU:HA	1.50	0.93
1:D:199:THR:HG22	1:D:200:TRP:H	1.32	0.93
1:D:199:THR:HG22	1:D:200:TRP:N	1.84	0.91
1:E:39:ASN:HB3	1:E:42:GLU:HG2	1.55	0.88
1:H:23:THR:HG22	1:H:63:GLN:HG2	1.54	0.88
1:F:127:ILE:HD12	1:F:202:ILE:CG2	2.04	0.87
1:F:123:ALA:H	1:F:124:GLU:HB2	1.10	0.87
1:C:166:THR:HG23	1:C:179:VAL:HG11	1.56	0.87
1:D:199:THR:O	1:D:200:TRP:CB	2.22	0.86
1:F:23:THR:HG22	1:F:63:GLN:HG2	1.58	0.86
1:B:186:VAL:HG23	1:B:187:LYS:HG3	1.59	0.85
1:F:122:GLY:C	1:F:124:GLU:CB	2.46	0.83
1:A:23:THR:HG22	1:A:63:GLN:HG2	1.60	0.83
1:E:189:ASP:HA	1:E:198:GLN:HA	1.61	0.82
1:C:186:VAL:HG23	1:C:187:LYS:HG3	1.62	0.82
1:F:40:ILE:HD11	1:F:82:VAL:HB	1.62	0.82
1:F:122:GLY:C	1:F:124:GLU:HB2	2.00	0.82
1:G:6:GLN:HG3	1:G:9:TYR:CE2	2.14	0.82
1:D:199:THR:CG2	1:D:200:TRP:H	1.92	0.82
1:B:23:THR:HG22	1:B:63:GLN:HG2	1.60	0.81
1:G:21:THR:HG22	1:G:65:THR:HG22	1.63	0.80
1:F:124:GLU:CA	1:F:124:GLU:OE2	2.30	0.80
1:A:205:LYS:O	1:A:206:LYS:CB	2.30	0.80
1:G:52:THR:OG1	1:G:53:PRO:HD3	1.82	0.78
1:D:201:THR:O	1:D:202:ILE:CB	2.30	0.78
1:D:121:LYS:CB	1:D:122:GLY:CA	2.61	0.78
2:C:225:MPD:H52	2:C:225:MPD:H12	1.65	0.78
1:G:165:GLY:N	1:G:166:THR:HA	1.99	0.77
1:E:127:ILE:HB	1:E:202:ILE:HG23	1.65	0.77
1:F:127:ILE:O	1:F:140:VAL:O	2.02	0.77
1:C:23:THR:HG22	1:C:63:GLN:HG2	1.66	0.75
1:F:192:ASN:ND2	1:F:196:GLU:H	1.83	0.75
1:H:123:ALA:HB2	1:H:190:SER:OG	1.87	0.74
1:F:51:VAL:HG22	1:F:68:ILE:HD13	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:ASP:O	1:E:167:THR:HG22	1.88	0.72
1:A:8:ARG:HH21	1:A:10:ILE:HG12	1.53	0.72
1:F:122:GLY:C	1:F:124:GLU:HB3	2.10	0.72
1:H:123:ALA:CB	1:H:124:GLU:HA	2.20	0.71
1:G:91:PRO:HG3	1:G:101:VAL:O	1.88	0.71
1:C:112:ARG:HH21	2:C:225:MPD:H4	1.56	0.71
1:B:87:LEU:HB3	1:B:105:THR:CG2	2.21	0.71
1:E:200:TRP:HA	1:E:201:THR:CB	2.22	0.70
1:F:170:LEU:HD11	1:F:173:PHE:HB2	1.71	0.70
1:G:146:ILE:HG13	1:G:175:PRO:HD3	1.71	0.70
1:F:127:ILE:HD12	1:F:202:ILE:HG22	1.74	0.70
1:F:18:LEU:HD13	1:F:20:ILE:HD11	1.74	0.70
1:D:8:ARG:CG	1:D:8:ARG:HH11	2.03	0.70
1:A:7:THR:OG1	2:A:225:MPD:H11	1.92	0.70
1:F:70:MET:HE3	1:F:111:TYR:CE1	2.27	0.70
1:B:192:ASN:ND2	1:B:196:GLU:H	1.89	0.70
1:F:192:ASN:HD21	1:F:196:GLU:H	1.38	0.69
1:G:23:THR:HG22	1:G:63:GLN:HG2	1.73	0.69
1:C:23:THR:HG23	4:C:230:HOH:O	1.94	0.68
1:D:21:THR:HG22	1:D:65:THR:HG22	1.75	0.68
1:B:12:ARG:NH1	1:B:117:LEU:HD22	2.08	0.68
1:G:184:ASN:HD22	1:G:184:ASN:C	1.97	0.68
1:G:106:LYS:O	1:G:107:LEU:HD23	1.94	0.67
1:C:112:ARG:NH2	2:C:225:MPD:H4	2.10	0.67
1:A:29:ARG:HG2	1:A:92:PRO:HG2	1.76	0.67
1:A:23:THR:HG23	4:A:310:HOH:O	1.94	0.67
1:C:155:GLY:HA2	1:C:186:VAL:HG21	1.75	0.66
1:A:6:GLN:HG2	2:A:225:MPD:H4	1.77	0.66
1:B:70:MET:HE1	1:B:111:TYR:CE1	2.31	0.66
