



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 08:03 AM BST

PDB ID : 6CBI
Title : PCNA in complex with inhibitor
Authors : Bruning, J.B.; Wegener, K.L.
Deposited on : 2018-02-03
Resolution : 2.75 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

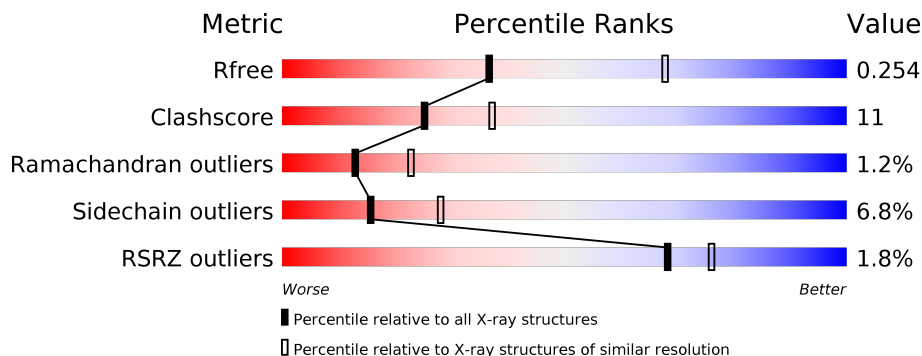
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.




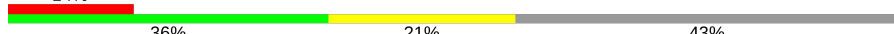

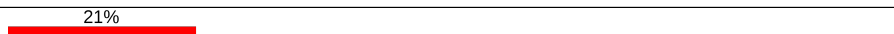
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 respectively. 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 $\leq 5\%$. 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	261	
1	B	261	
1	C	261	
1	D	261	
1	E	261	
1	F	261	

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Mol	Chain	Length	Quality of chain
2	H	14	
2	I	14	
2	J	14	
2	K	14	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11944 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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	248	Total	C	N	O	S	0	1	0
			1885	1186	311	372	16			
1	C	247	Total	C	N	O	S	0	1	0
			1882	1187	314	365	16			
1	E	255	Total	C	N	O	S	0	2	0
			1933	1216	317	384	16			
1	B	246	Total	C	N	O	S	0	1	0
			1867	1177	305	369	16			
1	D	249	Total	C	N	O	S	0	0	0
			1888	1190	308	374	16			
1	F	253	Total	C	N	O	S	0	1	0
			1921	1210	315	380	16			

- Molecule 2 is a protein called GLY-ARG-LYS-ARG-ARG-GLN-DAB-SER-MET-THR-GLU-PHE-TYR-HIS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	11	Total	C	N	O	S	0	0	0
			92	56	21	14	1			
2	I	8	Total	C	N	O	S	0	0	0
			61	38	10	12	1			
2	J	11	Total	C	N	O	S	0	0	0
			94	59	19	15	1			
2	K	11	Total	C	N	O	S	0	0	0
			99	62	21	15	1			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

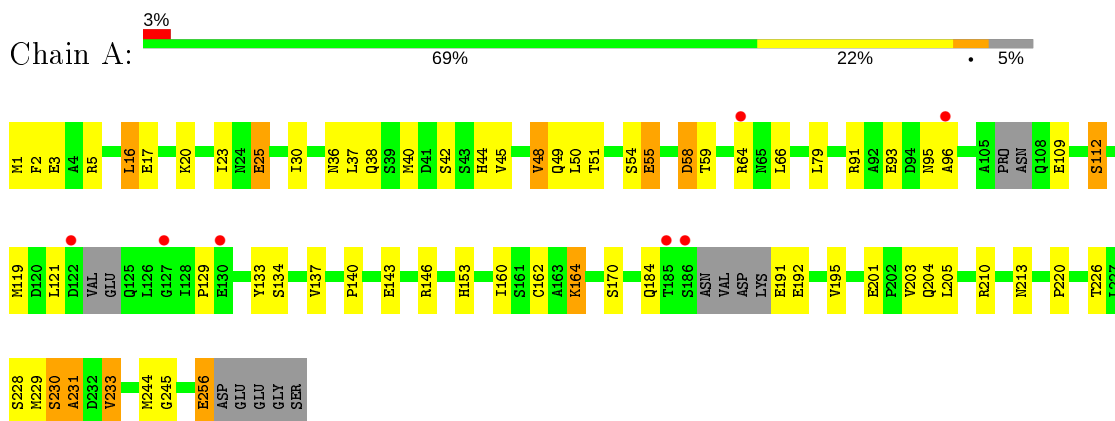
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	C	38	Total	O	0	0
			38	38		
4	E	38	Total	O	0	0
			38	38		
4	B	20	Total	O	0	0
			20	20		
4	D	28	Total	O	0	0
			28	28		
4	F	48	Total	O	0	0
			48	48		
4	H	2	Total	O	0	0
			2	2		
4	J	1	Total	O	0	0
			1	1		
4	K	4	Total	O	0	0
			4	4		

