Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 08:05 PM EDT

PDB ID	:	6FVL
Title	:	DNA polymerase sliding clamp from Escherichia coli with bound P7 peptide
Authors	:	Martiel, I.; Andre, C.; Olieric, V.; Guichard, G.; Burnouf, D.
Deposited on	:	2018-03-04
Resolution	:	1.98 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

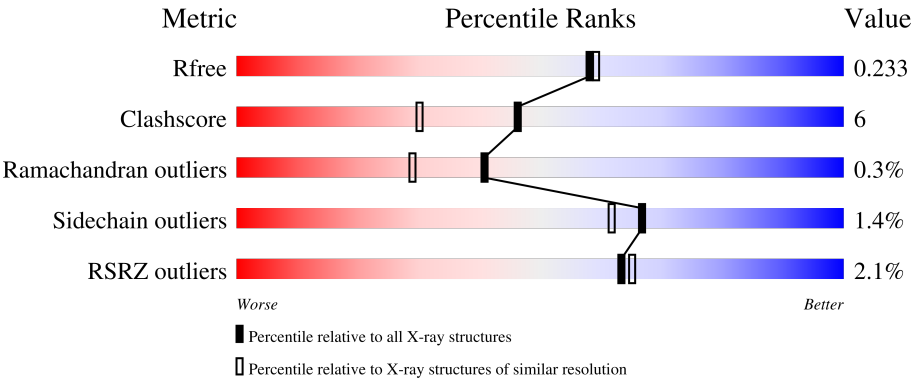
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 of 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 <=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	368	2% 89% 11%
1	B	368	87% 12%
1	C	368	2% 82% 17%
1	D	368	3% 82% 17%
2	H	6	100%

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Mol	Chain	Length	Quality of chain
2	I	6	100%
2	J	6	67% 33%
2	K	6	83% 17%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12038 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 Beta sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	4	0
			2818	1777	488	533	20			
1	B	364	Total	C	N	O	S	0	1	0
			2801	1765	491	526	19			
1	C	366	Total	C	N	O	S	0	4	0
			2814	1777	485	532	20			
1	D	365	Total	C	N	O	S	0	2	0
			2791	1766	485	521	19			

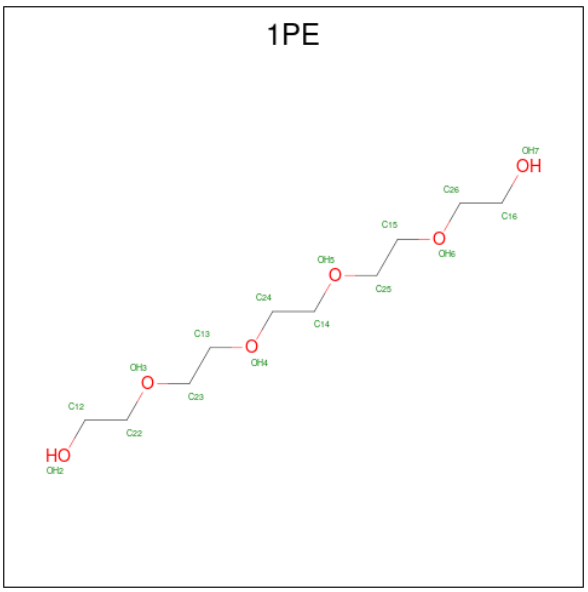
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P0A988
A	0	HIS	-	expression tag	UNP P0A988
B	-1	SER	-	expression tag	UNP P0A988
B	0	HIS	-	expression tag	UNP P0A988
C	-1	SER	-	expression tag	UNP P0A988
C	0	HIS	-	expression tag	UNP P0A988
D	-1	SER	-	expression tag	UNP P0A988
D	0	HIS	-	expression tag	UNP P0A988

- Molecule 2 is a protein called P7 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	6	Total	C	N	O	0	0	0
			51	35	6	10			
2	I	6	Total	C	N	O	0	0	0
			51	35	6	10			
2	J	6	Total	C	N	O	0	0	0
			51	35	6	10			
2	K	6	Total	C	N	O	0	0	0
			51	35	6	10			

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 10 6 4	0	0
3	B	1	Total C O 16 10 6	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 10 6 4	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 10 6 4	0	0
3	B	1	Total C O 13 8 5	0	0
3	C	1	Total C O 16 10 6	0	0
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C O 8 5 3	0	0