1:B:155:GLY:HA2	1:B:186:VAL:HG21	1.75	0.66
1:H:123:ALA:HB3	1:H:124:GLU:CA	2.24	0.65
1:B:130:GLN:HE21	1:B:132:ARG:HH12	1.43	0.65
1:G:114:LYS:HA	1:G:117:LEU:CD2	2.27	0.65
1:C:184:ASN:H	1:C:184:ASN:HD22	1.44	0.65
1:D:202:ILE:O	1:D:203:ASN:CB	2.46	0.64
1:C:44:ASP:OD1	1:C:46:ARG:HD3	1.97	0.64
1:D:23:THR:HG22	1:D:63:GLN:HG2	1.79	0.64
1:A:67:ARG:NH1	1:A:69:ILE:HD11	2.13	0.63
1:C:82:VAL:HG13	1:C:110:PHE:CD2	2.34	0.63
1:G:132:ARG:HE	1:G:138:MET:HG3	1.64	0.62
1:E:192:ASN:O	1:E:193:ASP:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ASN:HD21	1:E:48:THR:HG23	1.64	0.62
1:C:91:PRO:HG3	1:C:101:VAL:O	2.00	0.62
1:G:39:ASN:ND2	1:G:44:ASP:HB3	2.15	0.62
1:D:202:ILE:O	1:D:203:ASN:HB2	2.01	0.61
1:F:120:ARG:HD3	1:F:120:ARG:O	2.00	0.61
1:C:162:THR:O	1:C:166:THR:HB	2.01	0.61
1:D:30:THR:HG22	1:D:60:PRO:HD3	1.82	0.61
1:D:191:LEU:N	1:D:192:ASN:CB	2.64	0.60
1:H:4:VAL:HG21	1:H:107:LEU:HD11	1.81	0.60
1:B:182:LYS:HG2	1:B:184:ASN:HB2	1.84	0.60
1:H:88:GLN:OE1	1:H:104:ARG:HB2	2.01	0.60
1:G:192:ASN:C	1:G:192:ASN:HD22	2.04	0.60
1:B:23:THR:HG23	4:B:230:HOH:O	2.01	0.59
1:E:161:ALA:O	1:E:162:THR:HG23	2.02	0.59
1:G:40:ILE:CD1	1:G:40:ILE:H	2.09	0.59
1:F:70:MET:HE2	1:F:75:LEU:HD12	1.84	0.59
1:A:186:VAL:O	1:A:202:ILE:HG12	2.02	0.58
1:G:153:LEU:O	1:G:187:LYS:N	2.36	0.58
1:A:187:LYS:HB3	1:A:200:TRP:O	2.03	0.58
1:D:197:LEU:HD12	1:D:197:LEU:N	2.16	0.58
1:D:199:THR:CG2	1:D:200:TRP:N	2.49	0.58
1:H:191:LEU:O	1:H:192:ASN:HB3	2.03	0.58
1:B:87:LEU:HB3	1:B:105:THR:HG23	1.85	0.58
1:A:7:THR:H	2:A:225:MPD:H31	1.67	0.58
1:B:130:GLN:NE2	1:B:132:ARG:HH12	2.00	0.58
1:A:136:ARG:HH11	1:A:180:GLN:NE2	2.02	0.58
1:B:79:LYS:HA	1:B:116:LEU:HD11	1.84	0.58
1:C:70:MET:HE1	4:C:237:HOH:O	2.02	0.57
1:C:101:VAL:HG22	1:D:103:LEU:CD2	2.33	0.57
1:C:136:ARG:HH11	1:C:180:GLN:NE2	2.01	0.57
1:G:82:VAL:HG13	1:G:110:PHE:CE2	2.39	0.57
1:F:82:VAL:HG13	1:F:110:PHE:CD2	2.39	0.57
1:A:9:TYR:CE2	1:A:20:ILE:HD12	2.39	0.57
1:G:166:THR:HG23	1:G:168:GLN:O	2.04	0.57
1:B:136:ARG:HH11	1:B:180:GLN:HE22	1.52	0.57
1:B:182:LYS:C	1:B:184:ASN:H	2.06	0.57
1:D:30:THR:HG22	1:D:59:LYS:HA	1.87	0.56
1:E:99:ILE:HG12	1:F:105:THR:HG22	1.86	0.56
1:F:141:ASN:HB2	1:F:173:PHE:CE2	2.40	0.56
1:A:79:LYS:HA	1:A:116:LEU:HD11	1.88	0.56
1:H:82:VAL:HG22	1:H:146:ILE:HD13	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ASN:ND2	1:C:164:ASN:H	2.02	0.56
1:A:172:MET:HG2	1:A:174:MET:HE1	1.87	0.56
1:A:137:THR:HG22	4:A:251:HOH:O	2.06	0.56
1:B:70:MET:HE1	1:B:111:TYR:HE1	1.70	0.56
1:F:116:LEU:HB3	1:F:145:TYR:CE2	2.41	0.56
1:D:70:MET:HE1	1:D:75:LEU:HD12	1.88	0.56
1:B:192:ASN:C	1:B:192:ASN:HD22	2.09	0.55
1:B:82:VAL:HG13	1:B:110:PHE:CE2	2.40	0.55
1:F:120:ARG:HH12	1:F:124:GLU:HG2	1.71	0.55
