Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:42 AM GMT

PDB ID	:	2NTI
Title	:	Crystal structure of PCNA123 heterotrimer.
Authors	:	Hlinkova, V.; Ling, H.
Deposited on	:	2006-11-07
Resolution	:	2.50 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:

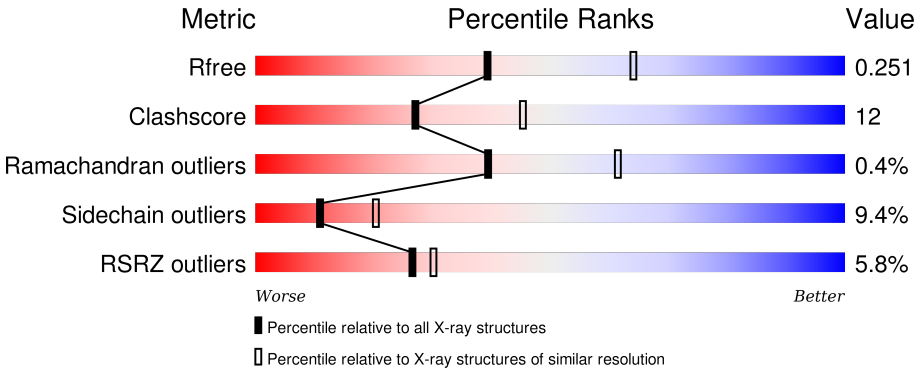
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	249	6% 74% 20% 5%
1	D	249	3% 73% 22% 5%
1	G	249	8% 64% 31% 5%
2	B	246	3% 78% 18% •
2	E	246	3% 77% 19% • •

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Mol	Chain	Length	Quality of chain
2	H	246	4% 76% 20%
3	C	244	9% 71% 25%
3	F	244	7% 80% 17%
3	I	244	8% 64% 30% 5%

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
4	BR	D	3039	-	-	X	-
4	BR	F	3024	-	-	X	-
4	BR	I	3032	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18488 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 DNA polymerase sliding clamp B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	249	Total	C	N	O	S	0	0	0
			1928	1227	310	382	9			
1	A	248	Total	C	N	O	S	0	0	0
			1914	1218	309	378	9			
1	G	249	Total	C	N	O	S	0	0	0
			1924	1225	310	380	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	2	VAL	PHE	ENGINEERED	UNP P57766
A	2	VAL	PHE	ENGINEERED	UNP P57766
G	2	VAL	PHE	ENGINEERED	UNP P57766

- Molecule 2 is a protein called DNA polymerase sliding clamp C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	244	Total	C	N	O	S	0	0	0
			1931	1241	302	383	5			
2	B	245	Total	C	N	O	S	0	0	0
			1935	1245	303	382	5			
2	H	246	Total	C	N	O	S	0	0	0
			1944	1249	304	386	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	INITIATING METHIONINE	UNP Q97Z84
B	1	MET	-	INITIATING METHIONINE	UNP Q97Z84
H	1	MET	-	INITIATING METHIONINE	UNP Q97Z84

- Molecule 3 is a protein called DNA polymerase sliding clamp A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	244	Total	C	N	O	S	0	0	0
			1934	1229	312	389	4			
3	C	244	Total	C	N	O	S	0	0	0
			1934	1229	312	389	4			
3	I	242	Total	C	N	O	S	0	0	0
			1917	1218	310	385	4			

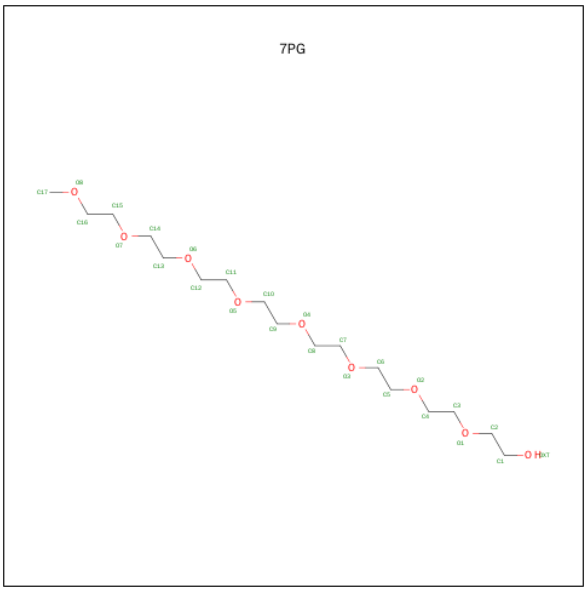
- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	Br	0	0
			2	2		
4	D	6	Total	Br	0	0
			6	6		
4	E	8	Total	Br	0	0
			8	8		
4	H	5	Total	Br	0	0
			5	5		
4	B	5	Total	Br	0	0
			5	5		
4	I	6	Total	Br	0	0
			6	6		
4	C	7	Total	Br	0	0
			7	7		
4	A	5	Total	Br	0	0
			5	5		
4	F	10	Total	Br	0	0
			10	10		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	K	0	0
			1	1		

- Molecule 6 is 2,5,8,11,14,17,20,23-OCTAOXAPENTACOSAN-25-OL (three-letter code: 7PG) (formula: $C_{17}H_{36}O_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C O 26 17 9	0	0

- Molecule 7 is water.

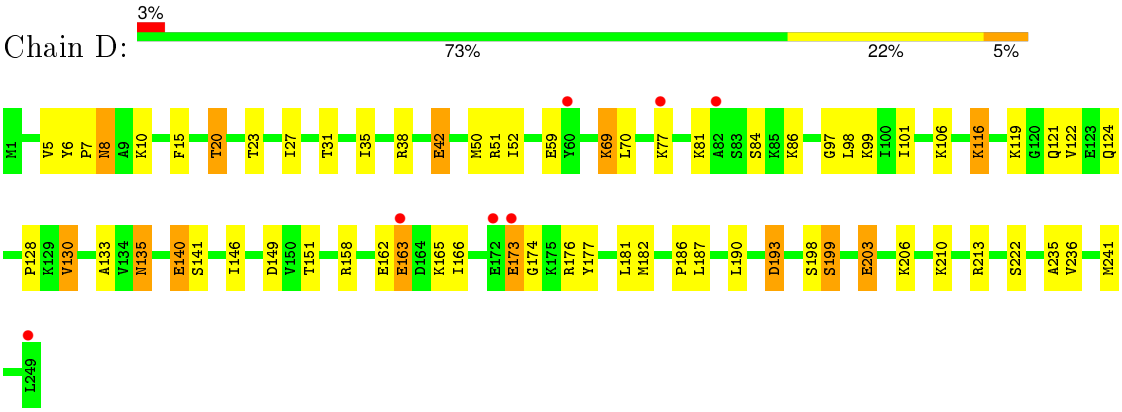
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	111	Total O 111 111	0	0
7	E	178	Total O 178 178	0	0
7	F	112	Total O 112 112	0	0
7	A	82	Total O 82 82	0	0
7	B	168	Total O 168 168	0	0
7	C	85	Total O 85 85	0	0
7	G	67	Total O 67 67	0	0
7	H	171	Total O 171 171	0	0
7	I	72	Total O 72 72	0	0

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.

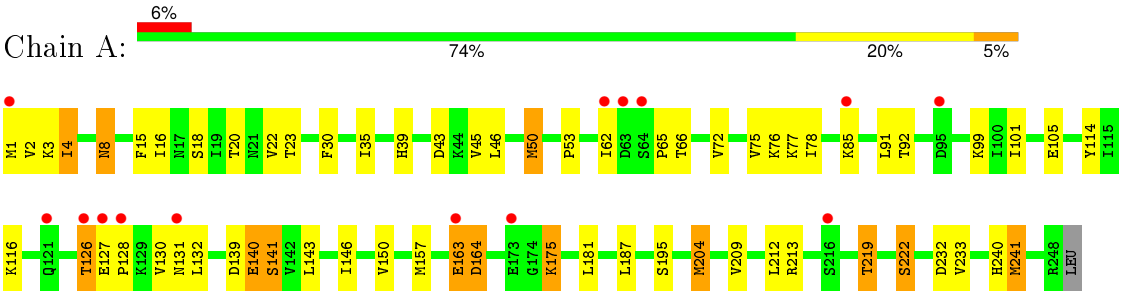
- Molecule 1: DNA polymerase sliding clamp B

Chain D:



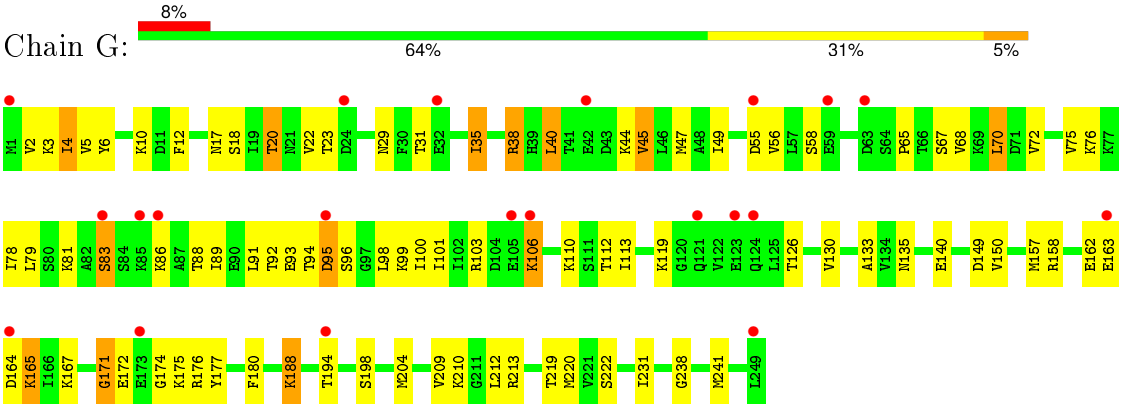
- Molecule 1: DNA polymerase sliding clamp B

