Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:00 PM GMT

PDB ID	:	1RO7
Title	:	Structural analysis of the sialyltransferase CstII from Campylobacter jejuni in complex with a substrate analogue, CMP-3FNeuAc.
Authors	:	Chiu, C.P.; Watts, A.G.; Lairson, L.L.; Gilbert, M.; Lim, D.; Wakarchuk, W.W.; Withers, S.G.; Strynadka, N.C.
Deposited on	:	2003-12-01
Resolution	:	1.80 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:

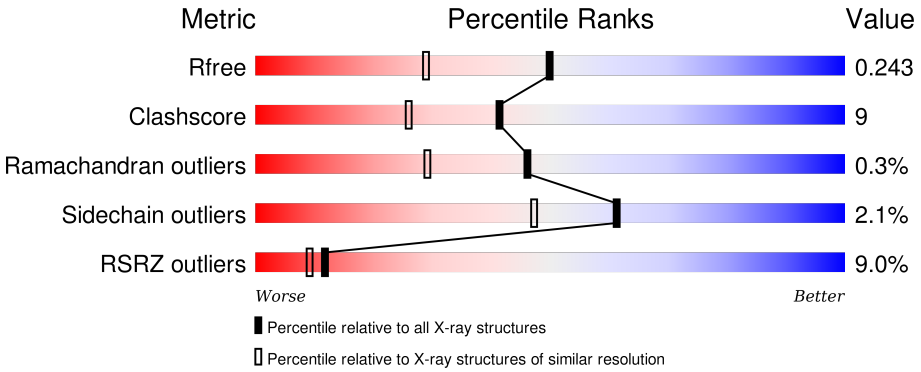
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	259	13% 82% 17% •
1	B	259	6% 72% 17% • 8%
1	C	259	8% 78% 13% • 6%
1	D	259	6% 81% 10% • 8%

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	CSF	C	1001	X	-	-	-
2	CSF	C	2001	X	-	-	-
2	CSF	C	3001	X	-	-	-
2	CSF	C	4001	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8668 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.

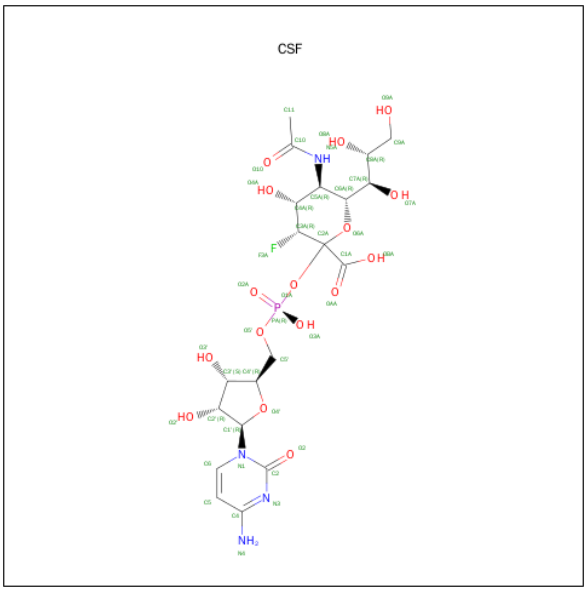
- Molecule 1 is a protein called alpha-2,3/8-sialyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	Se	0	0	0
			2155	1410	340	396	6	3			
1	B	237	Total	C	N	O	S	Se	0	0	0
			1985	1305	311	360	6	3			
1	C	243	Total	C	N	O	S	Se	0	0	0
			2032	1335	317	371	6	3			
1	D	238	Total	C	N	O	S	Se	0	0	0
			1990	1309	311	361	6	3			

There are 16 discrepancies between the modelled and reference sequences:

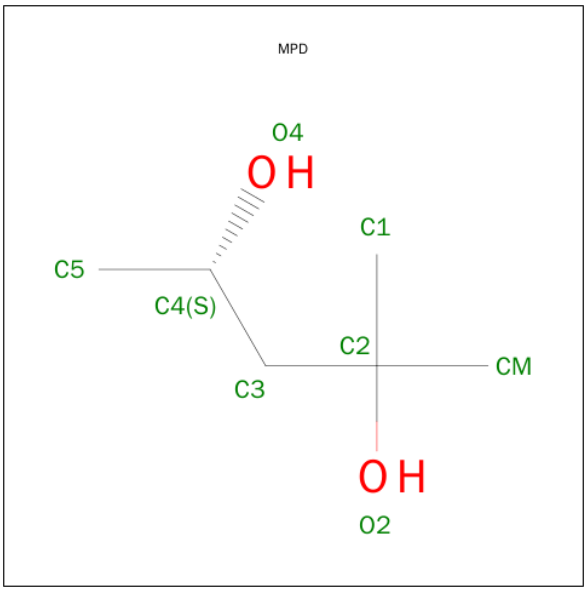
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LAK3
A	53	SER	ILE	ENGINEERED	UNP Q9LAK3
A	77	MSE	MET	MODIFIED RESIDUE	UNP Q9LAK3
A	136	MSE	MET	MODIFIED RESIDUE	UNP Q9LAK3
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LAK3
B	53	SER	ILE	ENGINEERED	UNP Q9LAK3
B	77	MSE	MET	MODIFIED RESIDUE	UNP Q9LAK3
B	136	MSE	MET	MODIFIED RESIDUE	UNP Q9LAK3
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LAK3
C	53	SER	ILE	ENGINEERED	UNP Q9LAK3
C	77	MSE	MET	MODIFIED RESIDUE	UNP Q9LAK3
C	136	MSE	MET	MODIFIED RESIDUE	UNP Q9LAK3
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LAK3
D	53	SER	ILE	ENGINEERED	UNP Q9LAK3
D	77	MSE	MET	MODIFIED RESIDUE	UNP Q9LAK3
D	136	MSE	MET	MODIFIED RESIDUE	UNP Q9LAK3