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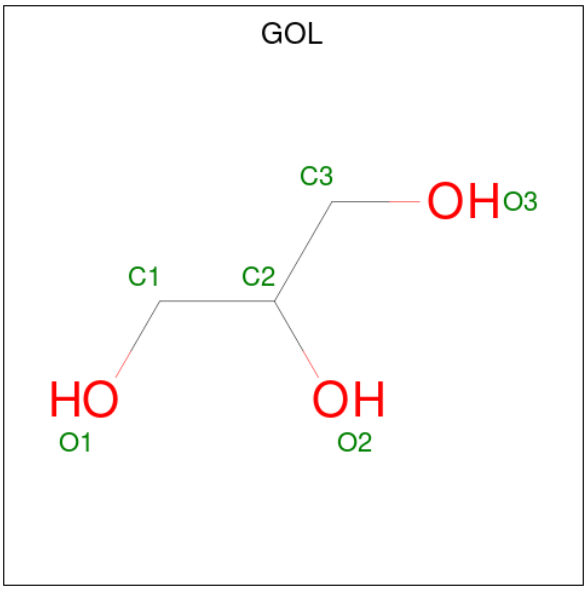
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 10 6 4	0	0
3	D	1	Total C O 7 4 3	0	0
3	I	1	Total C O 16 10 6	0	0
3	K	1	Total C O 16 10 6	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0

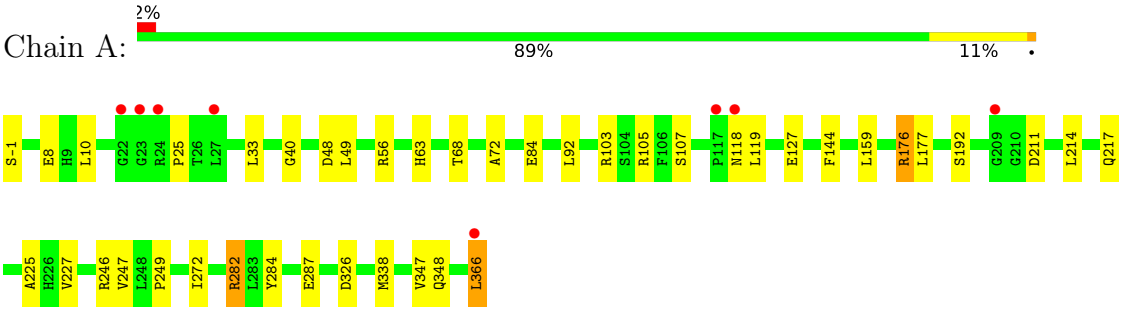
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	95	Total O 96 96	0	1
5	B	107	Total O 108 108	0	1
5	C	94	Total O 94 94	0	0
5	D	70	Total O 70 70	0	0
5	H	2	Total O 2 2	0	0
5	I	4	Total O 4 4	0	0
5	J	3	Total O 3 3	0	0
5	K	5	Total O 5 5	0	0

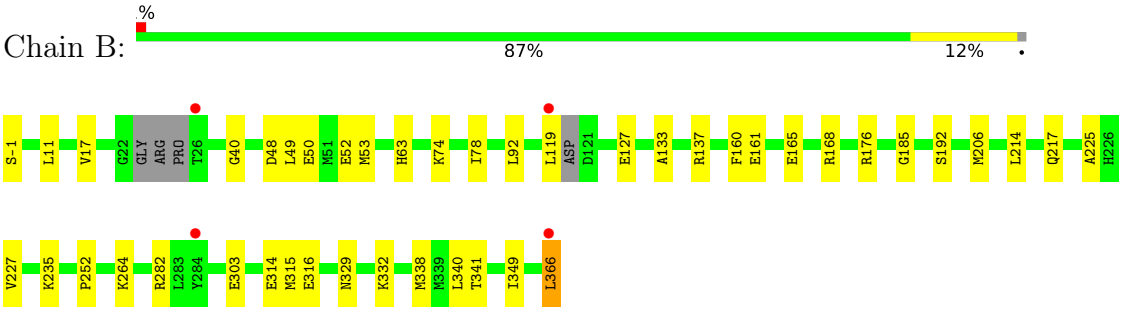
3 Residue-property plots (i)

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.