Chain A:



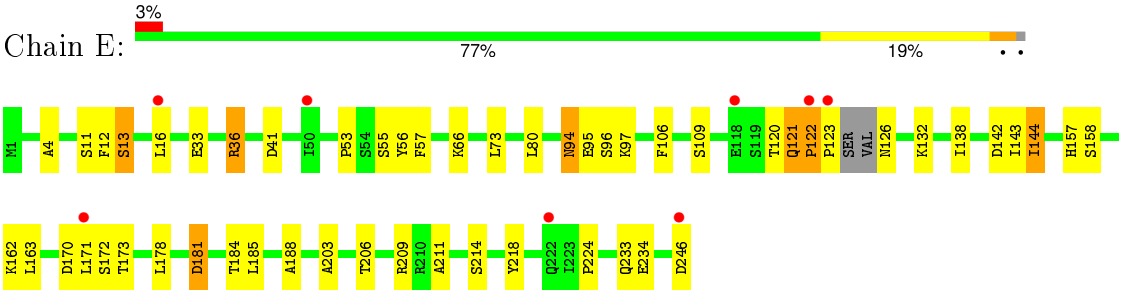
- Molecule 1: DNA polymerase sliding clamp B

Chain G:



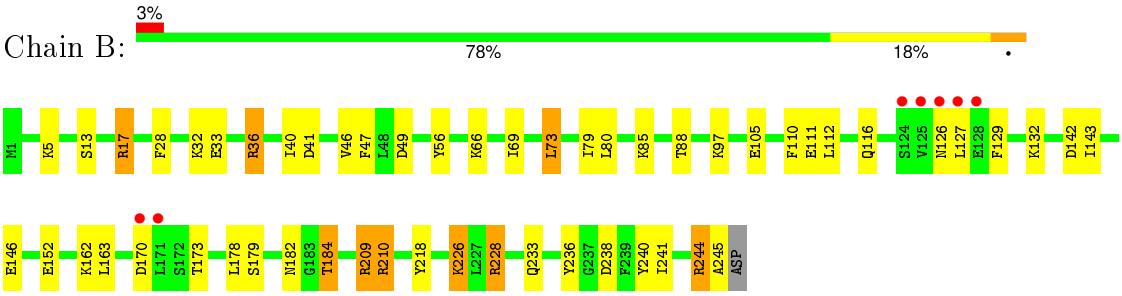
• Molecule 2: DNA polymerase sliding clamp C

Chain E:



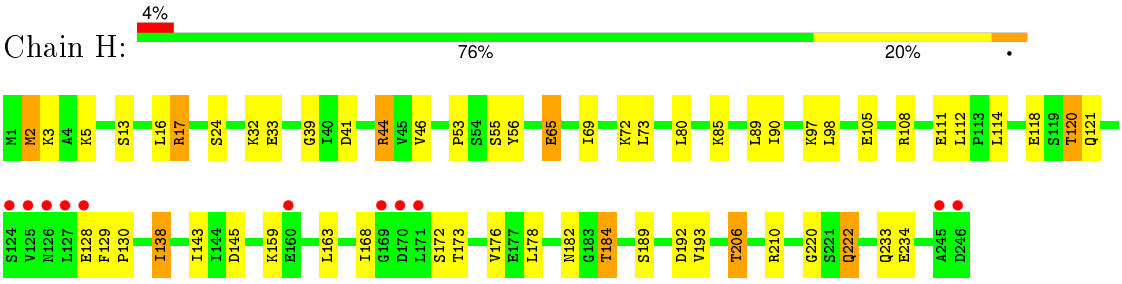
• Molecule 2: DNA polymerase sliding clamp C

Chain B:



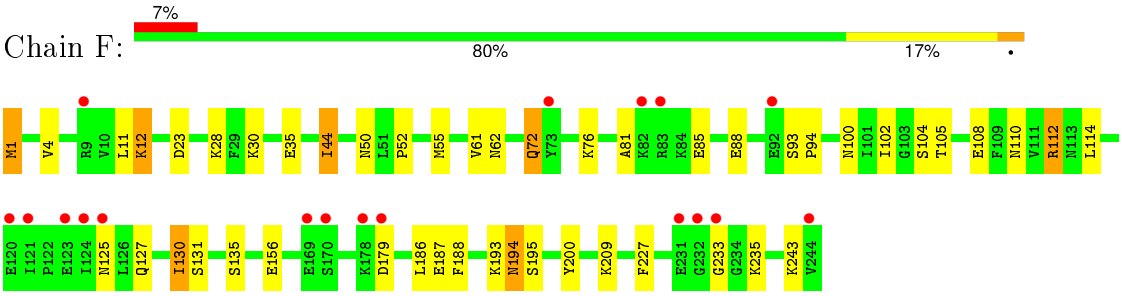
• Molecule 2: DNA polymerase sliding clamp C

Chain H:



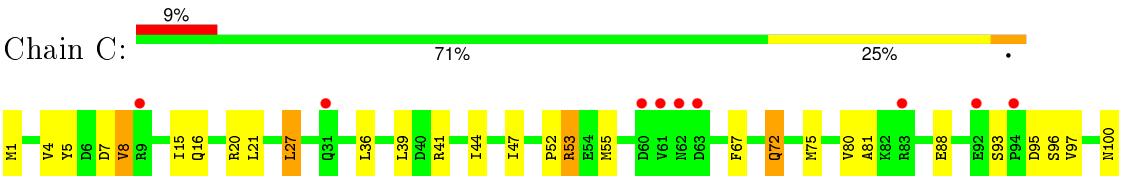
• Molecule 3: DNA polymerase sliding clamp A

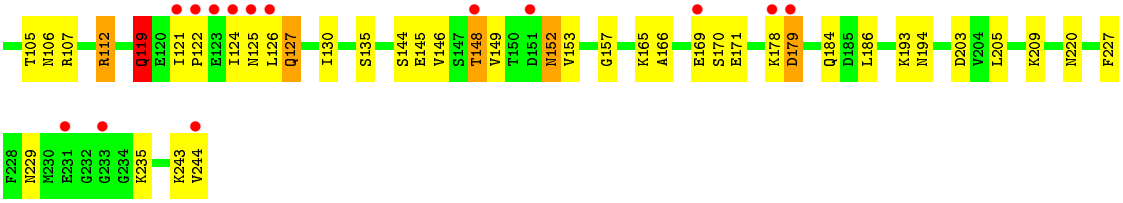
Chain F:



• Molecule 3: DNA polymerase sliding clamp A

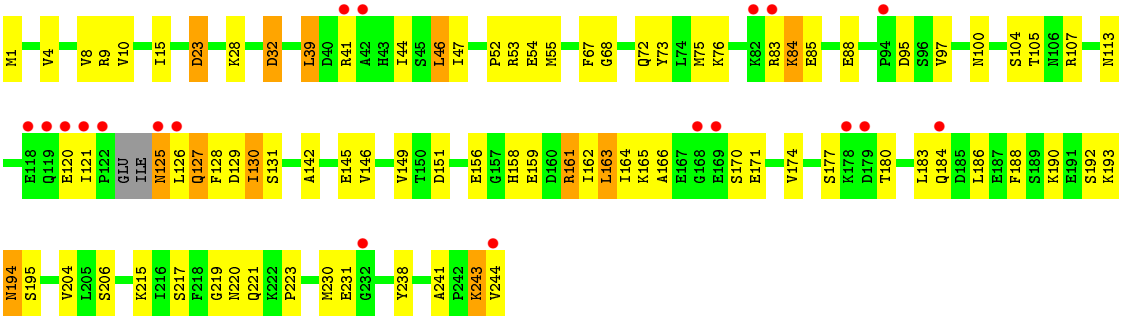
Chain C:





• Molecule 3: DNA polymerase sliding clamp A

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	148.14Å 222.33Å 80.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.20 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.00-2.50) 96.0 (29.20-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.251 0.214 , 0.251	Depositor DCC
R_{free} test set	1796 reflections (2.03%)	DCC
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 88412 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18488	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: K, 7PG, BR

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	0.49	1/1941 (0.1%)	0.56	0/2614
1	D	0.47	0/1955	0.58	0/2632
1	G	0.47	0/1951	0.56	0/2627
2	B	0.48	0/1970	0.62	1/2662 (0.0%)
2	E	0.47	0/1965	0.59	0/2652
2	H	0.47	0/1979	0.59	0/2673
3	C	0.46	0/1960	0.60	0/2641
3	F	0.44	0/1960	0.57	0/2641
3	I	0.51	1/1942 (0.1%)	0.56	0/2615
All	All	0.47	2/17623 (0.0%)	0.58	1/23757 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	GLU	CD-OE2	6.30	1.32	1.25
3	I	243	LYS	CE-NZ	5.87	1.63	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	73	LEU	CA-CB-CG	-5.15	103.46	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	171	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1914	0	1971	48	0
1	D	1928	0	1987	49	0
1	G	1924	0	1983	79	0
2	B	1935	0	1937	46	0
2	E	1931	0	1926	39	0
2	H	1944	0	1941	42	0
3	C	1934	0	1945	43	0
3	F	1934	0	1945	37	0
3	I	1917	0	1927	67	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
4	C	7	0	0	2	0
4	D	6	0	0	5	0
4	E	8	0	0	2	0
4	F	10	0	0	5	0
4	G	2	0	0	2	0
4	H	5	0	0	0	0
4	I	6	0	0	5	0
5	H	1	0	0	0	0
6	H	26	0	36	2	0
7	A	82	0	0	0	0
7	B	168	0	0	2	0
7	C	85	0	0	3	0
7	D	111	0	0	4	0
7	E	178	0	0	3	0
7	F	112	0	0	6	0
7	G	67	0	0	4	0
7	H	171	0	0	6	0
7	I	72	0	0	3	0
All	All	18488	0	17598	419	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 12.