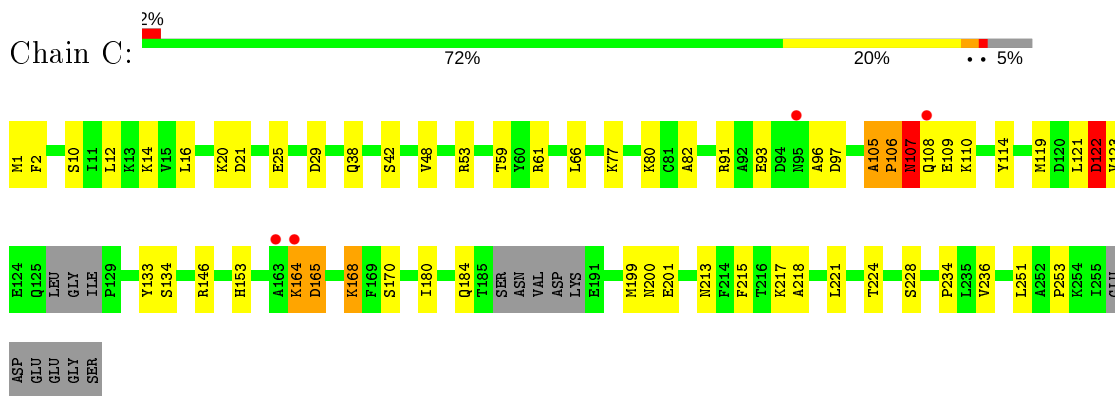
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

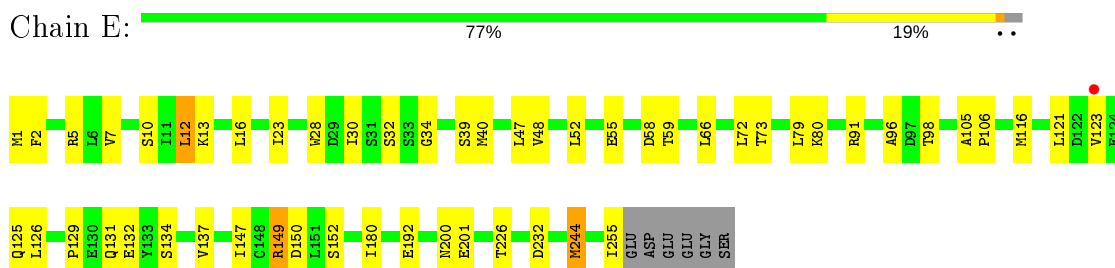
- Molecule 1: Proliferating cell nuclear antigen



- Molecule 1: Proliferating cell nuclear antigen

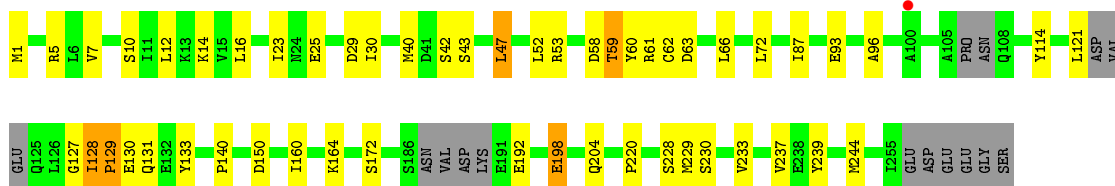


- Molecule 1: Proliferating cell nuclear antigen



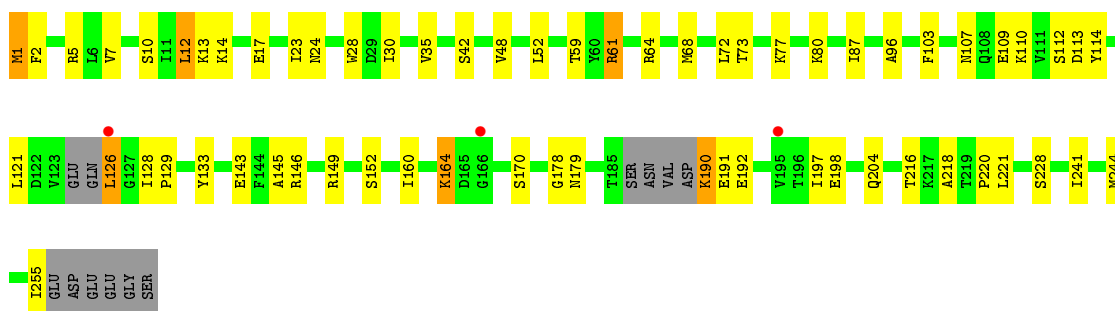
- Molecule 1: Proliferating cell nuclear antigen

Chain B:  74% 18% • 6%




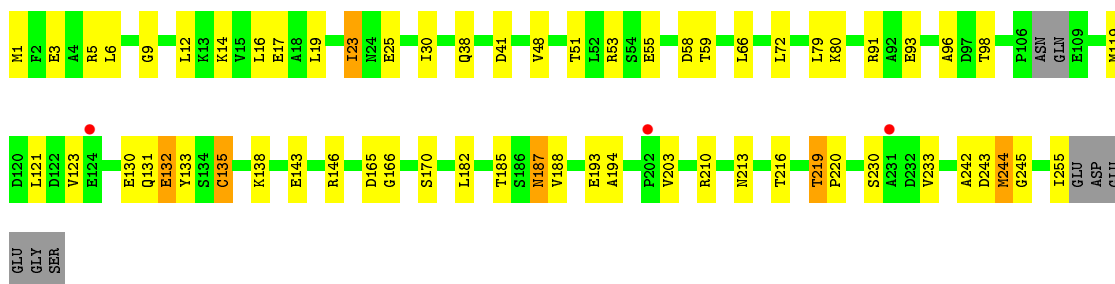
- Molecule 1: Proliferating cell nuclear antigen

