



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:39 am GMT

PDB ID : 3L88
Title : Crystal structure of the human Adenovirus type 21 fiber knob
Authors : Cupelli, K.; Jost, M.; Persson, B.D.; Stehle, T.
Deposited on : 2009-12-30
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

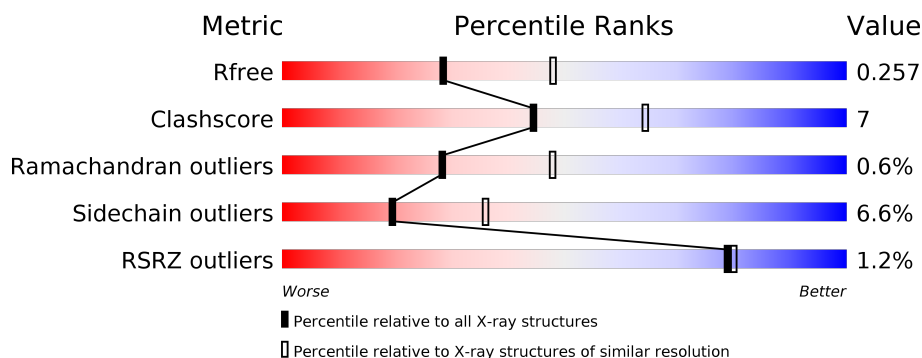
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



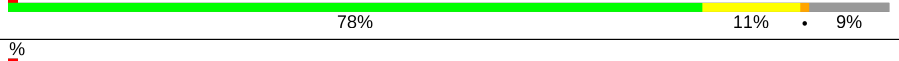
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 $\leq 5\%$. 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	201	<div> <div>74%</div> <div>15%</div> <div>9%</div> </div>
1	B	201	<div> <div>76%</div> <div>13%</div> <div>9%</div> </div>
1	C	201	<div> <div>80%</div> <div>10%</div> <div>8%</div> </div>
1	D	201	<div> <div>75%</div> <div>13%</div> <div>9%</div> </div>
1	E	201	<div> <div>75%</div> <div>14%</div> <div>9%</div> </div>
1	F	201	<div> <div>77%</div> <div>11%</div> <div>9%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	201	
1	H	201	
1	I	201	
1	J	201	
1	K	201	
1	L	201	

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	GOL	C	2	-	-	-	X
3	GOL	E	6	-	-	X	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 17174 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 Fiber protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1415	898	230	281	6			
1	B	183	Total	C	N	O	S	0	0	0
			1419	902	230	281	6			
1	C	184	Total	C	N	O	S	0	0	0
			1430	906	234	284	6			
1	D	183	Total	C	N	O	S	0	0	0
			1422	903	230	283	6			
1	E	183	Total	C	N	O	S	0	1	0
			1420	898	232	284	6			
1	F	183	Total	C	N	O	S	0	1	0
			1431	906	234	285	6			
1	G	183	Total	C	N	O	S	0	0	0
			1415	898	230	281	6			
1	H	183	Total	C	N	O	S	0	0	0
			1415	898	230	281	6			
1	I	183	Total	C	N	O	S	0	0	0
			1426	903	233	284	6			
1	J	182	Total	C	N	O	S	0	1	0
			1424	903	231	284	6			
1	K	183	Total	C	N	O	S	0	0	0
			1426	903	233	284	6			
1	L	182	Total	C	N	O	S	0	1	0
			1427	904	234	283	6			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

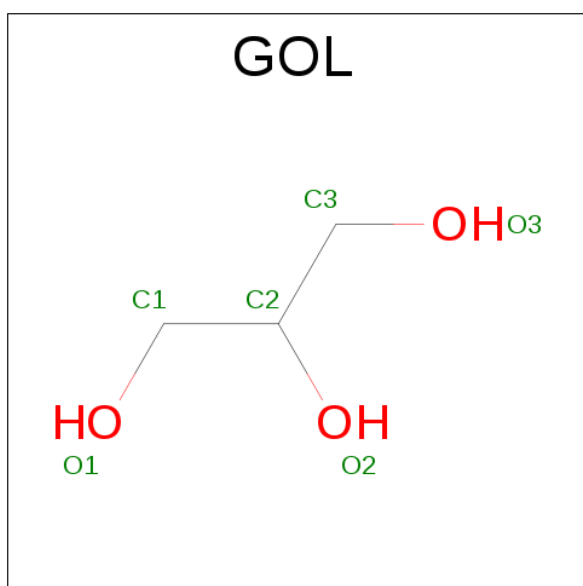
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	J	2	Total	Na	0	0
			2	2		
2	K	2	Total	Na	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total	Na	0	0
			1	1		
2	B	2	Total	Na	0	0
			2	2		
2	I	1	Total	Na	0	0
			1	1		
2	L	1	Total	Na	0	0
			1	1		
2	F	2	Total	Na	0	0
			2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	2	Total Cl 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0
5	B	2	Total O 2 2	0	0
5	C	3	Total O 3 3	0	0
5	D	5	Total O 5 5	0	0
5	E	6	Total O 6 6	0	0
5	F	6	Total O 6 6	0	0
5	G	8	Total O 8 8	0	0
5	H	5	Total O 5 5	0	0
5	I	8	Total O 8 8	0	0
5	J	6	Total O 6 6	0	0
5	K	11	Total O 11 11	0	0
5	L	2	Total O 2 2	0	0

3 Residue-property plots


These plots are drawn for all protein, RNA and DNA 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.