All (419) 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)
2:E:122:PRO:HB2	2:E:123:PRO:CD	1.79	1.13
2:E:122:PRO:HB2	2:E:123:PRO:HD3	1.30	1.10
1:G:89:ILE:HD11	1:G:100:ILE:HD11	1.34	1.05
2:B:17:ARG:HH11	2:B:17:ARG:HG2	1.23	1.03
1:G:56:VAL:HG11	1:G:238:GLY:HA3	1.40	0.99
3:F:233:GLY:O	4:F:3024:BR:BR	2.38	0.96
1:G:140:GLU:HG3	1:G:213:ARG:HA	1.47	0.94
2:H:138:ILE:H	2:H:138:ILE:HD12	1.34	0.92
1:A:53:PRO:HG3	4:A:3044:BR:BR	2.29	0.88
2:B:244:ARG:CG	2:B:244:ARG:HH11	1.87	0.88
3:I:4:VAL:HG22	3:I:88:GLU:HG2	1.55	0.88
2:H:17:ARG:HG2	2:H:17:ARG:HH11	1.38	0.87
3:I:142:ALA:HB1	3:I:174:VAL:HG11	1.56	0.86
1:G:18:SER:HB2	1:G:241:MET:HE2	1.58	0.85
1:D:42:GLU:HG3	1:A:39:HIS:HD1	1.42	0.85
2:E:16:LEU:HD12	2:E:80:LEU:HD11	1.59	0.85
3:I:156:GLU:HB3	3:I:163:LEU:HG	1.57	0.84
1:G:40:LEU:HD23	1:G:44:LYS:HD2	1.57	0.83
2:B:244:ARG:HG2	2:B:244:ARG:HH11	1.43	0.83
2:B:17:ARG:NH1	2:B:17:ARG:HG2	1.95	0.80
3:F:28:LYS:HD2	7:F:3051:HOH:O	1.81	0.80
2:H:178:LEU:HD23	2:H:184:THR:HG23	1.64	0.79
3:C:4:VAL:HG22	3:C:88:GLU:HG2	1.65	0.79
2:H:182:ASN:OD1	2:H:184:THR:HB	1.82	0.79
2:H:55:SER:HB3	2:H:233:GLN:HG2	1.65	0.79
1:A:18:SER:HB2	1:A:241:MET:HE2	1.65	0.79
1:A:140:GLU:HG3	1:A:213:ARG:HA	1.65	0.78
3:I:68:GLY:H	3:I:113:ASN:HD21	1.33	0.77
2:E:16:LEU:HD12	2:E:80:LEU:CD1	2.15	0.76
1:G:174:GLY:O	2:H:97:LYS:HE3	1.84	0.76
2:B:143:ILE:HD11	3:C:105:THR:HG21	1.68	0.76
3:C:112:ARG:HG2	3:C:112:ARG:HH11	1.51	0.75
2:B:5:LYS:HE3	2:B:88:THR:HG21	1.67	0.75
3:I:192:SER:HA	3:I:220:ASN:OD1	1.87	0.75
1:D:140:GLU:HG3	1:D:213:ARG:HA	1.67	0.75
1:G:18:SER:HB2	1:G:241:MET:CE	2.17	0.74
1:D:51:ARG:HD2	4:D:3028:BR:BR	2.41	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:SER:HB2	1:A:241:MET:CE	2.16	0.74
1:G:133:ALA:HB1	1:G:194:THR:HG22	1.69	0.74
2:E:143:ILE:HD11	3:F:105:THR:HG21	1.70	0.73
3:I:126:LEU:HD22	3:I:223:PRO:HD2	1.70	0.73
1:G:40:LEU:HD23	1:G:44:LYS:CD	2.18	0.73
2:E:224:PRO:HG3	4:E:3049:BR:BR	2.43	0.72
2:B:210:ARG:HH11	2:B:210:ARG:CG	2.03	0.71
1:G:99:LYS:HD3	1:G:101:ILE:HD11	1.72	0.71
3:I:129:ASP:HB3	3:I:190:LYS:HG2	1.70	0.71
1:G:75:VAL:HA	1:G:78:ILE:HD12	1.72	0.70
3:I:146:VAL:HG13	3:I:166:ALA:HB2	1.71	0.70
1:G:133:ALA:CB	1:G:194:THR:HG22	2.21	0.70
2:H:210:ARG:HD2	7:H:4005:HOH:O	1.90	0.70
3:I:107:ARG:HH21	3:I:107:ARG:HG3	1.57	0.70
2:B:178:LEU:HD23	2:B:184:THR:HG23	1.74	0.70
3:I:142:ALA:CB	3:I:174:VAL:HG11	2.22	0.69
1:A:3:LYS:HG3	1:A:92:THR:HG22	1.75	0.68
2:H:17:ARG:HG2	2:H:17:ARG:NH1	2.00	0.68
1:D:236:VAL:HG23	4:D:3039:BR:BR	2.49	0.68
2:E:94:ASN:ND2	2:E:97:LYS:H	1.93	0.67
1:A:22:VAL:HG12	1:A:23:THR:HG23	1.77	0.67
1:A:77:LYS:HB3	3:C:148:THR:HG21	1.77	0.67
2:H:178:LEU:HD23	2:H:184:THR:CG2	2.24	0.66
1:G:38:ARG:NH1	1:G:126:THR:O	2.29	0.66
3:I:130:ILE:HD11	3:I:186:LEU:HD11	1.77	0.66
2:E:122:PRO:CB	2:E:123:PRO:CD	2.65	0.66
1:D:8:ASN:HD22	1:D:8:ASN:C	2.00	0.65
1:A:8:ASN:C	1:A:8:ASN:HD22	2.00	0.64
2:B:228:ARG:HD3	2:B:238:ASP:OD2	1.96	0.64
3:I:159:GLU:HG3	3:I:188:PHE:CE2	2.32	0.64
3:F:4:VAL:HG22	3:F:88:GLU:HG2	1.77	0.64
1:G:100:ILE:HG23	1:G:113:ILE:HB	1.79	0.64
3:I:231:GLU:HA	3:I:231:GLU:OE2	1.98	0.64
1:A:219:THR:HG22	1:A:233:VAL:HB	1.80	0.63
2:E:97:LYS:HD3	4:E:3050:BR:BR	2.54	0.63
2:E:94:ASN:HD21	2:E:97:LYS:H	1.45	0.62
3:F:88:GLU:HB2	3:F:100:ASN:HB2	1.80	0.62
2:E:181:ASP:N	2:E:181:ASP:OD1	2.33	0.62
2:B:178:LEU:HA	2:B:184:THR:HG21	1.81	0.62
3:F:85:GLU:HB2	3:F:102:ILE:O	1.99	0.62
2:H:65:GLU:H	2:H:65:GLU:CD	2.02	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:LYS:HG2	2:B:179:SER:HB3	1.81	0.62
1:A:46:LEU:HB2	1:A:204:MET:HG3	1.82	0.62
2:B:56:TYR:HA	2:B:233:GLN:HE21	1.64	0.62
2:B:5:LYS:CE	2:B:88:THR:HG21	2.30	0.62
1:G:12:PHE:CZ	1:G:91:LEU:HD11	2.35	0.61
3:F:100:ASN:HD21	3:F:108:GLU:HG3	1.65	0.61
3:C:39:LEU:HD12	3:C:119:GLN:HG3	1.82	0.61
3:C:88:GLU:HB2	3:C:100:ASN:HB2	1.81	0.61
1:D:31:THR:HG22	1:D:122:VAL:HG21	1.81	0.61
2:H:39:GLY:HA2	2:H:120:THR:HG21	1.82	0.61
3:F:227:PHE:HZ	3:F:235:LYS:HE2	1.64	0.61
2:E:157:HIS:HD2	7:E:3068:HOH:O	1.83	0.61
2:E:36:ARG:HH21	2:E:121:GLN:HE22	1.49	0.61
1:G:2:VAL:H	1:G:93:GLU:HG2	1.66	0.61
1:A:139:ASP:OD1	1:A:141:SER:HB2	2.00	0.60
3:I:193:LYS:HE3	4:I:3007:BR:BR	2.55	0.60
3:F:62:ASN:HB2	7:F:3065:HOH:O	2.01	0.60
1:A:46:LEU:HB2	1:A:204:MET:CG	2.32	0.60
3:I:156:GLU:HB3	3:I:163:LEU:CG	2.30	0.60
2:H:143:ILE:HD11	2:H:176:VAL:HG21	1.83	0.60
1:G:78:ILE:HD11	3:I:149:VAL:HG11	1.83	0.60
3:F:100:ASN:HB3	3:F:102:ILE:HD11	1.84	0.60
1:D:133:ALA:O	1:D:193:ASP:HB2	2.01	0.59
1:G:101:ILE:HG12	1:G:112:THR:HG22	1.83	0.59
2:B:36:ARG:HD2	2:B:49:ASP:OD1	2.01	0.59
2:E:122:PRO:CB	2:E:123:PRO:HD3	2.16	0.59
2:H:222:GLN:HG3	7:H:4037:HOH:O	2.01	0.59
2:E:126:ASN:HB2	7:E:3151:HOH:O	2.03	0.59
1:D:210:LYS:HG2	4:D:3016:BR:BR	2.58	0.59
2:E:13:SER:HB2	2:E:80:LEU:HB3	1.84	0.59
1:A:72:VAL:O	1:A:76:LYS:HB2	2.03	0.59
1:G:72:VAL:O	1:G:76:LYS:HB2	2.02	0.58
3:I:39:LEU:HD12	3:I:46:LEU:HD12	1.84	0.58
2:B:210:ARG:HH11	2:B:210:ARG:HG3	1.67	0.58
2:E:144:ILE:HG22	2:E:206:THR:HG21	1.84	0.58
3:I:125:ASN:O	3:I:126:LEU:HG	2.04	0.58
1:G:31:THR:HG22	7:G:3103:HOH:O	2.04	0.58
3:I:244:VAL:HG23	4:I:3011:BR:BR	2.58	0.58
3:I:23:ASP:HB2	3:I:41:ARG:HH21	1.69	0.57
2:B:244:ARG:NH1	2:B:244:ARG:CG	2.56	0.57
1:D:186:PRO:HD3	2:E:106:PHE:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:16:LEU:HD12	2:H:80:LEU:HD11	1.86	0.57
3:F:130:ILE:HG13	3:F:131:SER:N	2.19	0.57
3:F:235:LYS:HD3	4:F:3024:BR:BR	2.59	0.57
1:G:20:THR:HG21	1:G:76:LYS:CE	2.34	0.57
2:E:16:LEU:CD1	2:E:80:LEU:HD11	2.31	0.57
1:G:175:LYS:HG2	2:H:112:LEU:HD23	1.86	0.57
3:F:50:ASN:ND2	4:F:3024:BR:BR	2.89	0.57
3:I:183:LEU:HD21	3:I:186:LEU:HD13	1.86	0.57
1:G:210:LYS:HG2	4:G:3052:BR:BR	2.60	0.56
1:A:4:ILE:HG13	1:A:35:ILE:HD11	1.87	0.56
1:G:149:ASP:HB3	1:G:177:TYR:CE1	2.40	0.56
1:G:6:TYR:HB3	1:G:89:ILE:HG22	1.87	0.56
3:I:88:GLU:HB2	3:I:100:ASN:HB2	1.87	0.56
1:D:15:PHE:HA	1:D:241:MET:HE2	1.88	0.56
1:G:140:GLU:HG3	1:G:213:ARG:CA	2.29	0.55
2:H:17:ARG:CG	2:H:17:ARG:HH11	2.13	0.55
1:G:89:ILE:HD11	1:G:100:ILE:CD1	2.24	0.54
3:C:149:VAL:HG11	3:C:170:SER:HB2	1.89	0.54
2:H:138:ILE:CD1	2:H:138:ILE:H	2.06	0.54
1:G:65:PRO:HB3	7:G:3103:HOH:O	2.08	0.54
3:I:10:VAL:CG1	3:I:230:MET:HE1	2.37	0.54
1:A:132:LEU:HD13	1:A:222:SER:HB2	1.90	0.54
1:A:150:VAL:HG11	1:A:157:MET:HB2	1.89	0.54
2:E:94:ASN:HD22	2:E:94:ASN:C	2.11	0.54