1:D:141:ASN:HB2	1:D:173:PHE:CE2	2.42	0.55
1:B:70:MET:CE	1:B:111:TYR:CE1	2.90	0.54
1:E:187:LYS:HA	1:E:201:THR:H	1.71	0.54
1:C:136:ARG:HH11	1:C:180:GLN:HE22	1.55	0.54
1:E:191:LEU:HA	1:E:195:GLY:O	2.07	0.54
1:D:191:LEU:CB	1:D:192:ASN:HA	2.38	0.54
1:E:184:ASN:H	1:E:184:ASN:ND2	2.04	0.54
1:B:82:VAL:HG13	1:B:110:PHE:CD2	2.43	0.54
1:C:162:THR:HG21	4:C:282:HOH:O	2.07	0.53
1:A:172:MET:HG2	1:A:174:MET:CE	2.38	0.53
1:G:1:SER:HB3	1:G:103:LEU:HD12	1.90	0.53
1:G:110:PHE:CD2	2:G:225:MPD:HM2	2.43	0.53
1:H:9:TYR:CE2	1:H:20:ILE:HG13	2.44	0.53
1:F:70:MET:CE	1:F:75:LEU:HD12	2.38	0.53
1:G:114:LYS:HA	1:G:117:LEU:HD22	1.89	0.53
1:G:192:ASN:ND2	1:G:196:GLU:H	2.06	0.53
1:E:75:LEU:HD12	1:E:111:TYR:CD2	2.44	0.52
1:H:123:ALA:CB	1:H:124:GLU:CA	2.85	0.52
1:B:136:ARG:HH11	1:B:180:GLN:NE2	2.08	0.52
1:F:123:ALA:H	1:F:124:GLU:CB	1.91	0.52
1:H:72:SER:OG	1:H:74:HIS:HD2	1.92	0.52
1:F:170:LEU:HD11	1:F:173:PHE:CB	2.40	0.52
1:G:82:VAL:HG13	1:G:110:PHE:CD2	2.45	0.52
1:A:192:ASN:HD21	1:A:196:GLU:HG3	1.73	0.52
1:E:48:THR:CG2	1:E:74:HIS:HE1	2.23	0.51
1:F:148:ALA:HB3	1:F:191:LEU:H	1.74	0.51
1:A:130:GLN:HE21	1:A:132:ARG:HH12	1.58	0.51
1:A:195:GLY:HA3	2:A:225:MPD:HM3	1.93	0.51
1:H:126:GLY:O	1:H:127:ILE:O	2.28	0.51
1:A:44:ASP:OD1	1:A:45:THR:N	2.44	0.51
1:E:202:ILE:HG22	1:E:203:ASN:N	2.25	0.51
1:D:70:MET:CE	1:D:111:TYR:CE1	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:LEU:HD12	1:G:188:VAL:HG12	1.93	0.51
1:G:168:GLN:C	1:G:170:LEU:H	2.14	0.50
1:C:34:GLN:HG3	1:C:54:SER:O	2.11	0.50
1:A:136:ARG:HH11	1:A:180:GLN:HE22	1.59	0.50
1:C:184:ASN:N	1:C:184:ASN:HD22	2.05	0.50
1:E:120:ARG:O	1:E:122:GLY:N	2.44	0.50
1:G:41:VAL:HG22	1:G:41:VAL:O	2.12	0.50
1:B:192:ASN:HB3	1:B:198:GLN:HE21	1.76	0.50
1:F:91:PRO:HG3	1:F:101:VAL:O	2.11	0.50
1:D:70:MET:HE1	1:D:111:TYR:CE1	2.46	0.50
1:E:12:ARG:HB2	1:E:15:GLU:HG3	1.94	0.50
1:C:163:ASP:O	1:C:167:THR:HG22	2.11	0.50
1:B:158:LYS:O	1:B:159:LYS:CB	2.60	0.50
1:A:169:LYS:HD3	1:A:179:VAL:CG1	2.41	0.50
1:E:48:THR:HG21	1:E:74:HIS:HE1	1.76	0.49
1:A:8:ARG:HG3	2:A:225:MPD:C1	2.42	0.49
1:G:154:ASP:CG	1:G:155:GLY:H	2.13	0.49
1:D:8:ARG:CG	1:D:8:ARG:NH1	2.70	0.49
1:G:154:ASP:CG	1:G:155:GLY:N	2.66	0.49
1:E:103:LEU:CD2	1:F:101:VAL:HG22	2.42	0.49
1:F:82:VAL:HG13	1:F:110:PHE:CE2	2.47	0.49
1:E:127:ILE:HD11	1:E:147:PHE:CD1	2.48	0.49
1:C:107:LEU:HD12	1:C:107:LEU:N	2.28	0.49
1:E:38:ASP:OD2	1:H:45:THR:HG21	2.13	0.49
1:C:44:ASP:OD1	1:C:46:ARG:CD	2.61	0.49
1:C:134:ASP:OD1	1:C:136:ARG:HG3	2.13	0.49
1:H:127:ILE:O	1:H:142:THR:HB	2.13	0.49
1:D:70:MET:CE	1:D:75:LEU:HD12	2.42	0.49
1:E:123:ALA:HA	1:E:199:THR:CB	2.43	0.49
1:E:127:ILE:HD11	1:E:147:PHE:CE1	2.47	0.49
