Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:17 AM GMT

PDB ID	:	2WKB
Title	:	CRYSTAL STRUCTURE OF MACROPHAGE MIGRATION INHIBITORY FACTOR FROM PLASMODIUM BERGHEI
Authors	:	Dobson, S.E.; Augustijn, K.D.; Brannigan, J.A.; Dodson, E.J.; Waters, A.P.; Wilkinson, A.J.
Deposited on	:	2009-06-08
Resolution	:	1.78 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:

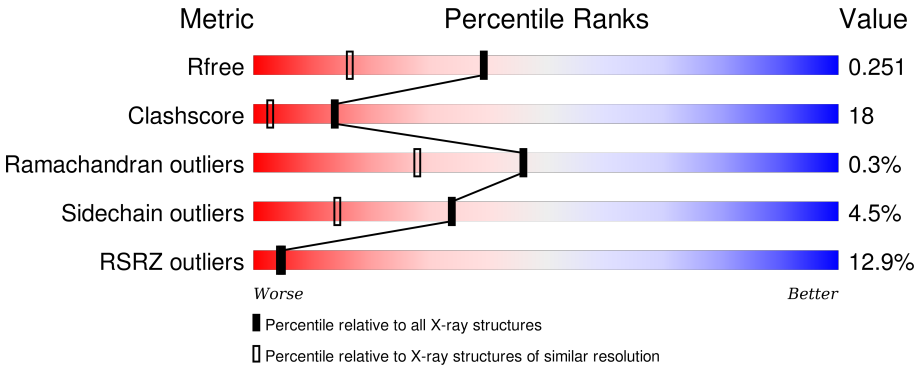
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.78 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	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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	125	18% 70% 15% • 14%
1	B	125	6% 72% 17% • 10%
1	C	125	12% 66% 24% • 7%
1	D	125	15% 63% 23% • 10%
1	E	125	10% 79% 12% • 6%

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Mol	Chain	Length	Quality of chain
1	F	125	8% 72% 18% 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
1	CME	C	2[B]	-	-	X	-
2	GOL	A	1116	-	-	-	X
2	GOL	A	1117	-	-	X	X
2	GOL	B	1116	-	-	X	X
2	GOL	E	1117	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5959 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 MACROPHAGE MIGRATION INHIBITORY FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	S	0	2	1
			857	543	143	165	6			
1	B	112	Total	C	N	O	S	0	1	1
			886	557	151	170	8			
1	C	116	Total	C	N	O	S	0	4	1
			933	585	159	180	9			
1	D	112	Total	C	N	O	S	0	4	1
			905	570	153	174	8			
1	E	117	Total	C	N	O	S	0	3	1
			928	579	160	181	8			
1	F	116	Total	C	N	O	S	0	1	1
			910	570	156	176	8			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	GLY	-	EXPRESSION TAG	UNP Q4YQW0
A	117	SER	-	EXPRESSION TAG	UNP Q4YQW0
A	118	ARG	-	EXPRESSION TAG	UNP Q4YQW0
A	119	SER	-	EXPRESSION TAG	UNP Q4YQW0
A	120	HIS	-	EXPRESSION TAG	UNP Q4YQW0
A	121	HIS	-	EXPRESSION TAG	UNP Q4YQW0
A	122	HIS	-	EXPRESSION TAG	UNP Q4YQW0
A	123	HIS	-	EXPRESSION TAG	UNP Q4YQW0
A	124	HIS	-	EXPRESSION TAG	UNP Q4YQW0
A	125	HIS	-	EXPRESSION TAG	UNP Q4YQW0
B	116	GLY	-	EXPRESSION TAG	UNP Q4YQW0
B	117	SER	-	EXPRESSION TAG	UNP Q4YQW0
B	118	ARG	-	EXPRESSION TAG	UNP Q4YQW0
B	119	SER	-	EXPRESSION TAG	UNP Q4YQW0
B	120	HIS	-	EXPRESSION TAG	UNP Q4YQW0
B	121	HIS	-	EXPRESSION TAG	UNP Q4YQW0
B	122	HIS	-	EXPRESSION TAG	UNP Q4YQW0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	123	HIS	-	EXPRESSION TAG	UNP Q4YQW0
B	124	HIS	-	EXPRESSION TAG	UNP Q4YQW0
B	125	HIS	-	EXPRESSION TAG	UNP Q4YQW0
C	116	GLY	-	EXPRESSION TAG	UNP Q4YQW0
C	117	SER	-	EXPRESSION TAG	UNP Q4YQW0
C	118	ARG	-	EXPRESSION TAG	UNP Q4YQW0
C	119	SER	-	EXPRESSION TAG	UNP Q4YQW0
C	120	HIS	-	EXPRESSION TAG	UNP Q4YQW0
C	121	HIS	-	EXPRESSION TAG	UNP Q4YQW0
C	122	HIS	-	EXPRESSION TAG	UNP Q4YQW0
C	123	HIS	-	EXPRESSION TAG	UNP Q4YQW0
C	124	HIS	-	EXPRESSION TAG	UNP Q4YQW0
C	125	HIS	-	EXPRESSION TAG	UNP Q4YQW0
D	116	GLY	-	EXPRESSION TAG	UNP Q4YQW0
D	117	SER	-	EXPRESSION TAG	UNP Q4YQW0
D	118	ARG	-	EXPRESSION TAG	UNP Q4YQW0
D	119	SER	-	EXPRESSION TAG	UNP Q4YQW0
D	120	HIS	-	EXPRESSION TAG	UNP Q4YQW0
D	121	HIS	-	EXPRESSION TAG	UNP Q4YQW0
D	122	HIS	-	EXPRESSION TAG	UNP Q4YQW0
D	123	HIS	-	EXPRESSION TAG	UNP Q4YQW0
D	124	HIS	-	EXPRESSION TAG	UNP Q4YQW0
D	125	HIS	-	EXPRESSION TAG	UNP Q4YQW0
E	116	GLY	-	EXPRESSION TAG	UNP Q4YQW0
E	117	SER	-	EXPRESSION TAG	UNP Q4YQW0
E	118	ARG	-	EXPRESSION TAG	UNP Q4YQW0
E	119	SER	-	EXPRESSION TAG	UNP Q4YQW0
E	120	HIS	-	EXPRESSION TAG	UNP Q4YQW0
E	121	HIS	-	EXPRESSION TAG	UNP Q4YQW0
E	122	HIS	-	EXPRESSION TAG	UNP Q4YQW0
E	123	HIS	-	EXPRESSION TAG	UNP Q4YQW0
E	124	HIS	-	EXPRESSION TAG	UNP Q4YQW0
E	125	HIS	-	EXPRESSION TAG	UNP Q4YQW0
F	116	GLY	-	EXPRESSION TAG	UNP Q4YQW0
F	117	SER	-	EXPRESSION TAG	UNP Q4YQW0
F	118	ARG	-	EXPRESSION TAG	UNP Q4YQW0
F	119	SER	-	EXPRESSION TAG	UNP Q4YQW0
F	120	HIS	-	EXPRESSION TAG	UNP Q4YQW0
F	121	HIS	-	EXPRESSION TAG	UNP Q4YQW0
F	122	HIS	-	EXPRESSION TAG	UNP Q4YQW0
F	123	HIS	-	EXPRESSION TAG	UNP Q4YQW0
F	124	HIS	-	EXPRESSION TAG	UNP Q4YQW0

