Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:48 AM GMT

PDB ID	:	2BR4
Title	:	CMCI-D160 MG-SAM
Authors	:	Oster, L.M.; Lester, D.R.; Terwisscha Van Scheltinga, A.; Svenda, M.; Genereux, C.; Andersson, I.
Deposited on	:	2005-05-01
Resolution	:	2.59 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

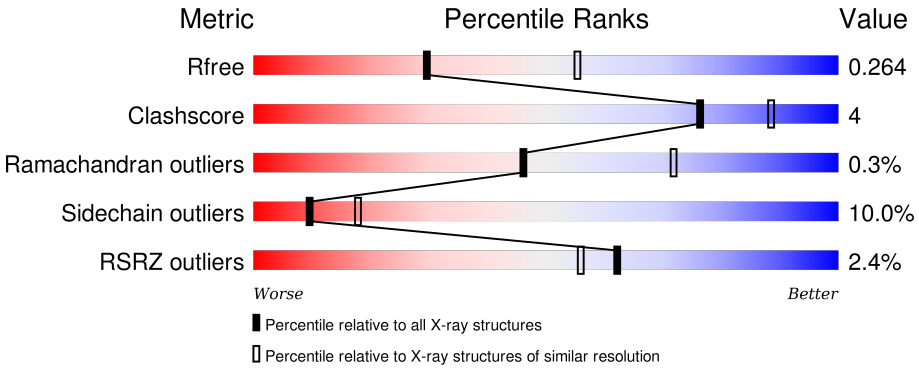
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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.



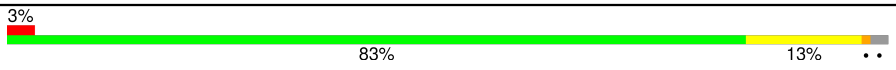
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	236	2% 77% 19%
1	B	236	% 80% 16%
1	C	236	% 78% 18%
1	D	236	2% 77% 19%
1	E	236	5% 80% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	236	

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	MG	D	300	-	-	-	X
3	SAM	A	301	-	-	-	X
3	SAM	B	301	-	-	-	X
3	SAM	E	301	-	-	-	X
3	SAM	F	301	-	-	-	X
5	P4C	D	500	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12075 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 CEPHALOSPORIN HYDROXYLASE CMCI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	1	0
			1912	1219	330	351	12			
1	B	232	Total	C	N	O	S	0	3	0
			1926	1227	331	356	12			
1	C	232	Total	C	N	O	S	0	2	0
			1923	1225	329	357	12			
1	D	230	Total	C	N	O	S	0	1	0
			1906	1214	327	353	12			
1	E	233	Total	C	N	O	S	0	2	0
			1930	1229	333	356	12			
1	F	231	Total	C	N	O	S	0	0	0
			1909	1217	328	352	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
B	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
C	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
D	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
E	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
F	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

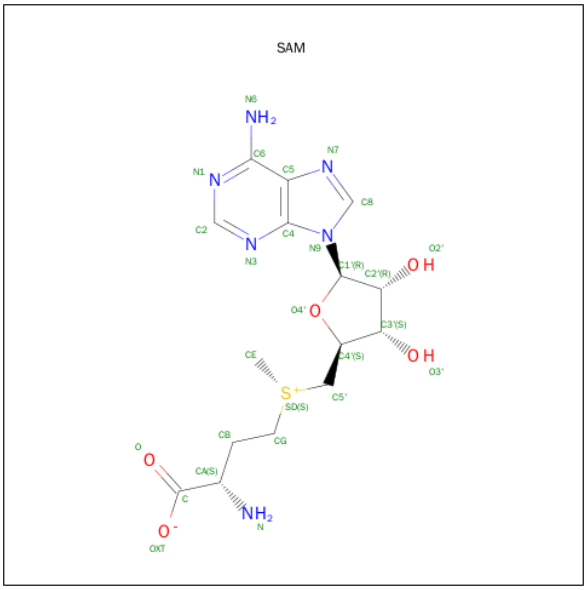
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

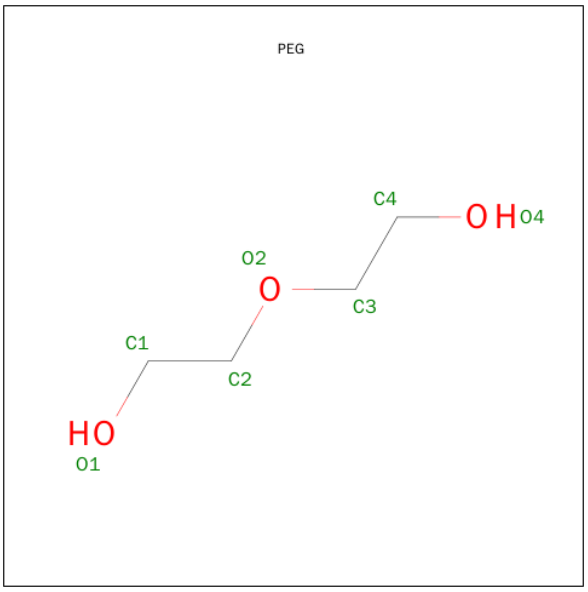
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