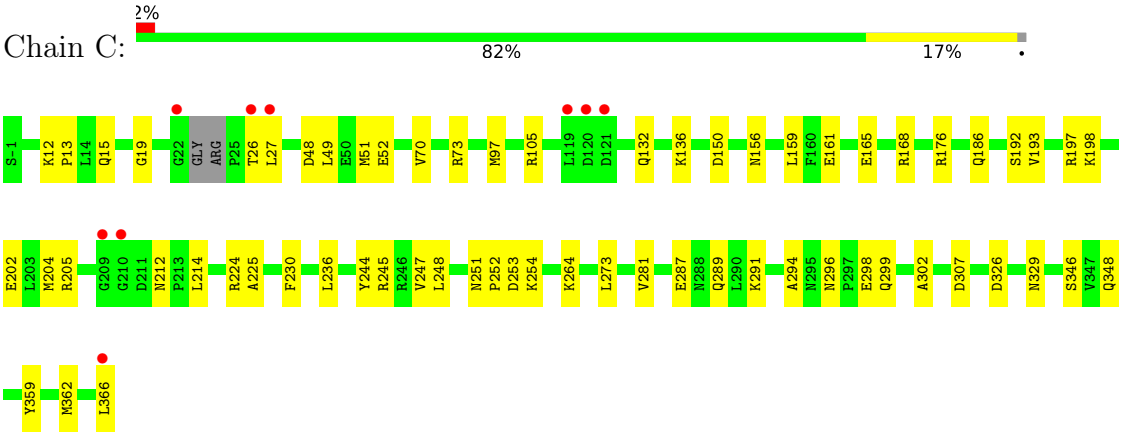
• Molecule 1: Beta sliding clamp



• Molecule 1: Beta sliding clamp

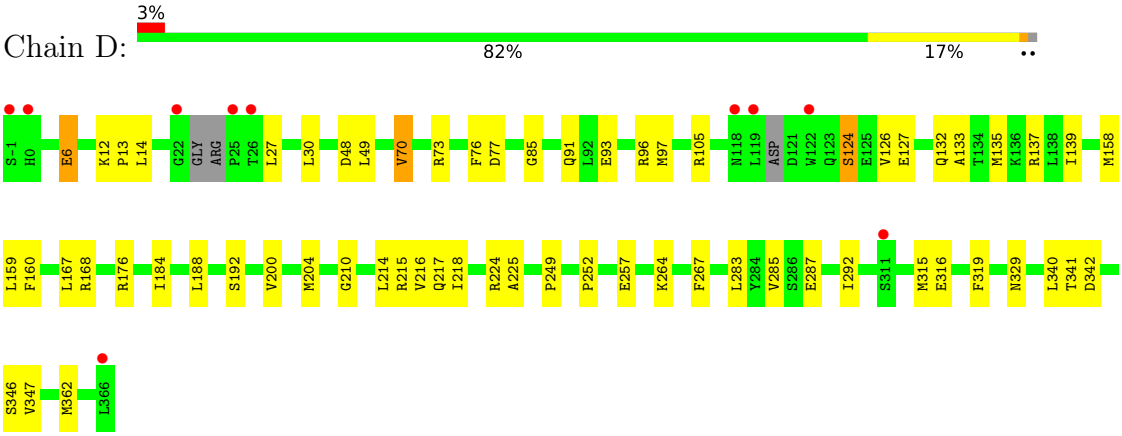


• Molecule 1: Beta sliding clamp



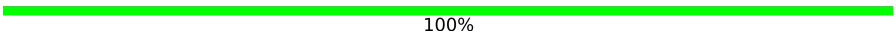
• Molecule 1: Beta sliding clamp

Chain D:



• Molecule 2: P7 peptide

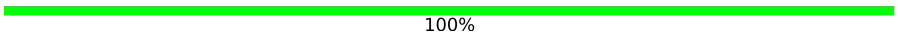
Chain H:



There are no outlier residues recorded for this chain.

• Molecule 2: P7 peptide

Chain I:



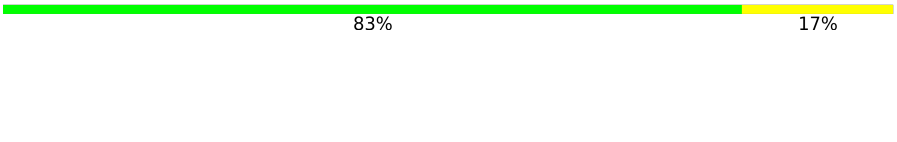
There are no outlier residues recorded for this chain.