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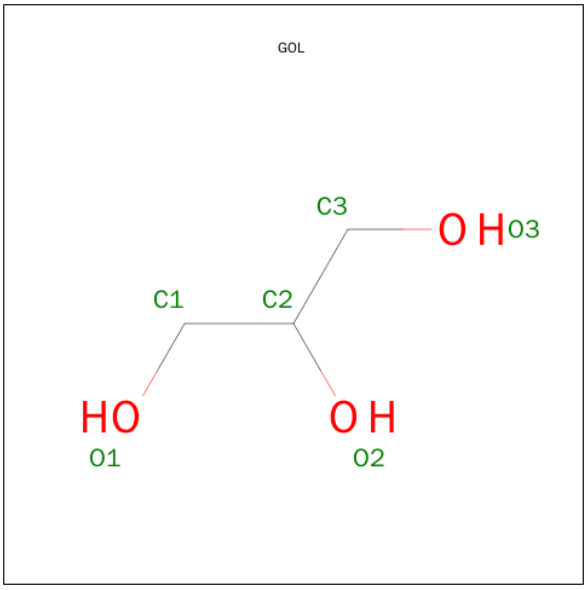
Chain	Residue	Modelled	Actual	Comment	Reference
F	125	HIS	-	EXPRESSION TAG	UNP Q4YQW0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	68	Total O 68 68	0	0

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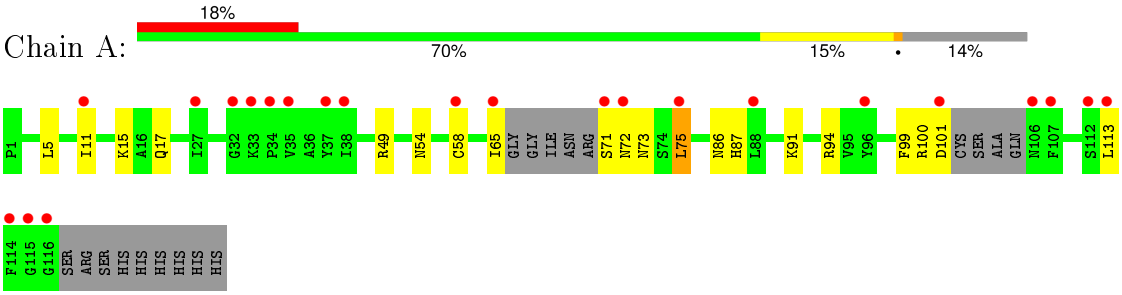
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	101	Total O 101 101	0	0
3	C	75	Total O 75 75	0	0
3	D	75	Total O 75 75	0	0
3	E	85	Total O 85 85	0	0
3	F	88	Total O 88 88	0	0

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.

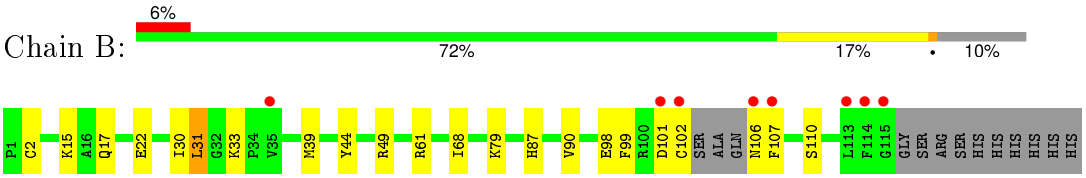
- Molecule 1: MACROPHAGE MIGRATION INHIBITORY FACTOR

Chain A:



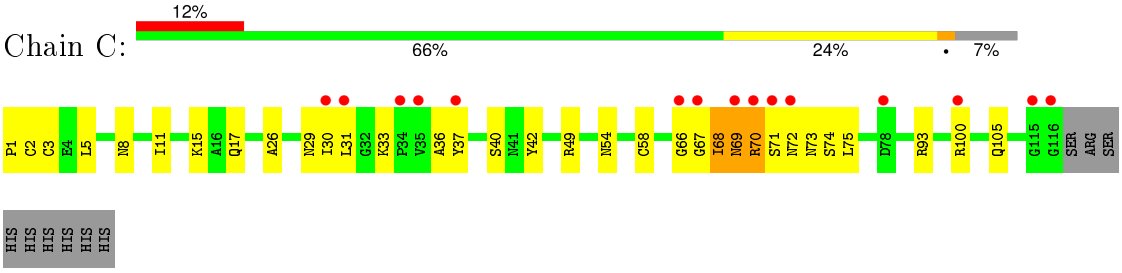
- Molecule 1: MACROPHAGE MIGRATION INHIBITORY FACTOR

Chain B:



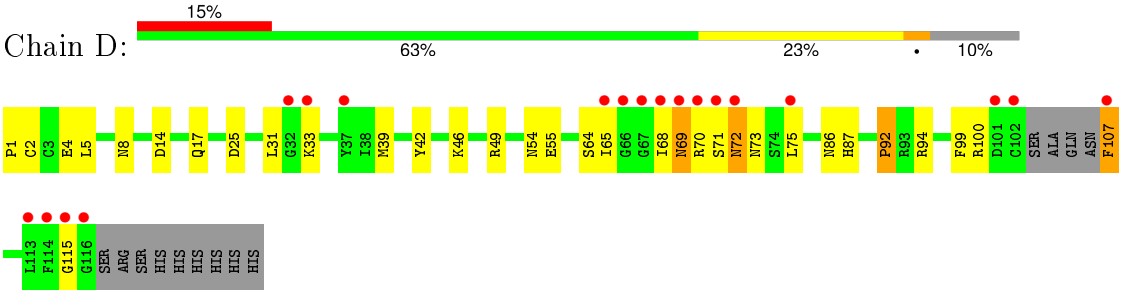
- Molecule 1: MACROPHAGE MIGRATION INHIBITORY FACTOR

Chain C:

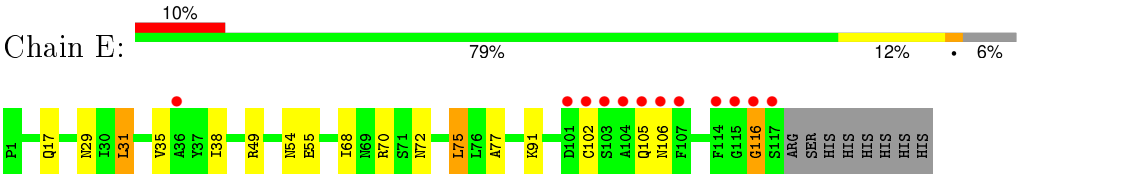


- Molecule 1: MACROPHAGE MIGRATION INHIBITORY FACTOR

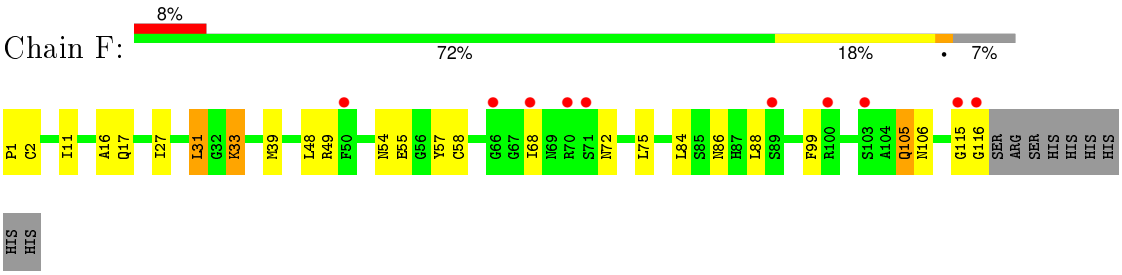
Chain D:



- Molecule 1: MACROPHAGE MIGRATION INHIBITORY FACTOR



• Molecule 1: MACROPHAGE MIGRATION INHIBITORY FACTOR



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.70Å 69.17Å 80.22Å 90.00° 118.20° 90.00°	Depositor
Resolution (Å)	70.71 – 1.78 49.44 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.4 (70.71-1.78) 99.4 (49.44-1.78)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.199 , 0.255 0.198 , 0.251	Depositor DCC
R_{free} test set	3657 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.5	EDS
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.022 for h,-k,-h-l 0.000 for -h-l,-k,l 0.000 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 72470 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5959	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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 42.78 % 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 1.9404e-04.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: GOL, CME