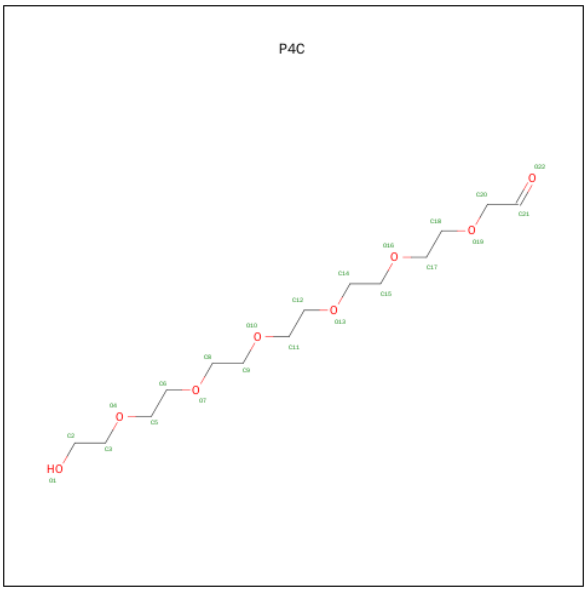
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 27 15 6 5 1	0	0
3	B	1	Total C N O S 27 15 6 5 1	0	0
3	C	1	Total C N O S 27 15 6 5 1	0	0
3	D	1	Total C N O S 26 15 6 4 1	0	0
3	E	1	Total C N O S 27 15 6 5 1	0	0
3	F	1	Total C N O S 27 15 6 5 1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0

- Molecule 5 is O-ACETALDEHYDYL-HEXAETHYLENE GLYCOL (three-letter code: P4C) (formula: $C_{14}H_{28}O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 22 14 8	0	0
5	B	1	Total C O 22 14 8	0	0
5	D	1	Total C O 22 14 8	0	0

- Molecule 6 is water.

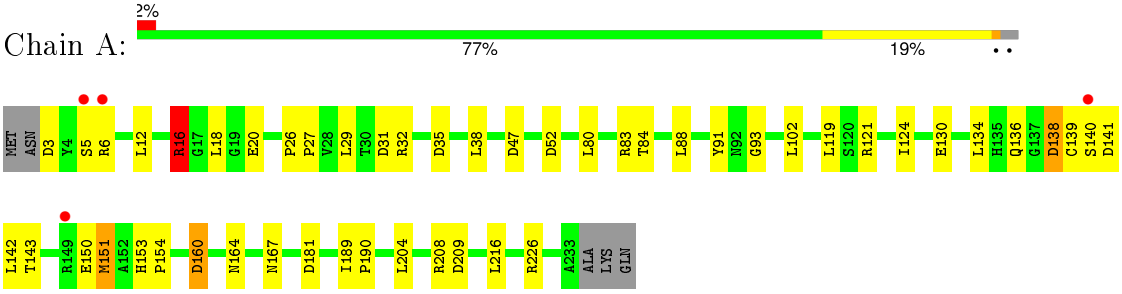
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	53	Total O 53 53	0	0
6	B	87	Total O 87 87	0	0
6	C	67	Total O 67 67	0	0
6	D	44	Total O 44 44	0	0
6	E	34	Total O 34 34	0	0
6	F	30	Total O 30 30	0	0

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.

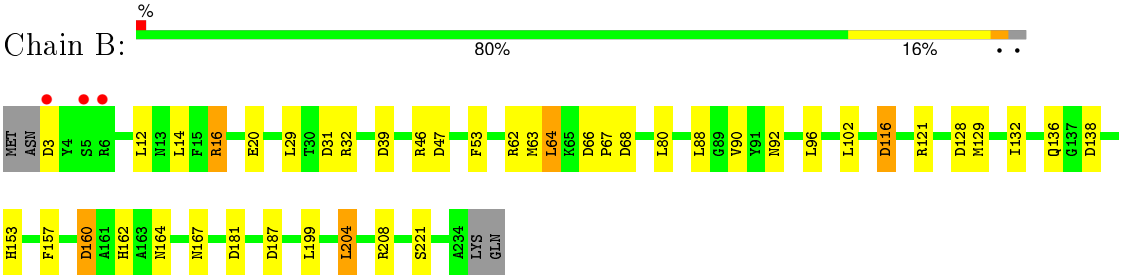
- Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain A:



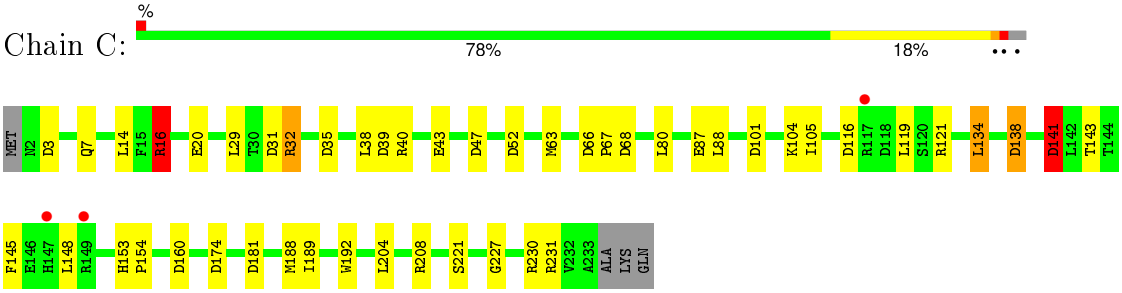
- Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain B:



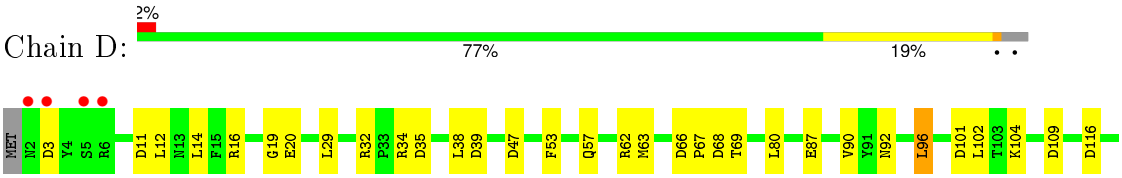
- Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain C:



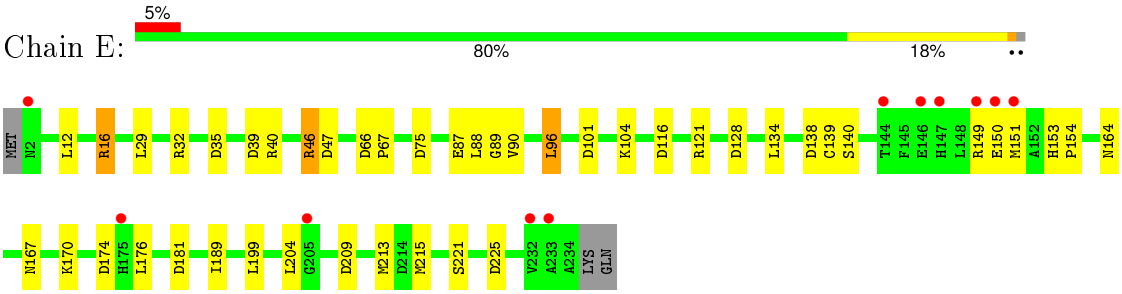
- Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain D:



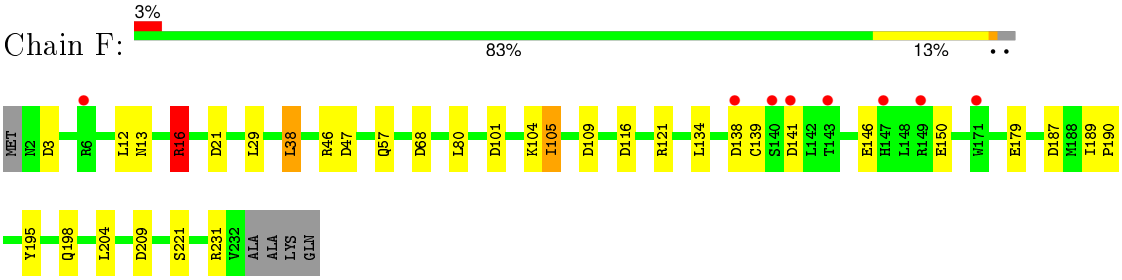
• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain E:



• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.54Å 102.36Å 181.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.30 – 2.59 51.18 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.6 (51.30-2.59) 99.6 (51.18-2.59)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.199 , 0.261 0.203 , 0.264	Depositor DCC
R_{free} test set	2700 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 53868 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12075	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: MG, PEG, P4C, SAM

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	0.41	0/1972	0.82	9/2681 (0.3%)
1	B	0.40	0/1993	0.82	12/2710 (0.4%)
1	C	0.40	0/1986	0.84	11/2701 (0.4%)
1	D	0.36	0/1965	0.82	10/2672 (0.4%)
1	E	0.37	0/1993	0.82	12/2710 (0.4%)
1	F	0.37	0/1964	0.80	12/2671 (0.4%)
All	All	0.39	0/11873	0.82	66/16145 (0.4%)

