Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:35 PM GMT

PDB ID	:	5AJI
Title	:	MscS D67R1 high resolution
Authors	:	Naismith, J.H.; Pliotas, C.
Deposited on	:	2015-02-24
Resolution	:	2.99 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:

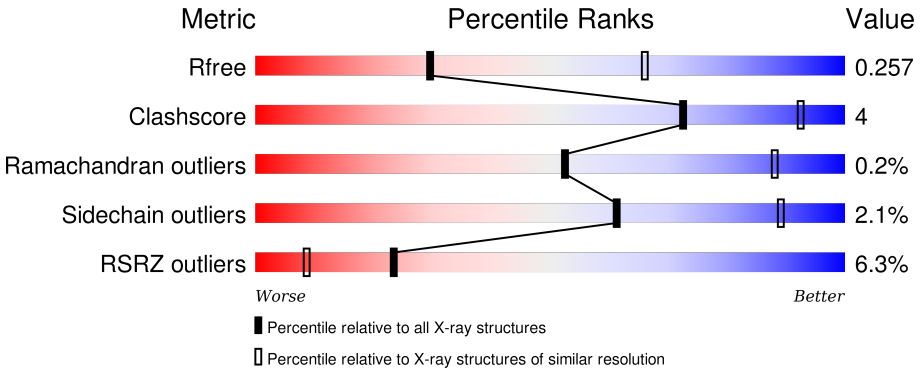
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.99 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	286	6% 82% 10% 8%
1	B	286	5% 80% 8% 11%
1	C	286	3% 77% 11% 11%
1	D	286	3% 81% 10% 8%
1	E	286	7% 82% 9% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	286	7% 79% 9% • 10%
1	G	286	8% 76% 12% 11%

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
3	HEX	A	501	-	-	-	X
3	HEX	B	500	-	-	-	X
3	HEX	C	500	-	-	-	X
3	HEX	C	501	-	-	-	X
3	HEX	D	501	-	-	-	X
3	HEX	E	500	-	-	-	X
3	HEX	E	501	-	-	-	X
3	HEX	F	500	-	-	-	X
3	HEX	F	501	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13963 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.

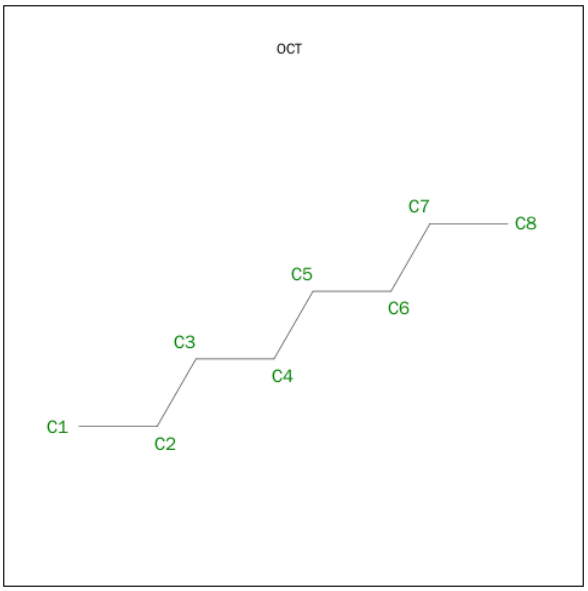
- Molecule 1 is a protein called SMALL-CONDUCTANCE MECHANOSENSITIVE CHANNEL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2022	1300	353	361	8			
1	B	255	Total	C	N	O	S	0	0	0
			1956	1257	341	350	8			
1	C	255	Total	C	N	O	S	0	0	0
			1956	1257	341	350	8			
1	D	263	Total	C	N	O	S	0	0	0
			2014	1295	351	360	8			
1	E	262	Total	C	N	O	S	0	0	0
			2003	1289	347	359	8			
1	F	256	Total	C	N	O	S	0	0	0
			1963	1262	342	351	8			
1	G	254	Total	C	N	O	S	0	0	0
			1945	1251	337	349	8			

There are 7 discrepancies between the modelled and reference sequences:

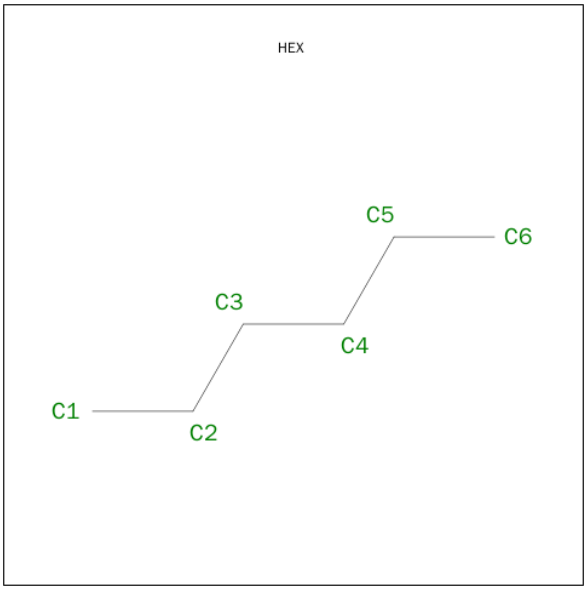
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	R1A	ASP	ENGINEERED MUTATION	UNP P0C0S2
B	67	R1A	ASP	ENGINEERED MUTATION	UNP P0C0S2
C	67	R1A	ASP	ENGINEERED MUTATION	UNP P0C0S2
D	67	R1A	ASP	ENGINEERED MUTATION	UNP P0C0S2
E	67	R1A	ASP	ENGINEERED MUTATION	UNP P0C0S2
F	67	R1A	ASP	ENGINEERED MUTATION	UNP P0C0S2
G	67	R1A	ASP	ENGINEERED MUTATION	UNP P0C0S2