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	0.98	0/863	0.87	0/1161
1	B	1.20	2/882 (0.2%)	1.01	0/1187
1	C	0.97	0/934	0.96	1/1259 (0.1%)
1	D	1.04	2/905 (0.2%)	0.98	4/1218 (0.3%)
1	E	1.18	1/925 (0.1%)	1.01	2/1246 (0.2%)
1	F	1.07	2/907 (0.2%)	0.92	0/1222
All	All	1.08	7/5416 (0.1%)	0.96	7/7293 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	77	ALA	CA-CB	5.80	1.64	1.52
1	F	58	CYS	CB-SG	-5.72	1.72	1.81
1	D	4	GLU	CB-CG	-5.63	1.41	1.52
1	F	55	GLU	CG-CD	5.37	1.60	1.51
1	B	44	TYR	CE1-CZ	5.23	1.45	1.38
1	B	90	VAL	CB-CG1	5.20	1.63	1.52
1	D	55	GLU	CG-CD	5.03	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	46	LYS	CD-CE-NZ	-5.60	98.82	111.70
1	E	70	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	D	94	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	C	93	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	25	ASP	CB-CG-OD1	5.26	123.04	118.30
1	D	14	ASP	CB-CG-OD1	5.20	122.98	118.30
1	E	31	LEU	CB-CG-CD1	5.14	119.73	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	857	0	847	23	0
1	B	886	0	881	35	0
1	C	933	0	921	82	0
1	D	905	0	896	43	0
1	E	928	0	915	30	0
1	F	910	0	903	27	0
2	A	12	0	16	5	0
2	B	12	0	15	6	0
2	C	6	0	7	3	0
2	D	6	0	8	2	0
2	E	6	0	8	2	0
2	F	6	0	8	1	0
3	A	68	0	0	1	0
3	B	101	0	0	1	0
3	C	75	0	0	2	0
3	D	75	0	0	3	0
3	E	85	0	0	3	0
3	F	88	0	0	7	0
All	All	5959	0	5425	201	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (201) 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:A:5:LEU:HD11	1:A:58[A]:CYS:SG	1.58	1.41
1:A:5:LEU:CD1	1:A:58[A]:CYS:SG	2.21	1.27
1:C:70:ARG:HG3	1:D:86:ASN:O	1.34	1.27
1:C:5:LEU:HD11	1:C:58[B]:CYS:SG	1.76	1.25
1:C:5:LEU:CD1	1:C:58[B]:CYS:SG	2.27	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69[A]:ASN:CG	1:C:72:ASN:HB2	1.69	1.11
1:D:100:ARG:HD3	1:E:106:ASN:HD22	1.10	1.11
1:D:99:PHE:O	1:E:106:ASN:HB2	1.49	1.10
1:C:68:ILE:HA	1:C:72:ASN:ND2	1.72	1.05
1:C:68:ILE:HA	1:C:72:ASN:HD22	1.20	1.00
1:A:99:PHE:O	1:B:106:ASN:HB2	1.62	0.99
1:C:69[B]:ASN:H	1:C:72:ASN:HB3	1.25	0.99
1:D:100:ARG:HD3	1:E:106:ASN:ND2	1.77	0.99
1:F:33:LYS:HD3	3:F:2032:HOH:O	1.63	0.99
1:C:69[A]:ASN:H	1:C:72:ASN:HB3	1.26	0.98
1:B:61:ARG:HH21	1:C:2[B]:CME:HZ3	1.28	0.97
1:D:39:MET:CE	1:F:48:LEU:HD11	1.93	0.97
1:D:107:PHE:HD2	3:F:2059:HOH:O	1.45	0.96
1:F:106:ASN:HB2	3:F:2079:HOH:O	1.63	0.96
1:B:61:ARG:HH21	1:C:2[B]:CME:CZ	1.77	0.96
1:D:39:MET:HE2	1:F:48:LEU:HD11	1.50	0.93
1:B:61:ARG:NH2	1:C:2[B]:CME:HZ3	1.83	0.93
1:B:30:ILE:HD11	1:B:79:LYS:HD2	1.50	0.93
1:C:5:LEU:HD11	1:C:58[B]:CYS:HG	1.22	0.92
1:D:107:PHE:N	1:D:107:PHE:HD1	1.70	0.90
2:E:1117:GOL:H31	3:E:2085:HOH:O	1.71	0.90
1:C:69[A]:ASN:O	1:C:72:ASN:HB3	1.72	0.89
1:D:73:ASN:HB2	3:D:2055:HOH:O	1.72	0.89
1:B:31:LEU:HB3	1:B:33:LYS:HG3	1.55	0.89
1:D:100:ARG:CD	1:E:106:ASN:ND2	2.36	0.88
1:B:31:LEU:HD11	1:B:68:ILE:HD13	1.56	0.88
1:D:99:PHE:O	1:E:106:ASN:CB	2.22	0.87
1:C:69[A]:ASN:ND2	1:C:72:ASN:HB2	1.90	0.85
1:E:29[B]:ASN:OD1	1:E:29[B]:ASN:O	1.94	0.85
1:D:100:ARG:NE	1:E:106:ASN:ND2	2.24	0.84
1:E:35:VAL:O	1:E:38:ILE:HG22	1.78	0.83
1:D:107:PHE:CD1	1:D:107:PHE:N	2.41	0.83
1:C:68:ILE:O	1:C:69[B]:ASN:OD1	1.96	0.82
1:C:69[B]:ASN:O	1:C:72:ASN:HB3	1.80	0.82
1:A:94:ARG:HG3	2:A:1117:GOL:O2	1.79	0.81
1:C:69[A]:ASN:HD22	1:C:71:SER:H	1.23	0.81
1:D:68:ILE:HG23	1:D:73:ASN:HD21	1.46	0.81
1:C:69[B]:ASN:N	1:C:72:ASN:HB3	1.96	0.80
1:C:69[A]:ASN:H	1:C:72:ASN:CB	1.94	0.79
1:C:70:ARG:CG	1:D:86:ASN:O	2.26	0.78
1:A:5:LEU:HD11	1:A:58[A]:CYS:HG	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69[A]:ASN:O	1:C:72:ASN:CB	2.31	0.77
1:B:31:LEU:HD11	1:B:68:ILE:CD1	2.14	0.76
1:C:69[A]:ASN:HD22	1:C:71:SER:N	1.83	0.76
1:B:31:LEU:CD1	1:B:68:ILE:HD13	2.16	0.76
1:C:68:ILE:CA	1:C:72:ASN:HD22	1.99	0.75
1:C:69[A]:ASN:ND2	1:C:72:ASN:N	2.36	0.73
1:C:69[A]:ASN:N	1:C:72:ASN:HB3	1.99	0.73
1:C:69[B]:ASN:H	1:C:72:ASN:CB	2.00	0.72
1:E:75:LEU:CD2	1:E:75:LEU:H	2.01	0.72
1:E:116:GLY:HA3	3:E:2083:HOH:O	1.89	0.72
1:B:30:ILE:CD1	1:B:79:LYS:HD2	2.19	0.72
1:C:26:ALA:O	1:C:30:ILE:HG12	1.90	0.72
1:D:100:ARG:HA	1:E:106:ASN:HB3	1.71	0.72
1:C:69[B]:ASN:O	1:C:72:ASN:N	2.23	0.71
1:B:61:ARG:NH2	1:C:2[B]:CME:CZ	2.48	0.71
1:C:69[B]:ASN:O	1:C:72:ASN:CB	2.38	0.70
1:A:5:LEU:HD12	1:A:58[A]:CYS:SG	2.30	0.69
1:D:65:ILE:HB	1:D:68:ILE:HD13	1.73	0.69
1:B:99:PHE:HB3	2:B:1116:GOL:H2	1.73	0.69
1:C:69[A]:ASN:O	1:C:72:ASN:N	2.25	0.68
1:F:72:ASN:HA	1:F:75:LEU:HD23	1.76	0.67
1:B:31:LEU:CD1	1:B:68:ILE:CD1	2.70	0.67
1:C:5:LEU:HD12	1:C:58[B]:CYS:SG	2.29	0.66
1:E:75:LEU:H	1:E:75:LEU:HD22	1.59	0.66
1:A:73:ASN:HD22	1:B:107:PHE:HZ	1.44	0.66
1:C:69[A]:ASN:OD1	1:C:72:ASN:HB2	1.94	0.66
1:C:31:LEU:CD2	1:C:33:LYS:HG2	2.26	0.66
1:C:69[A]:ASN:ND2	1:C:71:SER:H	1.93	0.64
1:D:107:PHE:CD2	3:F:2059:HOH:O	2.32	0.64
1:E:29[B]:ASN:OD1	1:E:29[B]:ASN:C	2.36	0.64
1:C:8:ASN:HB2	2:C:1116:GOL:H31	1.80	0.64
1:D:39:MET:HE3	1:F:48:LEU:HD11	1.76	0.64
1:A:113:LEU:HD11	3:A:2064:HOH:O	1.98	0.63
1:C:69[A]:ASN:ND2	1:C:71:SER:N	2.47	0.63
1:A:91:LYS:NZ	2:A:1117:GOL:H11	2.12	0.62
1:E:72:ASN:HA	1:E:75:LEU:HD23	1.83	0.61
1:B:68:ILE:HG22	2:B:1116:GOL:H12	1.82	0.61
1:D:75:LEU:HD22	3:D:2057:HOH:O	2.00	0.61
1:C:68:ILE:C	1:C:69[B]:ASN:OD1	2.39	0.60
1:C:29:ASN:HD22	1:C:30:ILE:HD13	1.65	0.60