Chain D:  71% 22% • 5%



- Molecule 1: Proliferating cell nuclear antigen

Chain F:  73% 21% • •

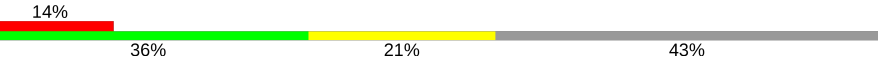


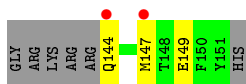
- Molecule 2: GLY-ARG-LYS-ARG-ARG-GLN-DAB-SER-MET-THR-GLU-PHE-TYR-HIS

Chain H:  50% 14% 14% 21%

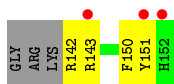


- Molecule 2: GLY-ARG-LYS-ARG-ARG-GLN-DAB-SER-MET-THR-GLU-PHE-TYR-HIS

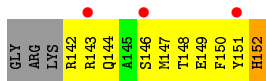
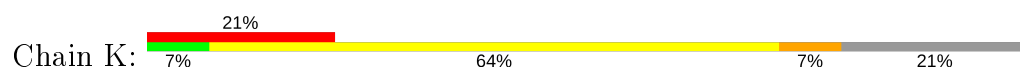
Chain I:  14% 36% 21% 43%



- Molecule 2: GLY-ARG-LYS-ARG-ARG-GLN-DAB-SER-MET-THR-GLU-PHE-TYR-HIS



- Molecule 2: GLY-ARG-LYS-ARG-ARG-GLN-DAB-SER-MET-THR-GLU-PHE-TYR-HIS



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.26Å 144.82Å 174.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.09 – 2.75 41.09 – 2.75	Depositor EDS
% Data completeness (in resolution range)	89.6 (41.09-2.75) 89.8 (41.09-2.75)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.208 , 0.252 0.209 , 0.254	Depositor DCC
R_{free} test set	2334 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtrriage
Anisotropy	0.331	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11944	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, DAB

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	0.32	0/1910	0.59	0/2576
1	B	0.37	0/1892	0.59	0/2552
1	C	0.37	0/1909	0.72	3/2577 (0.1%)
1	D	0.33	0/1912	0.60	1/2581 (0.0%)
1	E	0.32	0/1962	0.53	0/2655
1	F	0.36	0/1946	0.57	0/2632
2	H	0.34	0/85	0.57	0/109
2	I	0.45	0/53	0.51	0/67
2	J	0.47	0/87	0.75	0/112
2	K	0.45	0/93	0.48	0/120
All	All	0.35	0/11849	0.60	4/15981 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	105	ALA	C-N-CD	-20.59	75.31	120.60
1	C	106	PRO	CA-N-CD	-6.58	102.29	111.50
1	C	122	ASP	CB-CG-OD1	6.13	123.82	118.30
1	D	61	ARG	NE-CZ-NH1	-5.41	117.60	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1885	0	1876	51	0
1	B	1867	0	1859	30	0
1	C	1882	0	1889	38	1
1	D	1888	0	1877	48	0
1	E	1933	0	1904	35	0
1	F	1921	0	1907	44	1
2	H	92	0	84	2	0
2	I	61	0	51	3	0
2	J	94	0	86	10	0
2	K	99	0	91	12	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
4	A	33	0	0	15	0
4	B	20	0	0	9	0
4	C	38	0	0	14	0
4	D	28	0	0	4	0
4	E	38	0	0	5	0
4	F	48	0	0	15	0
4	H	2	0	0	0	0
4	J	1	0	0	0	0
4	K	4	0	0	1	0
All	All	11944	0	11624	250	1

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 11.