- Molecule 2 is CYTIDINE-5'-MONOPHOSPHATE-3-FLUORO-N-ACETYL-NEURAMINIC ACID (three-letter code: CSF) (formula: $C_{20}H_{30}FN_4O_{16}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	4	Total	C	F	N	O	P	0	0
			168	80	4	16	64	4		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is water.

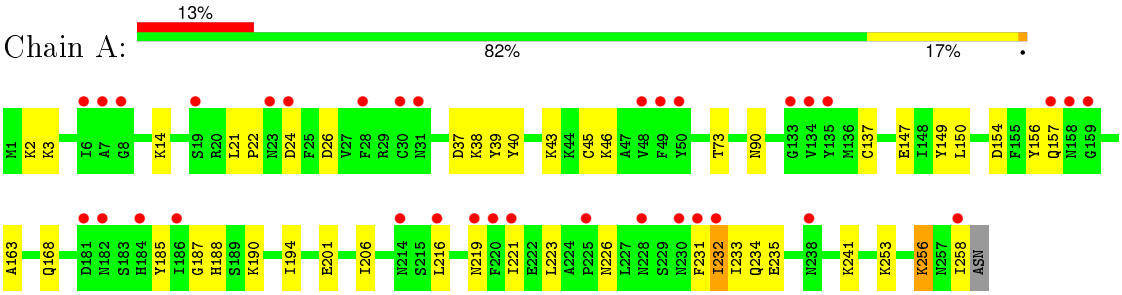
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	89	Total O 89 89	0	0
4	B	85	Total O 85 85	0	0
4	C	83	Total O 83 83	0	0
4	D	73	Total O 73 73	0	0

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.

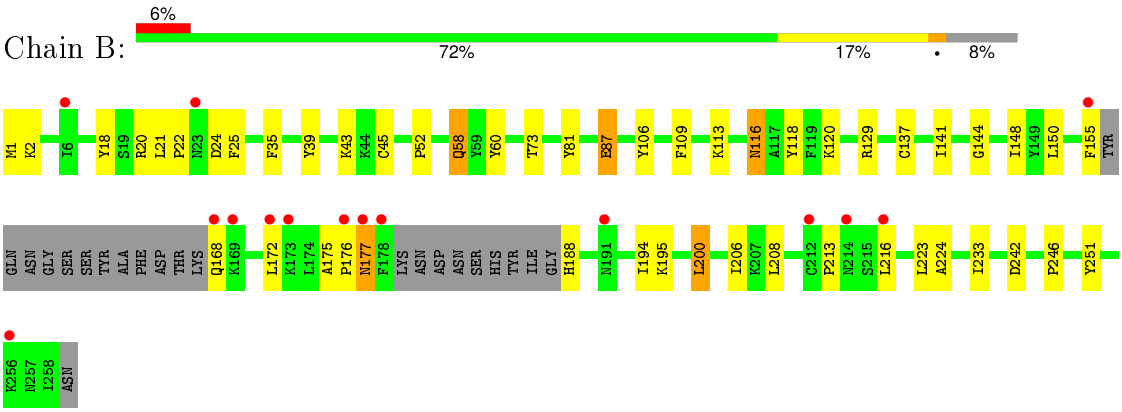
- Molecule 1: alpha-2,3/8-sialyltransferase

Chain A:



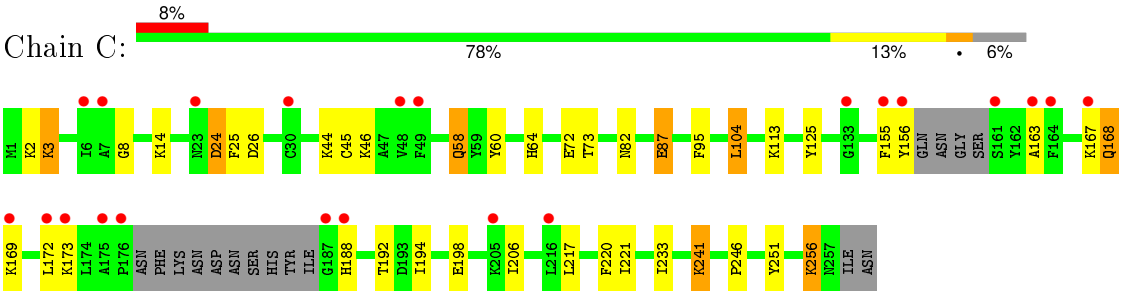
- Molecule 1: alpha-2,3/8-sialyltransferase