1:D:54:ASN:O	2:D:1116:GOL:H2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1116:GOL:H32	3:C:2041:HOH:O	2.02	0.59
1:C:68:ILE:HG22	1:C:73:ASN:HB3	1.85	0.59
1:F:27:ILE:O	1:F:31:LEU:HB2	2.02	0.59
1:D:49:ARG:HH11	1:E:17:GLN:NE2	2.01	0.58
1:C:69[A]:ASN:O	1:C:72:ASN:CA	2.52	0.58
1:B:101:ASP:HB2	2:B:1116:GOL:H32	1.86	0.58
1:C:31:LEU:HB2	3:C:2031:HOH:O	2.04	0.58
1:C:69[B]:ASN:O	1:C:72:ASN:CA	2.52	0.58
1:B:61:ARG:HH21	1:C:2[B]:CME:HZ2	1.68	0.57
1:F:2[B]:CME:SG	1:F:39:MET:CE	2.93	0.57
1:D:39:MET:HE3	1:F:57:TYR:HE2	1.69	0.57
1:D:100:ARG:NH2	1:E:102:CYS:HB2	2.20	0.56
1:A:73:ASN:ND2	1:B:107:PHE:HZ	2.03	0.56
1:F:105:GLN:HG3	1:F:106:ASN:OD1	2.06	0.56
1:C:54:ASN:O	2:C:1116:GOL:O2	2.23	0.56
1:C:69[B]:ASN:CA	1:C:72:ASN:HB3	2.37	0.55
1:A:91:LYS:HG3	2:A:1117:GOL:H31	1.88	0.55
1:D:65:ILE:HB	1:D:68:ILE:CD1	2.35	0.55
1:F:2[B]:CME:SG	1:F:39:MET:HE1	2.47	0.55
1:C:31:LEU:HG	1:C:33:LYS:HG2	1.89	0.54
1:B:49:ARG:HH11	1:C:17:GLN:NE2	2.06	0.54
1:F:86:ASN:HB2	3:F:2063:HOH:O	2.08	0.54
1:A:15:LYS:HE2	1:A:87:HIS:O	2.07	0.54
1:C:3:CYS:O	1:C:40:SER:HA	2.08	0.53
1:B:102:CYS:C	3:B:2096:HOH:O	2.45	0.53
1:D:100:ARG:CZ	1:E:106:ASN:HD21	2.22	0.52
1:E:75:LEU:HD22	1:E:75:LEU:N	2.24	0.52
1:A:72:ASN:OD1	1:A:75:LEU:HD23	2.09	0.52
1:C:69[B]:ASN:H	1:C:72:ASN:HD22	1.57	0.52
1:D:72:ASN:HD22	1:D:73:ASN:N	2.07	0.52
1:D:69:ASN:H	1:D:72:ASN:HD21	1.58	0.52
1:F:27:ILE:HG23	1:F:31:LEU:HD22	1.91	0.52
1:C:11:ILE:HD12	1:C:15:LYS:HG2	1.92	0.51
1:C:69[A]:ASN:H	1:C:72:ASN:HD22	1.59	0.51
1:A:49:ARG:HH11	1:B:17:GLN:NE2	2.08	0.51
1:D:8:ASN:O	2:D:1116:GOL:H31	2.11	0.51
1:F:68:ILE:HD13	1:F:99:PHE:HD1	1.76	0.50
1:D:17:GLN:NE2	1:F:49:ARG:HH11	2.09	0.50
1:B:98:GLU:OE2	1:C:2[B]:CME:OH	2.27	0.50
1:C:69[A]:ASN:ND2	1:C:72:ASN:CB	2.70	0.50
2:E:1117:GOL:C3	3:E:2085:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2[B]:CME:OH	1:D:64:SER:OG	2.26	0.49
1:A:54:ASN:HB2	1:B:17:GLN:NE2	2.27	0.49
1:D:100:ARG:CZ	1:E:106:ASN:ND2	2.74	0.49
1:B:31:LEU:CD1	1:B:68:ILE:HD11	2.42	0.49
1:E:49:ARG:HH11	1:F:17:GLN:NE2	2.10	0.48
1:E:54:ASN:HB2	1:F:17:GLN:NE2	2.28	0.48
1:F:2[B]:CME:SG	1:F:39:MET:HE3	2.53	0.48
1:A:17:GLN:NE2	1:C:49:ARG:HH11	2.11	0.48
1:C:5:LEU:HD23	1:C:42[B]:TYR:CD2	2.49	0.48
1:D:100:ARG:NH2	1:E:102:CYS:CB	2.77	0.48
1:B:31:LEU:HD13	1:B:68:ILE:HD11	1.96	0.48
1:C:31:LEU:HD23	1:C:33:LYS:HG2	1.95	0.48
1:F:11:ILE:HD11	1:F:16:ALA:HA	1.96	0.48
1:C:69[A]:ASN:C	1:C:72:ASN:HB3	2.33	0.47
1:E:31:LEU:HD11	1:E:68:ILE:HG12	1.95	0.47
1:C:69[B]:ASN:HB2	1:C:72:ASN:HB2	1.96	0.47
1:A:99:PHE:O	1:B:106:ASN:CB	2.50	0.47
1:D:5:LEU:HD23	1:D:42[A]:TYR:CD1	2.50	0.47
1:B:15:LYS:HE2	1:B:87:HIS:O	2.15	0.47
1:C:31:LEU:CG	1:C:33:LYS:HG2	2.45	0.46
1:B:2[B]:CME:SG	1:B:39:MET:HE1	2.55	0.46
1:A:100:ARG:HA	1:B:106:ASN:HB3	1.97	0.46
1:F:68:ILE:HD13	1:F:99:PHE:CD1	2.51	0.46
1:D:100:ARG:HH22	1:E:102:CYS:HB2	1.80	0.46
1:A:11:ILE:HB	1:A:15:LYS:HD3	1.98	0.46
1:E:75:LEU:CD2	1:E:75:LEU:N	2.77	0.46
1:D:69:ASN:C	1:D:69:ASN:HD22	2.19	0.45
1:C:69[A]:ASN:C	1:C:69[A]:ASN:ND2	2.70	0.45
1:C:29:ASN:ND2	1:C:30:ILE:HD13	2.31	0.45
1:C:36:ALA:HB1	1:C:37:TYR:HD2	1.81	0.45
1:C:5:LEU:HD13	1:C:58[B]:CYS:SG	2.42	0.45
1:C:11:ILE:HD11	1:C:42[B]:TYR:CE2	2.51	0.45
1:A:94:ARG:HG3	2:A:1117:GOL:HO2	1.80	0.44
1:F:1:PRO:C	1:F:2[B]:CME:SG	2.95	0.44
1:B:2[B]:CME:SG	1:B:39:MET:CE	3.05	0.44
1:B:101:ASP:HB2	2:B:1116:GOL:C3	2.47	0.44
1:C:69[A]:ASN:HD21	1:C:72:ASN:N	2.14	0.44
1:F:54:ASN:O	2:F:1116:GOL:O2	2.36	0.44
1:C:69[B]:ASN:N	1:C:72:ASN:HD22	2.16	0.43
1:E:55:GLU:OE1	1:E:91:LYS:HE3	2.18	0.43
1:C:69[A]:ASN:H	1:C:72:ASN:ND2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:GLU:OE2	1:B:87:HIS:NE2	2.51	0.43
1:E:55:GLU:OE1	1:E:91:LYS:CE	2.67	0.43
1:F:84:LEU:O	1:F:88:LEU:HB2	2.19	0.43
1:C:70:ARG:C	1:C:72:ASN:H	2.19	0.43
1:C:69[A]:ASN:C	1:C:69[A]:ASN:HD22	2.22	0.42
1:C:69[A]:ASN:CA	1:C:72:ASN:HB3	2.46	0.42
1:A:73:ASN:ND2	1:B:107:PHE:CZ	2.80	0.42
1:C:1:PRO:C	1:C:2[B]:CME:SG	2.88	0.42
1:D:92:PRO:HG2	1:E:116:GLY:H	1.85	0.42
1:B:68:ILE:HG22	2:B:1116:GOL:C1	2.49	0.42
1:D:68:ILE:HG13	1:D:73:ASN:OD1	2.20	0.42
1:D:1:PRO:HB3	1:D:64:SER:O	2.20	0.42
1:D:17:GLN:NE2	1:F:54:ASN:HB2	2.34	0.42
1:C:69[A]:ASN:O	1:C:73:ASN:N	2.50	0.41
1:C:5:LEU:CD2	1:C:42[B]:TYR:CD2	3.02	0.41
1:F:116:GLY:N	3:F:2087:HOH:O	2.53	0.41
1:C:69[A]:ASN:HD21	1:C:71:SER:C	2.23	0.41
1:F:115:GLY:HA2	3:F:2084:HOH:O	2.20	0.41
1:B:68:ILE:CG2	2:B:1116:GOL:H12	2.49	0.41
1:E:35:VAL:HB	1:E:38:ILE:HG21	2.02	0.41
1:D:86:ASN:HD22	1:D:87:HIS:CD2	2.39	0.41
1:C:69[A]:ASN:CG	1:C:72:ASN:CB	2.62	0.41
1:D:39:MET:CE	1:F:57:TYR:HE2	2.33	0.41
1:E:35:VAL:HB	1:E:38:ILE:CG2	2.51	0.41
1:A:17:GLN:NE2	1:C:54:ASN:HB2	2.35	0.41
1:A:91:LYS:CE	2:A:1117:GOL:H11	2.51	0.41
1:C:66:GLY:HA2	1:C:67:GLY:HA2	1.68	0.40
1:C:69[B]:ASN:C	1:C:72:ASN:HB3	2.33	0.40
1:D:75:LEU:HD13	3:D:2059:HOH:O	2.20	0.40
1:C:69[B]:ASN:O	1:C:73:ASN:N	2.47	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	102/125 (82%)	97 (95%)	5 (5%)	0	100 100
1	B	107/125 (86%)	106 (99%)	1 (1%)	0	100 100
1	C	116/125 (93%)	113 (97%)	3 (3%)	0	100 100
1	D	110/125 (88%)	107 (97%)	2 (2%)	1 (1%)	21 6
1	E	116/125 (93%)	112 (97%)	3 (3%)	1 (1%)	21 6
1	F	113/125 (90%)	110 (97%)	3 (3%)	0	100 100
All	All	664/750 (88%)	645 (97%)	17 (3%)	2 (0%)	46 28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	116	GLY
1	D	115	GLY