All (250) 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:107:ASN:O	1:C:109:GLU:N	1.87	1.08
1:C:107:ASN:O	1:C:107:ASN:ND2	1.97	0.97
1:A:256:GLU:O	2:I:144:GLN:N	1.99	0.94
1:F:58[B]:ASP:OD1	4:F:301:HOH:O	1.84	0.94
1:F:188:VAL:HG21	1:F:193:GLU:HB2	1.47	0.93
1:D:1:MET:H3	1:D:61:ARG:HH12	1.05	0.92
1:D:109:GLU:OE1	1:F:185:THR:HG22	1.70	0.91
1:D:129:PRO:HD2	2:J:151:TYR:HE1	1.34	0.91
1:B:198[B]:GLU:OE2	4:B:401:HOH:O	1.91	0.88
1:E:80:LYS:NZ	4:E:301:HOH:O	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HB3	1:D:61:ARG:NH1	1.76	0.81
1:A:143:GLU:OE1	1:A:146:ARG:NH2	2.14	0.80
1:B:5:ARG:HB3	1:B:59:THR:HG23	1.64	0.79
1:D:5:ARG:HB3	1:D:59:THR:HB	1.63	0.79
1:C:59:THR:OG1	4:C:301:HOH:O	2.01	0.77
1:E:132:GLU:OE2	1:E:200:ASN:ND2	2.18	0.76
1:F:185:THR:HB	4:F:316:HOH:O	1.85	0.76
1:E:129:PRO:HD2	2:K:151:TYR:CE1	2.22	0.75
1:F:188:VAL:CG2	1:F:193:GLU:HB2	2.16	0.75
1:B:10:SER:HB2	4:B:412:HOH:O	1.87	0.73
1:D:128:ILE:HA	2:J:151:TYR:CE1	2.24	0.73
1:E:129:PRO:HD2	2:K:151:TYR:HE1	1.53	0.73
1:F:53:ARG:HB2	1:F:244:MET:O	1.88	0.72
1:A:191:GLU:N	4:A:304:HOH:O	2.22	0.72
1:D:1:MET:N	1:D:61:ARG:HH12	1.85	0.72
1:F:143:GLU:OE1	1:F:146:ARG:NH2	2.23	0.72
1:C:77:LYS:NZ	4:C:306:HOH:O	2.24	0.71
1:A:205:LEU:HD12	1:A:229:MET:HG2	1.73	0.70
1:C:213:ASN:ND2	4:C:308:HOH:O	2.24	0.69
1:E:232:ASP:OD2	4:E:302:HOH:O	2.11	0.69
1:F:6:LEU:HD12	4:F:301:HOH:O	1.94	0.68
2:H:148:THR:O	2:H:152:HIS:HB3	1.93	0.68
1:C:105:ALA:HB3	1:C:110:LYS:HB3	1.75	0.67
1:C:29:ASP:OD2	4:C:302:HOH:O	2.12	0.67
1:F:53:ARG:NE	4:F:306:HOH:O	2.25	0.67
1:A:213:ASN:ND2	4:A:306:HOH:O	2.27	0.67
1:E:7:VAL:N	1:E:58[B]:ASP:OD2	2.27	0.67
1:C:119:MET:O	4:C:303:HOH:O	2.12	0.66
1:F:25:GLU:OE1	4:F:302:HOH:O	2.13	0.66
1:D:114:TYR:OH	4:D:401:HOH:O	2.14	0.65
1:B:150:ASP:OD1	4:B:402:HOH:O	2.13	0.65
1:B:30:ILE:HB	1:B:66:LEU:HB2	1.79	0.65
1:C:1:MET:SD	1:C:61:ARG:NH1	2.68	0.65
1:A:162:CYS:O	4:A:303:HOH:O	2.15	0.65
1:A:55:GLU:N	1:A:55:GLU:OE2	2.29	0.64
1:A:119:MET:SD	4:B:413:HOH:O	2.55	0.64
1:E:30:ILE:HB	1:E:66:LEU:HB2	1.79	0.64
1:A:30:ILE:HB	1:A:66:LEU:HB2	1.80	0.64
1:C:97:ASP:N	1:C:97:ASP:OD1	2.22	0.63
1:A:230:SER:HB2	1:A:233:VAL:H	1.63	0.63
1:F:93:GLU:HB2	1:F:96:ALA:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:GLU:OE2	4:B:403:HOH:O	2.15	0.63
1:C:165:ASP:OD1	1:C:165:ASP:N	2.30	0.63
1:D:255:ILE:N	2:J:143:ARG:O	2.31	0.63
1:F:216:THR:O	1:F:219:THR:OG1	2.16	0.63
1:A:184:GLN:HG3	1:A:195:VAL:O	1.98	0.62
1:F:132:GLU:OE2	1:F:132:GLU:HA	1.98	0.62
1:F:25:GLU:HB3	1:F:121:LEU:HD11	1.82	0.61
1:A:36[B]:ASN:ND2	1:A:50:LEU:O	2.34	0.60
1:B:93:GLU:HB2	1:B:96:ALA:HB2	1.83	0.60
1:A:162:CYS:HB3	4:A:303:HOH:O	2.00	0.60
1:A:95:ASN:HA	4:A:315:HOH:O	2.01	0.60
1:D:1:MET:N	1:D:61:ARG:NH1	2.48	0.60
1:B:172:SER:O	4:B:404:HOH:O	2.17	0.59
1:F:91:ARG:HD2	4:F:333:HOH:O	2.01	0.59
1:C:199:MET:O	4:C:304:HOH:O	2.16	0.59
1:D:129:PRO:HD2	2:J:151:TYR:CE1	2.25	0.59
1:B:23:ILE:HG13	1:B:72:LEU:HD12	1.84	0.59
1:E:16:LEU:HG	1:E:79:LEU:HD12	1.84	0.59
1:E:137:VAL:O	1:E:226:THR:HA	2.02	0.59
1:F:9:GLY:N	4:F:312:HOH:O	2.35	0.59
1:D:143:GLU:OE1	1:D:146:ARG:NH2	2.36	0.58
1:B:59:THR:OG1	4:B:405:HOH:O	2.17	0.58
1:D:121:LEU:O	4:D:402:HOH:O	2.17	0.58
1:D:126:LEU:HD11	2:J:151:TYR:O	2.03	0.58
1:F:19:LEU:HB3	1:F:23:ILE:HD11	1.86	0.58
1:C:121:LEU:O	1:C:122:ASP:OD1	2.21	0.58
1:D:23:ILE:HG13	1:D:72:LEU:HD12	1.86	0.58
1:A:230:SER:HB3	1:A:233:VAL:HG22	1.86	0.58
1:C:114:TYR:OH	4:C:305:HOH:O	2.17	0.57
1:E:34:GLY:O	4:E:303:HOH:O	2.17	0.57
1:F:59:THR:OG1	4:F:303:HOH:O	2.16	0.57
1:E:55:GLU:N	1:E:55:GLU:OE1	2.37	0.57
1:F:213:ASN:ND2	4:F:309:HOH:O	2.34	0.57