• Molecule 2: P7 peptide

Chain J:

• Molecule 2: P7 peptide

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.90Å 79.48Å 85.32Å 65.83° 75.16° 75.79°	Depositor
Resolution (Å)	57.05 – 1.98 57.05 – 1.98	Depositor EDS
% Data completeness (in resolution range)	65.4 (57.05-1.98) 65.5 (57.05-1.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 1.98Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.189 , 0.233 0.190 , 0.233	Depositor DCC
R_{free} test set	3791 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 57.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12038	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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, 0.333 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: 1PE, ACE, GOL, ALC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/2868	0.60	0/3891
1	B	0.36	0/2848	0.60	0/3856
1	C	0.35	0/2863	0.61	0/3882
1	D	0.39	0/2839	0.65	0/3848
2	H	0.38	0/37	0.69	0/46
2	I	0.38	0/37	0.71	0/46
2	J	0.42	0/37	0.52	0/46
2	K	0.38	0/37	0.84	0/46
All	All	0.36	0/11566	0.62	0/15661

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	2818	0	2783	29	0
1	B	2801	0	2794	31	0
1	C	2814	0	2783	38	0
1	D	2791	0	2772	52	0
2	H	51	0	49	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	51	0	49	0	0
2	J	51	0	49	3	0
2	K	51	0	49	2	0
3	A	33	0	42	0	0
3	B	73	0	94	3	0
3	C	31	0	40	2	0
3	D	17	0	21	0	0
3	I	16	0	22	0	0
3	K	16	0	22	0	0
4	A	12	0	16	0	0
4	B	12	0	16	2	0
4	D	6	0	8	0	0
4	H	6	0	8	0	0
4	I	6	0	8	0	0
5	A	96	0	0	5	0
5	B	108	0	0	1	0
5	C	94	0	0	3	0
5	D	70	0	0	1	0
5	H	2	0	0	0	0
5	I	4	0	0	0	0
5	J	3	0	0	0	0
5	K	5	0	0	0	0
All	All	12038	0	11625	147	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 6.