1:F:9:TYR:CE2	1:F:20:ILE:HG13	2.48	0.49
1:E:14:ASP:OD1	1:E:15:GLU:HG2	2.13	0.49
1:G:103:LEU:CD2	1:H:101:VAL:HG22	2.44	0.48
1:A:154:ASP:HB3	1:A:160:ILE:HD11	1.95	0.48
1:E:123:ALA:HA	1:E:199:THR:HB	1.95	0.48
1:H:122:GLY:O	1:H:123:ALA:C	2.51	0.48
1:F:148:ALA:HB1	1:F:191:LEU:HD13	1.95	0.48
1:E:75:LEU:N	1:E:75:LEU:HD23	2.27	0.48
1:A:192:ASN:OD1	1:A:196:GLU:HG3	2.14	0.48
1:A:137:THR:CG2	4:A:251:HOH:O	2.61	0.48
1:D:82:VAL:HG21	1:D:172:MET:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:ASP:HB3	1:E:198:GLN:HB2	1.96	0.48
1:A:55:PHE:CD1	1:D:69:ILE:HD11	2.48	0.48
1:B:84:TRP:CD2	1:B:106:LYS:HE2	2.49	0.48
1:G:40:ILE:N	1:G:40:ILE:HD13	2.15	0.47
1:E:199:THR:O	1:E:200:TRP:CB	2.62	0.47
1:G:30:THR:O	1:G:92:PRO:HG3	2.14	0.47
1:G:167:THR:O	1:G:168:GLN:CB	2.63	0.47
1:C:129:LEU:HD21	1:C:185:VAL:O	2.15	0.47
1:F:107:LEU:HD23	1:F:107:LEU:N	2.30	0.47
1:C:101:VAL:HG22	1:D:103:LEU:HD22	1.96	0.47
1:F:178:GLU:O	1:F:179:VAL:HB	2.15	0.47
1:F:170:LEU:O	1:F:172:MET:N	2.47	0.47
1:A:169:LYS:HD3	1:A:179:VAL:HG12	1.96	0.47
1:D:82:VAL:HG22	1:D:146:ILE:HD13	1.97	0.47
1:A:75:LEU:HD12	1:A:111:TYR:CD2	2.51	0.47
1:C:82:VAL:HG13	1:C:110:PHE:CE2	2.50	0.46
1:G:80:GLU:CB	1:G:146:ILE:HD12	2.45	0.46
1:E:39:ASN:CB	1:E:42:GLU:HG2	2.36	0.46
1:B:12:ARG:HD3	4:B:227:HOH:O	2.15	0.46
1:A:139:LEU:O	1:A:178:GLU:HA	2.16	0.46
1:F:127:ILE:CD1	1:F:202:ILE:HG22	2.45	0.46
1:F:170:LEU:HD13	1:F:171:LEU:N	2.31	0.46
1:G:42:GLU:O	1:G:44:ASP:N	2.39	0.46
1:C:192:ASN:HB3	1:C:198:GLN:HE21	1.80	0.46
1:G:137:THR:HG21	1:G:183:GLY:CA	2.45	0.46
1:G:125:GLU:HB3	1:G:204:LYS:HD2	1.98	0.46
1:F:27:LYS:HG2	1:F:61:ASN:OD1	2.16	0.46
1:G:40:ILE:HG12	1:G:41:VAL:N	2.32	0.45
1:F:141:ASN:ND2	1:F:143:THR:H	2.14	0.45
1:B:1:SER:OG	1:B:103:LEU:HD12	2.16	0.45
1:A:192:ASN:ND2	1:A:196:GLU:HG3	2.31	0.45
1:E:55:PHE:CE1	1:H:69:ILE:HD11	2.51	0.45
1:F:127:ILE:HD12	1:F:202:ILE:HG21	1.90	0.45
2:G:225:MPD:HM1	2:G:225:MPD:H4	1.70	0.45
1:B:166:THR:HG23	1:B:179:VAL:HG21	1.98	0.45
1:C:103:LEU:CD2	1:D:101:VAL:HG22	2.46	0.45
1:D:22:VAL:HG13	1:D:64:GLN:O	2.17	0.45
1:C:114:LYS:HG3	4:C:236:HOH:O	2.15	0.45
1:G:137:THR:HG23	1:G:181:VAL:O	2.17	0.45
1:B:170:LEU:HD12	1:B:170:LEU:HA	1.88	0.45
1:A:73:ASP:CG	1:A:73:ASP:O	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ASN:H	1:C:164:ASN:HD22	1.64	0.45
1:F:24:ASN:O	1:F:61:ASN:HA	2.17	0.45
1:C:84:TRP:CD2	1:C:106:LYS:HE3	2.51	0.45
1:E:141:ASN:HD22	1:E:143:THR:H	1.64	0.45
1:E:60:PRO:O	1:E:61:ASN:HB2	2.16	0.45
1:A:5:ASP:HB2	1:A:6:GLN:HG3	1.99	0.44
1:F:169:LYS:N	1:F:170:LEU:O	2.49	0.44
1:B:182:LYS:C	1:B:184:ASN:N	2.71	0.44
1:F:124:GLU:O	1:F:127:ILE:HD11	2.17	0.44
1:E:162:THR:O	1:E:163:ASP:HB3	2.17	0.44
1:G:146:ILE:HG12	1:G:174:MET:SD	2.56	0.44