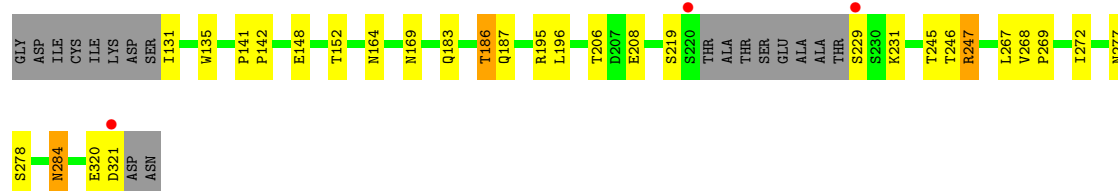
• Molecule 1: Fiber protein

Chain A: 




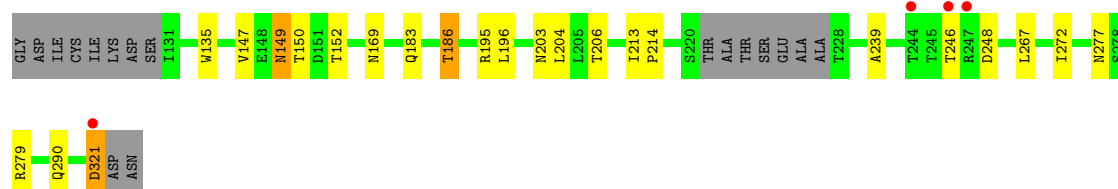
• Molecule 1: Fiber protein

Chain B: 



• Molecule 1: Fiber protein

Chain C: 



• Molecule 1: Fiber protein

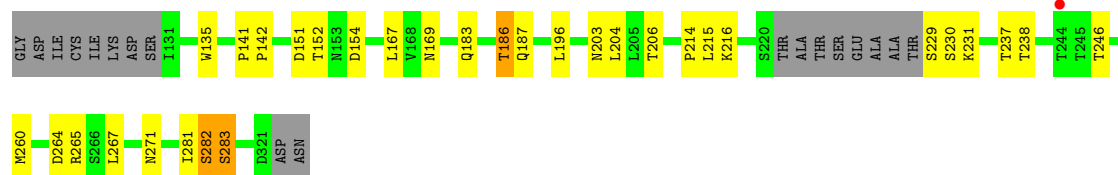
Chain D: 





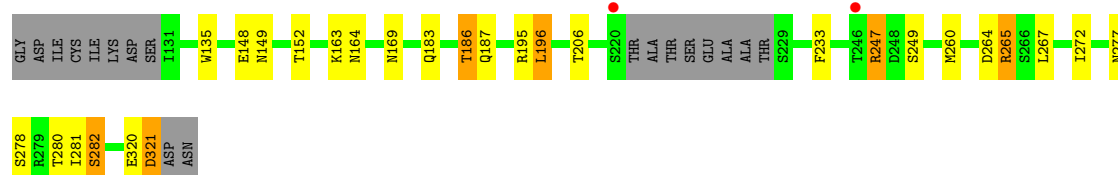
- Molecule 1: Fiber protein

Chain E: 75% 14% 9%



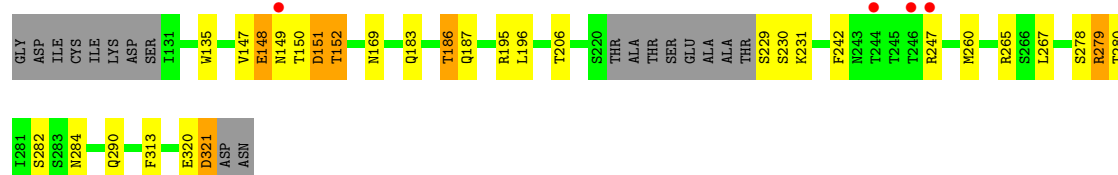
- Molecule 1: Fiber protein

Chain F: 77% 11% 9%



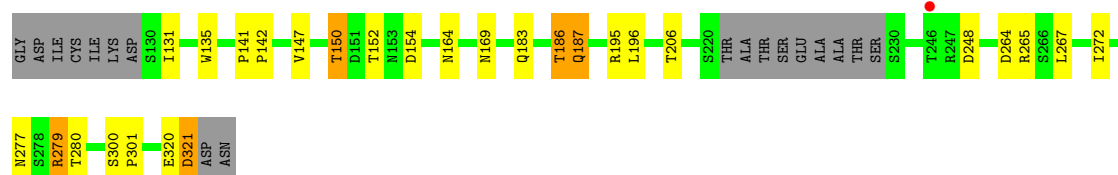
- Molecule 1: Fiber protein

Chain G: 76% 12% 9%



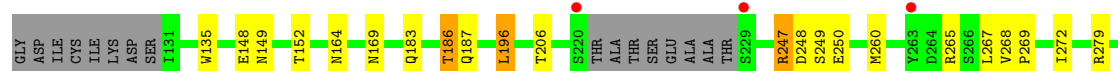
- Molecule 1: Fiber protein

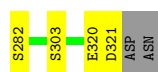
Chain H: 77% 11% 9%



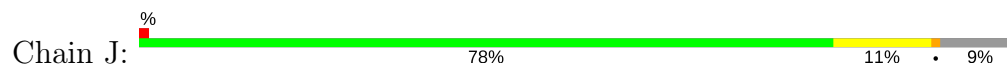
- Molecule 1: Fiber protein

Chain I: 78% 11% 9%

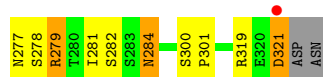
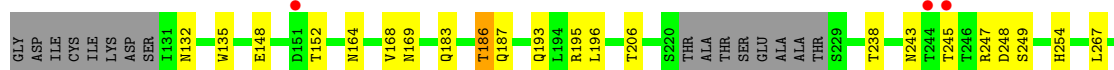
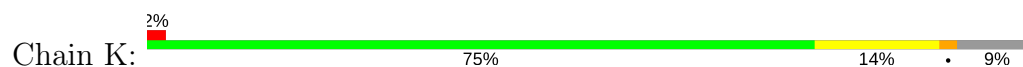