All (147) 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:D:184:ILE:HD11	1:D:188:LEU:HD11	1.52	0.91
1:B:366:LEU:HD22	4:B:409:GOL:H12	1.56	0.87
1:B:366:LEU:HD22	4:B:409:GOL:C1	2.12	0.79
1:D:362:MET:HE3	2:K:5:LEU:HA	1.64	0.79
1:A:249:PRO:HD2	1:A:348:GLN:HE21	1.49	0.77
1:A:-1:SER:HB3	1:A:92:LEU:HD12	1.65	0.77
1:C:296:ASN:OD1	1:C:298:GLU:HG2	1.88	0.73
1:A:118:ASN:ND2	5:A:501:HOH:O	2.23	0.71
1:C:176:ARG:NH1	1:C:326:ASP:OD2	2.22	0.71
1:A:177:LEU:HD13	1:A:247:VAL:HG21	1.73	0.69
1:B:127:GLU:HG2	1:B:217:GLN:HG2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:GLU:HG3	1:D:217:GLN:HG2	1.75	0.67
1:D:105:ARG:HH21	1:D:105:ARG:HG2	1.60	0.67
1:D:105:ARG:HG2	1:D:105:ARG:NH2	2.10	0.66
1:D:158:MET:HG2	1:D:160:PHE:CE1	2.31	0.65
1:A:56:ARG:NH2	5:A:503:HOH:O	2.29	0.65
1:A:127:GLU:HG2	1:A:217:GLN:HG2	1.79	0.64
1:D:264:LYS:HD2	1:D:329:ASN:OD1	1.98	0.63
1:B:214:LEU:HD11	1:B:225:ALA:HB1	1.81	0.62
1:B:282:ARG:NH1	1:B:316:GLU:OE2	2.33	0.62
1:D:267:PHE:CE1	1:D:283:LEU:HD21	2.35	0.62
1:D:139:ILE:HG12	1:D:158:MET:HE3	1.82	0.62
1:D:319:PHE:HZ	1:D:347:VAL:HG21	1.65	0.61
1:C:247:VAL:HG13	2:J:5:LEU:HD22	1.81	0.61
1:D:127:GLU:OE2	1:D:217:GLN:NE2	2.21	0.60
1:D:127:GLU:CG	1:D:217:GLN:HG2	2.31	0.59
1:D:285:VAL:HG22	1:D:315:MET:HG2	1.83	0.59
1:C:150:ASP:H	1:C:156:ASN:HD21	1.50	0.58
1:A:249:PRO:HD2	1:A:348:GLN:NE2	2.19	0.58
1:D:283:LEU:HD22	1:D:292:ILE:HG12	1.84	0.57
1:B:74:LYS:O	1:B:78:ILE:HD13	2.05	0.56
1:A:118:ASN:OD1	1:A:119:LEU:N	2.39	0.56
1:C:244:TYR:O	1:C:248:LEU:HD22	2.06	0.55
1:A:282:ARG:NH1	1:A:284:TYR:HB2	2.22	0.55
1:D:91:GLN:NE2	1:D:93:GLU:OE2	2.27	0.55
1:C:253:ASP:OD2	1:C:254:LYS:HG3	2.07	0.55
1:A:366:LEU:H	1:A:366:LEU:HD13	1.72	0.55
1:B:-1:SER:HB3	1:B:92:LEU:HD12	1.89	0.54
1:B:161:GLU:OE1	1:B:168:ARG:NH2	2.39	0.54
1:D:252:PRO:HA	1:D:341:THR:HG22	1.89	0.54
1:D:214:LEU:HD11	1:D:225:ALA:HB1	1.89	0.54
1:C:264:LYS:HD2	1:C:329:ASN:OD1	2.07	0.53
1:A:68:THR:HB	1:A:92:LEU:HD11	1.91	0.53
1:D:159:LEU:HD11	1:D:192:SER:HB3	1.90	0.53
1:D:73:ARG:O	1:D:73:ARG:HD3	2.09	0.53
1:A:105:ARG:HH12	1:A:107:SER:HB2	1.74	0.53
1:C:73:ARG:HH11	3:C:403:1PE:H252	1.72	0.52
1:C:299:GLN:O	1:D:96:ARG:NH1	2.39	0.51
1:D:346:SER:HB3	1:D:362:MET:CE	2.40	0.51
1:C:197[B]:ARG:NH1	5:C:504:HOH:O	2.36	0.51
1:D:6:GLU:OE2	1:D:85:GLY:HA2	2.10	0.51