1:E:40:MET:HE3	2:K:147:MET:HB2	1.86	0.57
1:C:134:SER:HB3	1:C:201:GLU:HG3	1.87	0.57
1:E:23:ILE:HG13	1:E:72:LEU:HD12	1.86	0.56
1:B:230:SER:HB2	1:B:233:VAL:HG11	1.86	0.56
1:D:160:ILE:O	1:D:204:GLN:HA	2.06	0.56
1:C:20:LYS:NZ	4:C:311:HOH:O	2.38	0.55
1:F:5:ARG:HD3	1:F:59:THR:HG23	1.87	0.55
1:E:23:ILE:HD13	1:E:48:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:147:MET:HE1	2:K:151:TYR:HD2	1.72	0.55
1:A:54:SER:OG	1:A:55:GLU:OE2	2.22	0.55
1:A:230:SER:CB	1:A:233:VAL:HG22	2.37	0.54
1:A:93:GLU:HB2	1:A:96:ALA:HB2	1.90	0.54
1:A:203:VAL:N	4:A:303:HOH:O	2.41	0.54
1:F:138:LYS:NZ	4:F:314:HOH:O	2.40	0.53
1:D:52:LEU:HD22	1:D:244:MET:HE2	1.90	0.53
1:D:23:ILE:HD13	1:D:48:VAL:HG11	1.90	0.53
1:A:153:HIS:ND1	4:A:310:HOH:O	2.34	0.53
1:F:23:ILE:HG12	1:F:72:LEU:HD12	1.90	0.53
1:F:17:GLU:OE1	1:F:80:LYS:NZ	2.40	0.52
1:A:230:SER:CB	1:A:233:VAL:H	2.22	0.52
1:C:107:ASN:HD22	1:C:109:GLU:H	1.57	0.52
1:A:91:ARG:NE	4:A:301:HOH:O	2.11	0.52
1:C:93:GLU:HB2	1:C:96:ALA:HB2	1.91	0.52
1:F:58[B]:ASP:OD1	1:F:58[B]:ASP:N	2.43	0.52
1:E:98:THR:HA	1:E:116:MET:O	2.10	0.51
1:D:255:ILE:CB	2:J:143:ARG:H	2.24	0.51
1:A:91:ARG:NH2	4:A:301:HOH:O	2.38	0.51
1:F:14:LYS:HD3	1:F:220:PRO:HB2	1.93	0.51
1:D:103:PHE:HB2	1:D:112:SER:HB2	1.93	0.51
1:D:30:ILE:HD11	1:D:68:MET:HE2	1.93	0.51
1:D:73:THR:HG22	1:D:77:LYS:NZ	2.26	0.50
1:F:131:GLN:HB3	4:F:304:HOH:O	2.11	0.50
1:F:187:ASN:HB3	4:F:316:HOH:O	2.11	0.50
1:D:110:LYS:HE3	1:F:143:GLU:OE2	2.11	0.50
1:E:58[B]:ASP:OD1	4:E:304:HOH:O	2.18	0.50
1:D:128:ILE:HA	2:J:151:TYR:CD1	2.46	0.50
1:C:168:LYS:HG2	4:C:316:HOH:O	2.12	0.50
1:E:47:LEU:HD12	1:E:126:LEU:HD12	1.94	0.50
1:F:131:GLN:HG2	4:F:315:HOH:O	2.10	0.50
1:B:7:VAL:HA	1:B:87:ILE:HD12	1.93	0.49
1:F:51:THR:O	1:F:245:GLY:HA3	2.13	0.49
1:A:44:HIS:ND1	4:A:311:HOH:O	2.35	0.49
1:B:160:ILE:O	1:B:204:GLN:HA	2.12	0.49
1:A:25:GLU:HB2	1:A:121:LEU:HD11	1.93	0.49
2:K:146:SER:O	2:K:149:GLU:HG2	2.13	0.49
1:B:128:ILE:O	1:B:129:PRO:O	2.31	0.49
1:A:16:LEU:HD13	1:A:79:LEU:CD1	2.43	0.48
1:D:149:ARG:O	1:D:152:SER:OG	2.29	0.48
1:F:188:VAL:HG11	1:F:194:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:TYR:CD2	1:D:178:GLY:HA3	2.48	0.48
1:B:133:TYR:CG	1:B:228:SER:HB3	2.49	0.48
1:B:229:MET:HA	4:B:410:HOH:O	2.13	0.48
1:B:61:ARG:HG2	1:B:62:CYS:N	2.28	0.48
1:A:58:ASP:N	1:A:58:ASP:OD1	2.45	0.48
1:D:113:ASP:OD1	4:D:403:HOH:O	2.20	0.48
1:E:40:MET:CE	2:K:147:MET:HB2	2.44	0.48
1:C:184:GLN:HB2	4:C:328:HOH:O	2.13	0.48
1:C:10:SER:O	1:C:14:LYS:HG3	2.13	0.48
1:D:218:ALA:HB1	1:D:221:LEU:HD12	1.96	0.48
2:K:144:GLN:OE1	4:K:201:HOH:O	2.20	0.47
1:B:14:LYS:HE3	4:B:412:HOH:O	2.14	0.47
1:D:14:LYS:HD2	1:D:220:PRO:HB2	1.97	0.47
1:E:10:SER:HA	1:E:13:LYS:HD3	1.97	0.47
1:A:2:PHE:O	1:A:91:ARG:HA	2.15	0.47
1:A:55:GLU:CD	1:A:55:GLU:H	2.16	0.47
1:C:133:TYR:O	1:C:200:ASN:ND2	2.48	0.47
1:A:205:LEU:HD11	1:A:230:SER:OG	2.14	0.47
1:B:25:GLU:HB3	1:B:121:LEU:HD11	1.97	0.47
1:D:2:PHE:CD1	1:D:30:ILE:HG21	2.49	0.47
1:F:133:TYR:HA	1:F:230:SER:OG	2.14	0.47
1:B:61:ARG:NH1	1:B:63:ASP:OD2	2.48	0.46
1:A:153:HIS:CE1	4:A:310:HOH:O	2.66	0.46
1:F:25:GLU:HG2	1:F:119:MET:SD	2.56	0.46
2:H:149:GLU:HG3	2:H:150:PHE:N	2.29	0.46
1:D:12:LEU:HD12	1:D:12:LEU:HA	1.77	0.46
1:A:220:PRO:HG2	4:A:323:HOH:O	2.15	0.46
1:B:128:ILE:HA	1:B:129:PRO:HD2	1.78	0.46
1:D:52:LEU:HD22	1:D:244:MET:CE	2.46	0.46
1:C:164:LYS:O	1:C:164:LYS:HG3	2.16	0.46
1:F:38:GLN:HA	1:F:48:VAL:O	2.16	0.46
1:A:38:GLN:HA	1:A:48:VAL:O	2.15	0.45
1:A:133:TYR:CG	1:A:228:SER:HB3	2.51	0.45
1:F:121:LEU:HD23	1:F:121:LEU:HA	1.86	0.45
1:B:140:PRO:HG3	1:B:192:GLU:O	2.16	0.45