Chain B:



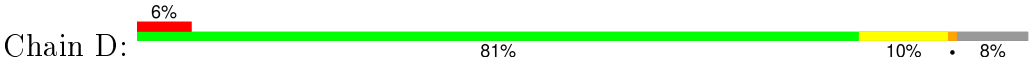
- Molecule 1: alpha-2,3/8-sialyltransferase

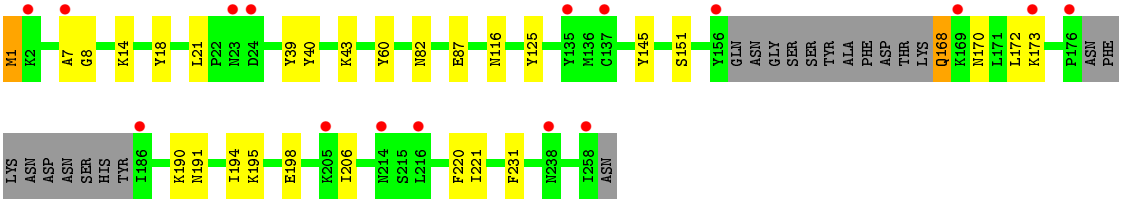
Chain C:



- Molecule 1: alpha-2,3/8-sialyltransferase

Chain D:




M1 K2 A7 G8 K14 Y18 L21 P22 N23 D24 Y39 Y40 K43 Y60 N82 E87 N116 Y125 Y135 M136 C137 Y145 S151 Y156 GLN ASN GLY SER SER TYR ALA PHE ASP THR LYS Q168 K169 N170 L171 L172 K173 P176 ASN PHE
LYS ASN ASP ASN SER HIS TYR I186 K190 N191 I194 K195 E198 K205 I206 N214 S215 L216 F220 I221 F231 N238 I258 ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.66Å 66.03Å 99.17Å 90.00° 94.42° 90.00°	Depositor
Resolution (Å)	29.64 – 1.80 29.63 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.64-1.80) 99.6 (29.63-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.248 0.214 , 0.243	Depositor DCC
R_{free} test set	5034 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 99667 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8668	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: MPD, CSF

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	0.35	0/2213	0.54	0/2982
1	B	0.36	0/2036	0.55	0/2740
1	C	0.36	0/2085	0.54	1/2806 (0.0%)
1	D	0.36	0/2041	0.54	1/2747 (0.0%)
All	All	0.36	0/8375	0.54	2/11275 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	8	GLY	N-CA-C	-5.21	100.07	113.10
1	C	8	GLY	N-CA-C	-5.18	100.16	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2155	0	2087	41	0
1	B	1985	0	1938	40	0
1	C	2032	0	1976	38	0
1	D	1990	0	1946	22	0
2	C	168	0	112	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	14	0	0
4	A	89	0	0	0	0
4	B	85	0	0	0	0
4	C	83	0	0	3	0
4	D	73	0	0	0	0
All	All	8668	0	8073	140	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 9.