3:I:177:SER:OG	3:I:180:THR:HG23	2.08	0.54
2:H:121:GLN:O	6:H:2001:7PG:H22	2.08	0.54
3:C:55:MET:HA	3:I:84:LYS:NZ	2.23	0.54
1:D:27:ILE:HG12	1:D:69:LYS:HG2	1.90	0.54
1:G:6:TYR:HB3	1:G:89:ILE:CG2	2.38	0.54
3:I:39:LEU:HD13	3:I:121:ILE:HG22	1.89	0.53
2:E:171:LEU:HD13	3:F:114:LEU:HD21	1.89	0.53
3:I:28:LYS:HE3	7:I:3097:HOH:O	2.08	0.53
2:E:120:THR:O	2:E:121:GLN:HB2	2.08	0.53
2:E:53:PRO:O	2:E:56:TYR:HB3	2.08	0.53
2:H:145:ASP:OD2	2:H:206:THR:HG21	2.09	0.53
1:D:165:LYS:HG2	1:D:182:MET:HE2	1.91	0.53
2:E:185:LEU:HD13	2:E:188:ALA:HB2	1.90	0.53
1:A:130:VAL:HG23	1:A:132:LEU:HG	1.91	0.53
3:F:44:ILE:HD11	3:F:200:TYR:CZ	2.44	0.52
2:E:11:SER:HB2	2:E:211:ALA:HA	1.91	0.52
2:H:172:SER:HB3	3:I:73:TYR:OH	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:164:ILE:HB	3:I:174:VAL:HG12	1.91	0.52
1:G:22:VAL:HG12	1:G:23:THR:HG23	1.91	0.52
2:E:142:ASP:OD2	2:E:209:ARG:NH2	2.43	0.52
3:F:52:PRO:O	3:F:55:MET:HG2	2.09	0.52
1:G:10:LYS:HA	1:G:83:SER:OG	2.10	0.52
1:A:204:MET:CE	1:A:204:MET:HA	2.40	0.52
1:A:78:ILE:HG23	3:C:145:GLU:HB3	1.91	0.52
2:B:13:SER:HB2	2:B:80:LEU:HB3	1.92	0.52
1:D:42:GLU:CG	1:A:39:HIS:HD1	2.19	0.51
3:I:32:ASP:N	3:I:32:ASP:OD1	2.43	0.51
1:G:56:VAL:CG1	1:G:238:GLY:HA3	2.27	0.51
2:B:244:ARG:HG3	2:B:244:ARG:HH11	1.71	0.51
3:C:16:GLN:HG3	7:C:3100:HOH:O	2.10	0.51
1:G:4:ILE:HD12	1:G:91:LEU:HD12	1.91	0.51
3:C:149:VAL:CG1	3:C:170:SER:HB2	2.41	0.51
1:G:68:VAL:HG11	1:G:98:LEU:HD13	1.93	0.51
1:D:116:LYS:H	1:D:116:LYS:NZ	2.08	0.51
1:G:212:LEU:HD11	1:G:231:ILE:HG21	1.93	0.51
3:C:20:ARG:HE	3:C:203:ASP:HA	1.75	0.51
3:F:1:MET:HG2	3:F:61:VAL:HG22	1.92	0.51
3:I:163:LEU:HD12	3:I:165:LYS:HD2	1.93	0.51
1:G:95:ASP:OD2	1:G:95:ASP:N	2.43	0.51
3:I:8:VAL:HG12	3:I:85:GLU:O	2.11	0.51
3:I:131:SER:OG	3:I:215:LYS:HE2	2.11	0.51
1:G:20:THR:HG21	1:G:76:LYS:NZ	2.26	0.50
3:F:193:LYS:HD3	4:F:3006:BR:BR	2.66	0.50
3:F:227:PHE:CE1	3:F:235:LYS:HG3	2.46	0.50
1:A:16:ILE:O	1:A:20:THR:HG23	2.12	0.50
1:G:150:VAL:HG11	1:G:157:MET:HB3	1.91	0.50
3:I:164:ILE:HB	3:I:174:VAL:CG1	2.41	0.50
1:G:17:ASN:O	1:G:20:THR:HG22	2.12	0.50
1:G:81:LYS:HB2	3:I:145:GLU:HG2	1.94	0.50
3:C:152:ASN:HB3	3:C:243:LYS:HE3	1.92	0.50
2:E:172:SER:HA	3:F:110:ASN:O	2.12	0.50
2:H:159:LYS:HD2	2:H:192:ASP:OD2	2.11	0.50
3:C:5:TYR:HE2	3:C:7:ASP:O	1.95	0.50
1:G:103:ARG:HD2	7:G:3106:HOH:O	2.11	0.50
1:G:12:PHE:CD2	1:G:89:ILE:HD13	2.46	0.50
1:D:162:GLU:O	1:D:163:GLU:HG2	2.11	0.50
3:I:129:ASP:HB2	3:I:192:SER:OG	2.12	0.50
2:E:181:ASP:OD1	7:E:3204:HOH:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:GLU:O	1:G:163:GLU:HG3	2.12	0.50
1:A:43:ASP:CG	1:A:45:VAL:HG13	2.32	0.49
3:C:8:VAL:HG21	3:C:81:ALA:CB	2.42	0.49
3:I:67:PHE:CD1	3:I:97:VAL:HG21	2.46	0.49
3:I:221:GLN:HA	7:I:3108:HOH:O	2.10	0.49
3:F:100:ASN:ND2	3:F:108:GLU:HG3	2.25	0.49
3:I:10:VAL:HG11	3:I:230:MET:HE1	1.95	0.49
3:I:159:GLU:HG3	3:I:188:PHE:CD2	2.47	0.49
1:G:163:GLU:OE2	1:G:165:LYS:HD2	2.13	0.49
2:B:210:ARG:NH1	2:B:210:ARG:CG	2.67	0.49
1:A:4:ILE:HD13	1:A:91:LEU:HB2	1.95	0.49
1:A:75:VAL:HA	1:A:78:ILE:HD12	1.94	0.49
1:G:29:ASN:O	1:G:35:ILE:HA	2.12	0.49
3:I:120:GLU:H	3:I:120:GLU:CD	2.15	0.49
2:B:245:ALA:HB2	7:B:3092:HOH:O	2.12	0.49
1:D:135:ASN:ND2	7:D:3086:HOH:O	2.45	0.49
3:F:156:GLU:HG3	3:F:193:LYS:HG3	1.95	0.48
1:D:70:LEU:HD21	1:D:98:LEU:HD22	1.93	0.48
1:D:173:GLU:O	1:D:176:ARG:NH2	2.45	0.48
3:I:192:SER:HB3	3:I:219:GLY:HA2	1.95	0.48
2:E:184:THR:HG21	3:F:105:THR:HG22	1.94	0.48
2:E:184:THR:CG2	3:F:105:THR:HG22	2.44	0.48
3:C:112:ARG:HG2	3:C:112:ARG:NH1	2.26	0.48
1:G:70:LEU:HD21	1:G:98:LEU:HD22	1.96	0.48
3:F:30:LYS:HE2	3:F:35:GLU:OE2	2.14	0.48
3:I:52:PRO:HB2	3:I:54:GLU:OE1	2.14	0.48
1:A:15:PHE:CD2	1:A:50:MET:HG3	2.48	0.48
2:E:122:PRO:HB2	2:E:123:PRO:HD2	1.82	0.48
3:I:107:ARG:NH2	3:I:107:ARG:HG3	2.23	0.48
1:A:126:THR:HG22	1:A:127:GLU:H	1.79	0.48
2:H:69:ILE:HG23	2:H:114:LEU:HD22	1.95	0.48
3:I:164:ILE:O	3:I:174:VAL:HG12	2.14	0.48
1:A:212:LEU:HD13	1:A:219:THR:HG21	1.96	0.47
3:C:75:MET:HE2	7:C:3100:HOH:O	2.14	0.47
2:B:132:LYS:HG2	4:B:3036:BR:BR	2.69	0.47
1:D:121:GLN:HG3	7:D:3140:HOH:O	2.15	0.47
2:B:146:GLU:HB3	3:C:80:VAL:HG13	1.96	0.47
3:I:15:ILE:HG22	3:I:75:MET:HG2	1.96	0.47
1:D:86:LYS:HD2	1:D:106:LYS:HB2	1.96	0.47
2:H:55:SER:HB3	2:H:233:GLN:CG	2.42	0.47
1:D:203:GLU:HG2	7:D:3045:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:ILE:CD1	3:C:105:THR:HG21	2.43	0.47
2:B:163:LEU:HB3	2:B:178:LEU:HB2	1.95	0.47
2:E:171:LEU:HB3	3:F:112:ARG:HB3	1.96	0.47
3:C:27:LEU:HD13	3:C:36:LEU:HD12	1.95	0.47
3:C:130:ILE:HD11	3:C:186:LEU:HD11	1.97	0.47
1:G:149:ASP:OD2	2:H:108:ARG:HD2	2.15	0.47
2:H:105:GLU:HB3	7:H:4130:HOH:O	2.15	0.47
2:B:178:LEU:HA	2:B:184:THR:CG2	2.45	0.47
1:G:38:ARG:HG3	1:G:38:ARG:O	2.15	0.47
2:H:89:LEU:HD23	2:H:90:ILE:N	2.30	0.47
3:F:104:SER:HB3	7:F:3137:HOH:O	2.14	0.47
3:F:23:ASP:OD1	3:C:41:ARG:HG2	2.15	0.47
3:F:72:GLN:HB2	7:F:3062:HOH:O	2.15	0.47
2:E:163:LEU:HB3	2:E:178:LEU:HB2	1.97	0.47
1:D:97:GLY:HA2	1:D:119:LYS:HE3	1.95	0.47
3:C:21:LEU:O	3:C:41:ARG:HG3	2.14	0.46
1:A:30:PHE:O	1:A:65:PRO:HA	2.16	0.46
2:B:244:ARG:NH1	2:B:244:ARG:HG3	2.30	0.46
1:D:42:GLU:HG3	1:A:39:HIS:ND1	2.19	0.46
2:B:228:ARG:HD2	2:B:236:TYR:HB2	1.96	0.46
3:C:146:VAL:HG13	3:C:166:ALA:HB2	1.97	0.46
3:F:30:LYS:HD3	7:F:3051:HOH:O	2.15	0.46
1:A:143:LEU:HB3	1:A:209:VAL:HG21	1.98	0.46
3:I:105:THR:OG1	3:I:107:ARG:NH2	2.49	0.46
2:H:44:ARG:O	6:H:2001:7PG:H121	2.16	0.46
1:D:203:GLU:CG	7:D:3045:HOH:O	2.62	0.46
2:E:203:ALA:O	2:E:206:THR:HG23	2.16	0.46
2:H:13:SER:HB2	2:H:80:LEU:HB3	1.96	0.46
1:D:15:PHE:HA	1:D:241:MET:CE	2.45	0.46
3:F:194:ASN:HD22	3:F:195:SER:H	1.62	0.46
1:A:99:LYS:HD3	1:A:101:ILE:HD11	1.99	0.46
1:D:35:ILE:HD11	1:D:52:ILE:HD12	1.99	0.46
1:A:18:SER:HB2	1:A:241:MET:HE3	1.93	0.45
3:I:54:GLU:HG3	4:I:3032:BR:BR	2.71	0.45
1:G:5:VAL:HG12	1:G:58:SER:OG	2.16	0.45
1:G:162:GLU:O	1:G:163:GLU:CG	2.65	0.45
2:B:146:GLU:OE2	3:C:107:ARG:HD3	2.16	0.45
1:A:2:VAL:HG22	1:A:62:ILE:HG22	1.99	0.45
2:B:209:ARG:NH1	7:B:3151:HOH:O	2.41	0.45
3:I:158:HIS:HB2	3:I:161:ARG:HG2	1.99	0.45
2:B:17:ARG:HH11	2:B:17:ARG:CG	2.08	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:80:LEU:CD2	2:H:89:LEU:HD11	2.47	0.45
3:F:131:SER:HB2	3:F:187:GLU:HB2	1.97	0.45
3:I:52:PRO:O	3:I:55:MET:HG2	2.16	0.45
2:B:226:LYS:HG3	2:B:240:TYR:CE2	2.52	0.45
1:G:40:LEU:CD1	1:G:47:MET:HB2	2.47	0.45
1:A:8:ASN:ND2	1:A:8:ASN:C	2.67	0.45