1:D:190:LYS:HA	1:D:190:LYS:HD2	1.38	0.45
1:A:37:LEU:HB3	1:A:50:LEU:HB3	1.97	0.45
1:E:2:PHE:O	1:E:91:ARG:HA	2.17	0.45
1:F:166:GLY:HA3	1:F:182:LEU:O	2.16	0.45
1:A:140:PRO:HG3	1:A:192:GLU:O	2.16	0.45
1:D:145:ALA:HA	1:D:216:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:VAL:HA	1:D:87:ILE:HG23	1.99	0.45
1:E:105:ALA:HB1	1:E:106:PRO:HD2	1.99	0.45
1:F:30:ILE:HB	1:F:66:LEU:HB2	1.98	0.45
1:A:36[A]:ASN:ND2	4:A:314:HOH:O	2.49	0.45
1:D:28:TRP:HE3	1:D:35:VAL:HG11	1.82	0.44
1:E:121:LEU:HA	1:E:121:LEU:HD23	1.85	0.44
1:E:7:VAL:HG23	1:E:58[B]:ASP:OD2	2.17	0.44
2:K:149:GLU:HG3	2:K:150:PHE:N	2.32	0.44
1:D:121:LEU:HA	1:D:121:LEU:HD23	1.89	0.44
1:D:126:LEU:HD11	2:J:151:TYR:C	2.37	0.44
1:E:147:ILE:HG23	1:E:180:ILE:HD12	2.00	0.44
1:F:135:CYS:HB2	1:F:203:VAL:HG23	1.98	0.44
1:F:3:GLU:HG2	4:F:303:HOH:O	2.17	0.44
2:K:147:MET:HE2	2:K:147:MET:HB3	1.79	0.44
1:A:230:SER:OG	1:A:231:ALA:N	2.45	0.44
1:D:109:GLU:OE1	1:F:185:THR:CG2	2.55	0.44
1:B:53:ARG:HG2	1:B:244:MET:O	2.17	0.44
1:A:40:MET:CE	2:I:147:MET:HB2	2.48	0.44
1:E:255:ILE:N	2:K:143:ARG:O	2.45	0.44
1:A:112:SER:HB3	1:C:180:ILE:HG12	1.99	0.44
1:E:5:ARG:HD3	4:E:306:HOH:O	2.18	0.44
1:A:134:SER:HB3	1:A:201:GLU:HG3	2.00	0.43
1:A:184:GLN:HA	1:A:195:VAL:O	2.17	0.43
1:B:237:VAL:HG12	1:B:239:TYR:HE1	1.82	0.43
1:E:39:SER:O	1:E:48:VAL:HG12	2.17	0.43
1:F:23:ILE:HG22	1:F:41:ASP:HA	2.00	0.43
1:C:93:GLU:HB3	4:C:314:HOH:O	2.17	0.43
1:D:126:LEU:HD13	1:D:126:LEU:HA	1.73	0.43
1:C:121:LEU:HA	1:C:121:LEU:HD23	1.49	0.43
1:F:16:LEU:HD22	1:F:79:LEU:HD12	2.00	0.43
1:A:160:ILE:O	1:A:204:GLN:HA	2.19	0.43
1:D:17:GLU:OE2	1:D:80:LYS:NZ	2.30	0.43
1:E:149:ARG:HG3	1:E:150:ASP:N	2.33	0.43
1:E:28:TRP:HE1	1:E:72:LEU:HD21	1.83	0.43
1:C:134:SER:HA	1:C:200:ASN:HB2	2.01	0.43
1:C:82:ALA:HA	4:C:313:HOH:O	2.18	0.43
1:A:45:VAL:O	2:I:147:MET:HG2	2.18	0.43
1:A:51:THR:O	1:A:245:GLY:HA3	2.19	0.42
1:C:21:ASP:OD2	1:C:217:LYS:NZ	2.39	0.42
1:E:149:ARG:O	1:E:152:SER:OG	2.32	0.42
1:B:121:LEU:HD23	1:B:121:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:VAL:O	1:A:226:THR:HA	2.19	0.42
1:A:203:VAL:HG23	4:A:303:HOH:O	2.19	0.42
1:C:12:LEU:HD12	1:C:12:LEU:HA	1.86	0.42
1:C:38:GLN:N	4:C:312:HOH:O	2.39	0.42
1:D:164:LYS:NZ	1:D:197:ILE:O	2.52	0.42
1:E:12:LEU:HD13	1:E:12:LEU:HA	1.92	0.42
1:A:164:LYS:O	1:A:164:LYS:HG3	2.19	0.42
1:E:52:LEU:HD22	1:E:244:MET:HE2	2.02	0.42
1:F:230:SER:HA	4:F:311:HOH:O	2.20	0.42
1:F:53:ARG:HG2	1:F:55:GLU:OE1	2.19	0.42
1:C:215:PHE:HE2	1:C:251:LEU:HB2	1.83	0.42
1:D:1:MET:HB2	1:D:2:PHE:H	1.55	0.42
1:A:3:GLU:CD	4:A:301:HOH:O	2.58	0.41
1:C:2:PHE:O	1:C:91:ARG:HA	2.19	0.41
1:D:10:SER:HA	1:D:13:LYS:HD3	2.01	0.41
1:D:255:ILE:CB	2:J:142:ARG:HA	2.50	0.41
1:C:228:SER:HB2	1:C:236:VAL:HB	2.02	0.41
1:E:134:SER:HB3	1:E:201:GLU:HG3	2.00	0.41
1:C:107:ASN:HD22	1:C:107:ASN:C	2.06	0.41
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.85	0.41
1:C:218:ALA:HB1	1:C:221:LEU:HD12	2.03	0.41
1:B:60:TYR:CD1	1:B:61:ARG:N	2.89	0.41
1:B:40:MET:HG3	1:B:47:LEU:HD12	2.03	0.41
1:B:14:LYS:HE2	1:B:220:PRO:HB3	2.02	0.41
1:C:234:PRO:HA	1:C:253:PRO:HD3	2.02	0.41
2:K:148:THR:O	2:K:152:HIS:HD2	2.04	0.41
1:D:220:PRO:HG2	4:D:410:HOH:O	2.20	0.41
1:E:255:ILE:CB	2:K:142:ARG:HA	2.50	0.41
2:J:150:PHE:HB2	2:J:151:TYR:H	1.67	0.40
1:A:17:GLU:OE2	1:A:20:LYS:NZ	2.54	0.40
1:A:5:ARG:HD3	1:A:59:THR:HG23	2.03	0.40
1:D:133:TYR:CG	1:D:228:SER:HB3	2.56	0.40
1:D:241:ILE:HG22	1:D:244:MET:HB2	2.04	0.40
1:C:153:HIS:NE2	4:C:307:HOH:O	2.24	0.40
1:E:47:LEU:CD1	1:E:126:LEU:HD12	2.50	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ARG:NH1	1:F:187:ASN:OD1[1_655]	2.04	0.16