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	97/110 (88%)	92 (95%)	5 (5%)	29 11
1	B	99/110 (90%)	97 (98%)	2 (2%)	63 47
1	C	104/110 (94%)	96 (92%)	8 (8%)	16 4
1	D	101/110 (92%)	93 (92%)	8 (8%)	15 4
1	E	103/110 (94%)	101 (98%)	2 (2%)	65 49
1	F	101/110 (92%)	98 (97%)	3 (3%)	48 29
All	All	605/660 (92%)	577 (95%)	28 (5%)	34 14

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ILE
1	A	71	SER
1	A	75	LEU
1	A	86	ASN
1	A	101	ASP
1	B	31	LEU
1	B	110	SER
1	C	68	ILE
1	C	69[A]	ASN
1	C	69[B]	ASN
1	C	70	ARG
1	C	74	SER
1	C	75	LEU
1	C	100	ARG
1	C	105	GLN
1	D	31	LEU
1	D	33	LYS
1	D	69	ASN
1	D	70	ARG
1	D	71	SER
1	D	72	ASN
1	D	92	PRO
1	D	107	PHE
1	E	75	LEU
1	E	105	GLN
1	F	31	LEU
1	F	33	LYS
1	F	105	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	54	ASN
1	A	86	ASN
1	B	17	GLN
1	B	54	ASN
1	C	17	GLN
1	C	29	ASN
1	C	54	ASN
1	C	72	ASN
1	D	17	GLN
1	D	54	ASN