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	ASP	CB-CG-OD2	7.87	125.38	118.30
1	C	3	ASP	CB-CG-OD2	7.73	125.26	118.30
1	C	16	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	E	128	ASP	CB-CG-OD2	6.82	124.44	118.30
1	C	52	ASP	CB-CG-OD2	6.81	124.43	118.30
1	B	39	ASP	CB-CG-OD2	6.66	124.29	118.30
1	C	47	ASP	CB-CG-OD2	6.56	124.20	118.30
1	C	116	ASP	CB-CG-OD2	6.52	124.17	118.30
1	F	3	ASP	CB-CG-OD2	6.40	124.06	118.30
1	E	47	ASP	CB-CG-OD2	6.33	123.99	118.30
1	F	16	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	138	ASP	CB-CG-OD2	6.08	123.78	118.30
1	B	47	ASP	CB-CG-OD2	6.07	123.76	118.30
1	E	39	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	174	ASP	CB-CG-OD2	6.05	123.75	118.30
1	E	35	ASP	CB-CG-OD2	6.05	123.75	118.30
1	D	138	ASP	CB-CG-OD2	6.03	123.73	118.30
1	C	39	ASP	CB-CG-OD2	5.99	123.69	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	138	ASP	CB-CG-OD2	5.98	123.69	118.30
1	B	187	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	138	ASP	CB-CG-OD2	5.84	123.55	118.30
1	A	3	ASP	CB-CG-OD2	5.76	123.49	118.30
1	E	116	ASP	CB-CG-OD2	5.75	123.47	118.30
1	E	181	ASP	CB-CG-OD2	5.74	123.46	118.30
1	C	68	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	11	ASP	CB-CG-OD2	5.68	123.41	118.30
1	D	47	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	209	ASP	CB-CG-OD2	5.66	123.40	118.30
1	D	160	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	52	ASP	CB-CG-OD2	5.64	123.38	118.30
1	F	116	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	160	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	181	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	35	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	128[A]	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	128[B]	ASP	CB-CG-OD2	5.48	123.23	118.30
1	F	109	ASP	CB-CG-OD2	5.47	123.22	118.30
1	E	75	ASP	CB-CG-OD2	5.46	123.21	118.30
1	C	141	ASP	CB-CG-OD2	5.46	123.21	118.30
1	D	101	ASP	CB-CG-OD2	5.45	123.20	118.30
1	E	225	ASP	CB-CG-OD2	5.44	123.19	118.30
1	D	39	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	116	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	35	ASP	CB-CG-OD2	5.40	123.16	118.30
1	F	138	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	209	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	31	ASP	CB-CG-OD2	5.33	123.10	118.30
1	D	109	ASP	CB-CG-OD2	5.30	123.07	118.30
1	F	68	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	3	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	68[A]	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	68[B]	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	31	ASP	CB-CG-OD2	5.25	123.03	118.30
1	F	47	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	35	ASP	CB-CG-OD2	5.23	123.01	118.30
1	F	187	ASP	CB-CG-OD2	5.21	122.99	118.30
1	F	141	ASP	CB-CG-OD2	5.21	122.99	118.30
1	F	101	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	141	ASP	CB-CG-OD2	5.14	122.93	118.30
1	E	174	ASP	CB-CG-OD2	5.08	122.88	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	101	ASP	CB-CG-OD2	5.07	122.86	118.30
1	F	209	ASP	CB-CG-OD2	5.07	122.87	118.30
1	D	209	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	16	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	F	21	ASP	CB-CG-OD2	5.03	122.82	118.30
1	B	3	ASP	CB-CG-OD2	5.01	122.81	118.30

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	1912	0	1819	20	0
1	B	1926	0	1825	21	0
1	C	1923	0	1819	19	0
1	D	1906	0	1803	12	0
1	E	1930	0	1831	13	0
1	F	1909	0	1812	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	27	0	22	6	0
3	B	27	0	22	0	0
3	C	27	0	22	0	0
3	D	26	0	22	0	0
3	E	27	0	22	1	0
3	F	27	0	22	1	0
4	A	7	0	10	0	0
4	B	7	0	10	3	0
4	D	7	0	10	0	0
5	A	22	0	25	1	0
5	B	22	0	23	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	22	0	24	0	0
6	A	53	0	0	1	0
6	B	87	0	0	2	0
6	C	67	0	0	0	0
6	D	44	0	0	0	0
6	E	34	0	0	0	0
6	F	30	0	0	0	0
All	All	12075	0	11143	88	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 4.