All (140) 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:256:LYS:H	1:C:256:LYS:HD2	1.40	0.86
1:C:44:LYS:HD2	1:C:72:GLU:HG3	1.62	0.82
1:C:14:LYS:HG3	1:C:163:ALA:HB1	1.62	0.81
1:D:168:GLN:HE21	1:D:168:GLN:N	1.82	0.76
1:A:154:ASP:HB3	1:A:157:GLN:HE21	1.51	0.75
1:C:14:LYS:HD2	1:C:163:ALA:O	1.87	0.74
1:B:1:MSE:HG3	1:B:144:GLY:O	1.89	0.73
1:C:246:PRO:HG2	1:C:251:TYR:CE1	2.25	0.71
1:A:256:LYS:NZ	1:A:256:LYS:H	1.88	0.70
1:A:14:LYS:HG3	1:A:163:ALA:HB1	1.73	0.69
1:C:194:ILE:O	1:C:198:GLU:HG3	1.93	0.69
1:B:118:TYR:OH	1:B:195:LYS:HG2	1.94	0.68
1:A:185:TYR:HB3	1:A:188:HIS:CD2	2.29	0.67
1:D:170:ASN:O	1:D:173:LYS:HG2	1.96	0.66
1:A:233:ILE:HD12	1:A:233:ILE:N	2.10	0.65
1:D:194:ILE:O	1:D:198:GLU:HG3	1.96	0.65
1:D:168:GLN:O	1:D:172:LEU:HD23	1.97	0.65
1:D:168:GLN:NE2	1:D:168:GLN:N	2.44	0.64
1:D:221:ILE:HD12	1:D:221:ILE:N	2.14	0.62
1:B:129:ARG:HH21	1:B:188:HIS:HE1	1.47	0.62
1:B:58:GLN:HA	1:B:58:GLN:HE21	1.66	0.61
1:C:188:HIS:O	1:C:192:THR:HB	2.00	0.61
1:C:155:PHE:CZ	1:C:194:ILE:HD11	2.35	0.61
1:A:2:LYS:HG2	1:A:24:ASP:OD2	2.01	0.60
1:D:14:LYS:HG2	1:D:40:TYR:CZ	2.36	0.60
1:A:256:LYS:HD2	1:A:256:LYS:H	1.64	0.60
1:A:190:LYS:HE2	1:A:216:LEU:HD21	1.82	0.60
1:C:256:LYS:CD	1:C:256:LYS:H	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:TYR:CE2	1:D:43:LYS:HG2	2.38	0.59
1:A:231:PHE:O	1:A:232:ILE:HB	2.03	0.58
1:C:58:GLN:HA	1:C:58:GLN:HE21	1.68	0.58
1:A:256:LYS:HZ3	1:A:256:LYS:H	1.51	0.58
1:C:241:LYS:HD3	4:C:4084:HOH:O	2.04	0.57
1:B:81:TYR:N	1:B:87:GLU:OE1	2.35	0.57
1:C:188:HIS:HA	4:C:4048:HOH:O	2.04	0.57
1:B:155:PHE:CZ	1:B:194:ILE:HD11	2.40	0.57
1:D:1:MSE:HB2	1:D:145:TYR:CE1	2.39	0.56
1:A:256:LYS:CD	1:A:256:LYS:H	2.19	0.56
1:B:18:TYR:CE2	1:B:233:ILE:HD11	2.39	0.56
1:B:35:PHE:CE2	1:B:168:GLN:HG2	2.40	0.56
1:A:216:LEU:HD12	1:A:219:ASN:HD22	1.71	0.55
1:A:37:ASP:OD2	1:A:38:LYS:HG3	2.07	0.55
1:A:258:ILE:HG13	1:A:258:ILE:O	2.06	0.54
1:A:253:LYS:O	1:A:256:LYS:HE2	2.07	0.54
1:B:52:PRO:HG2	1:B:87:GLU:HG2	1.89	0.53
1:C:44:LYS:CD	1:C:72:GLU:HG3	2.38	0.53
1:B:206:ILE:C	1:B:206:ILE:HD12	2.29	0.53
2:C:3001:CSF:O3A	2:C:3001:CSF:H3'	2.09	0.52
1:D:170:ASN:HA	1:D:173:LYS:HE3	1.91	0.52
1:B:113:LYS:HB3	1:B:113:LYS:HZ3	1.75	0.52
1:D:190:LYS:O	1:D:194:ILE:HG12	2.10	0.52
1:C:221:ILE:HD12	1:C:221:ILE:N	2.24	0.52
1:B:129:ARG:HH21	1:B:188:HIS:CE1	2.27	0.52
1:B:137:CYS:SG	1:B:150:LEU:HD21	2.50	0.52
1:C:241:LYS:HG2	1:C:241:LYS:O	2.10	0.51
1:D:191:ASN:HB3	1:D:195:LYS:NZ	2.24	0.51
1:B:2:LYS:HE2	1:B:25:PHE:C	2.30	0.51
1:B:206:ILE:O	1:B:206:ILE:HD12	2.11	0.51
1:A:39:TYR:CE2	1:A:43:LYS:HG2	2.45	0.51
1:A:206:ILE:C	1:A:206:ILE:HD12	2.31	0.51
1:C:2:LYS:HE3	1:C:24:ASP:OD1	2.10	0.51
1:A:256:LYS:HD2	1:A:256:LYS:N	2.26	0.50
1:D:220:PHE:HB2	1:D:221:ILE:HD12	1.93	0.50
1:A:14:LYS:HG2	1:A:40:TYR:CZ	2.46	0.50
1:A:21:LEU:HD12	1:A:22:PRO:HD2	1.94	0.50
1:A:233:ILE:HD12	1:A:233:ILE:H	1.74	0.50
1:A:256:LYS:NZ	1:A:256:LYS:N	2.59	0.50
1:C:2:LYS:HE2	1:C:25:PHE:C	2.32	0.50
1:A:201:GLU:HG3	1:A:206:ILE:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TYR:CE1	1:A:187:GLY:HA3	2.47	0.49
1:A:45:CYS:O	1:A:73:THR:HA	2.12	0.49
1:B:2:LYS:HE3	1:B:24:ASP:CG	2.32	0.49
1:C:156:TYR:OH	2:C:3001:CSF:H3A	2.13	0.49