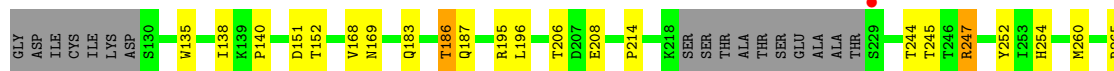
• Molecule 1: Fiber protein



• Molecule 1: Fiber protein



• Molecule 1: Fiber protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	85.00Å 63.92Å 209.35Å 90.00° 91.70° 90.00°	Depositor
Resolution (Å)	49.45 – 2.50 49.42 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.6 (49.45-2.50) 84.1 (49.42-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.259 0.234 , 0.257	Depositor DCC
R_{free} test set	3593 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , -6.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.187 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	17174	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, NA

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	0.27	0/1444	0.41	0/1970
1	B	0.27	0/1448	0.41	0/1975
1	C	0.27	0/1459	0.41	0/1989
1	D	0.26	0/1451	0.41	0/1979
1	E	0.32	0/1448	0.42	0/1975
1	F	0.28	0/1460	0.43	0/1990
1	G	0.27	0/1444	0.41	0/1969
1	H	0.27	0/1444	0.41	0/1970
1	I	0.27	0/1455	0.40	0/1983
1	J	0.27	0/1453	0.41	0/1981
1	K	0.28	0/1455	0.40	0/1983
1	L	0.28	0/1456	0.41	0/1985
All	All	0.28	0/17417	0.41	0/23749

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1415	0	1369	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1419	0	1380	25	0
1	C	1430	0	1392	24	0
1	D	1422	0	1382	28	0
1	E	1420	0	1371	31	0
1	F	1431	0	1388	26	0
1	G	1415	0	1363	22	0
1	H	1415	0	1369	18	0
1	I	1426	0	1387	17	0
1	J	1424	0	1381	24	0
1	K	1426	0	1387	22	0
1	L	1427	0	1384	29	0
2	B	2	0	0	0	0
2	F	2	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	1	0	0	0	0
3	C	6	0	8	3	0
3	E	12	0	16	8	0
3	F	6	0	8	0	0
4	J	2	0	0	1	0
5	A	5	0	0	0	0
5	B	2	0	0	0	0
5	C	3	0	0	0	0
5	D	5	0	0	0	0
5	E	6	0	0	2	0
5	F	6	0	0	1	0
5	G	8	0	0	2	1
5	H	5	0	0	0	0
5	I	8	0	0	1	0
5	J	6	0	0	0	0
5	K	11	0	0	1	0
5	L	2	0	0	0	0
All	All	17174	0	16585	251	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 7.