1:D:267:PHE:HE1	1:D:283:LEU:HD21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:MET:HE1	1:B:340:LEU:HD22	1.92	0.51
1:C:19:GLY:HA3	1:C:202:GLU:OE2	2.12	0.50
1:A:176:ARG:HD3	5:A:526:HOH:O	2.11	0.50
1:D:319:PHE:HZ	1:D:347:VAL:CG2	2.25	0.50
1:C:251:ASN:N	1:C:252:PRO:HD3	2.26	0.50
1:C:12:LYS:HA	1:C:15:GLN:HG3	1.94	0.50
1:C:136:LYS:HD2	1:C:204[B]:MET:SD	2.52	0.49
1:B:53:MET:SD	1:B:206:MET:HE3	2.52	0.49
1:D:249:PRO:HB2	1:D:252:PRO:HG3	1.94	0.49
1:C:13:PRO:HA	1:C:230:PHE:HE2	1.77	0.49
1:B:40:GLY:HA2	1:B:63:HIS:NE2	2.28	0.48
1:A:272:ILE:HD13	1:B:78:ILE:HD12	1.95	0.48
1:B:165:GLU:HG3	1:B:185:GLY:H	1.79	0.48
1:A:105:ARG:NH1	5:A:508:HOH:O	2.46	0.48
1:C:296:ASN:CG	1:C:298:GLU:HG2	2.35	0.47
1:C:132:GLN:HE21	1:C:212:ASN:HB3	1.80	0.46
1:C:73:ARG:NH1	3:C:403:1PE:H252	2.30	0.46
1:C:193:VAL:HB	1:C:236:LEU:HD13	1.97	0.46
1:D:285:VAL:CG2	1:D:315:MET:HG2	2.44	0.46
1:D:27:LEU:HB2	1:D:30:LEU:HG	1.97	0.46
1:C:70:VAL:HG11	1:C:97:MET:SD	2.55	0.46
1:C:289:GLN:NE2	1:C:307:ASP:OD1	2.49	0.46
1:A:48:ASP:O	1:A:49:LEU:HB2	2.15	0.46
1:A:105:ARG:HG3	1:B:303:GLU:HB3	1.98	0.46
1:A:144:PHE:CD1	1:A:326:ASP:HB3	2.50	0.46
1:B:264:LYS:HD2	1:B:329:ASN:OD1	2.15	0.46
1:D:362:MET:CE	2:K:5:LEU:HD12	2.46	0.46
1:B:338:MET:HG2	1:B:349:ILE:HG12	1.98	0.45
1:C:161:GLU:OE2	1:C:168:ARG:NH1	2.49	0.45
1:C:291:LYS:NZ	5:C:510:HOH:O	2.49	0.45
1:D:91:GLN:HE21	1:D:93:GLU:CD	2.15	0.45
1:B:11:LEU:HD23	1:B:11:LEU:HA	1.81	0.45
1:B:133:ALA:O	1:B:137:ARG:HG2	2.17	0.45
1:C:273:LEU:HD12	1:C:302:ALA:HB2	1.99	0.45
1:D:124:SER:O	5:D:501:HOH:O	2.21	0.45
1:A:33:LEU:HG	1:A:72:ALA:HB2	1.99	0.45
1:C:51:MET:HE1	1:C:198:LYS:HB3	1.99	0.45
1:A:214:LEU:HD11	1:A:225:ALA:HB1	1.99	0.45
1:D:139:ILE:HG21	1:D:204:MET:HB2	1.98	0.45
1:B:332:LYS:HZ2	3:B:402:1PE:H232	1.82	0.45
1:B:-1:SER:HB3	1:B:92:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:PRO:HA	1:B:341:THR:HG22	1.99	0.44
1:D:73:ARG:HD2	1:D:77:ASP:OD2	2.17	0.44
1:B:48:ASP:O	1:B:49:LEU:HB2	2.17	0.44
1:C:346:SER:HB3	1:C:362:MET:SD	2.57	0.44
1:B:332:LYS:HZ3	3:B:402:1PE:H221	1.81	0.44
1:C:247:VAL:CG1	2:J:5:LEU:HD22	2.48	0.44
1:B:17:VAL:HA	1:B:53:MET:HB3	2.00	0.44
1:C:48:ASP:O	1:C:49:LEU:HB2	2.18	0.44
1:C:214:LEU:HD11	1:C:225:ALA:HB1	2.00	0.44
1:A:105:ARG:NH1	1:A:107:SER:HB2	2.33	0.44
1:D:340:LEU:HD23	1:D:347:VAL:HG22	2.00	0.44
1:A:176:ARG:NH1	1:A:326:ASP:OD2	2.45	0.43
1:B:315:MET:HG2	1:B:316:GLU:N	2.32	0.43