1:C:156:TYR:HA	2:C:3001:CSF:H41	1.77	0.49
1:B:60:TYR:HB2	1:D:125:TYR:CE2	2.46	0.49
1:C:256:LYS:N	1:C:256:LYS:HD2	2.19	0.48
1:B:216:LEU:N	1:B:216:LEU:HD22	2.29	0.48
1:A:156:TYR:HA	2:C:1001:CSF:H41	1.77	0.48
1:D:206:ILE:HD12	1:D:206:ILE:C	2.33	0.47
1:C:168:GLN:O	1:C:172:LEU:HG	2.13	0.47
1:B:113:LYS:HB3	1:B:113:LYS:NZ	2.29	0.47
1:A:190:LYS:O	1:A:194:ILE:HG12	2.15	0.47
1:B:216:LEU:H	1:B:216:LEU:HD22	1.80	0.46
1:A:3:LYS:HE3	1:A:147:GLU:OE1	2.16	0.46
1:B:116:ASN:HD21	1:B:120:LYS:NZ	2.14	0.46
1:B:246:PRO:HG2	1:B:251:TYR:CE2	2.51	0.45
1:A:43:LYS:HE3	1:A:234:GLN:OE1	2.16	0.45
1:D:21:LEU:HD12	1:D:231:PHE:HB2	1.99	0.45
1:B:1:MSE:HA	1:B:1:MSE:HE2	1.98	0.45
1:A:216:LEU:HD12	1:A:219:ASN:ND2	2.32	0.45
1:B:21:LEU:HD12	1:B:22:PRO:HD2	1.99	0.45
1:D:190:LYS:HD3	1:D:220:PHE:CE2	2.52	0.45
1:B:168:GLN:HB3	1:B:242:ASP:OD2	2.17	0.45
1:A:221:ILE:N	1:A:221:ILE:HD12	2.32	0.45
1:B:141:ILE:HD12	1:B:200:LEU:HG	1.98	0.44
1:A:26:ASP:HB3	1:A:46:LYS:HB2	2.00	0.44
1:A:3:LYS:HD3	1:A:149:TYR:CE2	2.53	0.44
1:B:148:ILE:HB	1:B:208:LEU:HD23	1.99	0.44
1:C:217:LEU:CD1	1:C:221:ILE:HD13	2.48	0.44
1:C:60:TYR:CE2	1:C:64:HIS:HE1	2.36	0.43
1:B:39:TYR:CZ	1:B:43:LYS:HG2	2.53	0.43
1:D:7:ALA:HA	1:D:151:SER:O	2.18	0.43
1:B:168:GLN:O	1:B:172:LEU:HG	2.17	0.43
1:A:137:CYS:SG	1:A:150:LEU:HD21	2.59	0.43
1:A:223:LEU:N	1:A:223:LEU:HD12	2.33	0.43
1:C:95:PHE:CG	1:C:104:LEU:HD13	2.53	0.43
1:C:206:ILE:C	1:C:206:ILE:HD12	2.39	0.43
1:C:168:GLN:HE21	1:C:241:LYS:NZ	2.16	0.43
1:C:95:PHE:CD2	1:C:104:LEU:HD13	2.52	0.43
1:B:106:TYR:HA	1:B:109:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LYS:H	1:C:3:LYS:HD2	1.84	0.43
1:B:45:CYS:O	1:B:73:THR:HA	2.18	0.43
1:C:82:ASN:N	1:C:87:GLU:OE1	2.52	0.42
1:C:45:CYS:O	1:C:73:THR:HA	2.19	0.42
1:B:177:ASN:C	1:B:177:ASN:ND2	2.72	0.42
1:B:2:LYS:HE2	1:B:25:PHE:O	2.18	0.42
1:C:113:LYS:HD2	4:C:4028:HOH:O	2.19	0.42
1:B:113:LYS:CB	1:B:113:LYS:NZ	2.83	0.42
1:B:213:PRO:HB3	1:B:223:LEU:HD21	2.02	0.42
1:A:39:TYR:CZ	1:A:43:LYS:HG2	2.54	0.42
1:B:216:LEU:H	1:B:216:LEU:CD2	2.33	0.41
1:A:190:LYS:HE2	1:A:216:LEU:CD2	2.49	0.41
1:A:156:TYR:HA	2:C:1001:CSF:N4	2.36	0.41
1:A:168:GLN:HG3	1:A:241:LYS:O	2.20	0.41
1:C:220:PHE:HB2	1:C:221:ILE:HD12	2.03	0.41
1:A:43:LYS:CE	1:A:234:GLN:HE22	2.34	0.41
1:C:104:LEU:HA	1:C:104:LEU:HD12	1.87	0.41
1:C:125:TYR:CE2	1:D:60:TYR:HB2	2.55	0.41
1:C:26:ASP:HB3	1:C:46:LYS:HB2	2.03	0.41
1:D:82:ASN:N	1:D:87:GLU:OE2	2.48	0.41
1:B:177:ASN:C	1:B:177:ASN:HD22	2.23	0.41
1:A:201:GLU:HA	1:A:206:ILE:CD1	2.51	0.41
1:B:20:ARG:HD3	1:B:224:ALA:O	2.21	0.41
1:D:39:TYR:CZ	1:D:43:LYS:HG2	2.56	0.40
1:C:233:ILE:HD12	1:C:233:ILE:N	2.36	0.40
1:C:168:GLN:HG2	1:C:241:LYS:O	2.22	0.40
1:B:35:PHE:CZ	1:B:168:GLN:HG2	2.57	0.40
1:D:18:TYR:HD2	1:D:21:LEU:HD11	1.85	0.40
1:B:175:ALA:HA	1:B:176:PRO:HD2	1.96	0.40
1:C:169:LYS:O	1:C:173:LYS:HG3	2.21	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	256/259 (99%)	239 (93%)	15 (6%)	2 (1%)	24 8
1	B	231/259 (89%)	225 (97%)	6 (3%)	0	100 100
1	C	237/259 (92%)	229 (97%)	7 (3%)	1 (0%)	39 23
1	D	232/259 (90%)	225 (97%)	7 (3%)	0	100 100
All	All	956/1036 (92%)	918 (96%)	35 (4%)	3 (0%)	46 29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	24	ASP
1	A	226	ASN
1	A	232	ILE