All (251) 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:E:214:PRO:HB3	3:E:6:GOL:H32	1.37	1.06
1:J:231:LYS:NZ	4:J:2:CL:CL	2.29	1.03
1:B:247:ARG:HG2	1:B:247:ARG:HH11	1.21	1.02
1:F:247:ARG:HH11	1:F:247:ARG:HG3	1.25	1.00
1:E:204:LEU:H	3:E:6:GOL:H2	1.30	0.97
1:D:149:ASN:H	1:D:149:ASN:HD22	0.98	0.96
1:L:260:MET:HE2	1:L:265:ARG:CZ	1.95	0.96
1:J:149[C]:ASN:H	1:J:149[C]:ASN:HD22	1.07	0.94
1:C:214:PRO:HB3	3:C:2:GOL:H31	1.54	0.87
1:D:169:ASN:ND2	1:F:169:ASN:HD21	1.72	0.86
1:A:188:LYS:HE2	1:K:238:THR:OG1	1.75	0.86
1:F:247:ARG:CG	1:F:247:ARG:HH11	1.90	0.85
1:D:321:ASP:OD2	1:D:321:ASP:C	2.15	0.84
1:C:203:ASN:HA	3:C:2:GOL:H11	1.57	0.84
1:D:149:ASN:HD22	1:D:149:ASN:N	1.77	0.82
1:J:147:VAL:HG12	1:J:149[C]:ASN:ND2	1.95	0.81
1:D:149:ASN:H	1:D:149:ASN:ND2	1.79	0.80
1:L:260:MET:HE2	1:L:265:ARG:NH1	1.96	0.79
1:A:169:ASN:HD21	1:B:169:ASN:ND2	1.80	0.79
1:B:247:ARG:CG	1:B:247:ARG:HH11	1.95	0.79
1:G:148:GLU:HA	1:G:148:GLU:OE1	1.84	0.77
1:J:131:ILE:N	1:J:131:ILE:HD12	2.00	0.77
1:J:149[C]:ASN:N	1:J:149[C]:ASN:HD22	1.83	0.76
1:D:248:ASP:OD1	1:E:265:ARG:NH2	2.18	0.76
1:L:260:MET:CE	1:L:265:ARG:CZ	2.65	0.75
1:K:279:ARG:HA	5:K:12:HOH:O	1.86	0.75
1:J:147:VAL:CG1	1:J:149[C]:ASN:ND2	2.51	0.74
1:K:284:ASN:HD22	1:K:284:ASN:H	1.36	0.74
1:L:260:MET:CE	1:L:265:ARG:NH1	2.51	0.73
1:E:229:SER:C	1:E:231:LYS:H	1.91	0.72
1:J:149[C]:ASN:H	1:J:149[C]:ASN:ND2	1.86	0.72
1:A:169:ASN:ND2	1:C:169:ASN:HD21	1.89	0.71
1:B:247:ARG:NH1	1:B:247:ARG:HG2	2.02	0.70
1:H:169:ASN:HD21	1:I:169:ASN:ND2	1.90	0.69
1:J:147:VAL:HG12	1:J:149[C]:ASN:HD22	1.58	0.68
1:J:169:ASN:ND2	1:L:169:ASN:HD21	1.91	0.68
1:C:183:GLN:O	1:C:186:THR:HB	1.94	0.68
1:G:183:GLN:O	1:G:186:THR:HB	1.94	0.67
1:B:183:GLN:O	1:B:186:THR:HB	1.95	0.67
1:L:183:GLN:O	1:L:186:THR:HB	1.95	0.67
1:G:151:ASP:N	1:G:151:ASP:OD2	2.21	0.66
1:J:208:GLU:HB3	1:J:281:ILE:HD11	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ARG:HD3	1:B:247:ARG:C	2.15	0.66
1:I:183:GLN:O	1:I:186:THR:HB	1.96	0.66
1:D:169:ASN:HD22	1:F:169:ASN:HD21	1.41	0.65
1:F:260:MET:HE2	1:F:265:ARG:NH2	2.11	0.65
1:B:284:ASN:N	1:B:284:ASN:OD1	2.27	0.64
1:F:264:ASP:O	1:F:265:ARG:HB2	1.95	0.64
1:A:187:GLN:NE2	1:L:140:PRO:HA	2.13	0.64
1:J:183:GLN:O	1:J:186:THR:HB	1.96	0.64
1:L:208:GLU:HG2	1:L:281:ILE:HD11	1.80	0.64
1:H:183:GLN:O	1:H:186:THR:HB	1.98	0.64
1:D:183:GLN:O	1:D:186:THR:HB	1.96	0.64
1:E:183:GLN:O	1:E:186:THR:HB	1.97	0.64
1:F:183:GLN:O	1:F:186:THR:HB	1.97	0.64
1:J:147:VAL:CG1	1:J:149[C]:ASN:HD21	2.11	0.64
1:A:183:GLN:O	1:A:186:THR:HB	1.98	0.63
1:B:169:ASN:HD21	1:C:169:ASN:ND2	1.96	0.63
1:D:146:ILE:HG12	1:D:194:LEU:HD21	1.81	0.62
1:J:169:ASN:HD21	1:K:169:ASN:ND2	1.98	0.62
1:K:277:ASN:O	1:K:278:SER:HB3	1.98	0.62
1:K:183:GLN:O	1:K:186:THR:HB	1.98	0.62
1:G:169:ASN:HD21	1:H:169:ASN:ND2	1.97	0.62
1:G:169:ASN:ND2	1:I:169:ASN:HD21	1.97	0.61
1:B:208:GLU:OE2	1:B:284:ASN:ND2	2.31	0.61
1:E:281:ILE:O	1:E:281:ILE:HD12	2.00	0.61
1:F:247:ARG:CG	1:F:247:ARG:NH1	2.55	0.61
1:D:131:ILE:HD12	1:D:131:ILE:N	2.15	0.61
1:J:245:THR:OG1	1:J:246:THR:N	2.34	0.61
1:F:321:ASP:OD2	1:F:321:ASP:C	2.39	0.61
1:E:282:SER:O	1:E:283:SER:CB	2.49	0.60
1:D:208:GLU:HB3	1:D:281:ILE:HD11	1.83	0.59
1:G:147:VAL:O	1:G:150:THR:HG22	2.01	0.59
1:A:164:ASN:ND2	1:B:169:ASN:HD22	2.01	0.59
1:E:204:LEU:N	3:E:6:GOL:H2	2.10	0.59
1:F:281:ILE:O	1:F:282:SER:HB3	2.01	0.58
1:F:148:GLU:HG3	1:F:149:ASN:N	2.18	0.58
1:I:196:LEU:HD23	1:I:196:LEU:N	2.18	0.58
1:C:246:THR:HG23	1:C:246:THR:O	2.04	0.58
1:J:321:ASP:OD2	1:J:321:ASP:C	2.42	0.58
1:B:195:ARG:C	1:B:196:LEU:HD23	2.24	0.58
1:I:260:MET:HE3	1:I:265:ARG:CZ	2.34	0.57
1:K:282:SER:OG	1:K:284:ASN:ND2	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:195:ARG:C	1:L:196:LEU:HD23	2.25	0.57
1:D:169:ASN:HD21	1:E:169:ASN:ND2	2.03	0.57
1:E:229:SER:C	1:E:231:LYS:N	2.59	0.57
1:I:247:ARG:NH2	1:I:250:GLU:OE2	2.38	0.57
1:G:195:ARG:HG2	1:G:290:GLN:HE21	1.70	0.56
1:A:132:ASN:ND2	1:A:163:LYS:HE3	2.20	0.56
1:A:169:ASN:HD22	1:C:169:ASN:HD21	1.51	0.56
1:G:260:MET:HE1	1:G:265:ARG:CZ	2.34	0.56
1:A:132:ASN:HD22	1:A:163:LYS:HE3	1.70	0.55
1:E:216:LYS:HA	3:E:5:GOL:H31	1.89	0.55
1:B:164:ASN:ND2	1:C:169:ASN:HD22	2.04	0.55
1:J:280:THR:OG1	1:J:285:VAL:HB	2.06	0.55
1:G:313:PHE:HA	5:G:26:HOH:O	2.07	0.54
1:K:193:GLN:OE1	1:K:195:ARG:NH1	2.38	0.54
1:C:147:VAL:O	1:C:150:THR:HG22	2.08	0.54
1:F:260:MET:CE	1:F:265:ARG:CZ	2.85	0.54
1:A:186:THR:O	1:A:186:THR:CG2	2.55	0.54
1:K:196:LEU:HD23	1:K:196:LEU:N	2.22	0.54
1:A:147:VAL:HG13	1:L:214:PRO:HG2	1.88	0.54
1:C:195:ARG:HG2	1:C:290:GLN:HE21	1.73	0.54
1:C:248:ASP:OD1	1:C:248:ASP:N	2.36	0.54
1:H:164:ASN:ND2	1:I:169:ASN:HD22	2.06	0.54
1:D:146:ILE:HD11	1:D:174:LEU:HD11	1.90	0.53
1:G:186:THR:CG2	1:G:186:THR:O	2.57	0.53
1:K:247:ARG:N	1:K:247:ARG:HD3	2.22	0.53
1:C:321:ASP:C	1:C:321:ASP:OD2	2.46	0.53
1:A:196:LEU:N	1:A:196:LEU:HD23	2.24	0.53
1:K:169:ASN:HD21	1:L:169:ASN:ND2	2.06	0.53
1:B:247:ARG:CG	1:B:247:ARG:NH1	2.61	0.53
1:K:243:ASN:HD22	1:K:248:ASP:HB3	1.73	0.53
1:G:229:SER:C	1:G:231:LYS:H	2.12	0.52
1:I:303:SER:HA	5:I:28:HOH:O	2.08	0.52
1:C:204:LEU:H	3:C:2:GOL:H32	1.73	0.52
1:L:260:MET:HE3	1:L:265:ARG:HB3	1.91	0.52
1:E:154:ASP:HB3	5:E:42:HOH:O	2.10	0.52
1:G:152:THR:HG22	5:G:64:HOH:O	2.09	0.52
1:L:280:THR:OG1	1:L:285:VAL:HB	2.10	0.52
1:C:186:THR:O	1:C:186:THR:CG2	2.58	0.52
1:E:169:ASN:HD21	1:F:169:ASN:ND2	2.08	0.52
1:H:196:LEU:HD23	1:H:196:LEU:N	2.25	0.52
1:J:196:LEU:N	1:J:196:LEU:HD23	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:186:THR:O	1:I:186:THR:CG2	2.57	0.51