1:A:78:ILE:HD11	3:C:149:VAL:HG21	1.98	0.45
1:D:165:LYS:HE3	1:D:182:MET:HE2	1.99	0.45
3:I:204:VAL:HG11	3:I:238:TYR:CE1	2.52	0.45
3:C:127:GLN:HB2	3:C:127:GLN:HE21	1.64	0.45
3:C:67:PHE:CD1	3:C:97:VAL:HG21	2.53	0.45
2:B:210:ARG:NH1	2:B:210:ARG:HG2	2.31	0.44
3:C:209:LYS:HE3	4:C:3018:BR:BR	2.72	0.44
1:G:188:LYS:HG2	1:G:188:LYS:H	1.64	0.44
3:C:15:ILE:HG22	3:C:75:MET:HG2	1.99	0.44
1:G:172:GLU:HA	1:G:176:ARG:HG2	1.99	0.44
2:H:178:LEU:HA	2:H:184:THR:HG21	2.00	0.44
1:A:8:ASN:HD21	1:A:85:LYS:HA	1.83	0.44
2:H:69:ILE:HG21	2:H:98:LEU:HD13	1.99	0.44
1:A:146:ILE:HD11	1:A:181:LEU:HD21	2.00	0.44
1:D:77:LYS:H	1:D:77:LYS:HG2	1.62	0.44
2:B:210:ARG:HH11	2:B:210:ARG:HG2	1.80	0.44
3:I:44:ILE:HG23	3:I:241:ALA:HB3	2.00	0.44
1:G:18:SER:CB	1:G:241:MET:CE	2.91	0.43
3:I:156:GLU:O	3:I:163:LEU:HD23	2.18	0.43
1:D:20:THR:HA	1:D:23:THR:O	2.18	0.43
3:F:186:LEU:CD2	3:F:188:PHE:HB2	2.47	0.43
1:G:171:GLY:HA3	1:G:172:GLU:HA	1.74	0.43
3:F:209:LYS:NZ	4:F:3012:BR:BR	3.03	0.43
1:G:86:LYS:HB2	7:G:3069:HOH:O	2.17	0.43
1:A:78:ILE:HD11	3:C:149:VAL:CG2	2.48	0.43
3:C:205:LEU:HD23	3:C:205:LEU:HA	1.88	0.43
3:I:127:GLN:NE2	7:I:3101:HOH:O	2.52	0.43
1:A:175:LYS:HA	2:B:111:GLU:O	2.19	0.43
1:G:12:PHE:HZ	1:G:91:LEU:HD11	1.83	0.43
2:E:4:ALA:HB1	2:E:57:PHE:CD2	2.54	0.43
1:G:18:SER:CB	1:G:241:MET:HE3	2.49	0.43
1:D:173:GLU:HB2	1:D:174:GLY:H	1.69	0.43
2:B:142:ASP:OD2	2:B:209:ARG:NH2	2.52	0.43
2:E:132:LYS:HE3	2:E:218:TYR:OH	2.19	0.43
2:B:28:PHE:HB2	2:B:69:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:53:PRO:O	2:H:56:TYR:HB3	2.19	0.43
1:G:212:LEU:HD13	1:G:219:THR:HG21	2.01	0.42
2:H:111:GLU:HG3	7:H:4094:HOH:O	2.17	0.42
3:C:72:GLN:HB2	7:C:3064:HOH:O	2.19	0.42
3:I:220:ASN:O	3:I:221:GLN:HB2	2.19	0.42
2:H:129:PHE:HA	2:H:130:PRO:HD3	1.89	0.42
1:G:40:LEU:CD2	1:G:44:LYS:HD2	2.39	0.42
1:G:17:ASN:HD22	1:G:76:LYS:CE	2.32	0.42
3:C:55:MET:HA	3:I:84:LYS:HZ2	1.82	0.42
1:G:83:SER:O	1:G:83:SER:OG	2.37	0.42
3:C:130:ILE:HD13	3:C:157:GLY:HA3	2.02	0.42
3:C:193:LYS:H	3:C:220:ASN:ND2	2.18	0.42
2:H:16:LEU:HD12	2:H:80:LEU:CD1	2.48	0.42
1:A:175:LYS:HD2	2:B:112:LEU:CD2	2.49	0.42
1:G:79:LEU:CD2	1:G:100:ILE:HD13	2.49	0.42
3:C:93:SER:HB3	3:C:95:ASP:OD1	2.19	0.42
3:F:12:LYS:HE2	7:F:3134:HOH:O	2.19	0.42
1:G:4:ILE:HG23	1:G:91:LEU:HB2	2.01	0.42
1:D:31:THR:HG22	1:D:122:VAL:CG2	2.49	0.42
3:I:68:GLY:H	3:I:113:ASN:ND2	2.07	0.42
1:G:94:THR:HG22	1:G:95:ASP:N	2.34	0.42
1:A:143:LEU:HB3	1:A:209:VAL:CG2	2.49	0.42
1:D:99:LYS:HD2	1:D:101:ILE:HD11	2.01	0.42
2:H:32:LYS:HB2	7:H:4097:HOH:O	2.19	0.42
2:E:233:GLN:O	2:E:234:GLU:HB2	2.20	0.42
2:B:244:ARG:NH1	2:B:244:ARG:HG2	2.21	0.42
2:B:5:LYS:HE3	2:B:88:THR:CG2	2.42	0.42
1:G:76:LYS:HE2	4:G:3045:BR:BR	2.75	0.42
2:B:182:ASN:OD1	2:B:184:THR:HB	2.19	0.42
1:D:31:THR:HB	4:D:3015:BR:BR	2.75	0.42
1:G:3:LYS:HG3	1:G:92:THR:HG23	2.01	0.42
1:D:151:THR:HG21	1:D:206:LYS:HD2	2.01	0.42
2:H:5:LYS:HG3	2:H:90:ILE:HG12	2.02	0.42
1:G:20:THR:HG21	1:G:76:LYS:HE3	2.02	0.41
2:H:163:LEU:HB3	2:H:178:LEU:HB2	2.03	0.41
1:A:20:THR:HA	1:A:23:THR:O	2.20	0.41
3:C:227:PHE:CZ	3:C:235:LYS:HG2	2.54	0.41
1:G:45:VAL:HG22	1:G:204:MET:HG3	2.02	0.41
2:E:12:PHE:CE2	2:E:16:LEU:HD11	2.55	0.41
1:D:8:ASN:ND2	1:D:10:LYS:H	2.18	0.41
1:D:8:ASN:HD22	1:D:10:LYS:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:120:THR:HG22	7:H:4076:HOH:O	2.19	0.41
2:B:46:VAL:HG22	2:B:241:ILE:HG12	2.01	0.41
2:H:193:VAL:HG21	2:H:220:GLY:HA2	2.02	0.41
1:D:166:ILE:CD1	1:D:190:LEU:HD13	2.51	0.41
1:G:78:ILE:HD11	3:I:149:VAL:CG1	2.49	0.41
3:I:85:GLU:OE2	3:I:107:ARG:NH1	2.53	0.41
3:I:68:GLY:N	3:I:113:ASN:HD21	2.10	0.41
1:A:114:TYR:HB2	3:C:171:GLU:HG3	2.02	0.41
1:D:35:ILE:HG13	1:D:52:ILE:HB	2.03	0.41
3:I:194:ASN:ND2	3:I:195:SER:H	2.19	0.41
1:D:146:ILE:HD11	1:D:181:LEU:HD21	2.03	0.41
3:I:72:GLN:HG3	4:I:3048:BR:BR	2.76	0.41
1:D:235:ALA:HA	4:D:3039:BR:BR	2.76	0.41
1:D:128:PRO:HB2	1:D:130:VAL:HG22	2.01	0.41
3:C:244:VAL:HG22	4:C:3008:BR:BR	2.76	0.41
1:D:149:ASP:HB3	1:D:177:TYR:CE1	2.56	0.41
2:B:40:ILE:HG12	2:B:47:PHE:HD1	1.86	0.41
2:E:158:SER:HA	2:E:162:LYS:O	2.21	0.41
1:G:38:ARG:HB2	1:G:49:ILE:HG12	2.02	0.41
1:A:4:ILE:CD1	1:A:91:LEU:HB2	2.51	0.41
1:G:167:LYS:HG3	1:G:180:PHE:CE2	2.56	0.41
1:D:158:ARG:HG3	1:D:199:SER:HB3	2.03	0.41
2:H:168:ILE:O	2:H:168:ILE:HG22	2.21	0.41
1:D:81:LYS:HB3	1:D:81:LYS:HE2	1.78	0.41
1:D:6:TYR:HA	1:D:7:PRO:HD3	1.93	0.41
3:C:121:ILE:HG22	3:C:122:PRO:HD2	2.03	0.41
3:I:156:GLU:HB3	3:I:163:LEU:CD2	2.50	0.41
3:I:125:ASN:HB3	3:I:126:LEU:HD12	2.02	0.41
1:A:99:LYS:HE2	1:A:114:TYR:CE1	2.56	0.41
2:B:129:PHE:CG	2:B:218:TYR:HB3	2.56	0.41
2:B:218:TYR:HB2	2:B:226:LYS:HB3	2.01	0.41
1:D:5:VAL:HB	1:D:59:GLU:HB2	2.03	0.41
1:A:163:GLU:O	1:A:164:ASP:OD1	2.38	0.41
1:D:116:LYS:H	1:D:116:LYS:HZ2	1.68	0.41
3:I:53:ARG:HG3	4:I:3032:BR:BR	2.76	0.41
1:G:176:ARG:HE	1:G:176:ARG:HB3	1.74	0.41
1:G:106:LYS:HD3	1:G:106:LYS:HA	1.89	0.41
1:G:210:LYS:HE2	1:G:210:LYS:HB3	1.84	0.40
1:D:15:PHE:CD2	1:D:50:MET:HG3	2.56	0.40
1:G:70:LEU:CD2	1:G:98:LEU:HD22	2.50	0.40
2:H:2:MET:HG2	2:H:3:LYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:ILE:HG23	2:B:110:PHE:CD1	2.56	0.40
3:I:128:PHE:CG	3:I:217:SER:HB3	2.57	0.40
1:D:8:ASN:ND2	1:D:8:ASN:C	2.72	0.40
1:G:93:GLU:OE2	1:G:119:LYS:HE3	2.21	0.40
3:C:53:ARG:HG3	3:C:53:ARG:NH1	2.36	0.40
1:G:72:VAL:HA	1:G:75:VAL:HG22	2.04	0.40
3:C:52:PRO:O	3:C:55:MET:HG2	2.21	0.40
3:F:93:SER:HA	3:F:94:PRO:HD3	1.95	0.40
3:F:81:ALA:HA	3:F:85:GLU:OE2	2.21	0.40
3:I:73:TYR:O	3:I:76:LYS:HB2	2.21	0.40
1:A:232:ASP:OD1	1:A:240:HIS:HD2	2.04	0.40
1:G:94:THR:HG22	1:G:96:SER:H	1.87	0.40
2:B:218:TYR:CD1	2:B:226:LYS:HD2	2.57	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	246/249 (99%)	236 (96%)	8 (3%)	2 (1%)	24 41
1	D	247/249 (99%)	239 (97%)	7 (3%)	1 (0%)	39 61
1	G	247/249 (99%)	237 (96%)	10 (4%)	0	100 100
2	B	243/246 (99%)	237 (98%)	6 (2%)	0	100 100
2	E	240/246 (98%)	232 (97%)	6 (2%)	2 (1%)	24 41
2	H	244/246 (99%)	237 (97%)	7 (3%)	0	100 100
3	C	242/244 (99%)	227 (94%)	11 (4%)	4 (2%)	11 19
3	F	242/244 (99%)	231 (96%)	11 (4%)	0	100 100
3	I	238/244 (98%)	228 (96%)	10 (4%)	0	100 100
All	All	2189/2217 (99%)	2104 (96%)	76 (4%)	9 (0%)	39 61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	126	LEU
3	C	179	ASP
2	E	122	PRO
1	A	128	PRO
3	C	124	ILE
1	D	163	GLU
1	A	163	GLU
3	C	119	GLN
2	E	121	GLN