All (88) 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:C:16:ARG:HH11	1:C:16:ARG:HG2	1.29	0.96
1:A:164:ASN:HD21	1:A:167:ASN:HD22	1.23	0.84
1:B:16[B]:ARG:HH11	1:B:16[B]:ARG:HG2	1.49	0.76
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.51	0.76
1:F:16:ARG:HH11	1:F:16:ARG:HG2	1.50	0.76
1:C:16:ARG:HH11	1:C:16:ARG:CG	2.00	0.75
1:C:16:ARG:NH1	1:C:16:ARG:HG2	2.04	0.69
1:E:88:LEU:HD22	1:E:139:CYS:SG	2.34	0.67
1:D:143:THR:HG22	1:D:147:HIS:CE1	2.32	0.65
5:B:500:P4C:H171	6:B:2086:HOH:O	1.95	0.65
1:E:164:ASN:HD21	1:E:167:ASN:ND2	1.95	0.64
1:B:164:ASN:HD21	1:B:167:ASN:HD22	1.44	0.64
1:B:16[A]:ARG:NH1	1:B:16[A]:ARG:HB3	2.13	0.63
1:A:91:TYR:HB2	3:A:301:SAM:CE	2.29	0.62
5:A:500:P4C:H32	6:A:2043:HOH:O	2.00	0.60
1:E:139:CYS:SG	3:E:301:SAM:C2	2.91	0.58
1:D:188:MET:HG2	1:D:192:TRP:CZ2	2.38	0.58
1:E:164:ASN:HD21	1:E:167:ASN:HD22	1.49	0.58
1:A:139:CYS:HG	3:A:301:SAM:C2	2.16	0.57
1:A:153:HIS:HD2	1:A:181:ASP:OD2	1.87	0.57
1:B:16[A]:ARG:HD3	4:B:401:PEG:C3	2.35	0.56
1:B:64:LEU:HD23	1:B:64:LEU:N	2.22	0.55
1:A:91:TYR:HB2	3:A:301:SAM:HE2	1.88	0.54
1:D:62:ARG:O	1:D:92:ASN:ND2	2.40	0.54
1:F:139:CYS:SG	3:F:301:SAM:C2	2.96	0.54
1:D:19:GLY:HA2	1:F:195:TYR:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16[A]:ARG:HH22	5:B:500:P4C:H151	1.73	0.53
1:A:18:LEU:CD2	3:A:301:SAM:HE3	2.39	0.52
1:B:16[B]:ARG:HH11	1:B:16[B]:ARG:CG	2.22	0.52
1:B:153:HIS:HD2	1:B:181:ASP:OD2	1.93	0.52
1:F:16:ARG:HH11	1:F:16:ARG:CG	2.23	0.52
1:B:16[A]:ARG:HD3	4:B:401:PEG:H31	1.92	0.51
5:B:500:P4C:H152	1:C:16:ARG:NH2	2.26	0.51
1:D:192:TRP:HE1	1:F:13:ASN:ND2	2.09	0.51
1:C:31:ASP:C	1:C:32:ARG:HG3	2.31	0.51
1:A:91:TYR:HB2	3:A:301:SAM:HE1	1.93	0.50
1:C:138:ASP:HB3	1:C:141:ASP:OD2	2.11	0.50
1:A:88:LEU:HD22	1:A:139:CYS:SG	2.51	0.50
1:C:101:ASP:O	1:C:105:ILE:HG12	2.13	0.49
1:E:90:VAL:HG13	1:E:96:LEU:HD22	1.95	0.48
1:C:16:ARG:NH1	1:C:16:ARG:CG	2.66	0.48
1:C:204:LEU:HD22	1:F:38:LEU:HG	1.96	0.47
1:E:16[B]:ARG:HG2	1:E:16[B]:ARG:HH11	1.80	0.47
1:A:226:ARG:HD3	1:B:46:ARG:HD2	1.96	0.46
1:B:162:HIS:ND1	6:B:2058:HOH:O	2.36	0.46
1:D:90:VAL:HG13	1:D:96:LEU:HD22	1.98	0.46
1:C:88:LEU:HD21	1:C:145:PHE:CE2	2.51	0.46
1:D:66:ASP:HB2	1:D:67:PRO:CD	2.46	0.46
1:A:119:LEU:H	1:A:136:GLN:HE21	1.62	0.46
1:B:90:VAL:HG13	1:B:96:LEU:HD22	1.99	0.45
1:B:129:MET:HE2	1:B:132:ILE:HD12	1.98	0.45
1:E:213:MET:HG2	1:E:215:MET:CE	2.46	0.45
1:C:153:HIS:HA	1:C:154:PRO:C	2.37	0.45
1:E:153:HIS:HE1	1:E:176:LEU:O	2.00	0.45
1:A:189:ILE:HB	1:A:190:PRO:HD3	2.00	0.43
1:C:188:MET:HG2	1:C:192:TRP:CZ2	2.53	0.43
1:E:66:ASP:HB2	1:E:67:PRO:CD	2.49	0.43
1:D:167:ASN:HA	1:D:167:ASN:HD22	1.66	0.43
1:F:189:ILE:HB	1:F:190:PRO:HD3	2.01	0.43
1:A:160:ASP:HB3	3:A:301:SAM:HG1	2.01	0.43
1:D:68[A]:ASP:OD1	1:D:69:THR:N	2.52	0.43
1:E:153:HIS:HB3	1:E:154:PRO:HA	2.00	0.42
1:D:143:THR:CG2	1:D:147:HIS:CE1	3.00	0.42
1:B:116:ASP:O	1:B:136:GLN:HA	2.20	0.42
1:E:16[A]:ARG:HH11	1:E:16[A]:ARG:HB3	1.84	0.42
1:C:66:ASP:HB2	1:C:67:PRO:HD2	2.01	0.42
1:C:88:LEU:HD21	1:C:145:PHE:HE2	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HD13	1:B:204:LEU:HD22	2.02	0.42
1:B:88:LEU:HD11	1:B:157:PHE:CZ	2.55	0.42
1:A:84:THR:HG21	1:A:151:MET:HG3	2.01	0.41
1:E:153:HIS:HA	1:E:154:PRO:C	2.41	0.41
1:C:189:ILE:HD12	1:C:227:GLY:HA2	2.01	0.41
1:B:66:ASP:HB2	1:B:67:PRO:CD	2.51	0.41
1:F:16:ARG:NH1	1:F:16:ARG:CG	2.83	0.41
1:A:93:GLY:O	1:A:124:ILE:HD11	2.20	0.41
1:A:16:ARG:NH1	1:A:16:ARG:HG2	2.23	0.41
1:A:153:HIS:HA	1:A:154:PRO:C	2.41	0.41
1:C:105:ILE:HD11	1:F:105:ILE:HG21	2.03	0.41
1:D:116:ASP:O	1:D:136:GLN:HA	2.20	0.41
1:A:164:ASN:ND2	1:A:167:ASN:HD22	2.03	0.41
1:B:62:ARG:O	1:B:92:ASN:ND2	2.46	0.41
1:C:119:LEU:HD22	1:C:134:LEU:HG	2.03	0.40
1:B:199:LEU:HB2	1:C:20[A]:GLU:OE1	2.20	0.40
1:B:16[A]:ARG:CZ	1:B:16[A]:ARG:HB3	2.51	0.40
1:B:16[A]:ARG:HD3	4:B:401:PEG:H32	2.02	0.40
1:C:188:MET:HG3	1:C:192:TRP:CE2	2.56	0.40
1:A:26:PRO:HA	1:A:27:PRO:HD3	2.00	0.40
1:D:226:ARG:HD3	1:E:46:ARG:HD3	2.03	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	230/236 (98%)	218 (95%)	11 (5%)	1 (0%)	39 65
1	B	233/236 (99%)	225 (97%)	7 (3%)	1 (0%)	39 65
1	C	232/236 (98%)	226 (97%)	6 (3%)	0	100 100
1	D	229/236 (97%)	218 (95%)	10 (4%)	1 (0%)	39 65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	233/236 (99%)	226 (97%)	6 (3%)	1 (0%)	39 65
1	F	229/236 (97%)	217 (95%)	12 (5%)	0	100 100
All	All	1386/1416 (98%)	1330 (96%)	52 (4%)	4 (0%)	46 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	SER
1	E	89	GLY
1	D	53	PHE
1	B	53	PHE