5.3.2 Protein sidechains

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	234/232 (101%)	231 (99%)	3 (1%)	76 68
1	B	216/232 (93%)	211 (98%)	5 (2%)	58 42
1	C	220/232 (95%)	212 (96%)	8 (4%)	42 24
1	D	216/232 (93%)	213 (99%)	3 (1%)	74 65
All	All	886/928 (96%)	867 (98%)	19 (2%)	61 47

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	235	GLU
1	A	256	LYS
1	B	58	GLN
1	B	87	GLU

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Mol	Chain	Res	Type
1	B	116	ASN
1	B	177	ASN
1	B	200	LEU
1	C	3	LYS
1	C	58	GLN
1	C	87	GLU
1	C	104	LEU
1	C	167	LYS
1	C	168	GLN
1	C	241	LYS
1	C	256	LYS
1	D	1	MSE
1	D	116	ASN
1	D	168	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	69	GLN
1	A	128	GLN
1	A	157	GLN
1	A	158	ASN
1	A	177	ASN
1	A	180	ASN
1	A	219	ASN
1	A	228	ASN
1	A	257	ASN
1	B	51	ASN
1	B	58	GLN
1	B	111	GLN
1	B	116	ASN
1	B	128	GLN
1	B	177	ASN
1	B	188	HIS
1	C	32	GLN
1	C	58	GLN
1	C	67	GLN
1	C	90	ASN
1	C	128	GLN
1	C	168	GLN
1	C	228	ASN

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Mol	Chain	Res	Type
1	C	234	GLN
1	D	83	GLN
1	D	116	ASN
1	D	128	GLN
1	D	188	HIS
1	D	219	ASN
1	D	238	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

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MPD	B	401	-	6,7,7	0.42	0	7,10,10	0.46	0
2	CSF	C	1001	-	34,44,44	2.32	8 (23%)	41,67,67	2.22	11 (26%)
2	CSF	C	2001	-	34,44,44	2.43	8 (23%)	41,67,67	2.40	12 (29%)
2	CSF	C	3001	-	34,44,44	2.40	8 (23%)	41,67,67	2.48	15 (36%)
2	CSF	C	4001	-	34,44,44	2.51	9 (26%)	41,67,67	2.32	12 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	B	401	-	-	0/5/5/5	0/0/0/0
2	CSF	C	1001	-	1/1/14/15	0/23/75/75	0/3/3/3
2	CSF	C	2001	-	1/1/14/15	0/23/75/75	0/3/3/3
2	CSF	C	3001	-	1/1/14/15	0/23/75/75	0/3/3/3
2	CSF	C	4001	-	1/1/14/15	0/23/75/75	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3001	CSF	PA-O3A	-3.98	1.38	1.54
2	C	4001	CSF	PA-O3A	-3.84	1.38	1.54
2	C	2001	CSF	PA-O3A	-3.78	1.38	1.54
2	C	1001	CSF	PA-O3A	-3.33	1.40	1.54
2	C	2001	CSF	F3A-C3A	-2.20	1.36	1.39
2	C	1001	CSF	C5A-N5A	-2.12	1.42	1.45
2	C	4001	CSF	C5A-N5A	-2.11	1.42	1.45
2	C	3001	CSF	PA-O1A	2.10	1.66	1.60
2	C	1001	CSF	O6A-C2A	2.20	1.45	1.41
2	C	3001	CSF	C6A-C5A	2.22	1.56	1.53
2	C	4001	CSF	C6A-C5A	2.45	1.57	1.53
2	C	4001	CSF	O6A-C2A	2.68	1.46	1.41
2	C	2001	CSF	C6A-C5A	2.72	1.57	1.53
2	C	4001	CSF	C4-N3	3.09	1.41	1.35
2	C	1001	CSF	C4-N3	3.21	1.41	1.35
2	C	2001	CSF	O4'-C1'	3.27	1.45	1.41
2	C	1001	CSF	O4'-C1'	3.28	1.45	1.41
2	C	3001	CSF	C4-N3	3.37	1.41	1.35
2	C	2001	CSF	C4-N3	3.42	1.41	1.35
2	C	3001	CSF	O4'-C1'	3.99	1.46	1.41
2	C	4001	CSF	O4'-C1'	4.33	1.46	1.41
2	C	3001	CSF	C5-C4	4.97	1.52	1.40
2	C	1001	CSF	C5-C4	5.11	1.52	1.40
2	C	2001	CSF	C5-C4	5.14	1.52	1.40
2	C	1001	CSF	C3A-C4A	5.38	1.58	1.52
2	C	4001	CSF	C5-C4	5.47	1.53	1.40
2	C	4001	CSF	C3A-C4A	5.86	1.58	1.52
2	C	3001	CSF	C3A-C4A	5.93	1.58	1.52
2	C	2001	CSF	C3A-C4A	6.12	1.58	1.52
2	C	1001	CSF	C6-N1	7.65	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3001	CSF	C6-N1	7.66	1.46	1.35
2	C	2001	CSF	C6-N1	7.80	1.46	1.35
2	C	4001	CSF	C6-N1	8.07	1.47	1.35