1:F:186:THR:CG2	1:F:186:THR:O	2.57	0.51
1:L:260:MET:HE1	1:L:265:ARG:NH1	2.26	0.51
1:A:265:ARG:NH2	1:C:248:ASP:OD1	2.44	0.51
1:F:196:LEU:HD23	1:F:196:LEU:N	2.26	0.50
1:K:186:THR:O	1:K:186:THR:CG2	2.59	0.50
1:G:265:ARG:NH2	1:I:248:ASP:OD1	2.45	0.50
1:H:248:ASP:OD1	1:H:248:ASP:N	2.45	0.50
1:L:186:THR:O	1:L:186:THR:CG2	2.58	0.50
1:E:186:THR:CG2	1:E:186:THR:O	2.59	0.50
1:B:186:THR:CG2	1:B:186:THR:O	2.58	0.50
1:B:196:LEU:N	1:B:196:LEU:HD23	2.27	0.50
1:F:260:MET:HE2	1:F:265:ARG:CZ	2.42	0.50
1:A:169:ASN:HD21	1:B:169:ASN:HD22	1.56	0.49
1:A:188:LYS:HE3	1:K:238:THR:HG21	1.93	0.49
1:A:238:THR:HG23	1:E:142:PRO:HD2	1.93	0.49
1:E:281:ILE:HD12	1:E:281:ILE:C	2.33	0.49
1:D:242:PHE:HA	1:D:278:SER:HA	1.93	0.49
1:K:164:ASN:ND2	1:L:169:ASN:HD22	2.11	0.49
1:A:164:ASN:HD22	1:B:169:ASN:HD22	1.59	0.49
1:D:195:ARG:C	1:D:196:LEU:HD23	2.32	0.49
1:D:196:LEU:HD23	1:D:196:LEU:N	2.28	0.49
1:G:196:LEU:HD23	1:G:196:LEU:N	2.28	0.49
1:L:277:ASN:O	1:L:278:SER:HB3	2.12	0.49
1:D:147:VAL:HG12	1:D:149:ASN:ND2	2.28	0.49
1:J:186:THR:CG2	1:J:186:THR:O	2.60	0.48
1:E:216:LYS:HA	3:E:5:GOL:C3	2.43	0.48
1:E:196:LEU:N	1:E:196:LEU:HD23	2.27	0.48
1:E:215:LEU:N	3:E:6:GOL:O2	2.47	0.48
1:C:149:ASN:C	1:C:149:ASN:ND2	2.67	0.48
1:K:195:ARG:C	1:K:196:LEU:HD23	2.33	0.48
1:H:186:THR:O	1:H:186:THR:CG2	2.62	0.48
1:D:186:THR:O	1:D:186:THR:CG2	2.61	0.47
1:D:321:ASP:OD2	1:D:321:ASP:O	2.31	0.47
1:G:242:PHE:HA	1:G:278:SER:HA	1.97	0.47
1:B:277:ASN:O	1:B:278:SER:HB3	2.15	0.47
1:E:281:ILE:O	1:E:281:ILE:CD1	2.62	0.47
1:G:282:SER:OG	1:G:284:ASN:HB2	2.15	0.47
1:L:277:ASN:HA	1:L:288:ALA:HB3	1.97	0.47
1:I:248:ASP:OD1	1:I:248:ASP:N	2.48	0.47
1:G:169:ASN:HD22	1:I:164:ASN:ND2	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:149:ASN:ND2	1:L:247:ARG:HD3	2.30	0.46
1:A:243:ASN:HD22	1:A:248:ASP:HB3	1.80	0.46
1:A:260:MET:HE2	1:A:265:ARG:HB3	1.98	0.46
1:J:169:ASN:HD22	1:L:169:ASN:HD21	1.59	0.46
1:C:196:LEU:HD23	1:C:196:LEU:N	2.31	0.46
1:D:169:ASN:HD22	1:F:164:ASN:ND2	2.14	0.46
1:G:195:ARG:C	1:G:196:LEU:HD23	2.37	0.45
1:A:280:THR:O	1:A:280:THR:HG23	2.16	0.45
1:K:254:HIS:CD2	1:L:267:LEU:HD21	2.50	0.45
1:D:131:ILE:CD1	1:D:131:ILE:N	2.77	0.45
1:E:238:THR:CG2	1:H:187:GLN:NE2	2.80	0.45
1:F:265:ARG:HD2	1:F:265:ARG:N	2.30	0.45
1:L:244:THR:O	1:L:244:THR:CG2	2.64	0.45
1:F:280:THR:HG22	5:F:9:HOH:O	2.16	0.45
1:D:280:THR:OG1	1:D:281:ILE:N	2.49	0.45
1:A:187:GLN:NE2	1:L:138:ILE:O	2.49	0.45
1:J:248:ASP:N	1:J:248:ASP:OD1	2.50	0.44
1:J:260:MET:HE3	1:J:265:ARG:HB3	1.99	0.44
1:J:282:SER:OG	1:J:284:ASN:HB2	2.17	0.44
1:K:321:ASP:OD2	1:K:321:ASP:C	2.56	0.44
1:K:300:SER:HA	1:K:301:PRO:HD3	1.89	0.44
1:D:132:ASN:HD22	1:D:163:LYS:HB2	1.83	0.44
1:D:268:VAL:HA	1:D:269:PRO:HD3	1.86	0.43
1:A:277:ASN:O	1:A:279:ARG:N	2.48	0.43
1:G:169:ASN:HD21	1:H:169:ASN:HD22	1.65	0.43
1:L:244:THR:HG22	1:L:244:THR:O	2.18	0.43
1:L:245:THR:O	1:L:279:ARG:NH2	2.51	0.43
1:A:300:SER:HA	1:A:301:PRO:HD3	1.87	0.43
1:D:169:ASN:HD22	1:F:164:ASN:HD22	1.67	0.43
1:D:147:VAL:CG1	1:D:149:ASN:ND2	2.82	0.43
1:L:196:LEU:N	1:L:196:LEU:HD23	2.33	0.43
1:C:149:ASN:C	1:C:149:ASN:HD22	2.21	0.43
1:K:281:ILE:C	1:K:281:ILE:HD12	2.39	0.43
1:C:195:ARG:C	1:C:196:LEU:HD23	2.39	0.43
1:H:264:ASP:C	1:H:265:ARG:CG	2.87	0.43
1:J:195:ARG:C	1:J:196:LEU:HD23	2.39	0.43
1:G:229:SER:C	1:G:231:LYS:N	2.72	0.42
1:H:195:ARG:C	1:H:196:LEU:HD23	2.39	0.42
1:H:277:ASN:O	1:H:279:ARG:N	2.48	0.42
1:J:131:ILE:N	1:J:131:ILE:CD1	2.67	0.42
1:B:141:PRO:O	1:B:142:PRO:C	2.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:148:GLU:HA	1:I:148:GLU:OE1	2.19	0.42
1:F:148:GLU:HG3	1:F:149:ASN:H	1.82	0.42
1:L:320:GLU:O	1:L:321:ASP:C	2.58	0.42
1:A:138:ILE:HG23	1:C:239:ALA:HB2	2.02	0.42
1:E:169:ASN:HD21	1:F:169:ASN:HD22	1.68	0.42
1:H:147:VAL:HB	1:H:150:THR:HB	2.01	0.42
1:F:163:LYS:HG3	1:F:233:PHE:CE2	2.55	0.42
1:L:252:TYR:HB3	1:L:254:HIS:CE1	2.55	0.42
1:K:168:VAL:HG23	1:K:319:ARG:HB3	2.01	0.41
1:F:277:ASN:O	1:F:278:SER:HB3	2.20	0.41
1:K:132:ASN:HA	1:K:132:ASN:HD22	1.73	0.41
1:A:195:ARG:C	1:A:196:LEU:HD23	2.40	0.41
1:H:164:ASN:HD22	1:I:169:ASN:HD22	1.68	0.41
1:L:168:VAL:HG23	1:L:319:ARG:HB3	2.02	0.41
1:C:213:ILE:HA	1:C:214:PRO:HD3	1.90	0.41
1:D:213:ILE:HA	1:D:214:PRO:HD3	1.94	0.41
1:G:279:ARG:HD3	1:G:279:ARG:HA	1.89	0.41
1:A:237:THR:CG2	1:E:141:PRO:HD3	2.51	0.41
1:H:147:VAL:HG23	1:H:154:ASP:OD2	2.20	0.41
1:H:300:SER:HA	1:H:301:PRO:HD3	1.88	0.41
1:F:195[B]:ARG:C	1:F:196:LEU:HD23	2.41	0.41
1:B:268:VAL:HA	1:B:269:PRO:HD3	1.83	0.41
1:H:141:PRO:O	1:H:142:PRO:C	2.59	0.41
1:A:261:THR:O	1:A:265:ARG:HA	2.20	0.41
1:E:264:ASP:O	1:E:265:ARG:HB2	2.21	0.41
1:B:229:SER:C	1:B:231:LYS:H	2.24	0.41
1:E:203:ASN:HA	3:E:6:GOL:H2	2.03	0.41
1:E:260:MET:HE1	1:E:265:ARG:NE	2.36	0.41
1:I:268:VAL:HA	1:I:269:PRO:HD3	1.83	0.41
1:B:320:GLU:O	1:B:321:ASP:C	2.60	0.40
1:A:237:THR:HG21	1:E:141:PRO:HD3	2.02	0.40
1:E:204:LEU:H	3:E:6:GOL:C2	2.15	0.40
1:E:237:THR:CG2	1:E:237:THR:O	2.69	0.40
1:A:320:GLU:O	1:A:321:ASP:C	2.59	0.40
1:B:169:ASN:HD21	1:C:169:ASN:HD22	1.66	0.40
1:E:271:ASN:HB3	5:E:324:HOH:O	2.21	0.40
1:H:320:GLU:O	1:H:321:ASP:C	2.59	0.40
1:B:164:ASN:HD22	1:C:169:ASN:HD22	1.68	0.40
1:E:282:SER:O	1:E:283:SER:OG	2.35	0.40
1:I:320:GLU:O	1:I:321:ASP:C	2.60	0.40
1:A:164:ASN:ND2	1:B:169:ASN:ND2	2.67	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ASN:O	1:C:279:ARG:N	2.47	0.40
1:D:163:LYS:HG3	1:D:233:PHE:CE2	2.56	0.40
1:F:320:GLU:O	1:F:321:ASP:C	2.60	0.40
1:G:320:GLU:O	1:G:321:ASP:C	2.59	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)
5:G:64:HOH:O	5:G:64:HOH:O[2_555]	2.19	0.01