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Mol	Chain	Res	Type
1	D	69	ASN
1	D	72	ASN
1	D	87	HIS
1	E	17	GLN
1	E	54	ASN
1	E	105	GLN
1	E	106	ASN
1	F	17	GLN
1	F	54	ASN
1	F	86	ASN
1	F	105	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CME	A	2	1	8,9,10	0.64	0	6,9,11	3.50	1 (16%)
1	CME	B	2[A]	-	8,9,10	0.63	0	6,9,11	2.32	2 (33%)
1	CME	B	2[B]	-	8,9,10	0.69	0	6,9,11	3.92	2 (33%)
1	CME	C	2[A]	-	8,9,10	0.68	0	6,9,11	3.31	2 (33%)
1	CME	C	2[B]	-	8,9,10	1.02	0	6,9,11	5.73	2 (33%)
1	CME	D	2[A]	-	8,9,10	0.67	0	6,9,11	3.22	1 (16%)
1	CME	D	2[B]	-	8,9,10	0.76	0	6,9,11	4.84	3 (50%)
1	CME	E	2[A]	-	8,9,10	0.77	0	6,9,11	2.42	2 (33%)
1	CME	E	2[B]	-	8,9,10	0.62	0	6,9,11	2.28	1 (16%)
1	CME	F	2[A]	-	8,9,10	0.64	0	6,9,11	2.08	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CME	F	2[B]	-	8,9,10	0.70	0	6,9,11	4.94	1 (16%)

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
1	CME	A	2	1	-	0/5/8/10	0/0/0/0
1	CME	B	2[A]	-	-	0/5/8/10	0/0/0/0
1	CME	B	2[B]	-	-	0/5/8/10	0/0/0/0
1	CME	C	2[A]	-	-	0/5/8/10	0/0/0/0
1	CME	C	2[B]	-	-	0/5/8/10	0/0/0/0
1	CME	D	2[A]	-	-	0/5/8/10	0/0/0/0
1	CME	D	2[B]	-	-	0/5/8/10	0/0/0/0
1	CME	E	2[A]	-	-	0/5/8/10	0/0/0/0
1	CME	E	2[B]	-	-	0/5/8/10	0/0/0/0
1	CME	F	2[A]	-	-	0/5/8/10	0/0/0/0
1	CME	F	2[B]	-	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2[A]	CME	CZ-CE-SD	-4.55	102.04	113.16
1	C	2[B]	CME	CA-CB-SG	-3.95	99.90	114.23
1	D	2[B]	CME	CZ-CE-SD	-3.61	104.33	113.16
1	E	2[A]	CME	CZ-CE-SD	-2.98	105.88	113.16
1	D	2[B]	CME	O-C-CA	-2.37	119.31	125.49
1	B	2[B]	CME	CZ-CE-SD	-2.28	107.59	113.16
1	B	2[A]	CME	CZ-CE-SD	3.14	120.84	113.16
1	B	2[A]	CME	CB-SG-SD	4.38	112.49	103.95
1	E	2[A]	CME	CB-SG-SD	4.45	112.62	103.95
1	F	2[A]	CME	CB-SG-SD	4.55	112.82	103.95
1	E	2[B]	CME	CB-SG-SD	5.05	113.79	103.95
1	C	2[A]	CME	CB-SG-SD	6.42	116.45	103.95
1	D	2[A]	CME	CB-SG-SD	7.48	118.53	103.95
1	A	2	CME	CB-SG-SD	8.10	119.73	103.95
1	B	2[B]	CME	CB-SG-SD	8.90	121.30	103.95
1	D	2[B]	CME	CB-SG-SD	10.84	125.08	103.95
1	F	2[B]	CME	CB-SG-SD	11.78	126.90	103.95
1	C	2[B]	CME	CB-SG-SD	13.32	129.90	103.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	2[B]	CME	2	0
1	C	2[B]	CME	7	0
1	D	2[B]	CME	1	0
1	F	2[B]	CME	4	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	GOL	A	1116	-	5,5,5	0.80	0	5,5,5	1.40	1 (20%)
2	GOL	A	1117	-	5,5,5	1.03	0	5,5,5	1.34	1 (20%)
2	GOL	B	1115	-	5,5,5	0.37	0	5,5,5	0.67	0
2	GOL	B	1116	-	5,5,5	0.94	0	5,5,5	0.70	0
2	GOL	C	1116	-	5,5,5	1.18	1 (20%)	5,5,5	1.22	0
2	GOL	D	1116	-	5,5,5	0.42	0	5,5,5	1.72	1 (20%)
2	GOL	E	1117	-	5,5,5	0.53	0	5,5,5	0.99	0
2	GOL	F	1116	-	5,5,5	0.60	0	5,5,5	0.44	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	GOL	A	1116	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1117	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1115	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1116	-	-	0/4/4/4	0/0/0/0
2	GOL	C	1116	-	-	0/4/4/4	0/0/0/0
2	GOL	D	1116	-	-	0/4/4/4	0/0/0/0
2	GOL	E	1117	-	-	0/4/4/4	0/0/0/0
2	GOL	F	1116	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1116	GOL	O2-C2	-2.44	1.36	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1116	GOL	O2-C2-C1	-2.32	98.00	108.65
2	A	1117	GOL	C3-C2-C1	2.56	121.16	111.12
2	D	1116	GOL	O1-C1-C2	3.08	125.14	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1117	GOL	5	0
2	B	1116	GOL	6	0
2	C	1116	GOL	3	0
2	D	1116	GOL	2	0
2	E	1117	GOL	2	0
2	F	1116	GOL	1	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	106/125 (84%)	1.21	23 (21%) 1 1	14, 31, 57, 64	1 (0%)
1	B	111/125 (88%)	0.80	8 (7%) 18 17	12, 19, 43, 57	0
1	C	115/125 (92%)	0.84	15 (13%) 5 4	14, 28, 50, 53	0
1	D	111/125 (88%)	1.13	19 (17%) 2 2	13, 27, 59, 69	0
1	E	116/125 (92%)	1.03	12 (10%) 9 8	13, 21, 56, 65	0
1	F	115/125 (92%)	0.62	10 (8%) 13 12	15, 28, 47, 60	0
All	All	674/750 (89%)	0.94	87 (12%) 5 4	12, 26, 52, 69	1 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	117	SER	15.7
1	E	104	ALA	12.4
1	D	116	GLY	10.8
1	F	116	GLY	9.7
1	D	115	GLY	9.2
1	D	67	GLY	9.0
1	B	102	CYS	8.7
1	F	115	GLY	8.2
1	E	116	GLY	7.7
1	A	114	PHE	7.6
1	D	65	ILE	7.5
1	A	32	GLY	7.5
1	A	34	PRO	7.4
1	C	71	SER	7.3
1	A	115	GLY	6.7
1	C	35	VAL	6.6
1	A	33	LYS	6.6
1	C	116	GLY	6.5
1	A	113	LEU	6.5