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2001	CSF	O6A-C6A-C7A	-6.19	97.89	107.26
2	C	3001	CSF	O6A-C6A-C7A	-6.10	98.03	107.26
2	C	1001	CSF	O6A-C6A-C7A	-5.67	98.68	107.26
2	C	4001	CSF	O6A-C6A-C7A	-5.44	99.03	107.26
2	C	2001	CSF	O8A-C8A-C9A	-2.80	102.68	109.22
2	C	4001	CSF	O8A-C8A-C9A	-2.72	102.88	109.22
2	C	3001	CSF	C4A-C5A-C6A	-2.71	104.99	110.35
2	C	3001	CSF	O8A-C8A-C9A	-2.66	103.00	109.22
2	C	1001	CSF	O8A-C8A-C9A	-2.60	103.16	109.22
2	C	2001	CSF	O5'-PA-O2A	-2.48	100.01	109.62
2	C	2001	CSF	C4A-C5A-C6A	-2.43	105.54	110.35
2	C	4001	CSF	O5'-PA-O2A	-2.41	100.27	109.62
2	C	1001	CSF	C6A-C5A-N5A	-2.39	106.91	111.07
2	C	4001	CSF	C4A-C5A-C6A	-2.37	105.66	110.35
2	C	1001	CSF	O5'-PA-O2A	-2.33	100.58	109.62
2	C	4001	CSF	O4A-C4A-C5A	-2.16	105.25	109.66
2	C	3001	CSF	O5'-PA-O2A	-2.16	101.23	109.62
2	C	1001	CSF	O4A-C4A-C5A	-2.11	105.37	109.66
2	C	2001	CSF	C6A-C5A-N5A	-2.09	107.42	111.07
2	C	4001	CSF	C6A-C5A-N5A	-2.05	107.50	111.07
2	C	3001	CSF	O3A-PA-O2A	-2.04	101.47	112.53
2	C	3001	CSF	C6A-C5A-N5A	-2.02	107.54	111.07
2	C	3001	CSF	O4A-C4A-C5A	-2.00	105.57	109.66
2	C	2001	CSF	C5A-N5A-C10	2.15	128.62	123.10
2	C	4001	CSF	C4A-C5A-N5A	2.28	115.39	110.66
2	C	1001	CSF	C5A-N5A-C10	2.30	129.00	123.10
2	C	3001	CSF	O1A-PA-O2A	2.35	118.70	109.46
2	C	4001	CSF	C5A-N5A-C10	2.37	129.18	123.10
2	C	3001	CSF	C4A-C5A-N5A	2.44	115.72	110.66
2	C	3001	CSF	C5A-N5A-C10	2.45	129.39	123.10
2	C	2001	CSF	F3A-C3A-C4A	2.45	110.26	108.52
2	C	2001	CSF	C4A-C5A-N5A	2.62	116.09	110.66
2	C	1001	CSF	C4A-C5A-N5A	2.71	116.28	110.66
2	C	3001	CSF	C8A-C7A-C6A	3.60	120.25	113.01
2	C	2001	CSF	C8A-C7A-C6A	3.93	120.91	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1001	CSF	C7A-C6A-C5A	4.12	120.56	114.32
2	C	1001	CSF	C8A-C7A-C6A	4.12	121.30	113.01
2	C	4001	CSF	C8A-C7A-C6A	4.14	121.32	113.01
2	C	3001	CSF	O5'-C5'-C4'	4.15	124.43	109.12
2	C	2001	CSF	C2-N3-C4	4.51	121.97	115.61
2	C	3001	CSF	C2-N3-C4	4.57	122.06	115.61
2	C	1001	CSF	C2-N3-C4	4.58	122.07	115.61
2	C	4001	CSF	C2-N3-C4	4.78	122.36	115.61
2	C	4001	CSF	C7A-C6A-C5A	5.22	122.22	114.32
2	C	2001	CSF	C7A-C6A-C5A	5.37	122.46	114.32
2	C	3001	CSF	C7A-C6A-C5A	5.74	123.02	114.32
2	C	1001	CSF	C2A-O6A-C6A	7.28	125.06	114.36
2	C	4001	CSF	C2A-O6A-C6A	7.50	125.38	114.36
2	C	3001	CSF	C2A-O6A-C6A	7.64	125.59	114.36
2	C	2001	CSF	C2A-O6A-C6A	7.65	125.59	114.36