1:E:130:GLN:HE21	1:E:132:ARG:NH1	2.15	0.44
1:G:184:ASN:ND2	1:G:185:VAL:HG23	2.33	0.44
1:E:114:LYS:HA	1:E:117:LEU:HG	1.99	0.44
1:G:4:VAL:HB	1:G:9:TYR:OH	2.18	0.44
1:E:184:ASN:HD22	1:E:184:ASN:N	2.16	0.44
1:D:9:TYR:CE2	1:D:20:ILE:HG12	2.52	0.44
1:B:141:ASN:HB2	1:B:173:PHE:CE2	2.53	0.44
1:G:137:THR:HG21	1:G:183:GLY:HA2	2.00	0.44
1:F:127:ILE:HD12	1:F:202:ILE:CB	2.48	0.44
1:H:90:ILE:HA	1:H:91:PRO:HD2	1.89	0.44
1:A:75:LEU:N	1:A:75:LEU:HD23	2.31	0.43
1:G:201:THR:O	1:G:204:LYS:HE3	2.17	0.43
1:E:149:ILE:HG23	1:E:188:VAL:HG13	1.99	0.43
1:C:136:ARG:NH1	1:C:180:GLN:HE22	2.17	0.43
1:D:123:ALA:O	1:D:125:GLU:N	2.50	0.43
1:D:202:ILE:O	1:D:203:ASN:ND2	2.51	0.43
1:E:141:ASN:ND2	1:E:143:THR:H	2.15	0.43
1:C:169:LYS:CD	4:C:285:HOH:O	2.65	0.43
1:F:169:LYS:N	1:F:170:LEU:C	2.72	0.43
1:A:155:GLY:CA	1:A:186:VAL:HG21	2.48	0.43
1:D:70:MET:HE3	1:D:111:TYR:CE1	2.53	0.43
1:G:29:ARG:CB	1:G:92:PRO:HG2	2.49	0.43
1:E:6:GLN:HG2	1:E:9:TYR:CZ	2.54	0.43
1:G:52:THR:CB	1:G:53:PRO:HD3	2.49	0.43
1:B:192:ASN:HD21	1:B:196:GLU:H	1.61	0.43
1:B:130:GLN:HE21	1:B:132:ARG:NH1	2.14	0.43
1:E:184:ASN:HD22	1:E:185:VAL:N	2.17	0.43
1:H:75:LEU:HA	1:H:76:PRO:HD3	1.84	0.43
1:F:120:ARG:NH1	1:F:124:GLU:HG2	2.32	0.43
1:E:202:ILE:HD12	1:E:202:ILE:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:ALA:HB2	2:G:225:MPD:H51	2.01	0.43
1:E:184:ASN:ND2	1:E:184:ASN:N	2.65	0.43
1:B:162:THR:CG2	1:B:167:THR:OG1	2.67	0.43
1:H:144:PRO:HD2	1:H:145:TYR:CD1	2.54	0.43
1:B:18:LEU:HG	1:B:20:ILE:CD1	2.50	0.42
1:E:141:ASN:HD22	1:E:141:ASN:C	2.22	0.42
1:H:82:VAL:HG13	1:H:110:PHE:CD2	2.54	0.42
1:A:70:MET:HE3	1:A:111:TYR:CE1	2.54	0.42
1:E:53:PRO:HD2	1:E:66:LEU:HD23	2.02	0.42
1:H:123:ALA:HB1	1:H:147:PHE:CE2	2.55	0.42
1:B:192:ASN:ND2	1:B:194:TYR:H	2.17	0.42
1:F:120:ARG:O	1:F:121:LYS:C	2.58	0.42
1:A:8:ARG:HG3	2:A:225:MPD:H12	2.02	0.42
1:G:131:SER:C	1:G:132:ARG:HD2	2.40	0.42
1:C:12:ARG:NH2	4:C:238:HOH:O	2.50	0.42
1:B:70:MET:HB2	1:B:70:MET:HE3	1.63	0.42
1:E:120:ARG:C	1:E:122:GLY:N	2.73	0.42
1:B:121:LYS:HD2	1:B:121:LYS:HA	1.83	0.42
1:C:96:GLY:HA2	1:D:84:TRP:CH2	2.54	0.42
1:G:155:GLY:O	1:G:156:ASN:CB	2.68	0.42
1:C:82:VAL:C	1:C:83:TYR:CD1	2.93	0.42
1:F:70:MET:HE3	1:F:111:TYR:CZ	2.55	0.42
1:A:74:HIS:CD2	1:A:75:LEU:HD23	2.55	0.42
1:E:96:GLY:O	1:F:106:LYS:HE3	2.20	0.42
1:E:202:ILE:CG2	1:E:203:ASN:N	2.84	0.41
1:A:48:THR:HG21	1:A:75:LEU:HD21	2.01	0.41
1:D:8:ARG:HG2	1:D:8:ARG:NH1	2.08	0.41
1:B:158:LYS:O	1:B:159:LYS:HB3	2.21	0.41
1:G:184:ASN:C	1:G:184:ASN:ND2	2.68	0.41
1:G:192:ASN:ND2	1:G:194:TYR:H	2.18	0.41
1:H:30:THR:O	1:H:92:PRO:HG3	2.21	0.41
1:G:80:GLU:HB2	1:G:146:ILE:HD12	2.03	0.41
1:D:124:GLU:C	1:D:125:GLU:OE2	2.59	0.41