- Molecule 2 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 8 8	0	0
2	E	1	Total C 8 8	0	0

- Molecule 3 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



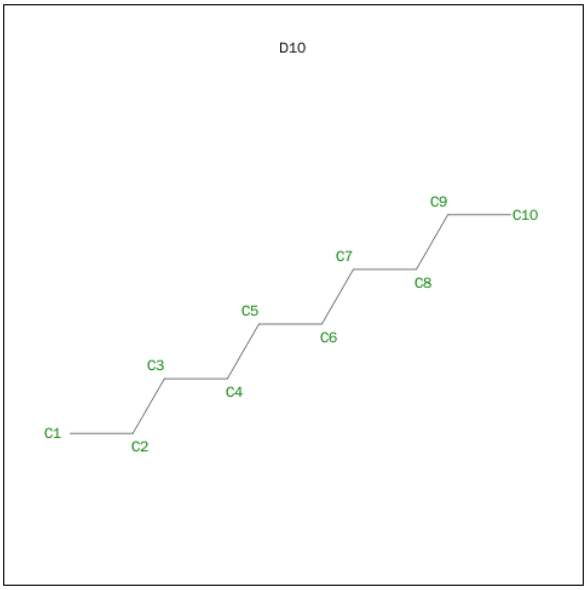
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 6 6	0	0
3	B	1	Total C 6 6	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 4 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



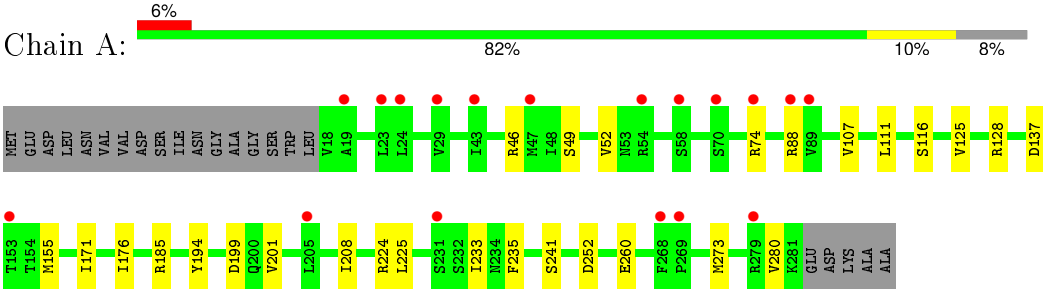
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C 8 8	0	0
4	D	1	Total C 10 10	0	0
4	G	1	Total C 10 10	0	0

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.

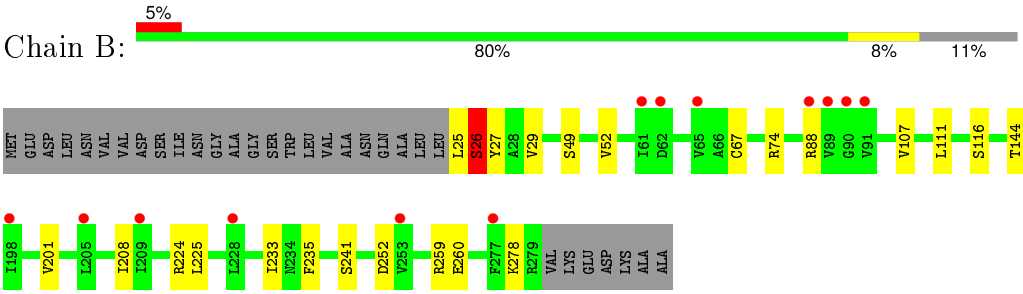
- Molecule 1: SMALL-CONDUCTANCE MECHANOSENSITIVE CHANNEL

Chain A:



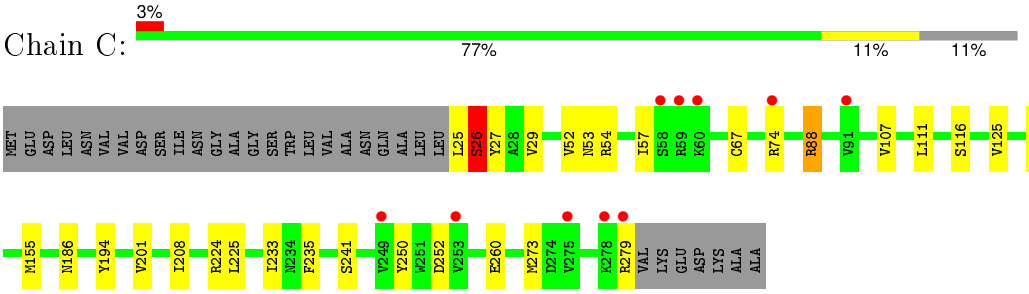
- Molecule 1: SMALL-CONDUCTANCE MECHANOSENSITIVE CHANNEL

Chain B:



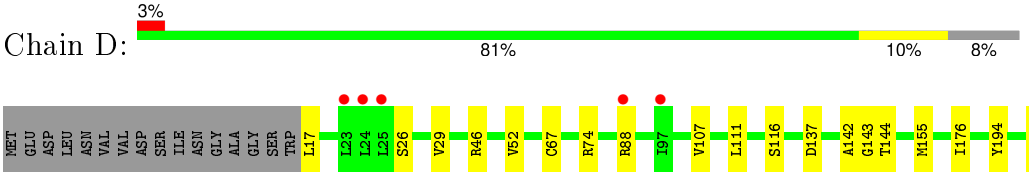
- Molecule 1: SMALL-CONDUCTANCE MECHANOSENSITIVE CHANNEL

Chain C:



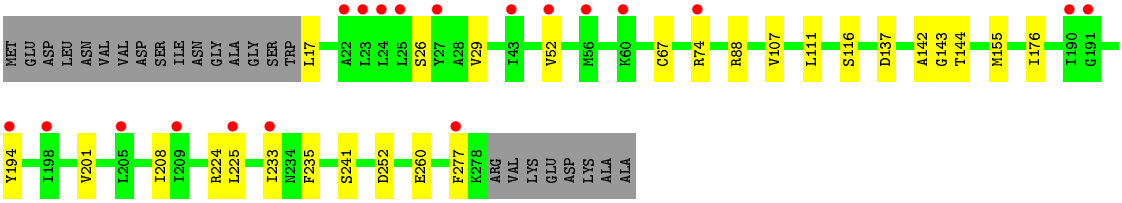
- Molecule 1: SMALL-CONDUCTANCE MECHANOSENSITIVE CHANNEL

Chain D:



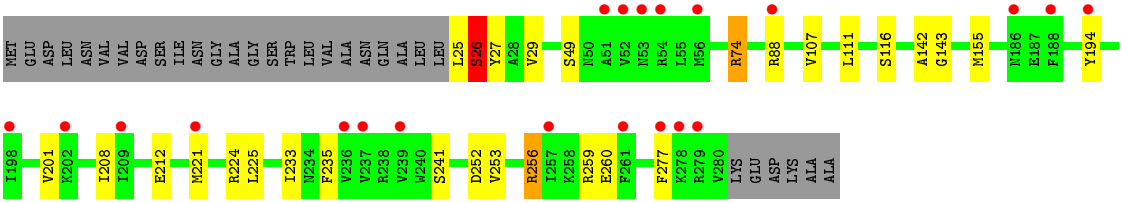
• Molecule 1: SMALL-CONDUCTANCE MECHANOSENSITIVE CHANNEL

Chain E:



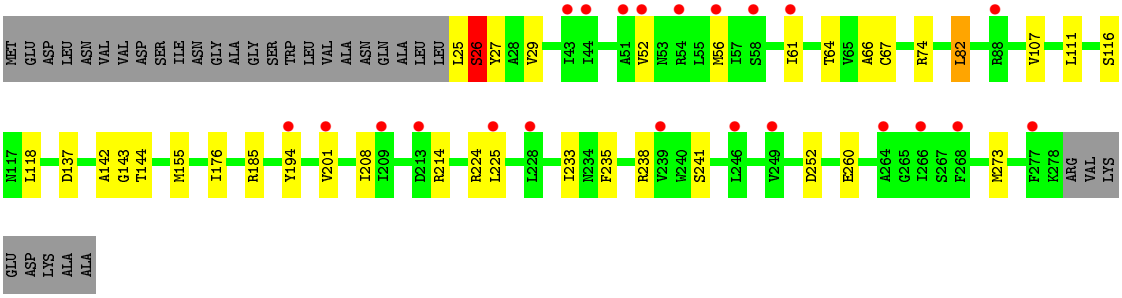
• Molecule 1: SMALL-CONDUCTANCE MECHANOSENSITIVE CHANNEL

Chain F:



• Molecule 1: SMALL-CONDUCTANCE MECHANOSENSITIVE CHANNEL

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	126.33Å 149.09Å 173.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.51 – 2.99 68.51 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (68.51-2.99) 99.6 (68.51-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.244 , 0.263 0.243 , 0.257	Depositor DCC
R_{free} test set	3401 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	90.8	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 63.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 66748 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13963	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: D10, HEX, OCT, R1A

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	0.39	0/2028	0.62	2/2748 (0.1%)
1	B	0.39	0/1962	0.58	0/2658
1	C	0.38	0/1962	0.61	1/2658 (0.0%)
1	D	0.41	1/2020 (0.0%)	0.61	1/2738 (0.0%)
1	E	0.39	0/2009	0.57	0/2724
1	F	0.41	0/1969	0.67	4/2668 (0.1%)
1	G	0.37	0/1951	0.65	4/2644 (0.2%)
All	All	0.39	1/13901 (0.0%)	0.62	12/18838 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	279	ARG	C-O	5.92	1.34	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	256	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	G	214	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	F	259	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	G	214	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	F	256	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	D	46	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	185	ARG	CG-CD-NE	6.32	125.06	111.80
1	G	82	LEU	CB-CG-CD1	-6.27	100.34	111.00
1	G	214	ARG	CG-CD-NE	6.13	124.68	111.80
1	F	256	ARG	CB-CG-CD	-5.87	96.33	111.60
1	A	171	ILE	CB-CA-C	-5.45	100.69	111.60
1	C	88	ARG	CA-CB-CG	5.18	124.81	113.40