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	179/201 (89%)	173 (97%)	6 (3%)	0	100	100
1	B	179/201 (89%)	170 (95%)	8 (4%)	1 (1%)	28	48
1	C	180/201 (90%)	170 (94%)	10 (6%)	0	100	100
1	D	179/201 (89%)	170 (95%)	8 (4%)	1 (1%)	28	48
1	E	180/201 (90%)	167 (93%)	10 (6%)	3 (2%)	11	18
1	F	180/201 (90%)	171 (95%)	8 (4%)	1 (1%)	28	48
1	G	179/201 (89%)	170 (95%)	7 (4%)	2 (1%)	17	29
1	H	179/201 (89%)	167 (93%)	10 (6%)	2 (1%)	17	29
1	I	179/201 (89%)	170 (95%)	9 (5%)	0	100	100
1	J	179/201 (89%)	172 (96%)	6 (3%)	1 (1%)	28	48
1	K	179/201 (89%)	174 (97%)	4 (2%)	1 (1%)	28	48
1	L	179/201 (89%)	172 (96%)	7 (4%)	0	100	100
All	All	2151/2412 (89%)	2046 (95%)	93 (4%)	12 (1%)	28	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	230	SER
1	H	150	THR
1	J	245	THR
1	B	148	GLU
1	F	282	SER
1	G	247	ARG
1	K	148	GLU
1	E	282	SER
1	E	283	SER
1	G	230	SER
1	D	281	ILE
1	H	131	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	161/182 (88%)	148 (92%)	13 (8%)	14	26
1	B	162/182 (89%)	149 (92%)	13 (8%)	14	27
1	C	164/182 (90%)	156 (95%)	8 (5%)	29	52
1	D	163/182 (90%)	152 (93%)	11 (7%)	19	35
1	E	162/182 (89%)	153 (94%)	9 (6%)	25	45
1	F	164/182 (90%)	152 (93%)	12 (7%)	16	31
1	G	160/182 (88%)	148 (92%)	12 (8%)	16	29
1	H	161/182 (88%)	151 (94%)	10 (6%)	21	39
1	I	164/182 (90%)	152 (93%)	12 (7%)	16	31
1	J	164/182 (90%)	155 (94%)	9 (6%)	25	46
1	K	164/182 (90%)	153 (93%)	11 (7%)	19	35
1	L	163/182 (90%)	154 (94%)	9 (6%)	25	46
All	All	1952/2184 (89%)	1823 (93%)	129 (7%)	19	36