1:B:87:LEU:HB3	1:B:105:THR:HG22	1.97	0.41
1:C:70:MET:HE1	1:C:111:TYR:CE1	2.56	0.41
1:E:55:PHE:CD1	1:H:69:ILE:HD11	2.56	0.41
1:F:141:ASN:HD22	1:F:141:ASN:C	2.23	0.41
1:G:155:GLY:O	1:G:156:ASN:HB2	2.21	0.41
1:D:172:MET:HE3	1:D:174:MET:SD	2.61	0.41
1:D:9:TYR:HB3	1:D:18:LEU:HD11	2.02	0.41
1:A:171:LEU:HA	1:A:171:LEU:HD23	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:THR:HB	1:G:49:PHE:H	1.70	0.41
1:G:8:ARG:HB2	1:G:108:LYS:HB2	2.03	0.41
1:B:104:ARG:HH22	1:D:73:ASP:CB	2.33	0.41
1:E:70:MET:HE3	1:E:111:TYR:CE1	2.56	0.40
1:H:72:SER:CB	1:H:74:HIS:HD2	2.34	0.40
1:B:153:LEU:HD23	1:B:159:LYS:HA	2.03	0.40
1:B:29:ARG:HB2	1:B:92:PRO:HG3	2.02	0.40
1:C:139:LEU:O	1:C:178:GLU:HA	2.22	0.40
1:E:9:TYR:CE2	1:E:20:ILE:HG12	2.55	0.40
1:G:34:GLN:HA	1:G:54:SER:O	2.22	0.40
1:G:4:VAL:HG21	1:G:107:LEU:CD1	2.52	0.40
1:E:162:THR:O	1:E:163:ASP:CB	2.69	0.40
1:E:184:ASN:H	1:E:184:ASN:HD22	1.66	0.40
1:E:130:GLN:NE2	1:E:132:ARG:HH12	2.20	0.40
1:G:168:GLN:C	1:G:170:LEU:N	2.75	0.40
1:C:163:ASP:HB3	4:C:283:HOH:O	2.21	0.40
1:H:38:ASP:HB2	1:H:84:TRP:HB2	2.04	0.40
1:G:192:ASN:HD21	1:G:196:GLU:H	1.67	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	204/224 (91%)	198 (97%)	5 (2%)	1 (0%)	34 41
1	B	203/224 (91%)	193 (95%)	7 (3%)	3 (2%)	13 12
1	C	204/224 (91%)	195 (96%)	7 (3%)	2 (1%)	19 21
1	D	153/224 (68%)	136 (89%)	11 (7%)	6 (4%)	4 2
1	E	188/224 (84%)	166 (88%)	15 (8%)	7 (4%)	4 2
1	F	156/224 (70%)	145 (93%)	8 (5%)	3 (2%)	10 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	181/224 (81%)	163 (90%)	17 (9%)	1 (1%)	30 36
1	H	143/224 (64%)	130 (91%)	7 (5%)	6 (4%)	3 1
All	All	1432/1792 (80%)	1326 (93%)	77 (5%)	29 (2%)	9 7

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	LYS
1	D	200	TRP
1	D	202	ILE
1	D	203	ASN
1	E	162	THR
1	F	124	GLU
1	G	156	ASN
1	H	121	LYS
1	H	123	ALA
1	B	158	LYS
1	C	134	ASP
1	F	121	LYS
1	H	124	GLU
1	H	141	ASN
1	B	121	LYS
1	D	124	GLU
1	D	199	THR
1	E	121	LYS
1	E	124	GLU
1	E	163	ASP
1	E	198	GLN
1	H	73	ASP
1	H	196	GLU
1	A	163	ASP
1	D	204	LYS
1	E	182	LYS
1	E	200	TRP
1	C	163	ASP
1	F	128	SER

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	170/189 (90%)	156 (92%)	14 (8%)	14 17
1	B	166/189 (88%)	153 (92%)	13 (8%)	16 19
1	C	165/189 (87%)	148 (90%)	17 (10%)	9 10
1	D	118/189 (62%)	105 (89%)	13 (11%)	8 8
1	E	141/189 (75%)	127 (90%)	14 (10%)	10 11
1	F	121/189 (64%)	107 (88%)	14 (12%)	7 7
1	G	128/189 (68%)	112 (88%)	16 (12%)	6 6
1	H	112/189 (59%)	100 (89%)	12 (11%)	8 9
All	All	1121/1512 (74%)	1008 (90%)	113 (10%)	9 11

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	7	THR
1	A	8	ARG
1	A	21	THR
1	A	22	VAL
1	A	87	LEU
1	A	105	THR
1	A	121	LYS
1	A	129	LEU