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	2022	0	2130	21	0
1	B	1956	0	2053	15	0
1	C	1956	0	2053	20	0
1	D	2014	0	2119	17	0
1	E	2003	0	2106	17	0
1	F	1963	0	2062	21	0
1	G	1945	0	2040	26	0
2	A	8	0	18	0	0
2	E	8	0	18	0	0
3	A	6	0	14	0	0
3	B	12	0	28	0	0
3	C	12	0	28	0	0
3	D	6	0	14	0	0
3	E	12	0	28	0	0
3	F	12	0	28	0	0
4	C	8	0	15	0	0
4	D	10	0	22	0	0
4	G	10	0	22	0	0
All	All	13963	0	14798	121	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 (121) 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:G:185:ARG:NH1	1:G:238:ARG:HD3	1.88	0.87
1:A:273:MET:HB2	1:G:273:MET:HE2	1.69	0.75
1:A:224:ARG:NH2	1:B:252:ASP:OD1	2.18	0.75
1:F:49:SER:OG	1:F:74:ARG:HG2	1.87	0.75
1:E:224:ARG:NH2	1:F:252:ASP:OD1	2.22	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:MET:HE3	1:D:273:MET:SD	2.31	0.70
1:F:49:SER:CB	1:F:74:ARG:HG2	2.23	0.69
1:C:224:ARG:NH2	1:D:252:ASP:OD1	2.28	0.67
1:G:25:LEU:O	1:G:27:TYR:N	2.31	0.64
1:C:25:LEU:O	1:C:27:TYR:N	2.30	0.64
1:B:25:LEU:O	1:B:27:TYR:N	2.31	0.64
1:G:56:MET:HG3	1:G:66:ALA:CB	2.28	0.63
1:F:25:LEU:O	1:F:27:TYR:N	2.31	0.63
1:B:224:ARG:NH2	1:C:252:ASP:OD1	2.34	0.61
1:D:224:ARG:NH2	1:E:252:ASP:OD1	2.34	0.61
1:A:194:TYR:HA	1:A:233:ILE:HD13	1.84	0.60
1:D:143:GLY:N	1:D:155:MET:HE3	2.17	0.59
1:D:194:TYR:HA	1:D:233:ILE:HD13	1.83	0.58
1:B:194:TYR:HA	1:B:233:ILE:HD13	1.85	0.58
1:A:143:GLY:N	1:A:155:MET:HE3	2.17	0.58
1:C:143:GLY:N	1:C:155:MET:HE3	2.19	0.58
1:F:194:TYR:HA	1:F:233:ILE:HD13	1.85	0.58
1:E:143:GLY:N	1:E:155:MET:HE3	2.19	0.58
1:C:194:TYR:HA	1:C:233:ILE:HD13	1.85	0.57
1:G:194:TYR:HA	1:G:233:ILE:HD13	1.84	0.57
1:E:194:TYR:HA	1:E:233:ILE:HD13	1.85	0.57
1:C:225:LEU:HD13	1:C:233:ILE:HG23	1.87	0.57
1:F:143:GLY:N	1:F:155:MET:HE3	2.19	0.57
1:B:225:LEU:HD13	1:B:233:ILE:HG23	1.87	0.57
1:G:225:LEU:HD13	1:G:233:ILE:HG23	1.87	0.57
1:D:67:R1A:O1	1:D:74:ARG:NH1	2.38	0.56
1:F:224:ARG:NH2	1:G:252:ASP:OD1	2.38	0.56
1:F:225:LEU:HD13	1:F:233:ILE:HG23	1.87	0.56
1:G:143:GLY:N	1:G:155:MET:HE3	2.21	0.56
1:E:225:LEU:HD13	1:E:233:ILE:HG23	1.87	0.55
1:E:67:R1A:O1	1:E:74:ARG:NH1	2.40	0.55
1:D:225:LEU:HD13	1:D:233:ILE:HG23	1.88	0.55
1:B:67:R1A:O1	1:B:74:ARG:NH1	2.40	0.54
1:G:67:R1A:O1	1:G:74:ARG:NH1	2.40	0.54
1:A:273:MET:CB	1:G:273:MET:HE2	2.37	0.54
1:A:225:LEU:HD13	1:A:233:ILE:HG23	1.89	0.53
1:C:67:R1A:O1	1:C:74:ARG:NH1	2.40	0.53
1:A:252:ASP:OD1	1:G:224:ARG:NH2	2.41	0.52
1:E:201:VAL:HG11	1:E:235:PHE:CE1	2.44	0.52
1:F:212:GLU:OE1	1:F:256:ARG:NH2	2.43	0.51
1:G:56:MET:HG3	1:G:66:ALA:HB1	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:VAL:HG11	1:C:235:PHE:CE1	2.47	0.50
1:A:201:VAL:HG11	1:A:235:PHE:CE1	2.47	0.50
1:B:201:VAL:HG11	1:B:235:PHE:CE1	2.47	0.50
1:D:201:VAL:HG11	1:D:235:PHE:CE1	2.47	0.49
1:G:201:VAL:HG11	1:G:235:PHE:CE1	2.47	0.49
1:C:186:ASN:ND2	1:C:250:TYR:HB2	2.28	0.49
1:F:253:VAL:HA	1:F:256:ARG:HH11	1.78	0.49
1:A:88:ARG:N	1:A:88:ARG:HD3	2.28	0.49
1:E:107:VAL:HG12	1:E:111:LEU:HD12	1.95	0.48
1:C:107:VAL:HG12	1:C:111:LEU:HD12	1.96	0.48
1:D:26:SER:O	1:D:29:VAL:HG22	2.13	0.48
1:F:26:SER:O	1:F:29:VAL:HG22	2.14	0.48
1:C:225:LEU:CD1	1:C:233:ILE:HG23	2.44	0.48