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	TRP
1	A	152	THR
1	A	186	THR
1	A	187	GLN
1	A	196	LEU
1	A	206	THR
1	A	219	SER
1	A	244	THR
1	A	246	THR
1	A	267	LEU
1	A	272	ILE
1	A	282	SER
1	A	321	ASP
1	B	131	ILE
1	B	135	TRP
1	B	152	THR
1	B	186	THR
1	B	187	GLN
1	B	206	THR
1	B	219	SER
1	B	245	THR
1	B	246	THR
1	B	247	ARG
1	B	267	LEU
1	B	272	ILE
1	B	284	ASN
1	C	135	TRP
1	C	149	ASN
1	C	152	THR
1	C	186	THR
1	C	206	THR
1	C	267	LEU
1	C	272	ILE
1	C	321	ASP
1	D	131	ILE
1	D	135	TRP
1	D	149	ASN
1	D	152	THR
1	D	167	LEU
1	D	186	THR
1	D	187	GLN
1	D	206	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	267	LEU
1	D	272	ILE
1	D	321	ASP
1	E	135	TRP
1	E	151	ASP
1	E	152	THR
1	E	167	LEU
1	E	186	THR
1	E	187	GLN
1	E	206	THR
1	E	246	THR
1	E	267	LEU
1	F	135	TRP
1	F	152	THR
1	F	186	THR
1	F	187	GLN
1	F	196	LEU
1	F	206	THR
1	F	247	ARG
1	F	249	SER
1	F	265	ARG
1	F	267	LEU
1	F	272	ILE
1	F	321	ASP
1	G	135	TRP
1	G	148	GLU
1	G	149	ASN
1	G	151	ASP
1	G	152	THR
1	G	186	THR
1	G	187	GLN
1	G	206	THR
1	G	267	LEU
1	G	279	ARG
1	G	280	THR
1	G	321	ASP
1	H	135	TRP
1	H	152	THR
1	H	186	THR
1	H	187	GLN
1	H	206	THR
1	H	267	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	272	ILE
1	H	279	ARG
1	H	280	THR
1	H	321	ASP
1	I	135	TRP
1	I	152	THR
1	I	186	THR
1	I	187	GLN
1	I	196	LEU
1	I	206	THR
1	I	247	ARG
1	I	249	SER
1	I	267	LEU
1	I	272	ILE
1	I	279	ARG
1	I	282	SER
1	J	131	ILE
1	J	135	TRP
1	J	152	THR
1	J	186	THR
1	J	187	GLN
1	J	206	THR
1	J	245	THR
1	J	267	LEU
1	J	321	ASP
1	K	135	TRP
1	K	152	THR
1	K	186	THR
1	K	187	GLN
1	K	206	THR
1	K	245	THR
1	K	249	SER
1	K	267	LEU
1	K	279	ARG
1	K	284	ASN
1	K	321	ASP
1	L	135	TRP
1	L	151	ASP
1	L	152	THR
1	L	186	THR
1	L	187	GLN
1	L	206	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	247	ARG
1	L	267	LEU
1	L	321	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	164	ASN
1	A	169	ASN
1	A	187	GLN
1	A	243	ASN
1	A	254	HIS
1	A	296	ASN
1	B	132	ASN
1	B	164	ASN
1	B	169	ASN
1	B	243	ASN
1	B	254	HIS
1	B	290	GLN
1	B	296	ASN
1	C	149	ASN
1	C	243	ASN
1	C	254	HIS
1	C	290	GLN
1	C	296	ASN
1	D	132	ASN
1	D	149	ASN
1	D	169	ASN
1	D	243	ASN
1	D	254	HIS
1	D	296	ASN
1	E	164	ASN
1	E	169	ASN
1	E	254	HIS
1	E	296	ASN
1	F	254	HIS
1	F	290	GLN
1	F	296	ASN
1	G	169	ASN
1	G	243	ASN
1	G	254	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	290	GLN
1	G	296	ASN
1	H	132	ASN
1	H	164	ASN
1	H	169	ASN
1	H	187	GLN
1	H	254	HIS
1	H	296	ASN
1	I	132	ASN
1	I	243	ASN
1	I	254	HIS
1	I	296	ASN
1	J	169	ASN
1	J	254	HIS
1	J	296	ASN
1	K	132	ASN
1	K	164	ASN
1	K	169	ASN
1	K	243	ASN
1	K	254	HIS
1	K	284	ASN
1	K	296	ASN
1	L	149	ASN
1	L	243	ASN
1	L	254	HIS
1	L	296	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 17 ligands modelled in this entry, 13 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	C	2	-	5,5,5	0.38	0	5,5,5	0.14	0
3	GOL	E	5	-	5,5,5	0.34	0	5,5,5	0.29	0
3	GOL	E	6	-	5,5,5	0.36	0	5,5,5	0.20	0
3	GOL	F	3	-	5,5,5	0.32	0	5,5,5	0.22	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
3	GOL	C	2	-	-	0/4/4/4	0/0/0/0
3	GOL	E	5	-	-	0/4/4/4	0/0/0/0
3	GOL	E	6	-	-	0/4/4/4	0/0/0/0
3	GOL	F	3	-	-	0/4/4/4	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.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	GOL	3	0
3	E	5	GOL	2	0
3	E	6	GOL	6	0