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	218/220 (99%)	200 (92%)	18 (8%)	14 26
1	D	220/220 (100%)	201 (91%)	19 (9%)	13 24
1	G	219/220 (100%)	195 (89%)	24 (11%)	8 14
2	B	219/220 (100%)	197 (90%)	22 (10%)	9 18
2	E	218/220 (99%)	200 (92%)	18 (8%)	14 26
2	H	220/220 (100%)	199 (90%)	21 (10%)	11 20
3	C	220/220 (100%)	195 (89%)	25 (11%)	7 13
3	F	220/220 (100%)	206 (94%)	14 (6%)	22 39
3	I	218/220 (99%)	194 (89%)	24 (11%)	8 14
All	All	1972/1980 (100%)	1787 (91%)	185 (9%)	11 20

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	8	ASN
1	D	20	THR
1	D	38	ARG
1	D	42	GLU

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Mol	Chain	Res	Type
1	D	69	LYS
1	D	84	SER
1	D	116	LYS
1	D	124	GLN
1	D	130	VAL
1	D	135	ASN
1	D	140	GLU
1	D	141	SER
1	D	173	GLU
1	D	187	LEU
1	D	193	ASP
1	D	198	SER
1	D	199	SER
1	D	203	GLU
1	D	222	SER
2	E	13	SER
2	E	33	GLU
2	E	36	ARG
2	E	41	ASP
2	E	55	SER
2	E	66	LYS
2	E	73	LEU
2	E	94	ASN
2	E	95	GLU
2	E	96	SER
2	E	109	SER
2	E	138	ILE
2	E	144	ILE
2	E	170	ASP
2	E	173	THR
2	E	181	ASP
2	E	214	SER
2	E	246	ASP
3	F	1	MET
3	F	11	LEU
3	F	12	LYS
3	F	44	ILE
3	F	72	GLN
3	F	76	LYS
3	F	112	ARG
3	F	125	ASN
3	F	127	GLN