1:B:49:SER:HA	1:B:52:VAL:HG22	1.96	0.48
1:B:88:ARG:N	1:B:88:ARG:HD3	2.29	0.48
1:F:201:VAL:HG11	1:F:235:PHE:CE1	2.48	0.48
1:A:107:VAL:HG12	1:A:111:LEU:HD12	1.96	0.48
1:E:225:LEU:CD1	1:E:233:ILE:HG23	2.44	0.48
1:G:26:SER:O	1:G:29:VAL:HG22	2.14	0.47
1:A:49:SER:HA	1:A:52:VAL:HG22	1.95	0.47
1:D:88:ARG:N	1:D:88:ARG:HD3	2.29	0.47
1:D:107:VAL:HG12	1:D:111:LEU:HD12	1.95	0.47
1:G:225:LEU:CD1	1:G:233:ILE:HG23	2.44	0.47
1:D:225:LEU:CD1	1:D:233:ILE:HG23	2.44	0.47
1:A:46:ARG:HD2	1:A:74:ARG:HH12	1.79	0.47
1:F:107:VAL:HG12	1:F:111:LEU:HD12	1.97	0.47
1:B:225:LEU:CD1	1:B:233:ILE:HG23	2.44	0.47
1:A:125:VAL:O	1:A:128:ARG:HG2	2.15	0.47
1:E:88:ARG:HD3	1:E:88:ARG:N	2.30	0.47
1:E:26:SER:O	1:E:29:VAL:HG12	2.15	0.46
1:G:107:VAL:HG12	1:G:111:LEU:HD12	1.96	0.46
1:F:225:LEU:CD1	1:F:233:ILE:HG23	2.45	0.46
1:A:199:ASP:OD1	1:B:259:ARG:NH2	2.48	0.46
1:A:225:LEU:CD1	1:A:233:ILE:HG23	2.45	0.46
1:D:143:GLY:N	1:D:155:MET:CE	2.78	0.46
1:F:88:ARG:N	1:F:88:ARG:HD3	2.31	0.46
1:B:107:VAL:HG12	1:B:111:LEU:HD12	1.97	0.46
1:C:279:ARG:HB3	1:D:277:PHE:HB2	1.98	0.46
1:C:54:ARG:HA	1:C:57:ILE:CG1	2.46	0.45
1:C:125:VAL:O	1:C:128:ARG:HG2	2.16	0.45
1:C:26:SER:O	1:C:29:VAL:HG12	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:VAL:HG11	1:B:278:LYS:HE2	1.98	0.45
1:C:143:GLY:N	1:C:155:MET:CE	2.79	0.45
1:A:143:GLY:N	1:A:155:MET:CE	2.79	0.45
1:B:26:SER:O	1:B:29:VAL:HG12	2.16	0.45
1:D:142:ALA:C	1:D:155:MET:CE	2.85	0.44
1:C:142:ALA:C	1:C:155:MET:CE	2.86	0.44
1:F:143:GLY:N	1:F:155:MET:CE	2.81	0.44
1:A:142:ALA:C	1:A:155:MET:CE	2.86	0.43
1:E:143:GLY:N	1:E:155:MET:CE	2.81	0.43
1:C:53:ASN:O	1:C:57:ILE:HG12	2.19	0.43
1:F:142:ALA:C	1:F:155:MET:CE	2.87	0.43
1:G:143:GLY:N	1:G:155:MET:CE	2.82	0.43
1:G:137:ASP:HB3	1:G:176:ILE:HB	2.02	0.42
1:F:208:ILE:HD11	1:F:260:GLU:HG3	2.02	0.42
1:C:208:ILE:HD11	1:C:260:GLU:HG3	2.02	0.42
1:A:208:ILE:HD11	1:A:260:GLU:HG3	2.02	0.42
1:G:52:VAL:HG13	1:G:56:MET:CE	2.50	0.41
1:E:208:ILE:HD11	1:E:260:GLU:HG3	2.02	0.41
1:E:137:ASP:HB3	1:E:176:ILE:HB	2.02	0.41
1:E:277:PHE:CE1	1:F:277:PHE:HZ	2.38	0.41
1:A:273:MET:HB2	1:G:273:MET:CE	2.43	0.41
1:G:56:MET:HB2	1:G:61:ILE:HD12	2.03	0.41
1:E:277:PHE:CE1	1:F:277:PHE:CZ	3.09	0.41
1:B:208:ILE:HD11	1:B:260:GLU:HG3	2.02	0.41
1:E:142:ALA:C	1:E:155:MET:CE	2.89	0.41
1:F:221:MET:HE3	1:F:221:MET:HB3	1.81	0.41
1:G:56:MET:HG3	1:G:66:ALA:HB2	2.02	0.40
1:G:142:ALA:C	1:G:155:MET:CE	2.89	0.40
1:D:208:ILE:HD11	1:D:260:GLU:HG3	2.03	0.40
1:A:137:ASP:HB3	1:A:176:ILE:HB	2.03	0.40
1:D:137:ASP:HB3	1:D:176:ILE:HB	2.03	0.40
1:G:64:THR:CG2	1:G:118:LEU:HD11	2.52	0.40
1:G:56:MET:HB2	1:G:61:ILE:CD1	2.51	0.40
1:G:208:ILE:HD11	1:G:260:GLU:HG3	2.04	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	261/286 (91%)	255 (98%)	6 (2%)	0	100	100
1	B	252/286 (88%)	247 (98%)	4 (2%)	1 (0%)	39	80
1	C	252/286 (88%)	247 (98%)	4 (2%)	1 (0%)	39	80
1	D	260/286 (91%)	253 (97%)	7 (3%)	0	100	100
1	E	259/286 (91%)	252 (97%)	7 (3%)	0	100	100
1	F	253/286 (88%)	248 (98%)	4 (2%)	1 (0%)	39	80
1	G	251/286 (88%)	245 (98%)	5 (2%)	1 (0%)	39	80
All	All	1788/2002 (89%)	1747 (98%)	37 (2%)	4 (0%)	52	88