1:D:126:VAL:HG13	1:D:218:ILE:HB	2.00	0.43
1:D:135:MET:HE3	1:D:216:VAL:HG21	2.00	0.43
1:B:332:LYS:NZ	3:B:402:1PE:H221	2.32	0.43
1:C:244:TYR:CD1	1:C:248:LEU:HD21	2.54	0.43
1:D:158:MET:HG2	1:D:160:PHE:HE1	1.78	0.43
1:C:281:VAL:HG12	1:C:294:ALA:HB2	1.99	0.43
1:A:10:LEU:HD12	1:A:10:LEU:HA	1.89	0.43
1:D:70:VAL:HG21	1:D:97:MET:CE	2.48	0.42
1:B:314:GLU:HG2	5:B:585:HOH:O	2.18	0.42
1:A:159:LEU:HD11	1:A:192[A]:SER:HB3	2.01	0.42
1:D:139:ILE:HG23	1:D:158:MET:CE	2.49	0.42
1:A:40:GLY:HA2	1:A:63:HIS:NE2	2.35	0.42
1:B:160:PHE:O	1:B:192:SER:HA	2.19	0.42
1:C:362:MET:CE	2:J:3:ALC:HB2	2.49	0.42
1:D:283:LEU:O	1:D:316:GLU:HA	2.20	0.42
1:B:52:GLU:OE2	1:B:119:LEU:HB2	2.20	0.42
1:C:244:TYR:HD2	5:C:548:HOH:O	2.03	0.42
1:C:26:THR:HG22	1:C:27:LEU:HD23	2.02	0.42
1:D:73:ARG:HD3	1:D:73:ARG:C	2.40	0.42
1:D:346:SER:HB3	1:D:362:MET:HE1	2.01	0.42
1:A:214:LEU:HD13	1:A:227:VAL:HG22	2.00	0.41
1:D:217:GLN:OE1	1:D:224:ARG:NH2	2.52	0.41
1:D:48:ASP:O	1:D:49:LEU:HB2	2.20	0.41
1:C:165:GLU:HA	1:C:186:GLN:O	2.20	0.41
1:B:214:LEU:HD13	1:B:227:VAL:HB	2.02	0.41
1:D:133:ALA:O	1:D:137:ARG:HG2	2.20	0.41
1:A:103:ARG:HB2	5:A:559:HOH:O	2.20	0.41
1:C:161:GLU:OE2	1:C:245:ARG:NH2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:GLN:HA	1:C:359:TYR:O	2.20	0.41
1:D:341:THR:OG1	1:D:342:ASP:N	2.54	0.41
1:A:8:GLU:OE2	1:A:84:GLU:HG3	2.21	0.41
1:A:338:MET:HG2	1:A:347:VAL:HG21	2.03	0.41
1:D:132:GLN:HG3	1:D:210:GLY:O	2.21	0.41
1:D:167:LEU:HD23	1:D:168:ARG:N	2.35	0.41
1:D:14:LEU:HB3	1:D:76:PHE:HD1	1.86	0.40
1:D:283:LEU:CD2	1:D:292:ILE:HG12	2.51	0.40
1:D:126:VAL:CG1	1:D:218:ILE:HB	2.51	0.40
1:B:50:GLU:HA	1:B:235:LYS:HD2	2.04	0.40
1:D:158:MET:CE	1:D:200:VAL:HG13	2.51	0.40
1:C:159:LEU:HD11	1:C:192:SER:HB3	2.03	0.40
1:D:12:LYS:HB3	1:D:13:PRO:HD3	2.02	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	370/368 (100%)	360 (97%)	7 (2%)	3 (1%)	19 9
1	B	359/368 (98%)	355 (99%)	4 (1%)	0	100 100
1	C	366/368 (100%)	357 (98%)	8 (2%)	1 (0%)	41 29
1	D	361/368 (98%)	355 (98%)	5 (1%)	1 (0%)	41 29
2	H	3/6 (50%)	3 (100%)	0	0	100 100
2	I	3/6 (50%)	3 (100%)	0	0	100 100
2	J	3/6 (50%)	3 (100%)	0	0	100 100
2	K	3/6 (50%)	3 (100%)	0	0	100 100
All	All	1468/1496 (98%)	1439 (98%)	24 (2%)	5 (0%)	41 29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	287	GLU
1	D	287	GLU
1	A	211	ASP
1	A	287	GLU
1	A	25	PRO