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, 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	183/201 (91%)	-0.24	1 (0%) 90 91	7, 17, 40, 55	0
1	B	183/201 (91%)	-0.32	3 (1%) 72 73	7, 17, 38, 57	0
1	C	184/201 (91%)	-0.24	4 (2%) 62 64	5, 17, 40, 74	0
1	D	183/201 (91%)	-0.25	0 100 100	7, 18, 45, 61	0
1	E	183/201 (91%)	-0.22	1 (0%) 90 91	7, 18, 48, 61	0
1	F	183/201 (91%)	-0.19	2 (1%) 80 81	7, 18, 44, 65	0
1	G	183/201 (91%)	-0.27	4 (2%) 62 64	7, 17, 45, 55	0
1	H	183/201 (91%)	-0.25	1 (0%) 90 91	7, 17, 41, 55	0
1	I	183/201 (91%)	-0.30	3 (1%) 72 73	7, 17, 40, 51	0
1	J	182/201 (90%)	-0.18	3 (1%) 72 73	7, 18, 43, 59	0
1	K	183/201 (91%)	-0.25	4 (2%) 62 64	7, 18, 47, 71	0
1	L	182/201 (90%)	-0.26	1 (0%) 90 91	7, 18, 41, 70	0
All	All	2195/2412 (91%)	-0.25	27 (1%) 79 80	5, 18, 46, 74	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	220	SER	4.8
1	J	229	SER	4.7
1	B	220	SER	4.6
1	L	229	SER	4.5
1	K	245	THR	4.4
1	K	244	THR	4.1
1	J	244	THR	3.9
1	C	244	THR	3.4
1	H	246	THR	3.2
1	I	263	TYR	3.1
1	A	220	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	244	THR	3.0
1	E	244	THR	3.0
1	G	247	ARG	2.9
1	C	247	ARG	2.8
1	G	149	ASN	2.5
1	C	321	ASP	2.3
1	K	151	ASP	2.3
1	F	246	THR	2.3
1	F	220	SER	2.2
1	G	246	THR	2.2
1	J	321	ASP	2.2
1	C	246	THR	2.1
1	K	321	ASP	2.1
1	B	229	SER	2.1
1	B	321	ASP	2.0
1	I	229	SER	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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	C	2	6/6	0.89	0.26	7.03	23,30,35,35	0
3	GOL	E	6	6/6	0.77	0.22	5.18	22,27,30,32	0
3	GOL	E	5	6/6	0.87	0.22	1.88	22,24,27,28	0
2	NA	J	8	1/1	0.84	0.21	1.31	52,52,52,52	0
2	NA	L	10	1/1	0.87	0.15	0.59	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CL	J	1	1/1	0.99	0.06	-2.59	31,31,31,31	0
2	NA	J	9	1/1	0.96	0.06	-2.88	20,20,20,20	0
2	NA	K	5	1/1	0.96	0.20	-	26,26,26,26	0
2	NA	K	4	1/1	0.97	0.15	-	25,25,25,25	0
2	NA	F	7	1/1	0.97	0.12	-	38,38,38,38	0
2	NA	B	1	1/1	0.95	0.08	-	23,23,23,23	0
4	CL	J	2	1/1	0.98	0.06	-	33,33,33,33	0
2	NA	I	11	1/1	0.99	0.06	-	19,19,19,19	0
3	GOL	F	3	6/6	0.86	0.19	-	39,42,44,44	0
2	NA	H	6	1/1	0.94	0.15	-	32,32,32,32	0
2	NA	F	2	1/1	0.96	0.15	-	22,22,22,22	0
2	NA	B	3	1/1	0.88	0.14	-	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.