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	26	SER
1	C	26	SER
1	F	26	SER
1	G	26	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	213/230 (93%)	211 (99%)	2 (1%)	84	95
1	B	206/230 (90%)	202 (98%)	4 (2%)	65	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	206/230 (90%)	200 (97%)	6 (3%)	50 84
1	D	212/230 (92%)	207 (98%)	5 (2%)	57 87
1	E	211/230 (92%)	206 (98%)	5 (2%)	57 87
1	F	207/230 (90%)	203 (98%)	4 (2%)	65 90
1	G	205/230 (89%)	200 (98%)	5 (2%)	57 87
All	All	1460/1610 (91%)	1429 (98%)	31 (2%)	61 89

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	SER
1	A	241	SER
1	B	26	SER
1	B	116	SER
1	B	144	THR
1	B	241	SER
1	C	26	SER
1	C	52	VAL
1	C	88	ARG
1	C	116	SER
1	C	144	THR
1	C	241	SER
1	D	17	LEU
1	D	52	VAL
1	D	116	SER
1	D	144	THR
1	D	241	SER
1	E	17	LEU
1	E	52	VAL
1	E	116	SER
1	E	144	THR
1	E	241	SER
1	F	26	SER
1	F	74	ARG
1	F	116	SER
1	F	241	SER
1	G	26	SER
1	G	82	LEU
1	G	116	SER
1	G	144	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	241	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	186	ASN
1	C	203	GLN
1	C	207	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

7 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	R1A	A	67	1	15,18,19	1.36	1 (6%)	16,27,29	3.01	4 (25%)
1	R1A	B	67	1	15,18,19	1.33	1 (6%)	16,27,29	2.89	4 (25%)
1	R1A	C	67	1	15,18,19	1.36	1 (6%)	16,27,29	2.83	4 (25%)
1	R1A	D	67	1	15,18,19	1.37	1 (6%)	16,27,29	2.87	4 (25%)
1	R1A	E	67	1	15,18,19	1.33	1 (6%)	16,27,29	3.05	4 (25%)
1	R1A	F	67	1	15,18,19	1.30	1 (6%)	16,27,29	3.11	5 (31%)
1	R1A	G	67	1	15,18,19	1.32	1 (6%)	16,27,29	2.87	5 (31%)

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	R1A	A	67	1	-	0/5/32/34	0/1/1/1
1	R1A	B	67	1	-	0/5/32/34	0/1/1/1
1	R1A	C	67	1	-	0/5/32/34	0/1/1/1
1	R1A	D	67	1	-	0/5/32/34	0/1/1/1
1	R1A	E	67	1	-	0/5/32/34	0/1/1/1
1	R1A	F	67	1	-	0/5/32/34	0/1/1/1
1	R1A	G	67	1	-	0/5/32/34	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	R1A	CE-SD	-4.28	1.76	1.81
1	D	67	R1A	CE-SD	-4.26	1.76	1.81
1	C	67	R1A	CE-SD	-4.25	1.76	1.81
1	G	67	R1A	CE-SD	-4.12	1.76	1.81
1	B	67	R1A	CE-SD	-4.08	1.76	1.81
1	E	67	R1A	CE-SD	-4.07	1.76	1.81
1	F	67	R1A	CE-SD	-4.02	1.76	1.81