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1001	CSF	C2A
2	C	3001	CSF	C2A
2	C	2001	CSF	C2A
2	C	4001	CSF	C2A

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	CSF	2	0
2	C	3001	CSF	3	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	255/259 (98%)	0.64	34 (13%)	4 3	17, 34, 63, 77	0
1	B	234/259 (90%)	0.37	15 (6%)	23 18	18, 29, 51, 63	0
1	C	240/259 (92%)	0.42	22 (9%)	11 8	21, 30, 56, 73	0
1	D	235/259 (90%)	0.42	16 (6%)	20 16	20, 32, 53, 65	0
All	All	964/1036 (93%)	0.47	87 (9%)	12 9	17, 31, 57, 77	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	156	TYR	7.5
1	B	178	PHE	7.2
1	C	187	GLY	6.6
1	D	186	ILE	5.6
1	B	23	ASN	5.6
1	A	158	ASN	5.6
1	B	176	PRO	5.2
1	A	230	ASN	5.1
1	A	23	ASN	5.0
1	B	172	LEU	4.9
1	A	6	ILE	4.9
1	C	188	HIS	4.8
1	C	164	PHE	4.1
1	A	184	HIS	4.0
1	C	163	ALA	4.0
1	A	228	ASN	4.0
1	A	24	ASP	3.9
1	B	177	ASN	3.9
1	A	30	CYS	3.6
1	A	49	PHE	3.5
1	D	23	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	169	LYS	3.5
1	A	232	ILE	3.4
1	A	258	ILE	3.4
1	D	214	ASN	3.4
1	A	159	GLY	3.4
1	A	219	ASN	3.4
1	D	238	ASN	3.3
1	A	231	PHE	3.2
1	D	2	LYS	3.2
1	A	220	PHE	3.2
1	B	169	LYS	3.2
1	C	173	LYS	3.1
1	A	28	PHE	3.1
1	D	176	PRO	3.1
1	C	156	TYR	3.0
1	B	214	ASN	2.9
1	A	7	ALA	2.9
1	A	48	VAL	2.9
1	A	238	ASN	2.9
1	C	161	SER	2.9
1	C	48	VAL	2.8
1	B	212	CYS	2.8
1	B	168	GLN	2.8
1	C	167	LYS	2.8
1	C	172	LEU	2.7
1	B	216	LEU	2.7
1	D	137	CYS	2.7
1	D	216	LEU	2.7
1	C	6	ILE	2.6
1	A	19	SER	2.6
1	A	157	GLN	2.6
1	C	23	ASN	2.5
1	B	256	LYS	2.5
1	D	169	LYS	2.5
1	C	155	PHE	2.5
1	D	24	ASP	2.5
1	D	258	ILE	2.4
1	A	133	GLY	2.4
1	A	135	TYR	2.4
1	C	49	PHE	2.4
1	A	186	ILE	2.4
1	A	181	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	6	ILE	2.4
1	C	30	CYS	2.4
1	B	191	ASN	2.3
1	C	216	LEU	2.3
1	A	214	ASN	2.3
1	C	133	GLY	2.3
1	D	7	ALA	2.3
1	A	221	ILE	2.3
1	A	182	ASN	2.3
1	B	173	LYS	2.3
1	C	175	ALA	2.2
1	C	176	PRO	2.2
1	A	216	LEU	2.2
1	D	173	LYS	2.2
1	C	7	ALA	2.2
1	C	205	LYS	2.2
1	D	205	LYS	2.2
1	A	50	TYR	2.1
1	B	155	PHE	2.1
1	A	31	ASN	2.1
1	A	8	GLY	2.1
1	A	225	PRO	2.1
1	A	134	VAL	2.1
1	D	135	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MPD	B	401	8/8	0.82	0.17	1.61	40,46,47,48	0
2	CSF	C	2001	42/42	0.80	0.20	0.66	39,49,60,61	0
2	CSF	C	3001	42/42	0.81	0.18	0.16	36,43,48,49	0
2	CSF	C	4001	42/42	0.87	0.15	0.04	37,41,45,49	0
2	CSF	C	1001	42/42	0.91	0.14	-0.34	21,29,37,40	0

6.5 Other polymers (i)

There are no such residues in this entry.