1	A	137	THR
1	A	169	LYS
1	A	174	MET
1	A	191	LEU
1	A	196	GLU
1	B	5	ASP
1	B	8	ARG
1	B	21	THR
1	B	22	VAL
1	B	82	VAL
1	B	87	LEU
1	B	107	LEU
1	B	129	LEU
1	B	137	THR

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Mol	Chain	Res	Type
1	B	162	THR
1	B	170	LEU
1	B	191	LEU
1	B	192	ASN
1	C	8	ARG
1	C	18	LEU
1	C	21	THR
1	C	34	GLN
1	C	40	ILE
1	C	50	VAL
1	C	82	VAL
1	C	87	LEU
1	C	107	LEU
1	C	129	LEU
1	C	137	THR
1	C	162	THR
1	C	163	ASP
1	C	164	ASN
1	C	167	THR
1	C	170	LEU
1	C	184	ASN
1	D	5	ASP
1	D	8	ARG
1	D	15	GLU
1	D	18	LEU
1	D	22	VAL
1	D	50	VAL
1	D	82	VAL
1	D	87	LEU
1	D	141	ASN
1	D	193	ASP
1	D	197	LEU
1	D	200	TRP
1	D	201	THR
1	E	5	ASP
1	E	18	LEU
1	E	22	VAL
1	E	23	THR
1	E	82	VAL
1	E	87	LEU
1	E	105	THR
1	E	107	LEU

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Mol	Chain	Res	Type
1	E	141	ASN
1	E	162	THR
1	E	167	THR
1	E	184	ASN
1	E	188	VAL
1	E	203	ASN
1	F	18	LEU
1	F	22	VAL
1	F	30	THR
1	F	41	VAL
1	F	82	VAL
1	F	87	LEU
1	F	120	ARG
1	F	124	GLU
1	F	128	SER
1	F	138	MET
1	F	141	ASN
1	F	170	LEU
1	F	192	ASN
1	F	203	ASN
1	G	6	GLN
1	G	8	ARG
1	G	18	LEU
1	G	22	VAL
1	G	40	ILE
1	G	82	VAL
1	G	87	LEU
1	G	117	LEU
1	G	137	THR
1	G	152	LEU
1	G	156	ASN
1	G	184	ASN
1	G	189	ASP
1	G	192	ASN
1	G	202	ILE
1	G	203	ASN
1	H	5	ASP
1	H	8	ARG
1	H	18	LEU
1	H	21	THR
1	H	22	VAL
1	H	25	ASN

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Mol	Chain	Res	Type
1	H	82	VAL
1	H	87	LEU
1	H	105	THR
1	H	107	LEU
1	H	127	ILE
1	H	143	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	39	ASN
1	A	61	ASN
1	A	130	GLN
1	A	180	GLN
1	B	34	GLN
1	B	63	GLN
1	B	130	GLN
1	B	180	GLN
1	B	192	ASN
1	B	198	GLN
1	C	63	GLN
1	C	164	ASN
1	C	180	GLN
1	C	184	ASN
1	C	198	GLN
1	D	6	GLN
1	D	25	ASN
1	D	39	ASN
1	D	61	ASN
1	D	63	GLN
1	D	64	GLN
1	D	74	HIS
1	D	141	ASN
1	E	39	ASN
1	E	63	GLN
1	E	64	GLN
1	E	130	GLN
1	E	141	ASN
1	E	184	ASN
1	F	6	GLN
1	F	64	GLN

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Mol	Chain	Res	Type
1	F	130	GLN
1	F	141	ASN
1	F	192	ASN
1	F	203	ASN
1	G	6	GLN
1	G	34	GLN
1	G	39	ASN
1	G	63	GLN
1	G	130	GLN
1	G	156	ASN
1	G	180	GLN
1	G	184	ASN
1	G	192	ASN
1	G	198	GLN
1	G	203	ASN
1	H	25	ASN
1	H	74	HIS

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	$\#\|Z\|>2$
2	MPD	A	225	-	6,7,7	0.28	0	7,10,10	0.53	0
3	PO4	A	226	-	4,4,4	0.39	0	6,6,6	0.27	0
2	MPD	C	225	-	6,7,7	0.28	0	7,10,10	0.48	0
2	MPD	G	225	-	6,7,7	0.28	0	7,10,10	0.57	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
2	MPD	A	225	-	-	0/5/5/5	0/0/0/0
3	PO4	A	226	-	-	0/0/0/0	0/0/0/0
2	MPD	C	225	-	1/1/2/2	0/5/5/5	0/0/0/0
2	MPD	G	225	-	1/1/2/2	0/5/5/5	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	225	MPD	C4
2	C	225	MPD	C4