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	67	R1A	C7-C5-C4	-6.48	105.38	112.75
1	F	67	R1A	C7-C5-C4	-6.29	105.60	112.75
1	A	67	R1A	C7-C5-C4	-6.14	105.76	112.75
1	D	67	R1A	C6-C5-C4	-4.37	107.77	112.75
1	B	67	R1A	C6-C5-C4	-4.30	107.86	112.75
1	G	67	R1A	C6-C5-C4	-4.23	107.94	112.75
1	C	67	R1A	C6-C5-C4	-4.09	108.10	112.75
1	F	67	R1A	C5-C4-C3	-3.09	111.25	113.70
1	G	67	R1A	C5-C4-C3	-2.98	111.33	113.70
1	B	67	R1A	C5-C4-C3	-2.92	111.38	113.70
1	D	67	R1A	C5-C4-C3	-2.92	111.39	113.70
1	C	67	R1A	C5-C4-C3	-2.80	111.48	113.70
1	A	67	R1A	C5-C4-C3	-2.79	111.49	113.70
1	E	67	R1A	C5-C4-C3	-2.59	111.65	113.70
1	G	67	R1A	C4-C5-N1	2.04	101.20	99.29
1	F	67	R1A	C4-C5-N1	2.19	101.35	99.29
1	A	67	R1A	C7-C5-N1	2.24	113.36	109.61
1	F	67	R1A	C7-C5-N1	2.32	113.49	109.61
1	E	67	R1A	C7-C5-N1	2.40	113.64	109.61
1	C	67	R1A	C6-C5-N1	2.75	114.23	109.61
1	G	67	R1A	C6-C5-N1	2.77	114.26	109.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	67	R1A	C6-C5-N1	2.88	114.45	109.61
1	D	67	R1A	C6-C5-N1	2.94	114.54	109.61
1	A	67	R1A	CE-SD-SG	8.92	113.14	103.76
1	E	67	R1A	CE-SD-SG	8.93	113.15	103.76
1	D	67	R1A	CE-SD-SG	9.05	113.27	103.76
1	G	67	R1A	CE-SD-SG	9.06	113.28	103.76
1	C	67	R1A	CE-SD-SG	9.08	113.31	103.76
1	F	67	R1A	CE-SD-SG	9.19	113.42	103.76
1	B	67	R1A	CE-SD-SG	9.23	113.47	103.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	67	R1A	1	0
1	C	67	R1A	1	0
1	D	67	R1A	1	0
1	E	67	R1A	1	0
1	G	67	R1A	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