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Mol	Chain	Res	Type
3	F	130	ILE
3	F	135	SER
3	F	179	ASP
3	F	194	ASN
3	F	243	LYS
1	A	1	MET
1	A	4	ILE
1	A	8	ASN
1	A	50	MET
1	A	66	THR
1	A	116	LYS
1	A	126	THR
1	A	131	ASN
1	A	140	GLU
1	A	141	SER
1	A	164	ASP
1	A	175	LYS
1	A	187	LEU
1	A	195	SER
1	A	204	MET
1	A	219	THR
1	A	222	SER
1	A	241	MET
2	B	17	ARG
2	B	32	LYS
2	B	33	GLU
2	B	36	ARG
2	B	41	ASP
2	B	66	LYS
2	B	73	LEU
2	B	85	LYS
2	B	97	LYS
2	B	105	GLU
2	B	116	GLN
2	B	126	ASN
2	B	127	LEU
2	B	152	GLU
2	B	170	ASP
2	B	173	THR
2	B	184	THR
2	B	209	ARG
2	B	210	ARG

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Mol	Chain	Res	Type
2	B	226	LYS
2	B	228	ARG
2	B	244	ARG
3	C	1	MET
3	C	8	VAL
3	C	27	LEU
3	C	44	ILE
3	C	47	ILE
3	C	53	ARG
3	C	72	GLN
3	C	96	SER
3	C	106	ASN
3	C	112	ARG
3	C	119	GLN
3	C	125	ASN
3	C	127	GLN
3	C	135	SER
3	C	144	SER
3	C	148	THR
3	C	152	ASN
3	C	153	VAL
3	C	165	LYS
3	C	169	GLU
3	C	178	LYS
3	C	179	ASP
3	C	184	GLN
3	C	194	ASN
3	C	229	ASN
1	G	4	ILE
1	G	20	THR
1	G	35	ILE
1	G	38	ARG
1	G	40	LEU
1	G	45	VAL
1	G	55	ASP
1	G	67	SER
1	G	70	LEU
1	G	83	SER
1	G	88	THR
1	G	95	ASP
1	G	106	LYS
1	G	110	LYS

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Mol	Chain	Res	Type
1	G	130	VAL
1	G	135	ASN
1	G	158	ARG
1	G	164	ASP
1	G	165	LYS
1	G	188	LYS
1	G	198	SER
1	G	209	VAL
1	G	220	MET
1	G	222	SER
2	H	2	MET
2	H	17	ARG
2	H	24	SER
2	H	33	GLU
2	H	41	ASP
2	H	44	ARG
2	H	46	VAL
2	H	65	GLU
2	H	72	LYS
2	H	73	LEU
2	H	85	LYS
2	H	118	GLU
2	H	120	THR
2	H	128	GLU
2	H	138	ILE
2	H	173	THR
2	H	184	THR
2	H	189	SER
2	H	206	THR
2	H	222	GLN
2	H	234	GLU
3	I	1	MET
3	I	9	ARG
3	I	23	ASP
3	I	32	ASP
3	I	39	LEU
3	I	46	LEU
3	I	47	ILE
3	I	83	ARG
3	I	84	LYS
3	I	95	ASP
3	I	104	SER

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Mol	Chain	Res	Type
3	I	125	ASN
3	I	127	GLN
3	I	130	ILE
3	I	151	ASP
3	I	161	ARG
3	I	162	ILE
3	I	163	LEU
3	I	170	SER
3	I	171	GLU
3	I	184	GLN
3	I	194	ASN
3	I	206	SER
3	I	243	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	8	ASN
1	D	17	ASN
1	D	21	ASN
1	D	131	ASN
1	D	135	ASN
2	E	64	GLN
2	E	94	ASN
2	E	121	GLN
2	E	157	HIS
2	E	161	ASN
2	E	233	GLN
3	F	100	ASN
3	F	127	GLN
3	F	194	ASN
3	F	229	ASN
1	A	8	ASN
1	A	17	ASN
1	A	21	ASN
1	A	124	GLN
1	A	240	HIS
2	B	27	ASN
2	B	64	GLN
2	B	116	GLN
2	B	126	ASN
2	B	233	GLN