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	225	MPD	6	0
2	C	225	MPD	3	0
2	G	225	MPD	3	0

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	206/224 (91%)	0.46	2 (0%) 84 88	27, 41, 66, 81	0
1	B	205/224 (91%)	0.16	1 (0%) 91 94	35, 51, 78, 95	0
1	C	206/224 (91%)	0.22	1 (0%) 91 94	29, 45, 67, 104	0
1	D	161/224 (71%)	0.52	7 (4%) 39 48	33, 55, 122, 150	0
1	E	194/224 (86%)	0.78	27 (13%) 4 6	39, 75, 127, 162	0
1	F	166/224 (74%)	0.89	27 (16%) 2 4	20, 74, 122, 146	0
1	G	193/224 (86%)	0.60	20 (10%) 8 12	68, 93, 121, 140	0
1	H	153/224 (68%)	0.57	11 (7%) 18 26	46, 71, 117, 139	0
All	All	1484/1792 (82%)	0.51	96 (6%) 22 30	20, 61, 117, 162	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	179	VAL	7.1
1	F	144	PRO	5.9
1	E	188	VAL	5.9
1	G	179	VAL	5.5
1	F	127	ILE	5.5
1	F	123	ALA	5.4
1	H	127	ILE	5.4
1	F	200	TRP	5.3
1	F	126	GLY	5.3
1	E	151	SER	5.2
1	E	200	TRP	5.2
1	G	129	LEU	5.1
1	H	173	PHE	4.9
1	F	125	GLU	4.5
1	E	121	LYS	4.5
1	F	142	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	187	LYS	4.0
1	G	181	VAL	3.9
1	E	191	LEU	3.9
1	F	176	GLY	3.8
1	E	161	ALA	3.7
1	G	153	LEU	3.6
1	F	139	LEU	3.6
1	F	198	GLN	3.5
1	H	31	PHE	3.5
1	H	1	SER	3.5
1	E	126	GLY	3.5
1	D	148	ALA	3.4
1	E	145	TYR	3.4
1	E	194	TYR	3.2
1	F	175	PRO	3.2
1	E	162	THR	3.2
1	D	201	THR	3.2
1	G	137	THR	3.1
1	G	139	LEU	3.1
1	H	170	LEU	3.1
1	E	149	ILE	3.1
1	E	117	LEU	3.1
1	G	201	THR	3.1
1	H	62	GLY	3.0
1	F	1	SER	3.0
1	F	128	SER	2.9
1	G	61	ASN	2.9
1	G	55	PHE	2.8
1	E	197	LEU	2.8
1	E	202	ILE	2.8
1	E	198	GLN	2.7
1	F	131	SER	2.7
1	F	199	THR	2.7
1	E	192	ASN	2.7
1	H	148	ALA	2.6
1	G	134	ASP	2.6
1	F	138	MET	2.6
1	A	75	LEU	2.6
1	C	162	THR	2.6
1	E	141	ASN	2.6
1	H	140	VAL	2.6
1	E	147	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	189	ASP	2.5
1	F	148	ALA	2.5
1	F	129	LEU	2.5
1	G	167	THR	2.5
1	E	140	VAL	2.5
1	E	185	VAL	2.5
1	F	145	TYR	2.5
1	F	197	LEU	2.5
1	G	203	ASN	2.5
1	G	200	TRP	2.5
1	E	201	THR	2.4
1	H	171	LEU	2.4
1	D	176	GLY	2.4
1	D	147	PHE	2.4
1	G	48	THR	2.4
1	G	100	ALA	2.3
1	F	119	GLY	2.3
1	F	202	ILE	2.3
1	G	198	GLN	2.3
1	D	191	LEU	2.3
1	G	82	VAL	2.3
1	F	122	GLY	2.3
1	G	124	GLU	2.2
1	E	128	SER	2.2
1	D	196	GLU	2.2
1	G	150	GLY	2.2
1	H	174	MET	2.2
1	A	70	MET	2.2
1	B	200	TRP	2.2
1	E	129	LEU	2.2
1	G	189	ASP	2.1
1	E	82	VAL	2.1
1	D	72	SER	2.1
1	E	166	THR	2.1
1	F	140	VAL	2.1
1	F	170	LEU	2.1
1	F	130	GLN	2.1
1	H	172	MET	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
2	MPD	G	225	8/8	0.89	0.26	4.52	78,86,90,98	0
2	MPD	C	225	8/8	0.88	0.20	4.02	42,59,78,81	0
3	PO4	A	226	5/5	0.83	0.20	1.93	135,136,137,138	0
2	MPD	A	225	8/8	0.91	0.25	1.74	72,86,90,94	0

6.5 Other polymers (i)

There are no such residues in this entry.