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	204/207 (99%)	182 (89%)	22 (11%)	8 15
1	B	206/207 (100%)	190 (92%)	16 (8%)	16 30
1	C	206/207 (100%)	183 (89%)	23 (11%)	7 13
1	D	204/207 (99%)	180 (88%)	24 (12%)	6 12
1	E	206/207 (100%)	185 (90%)	21 (10%)	9 17
1	F	204/207 (99%)	186 (91%)	18 (9%)	12 24
All	All	1230/1242 (99%)	1106 (90%)	124 (10%)	9 17

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	6	ARG
1	A	12	LEU
1	A	16	ARG
1	A	20	GLU
1	A	29	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	32	ARG
1	A	80	LEU
1	A	83	ARG
1	A	102	LEU
1	A	121	ARG
1	A	130	GLU
1	A	134	LEU
1	A	138	ASP
1	A	142	LEU
1	A	143	THR
1	A	150	GLU
1	A	151	MET
1	A	160	ASP
1	A	204	LEU
1	A	208	ARG
1	A	216	LEU
1	B	12	LEU
1	B	14	LEU
1	B	16[A]	ARG
1	B	16[B]	ARG
1	B	20	GLU
1	B	29	LEU
1	B	32	ARG
1	B	63	MET
1	B	64	LEU
1	B	80	LEU
1	B	102	LEU
1	B	121	ARG
1	B	160	ASP
1	B	204	LEU
1	B	208	ARG
1	B	221	SER
1	C	7	GLN
1	C	14	LEU
1	C	16	ARG
1	C	29	LEU
1	C	32	ARG
1	C	38	LEU
1	C	40	ARG
1	C	43	GLU
1	C	63	MET
1	C	80	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	87	GLU
1	C	104	LYS
1	C	121	ARG
1	C	134	LEU
1	C	138	ASP
1	C	141	ASP
1	C	143	THR
1	C	148	LEU
1	C	160	ASP
1	C	208	ARG
1	C	221	SER
1	C	230	ARG
1	C	231	ARG
1	D	12	LEU
1	D	14	LEU
1	D	16	ARG
1	D	20	GLU
1	D	29	LEU
1	D	32	ARG
1	D	34	ARG
1	D	38	LEU
1	D	57	GLN
1	D	63	MET
1	D	80	LEU
1	D	87	GLU
1	D	96	LEU
1	D	102	LEU
1	D	104	LYS
1	D	121	ARG
1	D	127	SER
1	D	140	SER
1	D	141	ASP
1	D	160	ASP
1	D	179	GLU
1	D	188	MET
1	D	204	LEU
1	D	208	ARG
1	E	12	LEU
1	E	16[A]	ARG
1	E	16[B]	ARG
1	E	29	LEU
1	E	32	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	40	ARG
1	E	46	ARG
1	E	87	GLU
1	E	96	LEU
1	E	104	LYS
1	E	121	ARG
1	E	134	LEU
1	E	140	SER
1	E	149	ARG
1	E	150	GLU
1	E	151	MET
1	E	170	LYS
1	E	189	ILE
1	E	199	LEU
1	E	204	LEU
1	E	221	SER
1	F	12	LEU
1	F	16	ARG
1	F	29	LEU
1	F	38	LEU
1	F	46	ARG
1	F	57	GLN
1	F	80	LEU
1	F	104	LYS
1	F	105	ILE
1	F	121	ARG
1	F	134	LEU
1	F	146	GLU
1	F	150	GLU
1	F	179	GLU
1	F	198	GLN
1	F	204	LEU
1	F	221	SER
1	F	231	ARG