15 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	OCT	A	401	-	7,7,7	0.39	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEX	A	501	-	5,5,5	0.52	0	4,4,4	0.15	0
3	HEX	B	500	-	5,5,5	0.47	0	4,4,4	0.25	0
3	HEX	B	501	-	5,5,5	0.42	0	4,4,4	0.23	0
4	D10	C	402	-	7,7,9	0.45	0	6,6,8	0.27	0
3	HEX	C	500	-	5,5,5	0.40	0	4,4,4	0.21	0
3	HEX	C	501	-	5,5,5	0.47	0	4,4,4	0.19	0
4	D10	D	404	-	9,9,9	0.36	0	8,8,8	0.40	0
3	HEX	D	501	-	5,5,5	0.38	0	4,4,4	0.13	0
2	OCT	E	406	-	7,7,7	0.45	0	6,6,6	0.21	0
3	HEX	E	500	-	5,5,5	0.49	0	4,4,4	0.05	0
3	HEX	E	501	-	5,5,5	0.45	0	4,4,4	0.07	0
3	HEX	F	500	-	5,5,5	0.44	0	4,4,4	0.25	0
3	HEX	F	501	-	5,5,5	0.40	0	4,4,4	0.08	0
4	D10	G	408	-	9,9,9	0.32	0	8,8,8	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	OCT	A	401	-	-	0/5/5/5	0/0/0/0
3	HEX	A	501	-	-	0/3/3/3	0/0/0/0
3	HEX	B	500	-	-	0/3/3/3	0/0/0/0
3	HEX	B	501	-	-	0/3/3/3	0/0/0/0
4	D10	C	402	-	-	0/5/5/7	0/0/0/0
3	HEX	C	500	-	-	0/3/3/3	0/0/0/0
3	HEX	C	501	-	-	0/3/3/3	0/0/0/0
4	D10	D	404	-	-	0/7/7/7	0/0/0/0
3	HEX	D	501	-	-	0/3/3/3	0/0/0/0
2	OCT	E	406	-	-	0/5/5/5	0/0/0/0
3	HEX	E	500	-	-	0/3/3/3	0/0/0/0
3	HEX	E	501	-	-	0/3/3/3	0/0/0/0
3	HEX	F	500	-	-	0/3/3/3	0/0/0/0
3	HEX	F	501	-	-	0/3/3/3	0/0/0/0
4	D10	G	408	-	-	0/7/7/7	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	263/286 (91%)	0.58	18 (6%) 20 7	80, 110, 171, 231	0
1	B	254/286 (88%)	0.55	15 (5%) 26 10	75, 105, 160, 215	0
1	C	254/286 (88%)	0.52	10 (3%) 43 18	76, 111, 159, 189	0
1	D	262/286 (91%)	0.47	8 (3%) 52 24	74, 106, 158, 216	0
1	E	261/286 (91%)	0.54	19 (7%) 18 6	72, 100, 162, 258	0
1	F	255/286 (89%)	0.68	21 (8%) 14 5	75, 108, 154, 170	0
1	G	253/286 (88%)	0.67	22 (8%) 13 4	80, 114, 166, 197	0
All	All	1802/2002 (90%)	0.57	113 (6%) 23 9	72, 108, 163, 258	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	LEU	6.9
1	G	266	ILE	4.9
1	D	23	LEU	4.8
1	F	56	MET	4.8
1	B	194	TYR	4.7
1	D	25	LEU	4.4
1	C	279	ARG	4.2
1	F	54	ARG	4.2
1	C	58	SER	4.1
1	E	23	LEU	4.0
1	G	54	ARG	4.0
1	A	279	ARG	3.9
1	E	25	LEU	3.8
1	G	51	ALA	3.7
1	B	88	ARG	3.7
1	F	279	ARG	3.7
1	E	277	PHE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	253	VAL	3.6
1	G	52	VAL	3.5
1	F	198	ILE	3.5
1	D	279	ARG	3.3
1	F	88	ARG	3.3
1	F	239	VAL	3.3
1	A	29	VAL	3.2
1	E	24	LEU	3.2
1	D	278	LYS	3.1
1	B	91	VAL	3.1
1	E	190	ILE	3.1
1	A	54	ARG	3.1
1	G	201	VAL	3.1
1	D	24	LEU	3.1
1	F	257	ILE	3.1
1	F	237	VAL	3.0
1	F	277	PHE	3.0
1	G	225	LEU	3.0
1	B	277	PHE	3.0
1	A	24	LEU	2.9
1	F	52	VAL	2.9
1	E	209	ILE	2.8
1	G	61	ILE	2.8
1	B	228	LEU	2.8
1	G	88	ARG	2.8
1	A	268	PHE	2.8
1	E	27	TYR	2.8
1	F	186	ASN	2.8
1	B	89	VAL	2.8
1	G	44	ILE	2.7
1	C	278	LYS	2.7
1	F	51	ALA	2.7
1	B	205	LEU	2.6
1	C	59	ARG	2.6
1	F	209	ILE	2.6
1	F	221	MET	2.6
1	E	56	MET	2.6
1	A	205	LEU	2.5
1	G	228	LEU	2.5
1	E	43	ILE	2.5
1	D	225	LEU	2.5
1	C	91	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	60	LYS	2.5
1	B	90	GLY	2.5
1	F	53	ASN	2.5
1	A	89	VAL	2.5
1	B	61	ILE	2.5
1	A	88	ARG	2.5
1	A	58	SER	2.5
1	A	43	ILE	2.4
1	F	202	LYS	2.4
1	E	198	ILE	2.4
1	B	198	ILE	2.4
1	E	233	ILE	2.3
1	E	191	GLY	2.3
1	G	249	VAL	2.3
1	A	153	THR	2.3
1	B	65	VAL	2.3
1	G	194	TYR	2.3
1	G	56	MET	2.3
1	D	88	ARG	2.3
1	F	188	PHE	2.3
1	G	239	VAL	2.3
1	G	246	LEU	2.3
1	G	58	SER	2.3
1	A	269	PRO	2.3
1	G	209	ILE	2.3
1	A	47	MET	2.2
1	C	249	VAL	2.2
1	F	261	PHE	2.2
1	G	43	ILE	2.2
1	A	74	ARG	2.2
1	G	277	PHE	2.2
1	A	231	SER	2.2
1	E	194	TYR	2.2
1	E	22	ALA	2.1
1	F	236	VAL	2.1
1	C	74	ARG	2.1
1	E	52	VAL	2.1
1	E	225	LEU	2.1
1	G	213	ASP	2.1
1	E	74	ARG	2.1
1	B	209	ILE	2.1
1	B	253	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	275	VAL	2.1
1	D	97	ILE	2.1
1	G	264	ALA	2.1
1	E	60	LYS	2.1
1	G	268	PHE	2.1
1	B	62	ASP	2.0
1	E	205	LEU	2.0
1	A	70	SER	2.0
1	A	19	ALA	2.0
1	F	278	LYS	2.0
1	B	153	THR	2.0
1	F	194	TYR	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	R1A	A	67	18/19	0.91	0.30	-	148,189,195,202	0
1	R1A	B	67	18/19	0.88	0.20	-	131,174,185,186	0
1	R1A	D	67	18/19	0.89	0.23	-	122,179,191,192	0
1	R1A	F	67	18/19	0.90	0.27	-	132,179,187,190	0
1	R1A	C	67	18/19	0.88	0.34	-	130,168,176,181	0
1	R1A	E	67	18/19	0.88	0.29	-	126,183,193,199	0
1	R1A	G	67	18/19	0.87	0.21	-	102,170,180,191	0

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	HEX	A	501	6/6	0.71	0.60	15.29	88,91,93,94	0
3	HEX	F	500	6/6	0.73	0.58	13.40	88,92,94,95	0
3	HEX	E	501	6/6	0.65	0.60	12.41	89,94,96,96	0
3	HEX	F	501	6/6	0.84	0.47	7.43	97,103,105,105	0
3	HEX	D	501	6/6	0.77	0.45	5.89	90,94,97,98	0
3	HEX	B	500	6/6	0.79	0.53	4.97	81,85,86,87	0
3	HEX	C	501	6/6	0.82	0.39	2.76	95,98,103,105	0
3	HEX	E	500	6/6	0.80	0.34	2.68	83,85,87,87	0
3	HEX	C	500	6/6	0.87	0.35	2.14	83,87,90,90	0
3	HEX	B	501	6/6	0.77	0.35	1.36	90,91,96,98	0
4	D10	D	404	10/10	0.71	0.27	-	112,114,118,118	0
2	OCT	A	401	8/8	0.77	0.26	-	102,111,114,115	0
4	D10	C	402	8/10	0.58	0.36	-	103,119,122,123	0
4	D10	G	408	10/10	0.77	0.24	-	108,121,124,124	0
2	OCT	E	406	8/8	0.47	0.42	-	109,117,123,125	0

6.5 Other polymers

There are no such residues in this entry.