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Mol	Chain	Res	Type	RSRZ
1	D	68	ILE	6.2
1	E	107	PHE	6.2
1	C	70	ARG	6.1
1	D	71	SER	6.0
1	E	105	GLN	6.0
1	B	107	PHE	5.8
1	E	103	SER	5.8
1	B	114	PHE	5.8
1	B	115	GLY	5.8
1	D	66	GLY	5.7
1	D	107	PHE	5.5
1	F	71	SER	5.2
1	F	70	ARG	5.0
1	C	67	GLY	5.0
1	D	37	TYR	4.8
1	C	69[A]	ASN	4.5
1	A	65	ILE	4.4
1	D	33	LYS	4.4
1	D	70	ARG	4.1
1	A	107	PHE	3.9
1	C	34	PRO	3.9
1	B	113	LEU	3.9
1	B	101	ASP	3.9
1	D	102	CYS	3.8
1	A	58[A]	CYS	3.8
1	D	114	PHE	3.8
1	D	75	LEU	3.7
1	A	37	TYR	3.6
1	C	31	LEU	3.5
1	A	75	LEU	3.4
1	E	102	CYS	3.3
1	E	106	ASN	3.3
1	A	35	VAL	3.2
1	A	72	ASN	3.2
1	B	106	ASN	3.1
1	D	101	ASP	3.1
1	E	36	ALA	3.1
1	A	11	ILE	3.0
1	A	101	ASP	3.0
1	C	66	GLY	3.0
1	E	101	ASP	3.0
1	E	114	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	106	ASN	2.9
1	C	115	GLY	2.9
1	C	37	TYR	2.9
1	D	32	GLY	2.7
1	A	38	ILE	2.6
1	F	68	ILE	2.6
1	F	89	SER	2.6
1	D	72	ASN	2.5
1	A	112	SER	2.5
1	C	100	ARG	2.5
1	E	115	GLY	2.5
1	F	100	ARG	2.4
1	C	72	ASN	2.4
1	A	88	LEU	2.4
1	A	27	ILE	2.4
1	A	71	SER	2.4
1	C	78	ASP	2.3
1	D	113	LEU	2.3
1	A	96	TYR	2.3
1	D	69	ASN	2.3
1	F	103	SER	2.3
1	B	35	VAL	2.1
1	A	116	GLY	2.1
1	F	66	GLY	2.1
1	C	30	ILE	2.0
1	F	50	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CME	E	2[A]	10/11	0.92	0.17	-	16,22,38,39	7
1	CME	C	2[B]	10/11	0.86	0.20	-	22,26,38,38	7
1	CME	D	2[B]	10/11	0.88	0.15	-	28,31,43,44	7
1	CME	A	2	10/11	0.75	0.17	-	29,33,46,48	0
1	CME	F	2[A]	10/11	0.85	0.22	-	17,21,23,25	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CME	F	2[B]	10/11	0.85	0.22	-	21,25,34,39	7
1	CME	D	2[A]	10/11	0.88	0.15	-	26,29,30,31	7
1	CME	B	2[A]	10/11	0.91	0.17	-	13,17,20,20	7
1	CME	B	2[B]	10/11	0.91	0.17	-	17,20,36,37	7
1	CME	E	2[B]	10/11	0.92	0.17	-	16,18,23,24	7
1	CME	C	2[A]	10/11	0.86	0.20	-	17,23,24,26	7

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	GOL	A	1117	6/6	0.77	0.33	7.52	37,40,45,47	0
2	GOL	A	1116	6/6	0.81	0.18	3.06	37,43,44,45	0
2	GOL	E	1117	6/6	0.81	0.16	2.75	28,42,46,46	0
2	GOL	B	1116	6/6	0.95	0.28	2.19	25,38,40,41	0
2	GOL	D	1116	6/6	0.88	0.15	1.83	30,39,40,46	0
2	GOL	C	1116	6/6	0.73	0.17	1.66	39,46,47,47	0
2	GOL	F	1116	6/6	0.75	0.14	1.47	44,53,53,55	0
2	GOL	B	1115	6/6	0.76	0.21	0.86	40,52,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.