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	111	GLN
1	A	131	ASN
1	A	136	GLN
1	A	153	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	162	HIS
1	A	164	ASN
1	A	198	GLN
1	B	153	HIS
1	B	164	ASN
1	C	25	HIS
1	C	74	HIS
1	C	162	HIS
1	D	147	HIS
1	D	167	ASN
1	E	8	ASN
1	E	111	GLN
1	E	131	ASN
1	E	164	ASN
1	E	175	HIS
1	F	13	ASN
1	F	25	HIS
1	F	131	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SAM	A	301	-	21,29,29	1.08	2 (9%)	17,42,42	3.19	3 (17%)
4	PEG	A	401	-	6,6,6	0.43	0	5,5,5	0.19	0
5	P4C	A	500	-	21,21,21	1.56	3 (14%)	19,20,20	3.27	4 (21%)
3	SAM	B	301	-	21,29,29	1.11	2 (9%)	17,42,42	3.19	3 (17%)
4	PEG	B	401	-	6,6,6	0.39	0	5,5,5	0.37	0
5	P4C	B	500	2	21,21,21	1.60	3 (14%)	19,20,20	3.54	3 (15%)
3	SAM	C	301	-	21,29,29	1.11	2 (9%)	17,42,42	3.21	2 (11%)
3	SAM	D	301	-	22,28,29	1.08	2 (9%)	18,40,42	3.13	2 (11%)
4	PEG	D	401	-	6,6,6	0.42	0	5,5,5	0.24	0
5	P4C	D	500	-	21,21,21	1.57	3 (14%)	19,20,20	3.59	5 (26%)
3	SAM	E	301	-	21,29,29	1.12	2 (9%)	17,42,42	3.13	3 (17%)
3	SAM	F	301	-	21,29,29	1.16	2 (9%)	17,42,42	3.05	1 (5%)