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	241/261 (92%)	230 (95%)	7 (3%)	4 (2%)	9	16
1	B	239/261 (92%)	230 (96%)	6 (2%)	3 (1%)	12	21
1	C	242/261 (93%)	233 (96%)	5 (2%)	4 (2%)	9	16
1	D	243/261 (93%)	233 (96%)	7 (3%)	3 (1%)	13	23
1	E	255/261 (98%)	243 (95%)	11 (4%)	1 (0%)	34	53
1	F	250/261 (96%)	241 (96%)	7 (3%)	2 (1%)	19	34
2	H	8/14 (57%)	6 (75%)	1 (12%)	1 (12%)	0	0
2	I	5/14 (36%)	5 (100%)	0	0	100	100
2	J	8/14 (57%)	6 (75%)	2 (25%)	0	100	100
2	K	8/14 (57%)	7 (88%)	1 (12%)	0	100	100
All	All	1499/1622 (92%)	1434 (96%)	47 (3%)	18 (1%)	13	23

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLU
1	A	230	SER
1	A	231	ALA
1	C	106	PRO
1	C	107	ASN
1	C	108	GLN
1	E	96	ALA
1	B	127	GLY
1	B	129	PRO
1	D	107	ASN
1	F	242	ALA
2	H	150	PHE
1	D	96	ALA
1	A	129	PRO