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Mol	Chain	Res	Type
3	C	16	GLN
3	C	100	ASN
3	C	127	GLN
3	C	184	GLN
3	C	194	ASN
3	C	220	ASN
3	C	225	GLN
3	C	229	ASN
1	G	17	ASN
1	G	21	ASN
1	G	135	ASN
2	H	27	ASN
3	I	100	ASN
3	I	113	ASN
3	I	184	GLN
3	I	194	ASN
3	I	229	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 56 ligands modelled in this entry, 55 are monoatomic - leaving 1 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	$\#\|Z\|>2$
6	7PG	H	2001	5	25,25,25	0.73	0	24,24,24	0.50	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
6	7PG	H	2001	5	-	0/23/23/23	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	2001	7PG	2	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	248/249 (99%)	0.20	14 (5%)	28	31	24, 43, 66, 84	0
1	D	249/249 (100%)	0.19	7 (2%)	56	61	22, 38, 58, 73	0
1	G	249/249 (100%)	0.39	21 (8%)	14	14	24, 44, 67, 77	0
2	B	245/246 (99%)	-0.13	7 (2%)	55	60	18, 32, 47, 65	0
2	E	244/246 (99%)	0.14	8 (3%)	50	55	18, 30, 48, 67	0
2	H	246/246 (100%)	-0.02	11 (4%)	37	42	19, 31, 50, 78	0
3	C	244/244 (100%)	0.41	23 (9%)	11	11	27, 42, 65, 80	0
3	F	244/244 (100%)	0.42	18 (7%)	17	19	27, 40, 66, 88	0
3	I	242/244 (99%)	0.42	19 (7%)	15	17	29, 44, 64, 84	0
All	All	2211/2217 (99%)	0.22	128 (5%)	26	30	18, 38, 63, 88	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	82	LYS	8.3
2	H	125	VAL	7.2
3	I	244	VAL	7.1
2	E	122	PRO	7.0
3	C	123	GLU	6.7
2	H	246	ASP	6.6
3	C	125	ASN	5.8
3	I	179	ASP	5.7
2	E	246	ASP	5.7
1	G	1	MET	5.5
1	A	1	MET	5.4
3	C	169	GLU	5.4
3	I	125	ASN	5.3
3	I	232	GLY	5.3
2	H	124	SER	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	125	VAL	5.2
3	F	179	ASP	5.1
3	C	124	ILE	5.1
1	A	63	ASP	4.7
3	I	120	GLU	4.7
1	G	249	LEU	4.6
3	C	62	ASN	4.5
2	H	170	ASP	4.5
3	I	122	PRO	4.5
3	C	122	PRO	4.5
2	E	171	LEU	4.5
2	B	124	SER	4.4
3	F	178	LYS	4.3
1	D	249	LEU	4.3
3	F	169	GLU	4.3
3	C	178	LYS	4.2
3	C	244	VAL	4.1
3	C	83	ARG	4.0
2	E	123	PRO	4.0
3	F	83	ARG	4.0
3	C	61	VAL	4.0
2	H	245	ALA	3.9
2	B	126	ASN	3.9
1	G	85	LYS	3.8
2	H	171	LEU	3.8
3	C	179	ASP	3.8
3	I	119	GLN	3.8
3	I	184	GLN	3.8
1	A	128	PRO	3.7
3	C	121	ILE	3.7
3	F	125	ASN	3.7
1	A	173	GLU	3.7
3	I	169	GLU	3.7
3	C	92	GLU	3.6
3	F	123	GLU	3.6
3	C	233	GLY	3.4
2	B	128	GLU	3.4
3	F	121	ILE	3.4
1	A	126	THR	3.3
3	I	126	LEU	3.2
2	H	126	ASN	3.2
1	A	163	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	127	GLU	3.1
2	H	169	GLY	3.1
1	G	124	GLN	3.0
3	C	9	ARG	3.0
1	G	63	ASP	2.9
3	C	60	ASP	2.9
1	G	32	GLU	2.9
3	F	73	TYR	2.9
1	A	121	GLN	2.9
1	A	95	ASP	2.8
1	G	163	GLU	2.8
1	A	131	ASN	2.8
3	F	120	GLU	2.7
3	I	118	GLU	2.7
3	F	232	GLY	2.7
1	G	55	ASP	2.7
1	G	123	GLU	2.7
1	G	121	GLN	2.7
3	F	170	SER	2.7
1	D	60	TYR	2.7
2	E	118	GLU	2.7
1	A	62	ILE	2.7
1	A	85	LYS	2.7
3	I	82	LYS	2.6
3	I	83	ARG	2.5
1	D	172	GLU	2.5
1	G	105	GLU	2.5
3	C	31	GLN	2.5
3	C	231	GLU	2.5
1	G	83	SER	2.5
3	C	94	PRO	2.5
3	F	231	GLU	2.5
1	G	106	LYS	2.4
3	C	148	THR	2.4
1	G	173	GLU	2.4
1	G	86	LYS	2.4
3	F	233	GLY	2.4
1	G	24	ASP	2.4
2	H	128	GLU	2.4
3	F	9	ARG	2.3
2	B	170	ASP	2.3
1	D	173	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	92	GLU	2.3
2	E	16	LEU	2.3
1	G	95	ASP	2.3
3	C	63	ASP	2.3
1	D	82	ALA	2.2
3	F	124	ILE	2.2
3	C	151	ASP	2.2
2	B	171	LEU	2.2
1	D	163	GLU	2.2
2	H	160	GLU	2.2
3	I	178	LYS	2.2
3	I	94	PRO	2.2
1	G	164	ASP	2.2
3	F	244	VAL	2.2
1	G	194	THR	2.2
3	I	41	ARG	2.2
2	H	127	LEU	2.1
3	I	121	ILE	2.1
2	B	127	LEU	2.1
3	I	168	GLY	2.1
3	I	42	ALA	2.1
1	A	216	SER	2.1
2	E	222	GLN	2.1
1	G	59	GLU	2.1
3	C	126	LEU	2.0
1	A	64	SER	2.0
2	E	50	ILE	2.0
1	D	77	LYS	2.0
1	G	42	GLU	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
6	7PG	H	2001	26/26	0.82	0.21	0.34	43,57,65,66	0
4	BR	D	3039	1/1	0.95	0.15	0.25	66,66,66,66	1
4	BR	A	3046	1/1	0.91	0.14	-0.26	64,64,64,64	1
4	BR	A	3047	1/1	0.96	0.12	-0.79	47,47,47,47	1
4	BR	B	3036	1/1	0.93	0.12	-0.95	52,52,52,52	1
4	BR	E	3001	1/1	0.98	0.08	-1.17	36,36,36,36	1
4	BR	H	3051	1/1	0.95	0.07	-1.30	56,56,56,56	1
4	BR	C	3029	1/1	0.99	0.10	-1.59	50,50,50,50	1
4	BR	E	3017	1/1	0.96	0.07	-1.76	56,56,56,56	1
4	BR	F	3023	1/1	0.96	0.10	-2.13	37,37,37,37	1
4	BR	D	3037	1/1	0.89	0.16	-	52,52,52,52	1
4	BR	A	3033	1/1	0.95	0.21	-	52,52,52,52	1
4	BR	E	3050	1/1	0.91	0.12	-	60,60,60,60	1
4	BR	F	3002	1/1	0.99	0.05	-	40,40,40,40	1
4	BR	C	3009	1/1	0.99	0.04	-	53,53,53,53	1
4	BR	I	3032	1/1	0.84	0.12	-	63,63,63,63	1
4	BR	F	3006	1/1	0.94	0.11	-	42,42,42,42	1
4	BR	E	3040	1/1	0.97	0.06	-	65,65,65,65	1
4	BR	H	3014	1/1	0.99	0.04	-	39,39,39,39	1
4	BR	F	3021	1/1	0.92	0.11	-	63,63,63,63	1
4	BR	C	3018	1/1	0.95	0.12	-	57,57,57,57	1
4	BR	F	3041	1/1	0.93	0.11	-	50,50,50,50	1
4	BR	H	3020	1/1	0.92	0.07	-	49,49,49,49	1
4	BR	H	3025	1/1	0.98	0.05	-	49,49,49,49	1
4	BR	G	3045	1/1	0.91	0.16	-	52,52,52,52	1
4	BR	I	3003	1/1	0.94	0.12	-	50,50,50,50	1
4	BR	F	3024	1/1	0.97	0.05	-	40,40,40,40	1
4	BR	D	3016	1/1	0.95	0.09	-	51,51,51,51	1
4	BR	E	3022	1/1	0.99	0.10	-	42,42,42,42	1
4	BR	I	3019	1/1	0.93	0.13	-	56,56,56,56	1
4	BR	F	3005	1/1	0.99	0.05	-	44,44,44,44	1
4	BR	A	3044	1/1	0.95	0.24	-	56,56,56,56	1
4	BR	B	3031	1/1	0.93	0.14	-	63,63,63,63	1
4	BR	F	3030	1/1	0.99	0.05	-	53,53,53,53	1
4	BR	G	3052	1/1	0.93	0.11	-	48,48,48,48	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	BR	E	3010	1/1	0.87	0.17	-	50,50,50,50	1
4	BR	B	3038	1/1	0.95	0.12	-	40,40,40,40	1
4	BR	D	3015	1/1	0.95	0.09	-	40,40,40,40	1
4	BR	F	3034	1/1	0.98	0.07	-	51,51,51,51	1
4	BR	B	3053	1/1	0.98	0.07	-	51,51,51,51	1
4	BR	E	3049	1/1	0.95	0.14	-	56,56,56,56	1
4	BR	C	3042	1/1	0.95	0.06	-	52,52,52,52	1
4	BR	F	3012	1/1	0.95	0.08	-	43,43,43,43	1
4	BR	C	3008	1/1	0.98	0.05	-	40,40,40,40	1
4	BR	I	3011	1/1	0.96	0.07	-	53,53,53,53	1
4	BR	D	3028	1/1	0.91	0.14	-	58,58,58,58	1
4	BR	I	3007	1/1	0.98	0.07	-	44,44,44,44	1
4	BR	H	3004	1/1	0.94	0.09	-	50,50,50,50	1
4	BR	E	3013	1/1	0.99	0.09	-	46,46,46,46	1
5	K	H	4001	1/1	0.70	0.22	-	122,122,122,122	0
4	BR	I	3048	1/1	0.88	0.17	-	60,60,60,60	1
4	BR	A	3043	1/1	0.86	0.11	-	52,52,52,52	1
4	BR	C	3054	1/1	0.94	0.15	-	60,60,60,60	1
4	BR	D	3027	1/1	0.94	0.08	-	53,53,53,53	1
4	BR	C	3035	1/1	0.94	0.11	-	50,50,50,50	1
4	BR	B	3026	1/1	0.97	0.13	-	65,65,65,65	1

6.5 Other polymers (i)

There are no such residues in this entry.