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	SAM	A	301	-	-	0/8/33/33	0/3/3/3
4	PEG	A	401	-	-	0/4/4/4	0/0/0/0
5	P4C	A	500	-	-	0/18/19/19	0/0/0/0
3	SAM	B	301	-	-	0/8/33/33	0/3/3/3
4	PEG	B	401	-	-	0/4/4/4	0/0/0/0
5	P4C	B	500	2	-	0/18/19/19	0/0/0/0
3	SAM	C	301	-	-	0/8/33/33	0/3/3/3
3	SAM	D	301	-	-	0/8/31/33	0/3/3/3
4	PEG	D	401	-	-	0/4/4/4	0/0/0/0
5	P4C	D	500	-	-	0/18/19/19	0/0/0/0
3	SAM	E	301	-	-	0/8/33/33	0/3/3/3
3	SAM	F	301	-	-	0/8/33/33	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	500	P4C	C20-C21	-5.36	1.19	1.47
5	A	500	P4C	C20-C21	-5.36	1.19	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	P4C	C20-C21	-5.35	1.19	1.47
5	A	500	P4C	C3-C2	-3.04	1.32	1.49
5	B	500	P4C	C3-C2	-2.97	1.32	1.49
5	D	500	P4C	C3-C2	-2.85	1.33	1.49
5	B	500	P4C	O19-C20	-2.80	1.33	1.42
5	D	500	P4C	O19-C20	-2.73	1.33	1.42
5	A	500	P4C	O19-C20	-2.63	1.34	1.42
3	D	301	SAM	C2-N1	2.17	1.38	1.33
3	B	301	SAM	C2-N1	2.26	1.38	1.33
3	C	301	SAM	C2-N1	2.31	1.38	1.33
3	A	301	SAM	C2-N1	2.32	1.38	1.33
3	E	301	SAM	C2-N1	2.35	1.38	1.33
3	F	301	SAM	C2-N1	2.52	1.38	1.33
3	B	301	SAM	C2-N3	3.37	1.38	1.32
3	A	301	SAM	C2-N3	3.38	1.38	1.32
3	D	301	SAM	C2-N3	3.38	1.38	1.32
3	C	301	SAM	C2-N3	3.40	1.38	1.32
3	E	301	SAM	C2-N3	3.44	1.38	1.32
3	F	301	SAM	C2-N3	3.61	1.38	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	301	SAM	N3-C2-N1	-12.57	119.27	128.89
3	C	301	SAM	N3-C2-N1	-12.48	119.34	128.89
3	B	301	SAM	N3-C2-N1	-12.40	119.40	128.89
3	A	301	SAM	N3-C2-N1	-12.34	119.45	128.89
3	E	301	SAM	N3-C2-N1	-11.99	119.71	128.89
3	F	301	SAM	N3-C2-N1	-11.96	119.74	128.89
3	C	301	SAM	C1'-N9-C4	-2.88	122.60	126.94
3	A	301	SAM	C1'-N9-C4	-2.58	123.05	126.94
3	B	301	SAM	C1'-N9-C4	-2.37	123.36	126.94
3	E	301	SAM	C1'-N9-C4	-2.22	123.59	126.94
3	D	301	SAM	O4'-C1'-N9	2.03	112.35	108.10
3	B	301	SAM	O4'-C1'-N9	2.03	112.36	108.10
3	A	301	SAM	O4'-C1'-N9	2.04	112.36	108.10
5	D	500	P4C	C5-O4-C3	2.12	122.44	113.31
5	A	500	P4C	C5-O4-C3	2.38	123.54	113.31
5	D	500	P4C	O1-C2-C3	2.45	127.19	112.03
5	A	500	P4C	O1-C2-C3	2.53	127.67	112.03
5	A	500	P4C	C20-O19-C18	2.59	120.76	112.37
5	D	500	P4C	O4-C3-C2	2.67	122.72	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	301	SAM	O4'-C1'-N9	2.72	113.78	108.10
5	D	500	P4C	C20-O19-C18	3.07	122.31	112.37
5	B	500	P4C	O1-C2-C3	3.09	131.08	112.03
5	B	500	P4C	C20-O19-C18	3.43	123.47	112.37
5	A	500	P4C	O19-C20-C21	13.42	168.30	109.04
5	B	500	P4C	O19-C20-C21	14.53	173.24	109.04
5	D	500	P4C	O19-C20-C21	14.70	173.96	109.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	SAM	6	0
5	A	500	P4C	1	0
4	B	401	PEG	3	0
5	B	500	P4C	3	0
3	E	301	SAM	1	0
3	F	301	SAM	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	231/236 (97%)	-0.11	4 (1%)	73 68	16, 25, 54, 64	0
1	B	232/236 (98%)	-0.13	3 (1%)	79 75	16, 23, 42, 70	0
1	C	232/236 (98%)	-0.05	3 (1%)	79 75	17, 25, 44, 49	0
1	D	230/236 (97%)	-0.02	4 (1%)	73 68	19, 26, 39, 82	0
1	E	233/236 (98%)	0.17	11 (4%)	35 28	18, 27, 55, 68	0
1	F	231/236 (97%)	0.17	8 (3%)	48 40	19, 27, 50, 59	0
All	All	1389/1416 (98%)	0.01	33 (2%)	62 56	16, 26, 48, 82	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	SER	4.9
1	C	149	ARG	4.1
1	F	149	ARG	4.1
1	F	147	HIS	3.8
1	A	149	ARG	3.7
1	F	140	SER	3.6
1	E	146	GLU	3.6
1	E	147	HIS	3.6
1	D	3	ASP	3.5
1	D	2	ASN	3.2
1	B	6	ARG	3.2
1	E	149	ARG	3.2
1	D	6	ARG	3.1
1	D	5	SER	3.0
1	E	150	GLU	3.0
1	E	151	MET	3.0
1	E	2	ASN	2.5
1	F	143	THR	2.4
1	C	117	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	6	ARG	2.4
1	E	144	THR	2.3
1	E	175	HIS	2.3
1	C	147	HIS	2.2
1	F	6	ARG	2.2
1	E	232	VAL	2.2
1	E	205	GLY	2.2
1	E	233	ALA	2.2
1	F	141	ASP	2.1
1	F	138	ASP	2.1
1	A	5	SER	2.1
1	A	140	SER	2.1
1	B	3	ASP	2.1
1	F	171	TRP	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	MG	D	300	1/1	0.49	0.43	11.98	79,79,79,79	0
3	SAM	A	301	27/27	0.76	0.38	5.20	87,90,91,91	0
3	SAM	E	301	27/27	0.83	0.27	3.43	89,91,91,91	0
5	P4C	D	500	22/22	0.83	0.22	3.05	72,73,77,78	0
3	SAM	B	301	27/27	0.87	0.22	2.64	60,63,67,68	0
3	SAM	F	301	27/27	0.80	0.32	2.04	90,92,92,93	0
2	MG	C	300	1/1	0.92	0.20	1.81	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	P4C	B	500	22/22	0.90	0.23	1.49	59,61,67,69	0
3	SAM	D	301	26/27	0.87	0.20	1.44	68,73,77,77	0
3	SAM	C	301	27/27	0.87	0.23	1.33	74,78,81,82	0
4	PEG	A	401	7/7	0.92	0.24	1.14	55,55,56,56	0
5	P4C	A	500	22/22	0.89	0.22	1.13	68,71,72,72	0
4	PEG	B	401	7/7	0.90	0.22	0.85	50,51,51,52	0
2	MG	A	300	1/1	0.60	0.26	-	95,95,95,95	0
2	MG	F	300	1/1	0.75	0.22	-	91,91,91,91	0
2	MG	B	300	1/1	0.75	0.19	-	53,53,53,53	0
2	MG	E	300	1/1	0.05	0.47	-	93,93,93,93	0
4	PEG	D	401	7/7	0.89	0.24	-	74,74,75,75	0

6.5 Other polymers

There are no such residues in this entry.