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Mol	Chain	Res	Type
1	D	191	GLU
1	B	128	ILE
1	F	187	ASN
1	C	122	ASP

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	209/228 (92%)	192 (92%)	17 (8%)	11	21
1	B	207/228 (91%)	193 (93%)	14 (7%)	16	28
1	C	209/228 (92%)	194 (93%)	15 (7%)	14	25
1	D	209/228 (92%)	197 (94%)	12 (6%)	20	36
1	E	212/228 (93%)	201 (95%)	11 (5%)	23	39
1	F	213/228 (93%)	197 (92%)	16 (8%)	13	23
2	H	9/12 (75%)	8 (89%)	1 (11%)	6	10
2	I	6/12 (50%)	5 (83%)	1 (17%)	2	3
2	J	9/12 (75%)	9 (100%)	0	100	100
2	K	10/12 (83%)	9 (90%)	1 (10%)	7	13
All	All	1293/1416 (91%)	1205 (93%)	88 (7%)	16	28

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	LEU
1	A	23	ILE
1	A	25	GLU
1	A	42	SER
1	A	48	VAL
1	A	49	GLN
1	A	55	GLU
1	A	58	ASP

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Mol	Chain	Res	Type
1	A	64	ARG
1	A	112	SER
1	A	164	LYS
1	A	170	SER
1	A	210	ARG
1	A	233	VAL
1	A	244	MET
1	A	256	GLU
1	C	16	LEU
1	C	25	GLU
1	C	42	SER
1	C	48	VAL
1	C	66	LEU
1	C	80	LYS
1	C	107	ASN
1	C	122	ASP
1	C	123	VAL
1	C	146	ARG
1	C	164	LYS
1	C	165	ASP
1	C	168	LYS
1	C	170	SER
1	C	224	THR
1	E	1	MET
1	E	12	LEU
1	E	32	SER
1	E	59	THR
1	E	73	THR
1	E	123	VAL
1	E	125	GLN
1	E	131	GLN
1	E	149	ARG
1	E	192	GLU
1	E	244	MET
1	B	1	MET
1	B	12	LEU
1	B	16	LEU
1	B	29	ASP
1	B	42	SER
1	B	43	SER
1	B	47	LEU
1	B	58	ASP

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Mol	Chain	Res	Type
1	B	59	THR
1	B	130	GLU
1	B	131	GLN
1	B	164	LYS
1	B	198[A]	GLU
1	B	198[B]	GLU
1	D	1	MET
1	D	12	LEU
1	D	24	ASN
1	D	42	SER
1	D	64	ARG
1	D	126	LEU
1	D	164	LYS
1	D	170	SER
1	D	179	ASN
1	D	190	LYS
1	D	192	GLU
1	D	198	GLU
1	F	1	MET
1	F	12	LEU
1	F	23	ILE
1	F	98	THR
1	F	123	VAL
1	F	130	GLU
1	F	132	GLU
1	F	135	CYS
1	F	165	ASP
1	F	170	SER
1	F	210	ARG
1	F	219	THR
1	F	233	VAL
1	F	243	ASP
1	F	244	MET
1	F	255	ILE
2	H	152	HIS
2	I	149	GLU
2	K	152	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	K	152	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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
2	DAB	I	145	2	5,6,7	1.04	0	1,6,8	0.41	0
2	DAB	J	145	2	5,6,7	0.90	0	1,6,8	0.45	0
2	DAB	H	145	2	5,6,7	0.86	0	1,6,8	0.40	0
2	DAB	K	145	2	5,6,7	0.93	0	1,6,8	0.20	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	DAB	I	145	2	-	1/4/5/7	-
2	DAB	J	145	2	-	1/4/5/7	-
2	DAB	H	145	2	-	1/4/5/7	-
2	DAB	K	145	2	-	1/4/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	145	DAB	CA-CB-CG-ND
2	J	145	DAB	CA-CB-CG-ND
2	H	145	DAB	CA-CB-CG-ND

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Mol	Chain	Res	Type	Atoms
2	K	145	DAB	CA-CB-CG-ND

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	D	301	-	4,4,4	0.14	0	6,6,6	0.07	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	248/261 (95%)	0.13	7 (2%) 53 62	41, 64, 101, 120	0
1	B	246/261 (94%)	0.05	1 (0%) 92 95	44, 63, 94, 117	0
1	C	247/261 (94%)	-0.04	4 (1%) 72 79	32, 48, 88, 109	0
1	D	249/261 (95%)	-0.08	3 (1%) 79 85	35, 54, 94, 112	0
1	E	255/261 (97%)	-0.14	1 (0%) 92 95	30, 48, 91, 132	0
1	F	253/261 (96%)	0.01	3 (1%) 79 85	34, 52, 87, 144	0
2	H	10/14 (71%)	-0.27	0 100 100	51, 67, 95, 100	0
2	I	7/14 (50%)	1.70	2 (28%) 0 0	96, 101, 104, 104	0
2	J	10/14 (71%)	1.25	3 (30%) 0 0	79, 89, 111, 121	0
2	K	10/14 (71%)	1.34	3 (30%) 0 0	66, 83, 105, 105	0
All	All	1535/1622 (94%)	0.01	27 (1%) 68 76	30, 55, 97, 144	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	124	GLU	5.3
1	A	127	GLY	5.1
1	C	95	ASN	4.3
2	J	143	ARG	4.1
1	C	164	LYS	3.3
2	J	151	TYR	3.2
1	C	108	GLN	3.0
1	A	64	ARG	2.8
1	E	123	VAL	2.7
1	D	166	GLY	2.6
1	A	185	THR	2.6
1	F	231	ALA	2.6
1	A	96	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	100	ALA	2.4
1	D	195	VAL	2.4
1	C	163	ALA	2.4
1	F	202	PRO	2.3
1	A	122	ASP	2.3
2	K	151	TYR	2.3
2	I	147	MET	2.2
2	K	146	SER	2.2
1	D	126	LEU	2.2
2	K	143	ARG	2.2
1	A	130	GLU	2.2
2	I	144	GLN	2.2
1	A	186	SER	2.1
2	J	152	HIS	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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
2	DAB	K	145	7/8	0.82	0.29	64,76,83,86	0
2	DAB	I	145	7/8	0.86	0.40	92,105,115,120	0
2	DAB	J	145	7/8	0.89	0.19	75,78,87,93	0
2	DAB	H	145	7/8	0.97	0.12	55,59,64,66	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(\AA^2)	Q<0.9
3	SO4	B	301	5/5	0.90	0.23	73,79,89,98	5
3	SO4	D	301	5/5	0.91	0.17	69,71,82,92	5

6.5 Other polymers [i](#)

There are no such residues in this entry.