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	301/315 (96%)	297 (99%)	4 (1%)	69	64
1	B	302/315 (96%)	300 (99%)	2 (1%)	84	83
1	C	301/315 (96%)	296 (98%)	5 (2%)	60	53
1	D	296/315 (94%)	290 (98%)	6 (2%)	55	48
2	H	4/4 (100%)	4 (100%)	0	100	100
2	I	4/4 (100%)	4 (100%)	0	100	100
2	J	4/4 (100%)	4 (100%)	0	100	100
2	K	4/4 (100%)	4 (100%)	0	100	100
All	All	1216/1276 (95%)	1199 (99%)	17 (1%)	67	62

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	ARG
1	A	246	ARG
1	A	282	ARG
1	A	366	LEU
1	B	176	ARG
1	B	366	LEU
1	C	52	GLU
1	C	105	ARG
1	C	205	ARG

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Mol	Chain	Res	Type
1	C	224	ARG
1	C	366	LEU
1	D	6	GLU
1	D	70	VAL
1	D	124	SER
1	D	176	ARG
1	D	215	ARG
1	D	257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	348	GLN
1	B	91	GLN
1	B	226	HIS
1	C	32	ASN
1	C	156	ASN
1	D	348	GLN

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	ALC	J	3	2	9,11,12	0.28	0	10,13,15	0.38	0
2	ALC	H	3	2	9,11,12	0.23	0	10,13,15	0.54	0
2	ALC	I	3	2	9,11,12	0.25	0	10,13,15	0.64	0
2	ALC	K	3	2	9,11,12	0.22	0	10,13,15	0.46	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	ALC	J	3	2	-	4/5/14/16	0/1/1/1
2	ALC	H	3	2	-	3/5/14/16	0/1/1/1
2	ALC	I	3	2	-	4/5/14/16	0/1/1/1
2	ALC	K	3	2	-	4/5/14/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	3	ALC	CA-CB-CG-CD2
2	H	3	ALC	CA-CB-CG-CD1
2	I	3	ALC	O-C-CA-CB
2	I	3	ALC	CA-CB-CG-CD2
2	I	3	ALC	CA-CB-CG-CD1
2	J	3	ALC	N-CA-CB-CG
2	J	3	ALC	CA-CB-CG-CD2
2	K	3	ALC	CA-CB-CG-CD2
2	K	3	ALC	CA-CB-CG-CD1
2	J	3	ALC	CA-CB-CG-CD1
2	J	3	ALC	C-CA-CB-CG
2	K	3	ALC	N-CA-CB-CG
2	K	3	ALC	C-CA-CB-CG
2	H	3	ALC	N-CA-CB-CG
2	I	3	ALC	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	3	ALC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

24 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	1PE	C	402	-	6,6,15	0.13	0	5,5,14	0.22	0
3	1PE	D	402	-	6,6,15	0.11	0	5,5,14	0.19	0
3	1PE	B	406	-	9,9,15	0.09	0	8,8,14	0.16	0
3	1PE	I	101	-	15,15,15	0.10	0	14,14,14	0.19	0
3	1PE	B	407	-	12,12,15	0.13	0	11,11,14	0.13	0
4	GOL	H	101	-	5,5,5	0.05	0	5,5,5	0.21	0
4	GOL	I	102	-	5,5,5	0.08	0	5,5,5	0.24	0
3	1PE	B	401	-	9,9,15	0.10	0	8,8,14	0.22	0
4	GOL	A	404	-	5,5,5	0.05	0	5,5,5	0.19	0
4	GOL	B	409	-	5,5,5	0.06	0	5,5,5	0.22	0
3	1PE	K	101	-	15,15,15	0.12	0	14,14,14	0.14	0
4	GOL	B	408	-	5,5,5	0.05	0	5,5,5	0.19	0
3	1PE	A	402	-	6,6,15	0.16	0	5,5,14	0.20	0
3	1PE	B	403	-	6,6,15	0.08	0	5,5,14	0.21	0
4	GOL	D	403	-	5,5,5	0.05	0	5,5,5	0.26	0
3	1PE	B	404	-	9,9,15	0.10	0	8,8,14	0.16	0
3	1PE	A	403	-	12,12,15	0.16	0	11,11,14	0.14	0
4	GOL	A	405	-	5,5,5	0.06	0	5,5,5	0.24	0
3	1PE	C	403	-	7,7,15	0.20	0	6,6,14	0.13	0
3	1PE	B	402	-	15,15,15	0.17	0	14,14,14	0.15	0
3	1PE	C	401	-	15,15,15	0.13	0	14,14,14	0.11	0
3	1PE	B	405	-	6,6,15	0.12	0	5,5,14	0.22	0
3	1PE	D	401	-	9,9,15	0.17	0	8,8,14	0.13	0
3	1PE	A	401	-	12,12,15	0.15	0	11,11,14	0.18	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	1PE	C	402	-	-	2/4/4/13	-
3	1PE	D	402	-	-	1/4/4/13	-
3	1PE	B	406	-	-	3/7/7/13	-
3	1PE	I	101	-	-	6/13/13/13	-
3	1PE	B	407	-	-	2/10/10/13	-
4	GOL	H	101	-	-	0/4/4/4	-
4	GOL	I	102	-	-	0/4/4/4	-
3	1PE	B	401	-	-	0/7/7/13	-
4	GOL	A	404	-	-	0/4/4/4	-
4	GOL	B	409	-	-	2/4/4/4	-
3	1PE	K	101	-	-	3/13/13/13	-
4	GOL	B	408	-	-	0/4/4/4	-
3	1PE	A	402	-	-	2/4/4/13	-
3	1PE	B	403	-	-	1/4/4/13	-
4	GOL	D	403	-	-	0/4/4/4	-
3	1PE	B	404	-	-	1/7/7/13	-
3	1PE	A	403	-	-	0/10/10/13	-
4	GOL	A	405	-	-	0/4/4/4	-
3	1PE	C	403	-	-	2/5/5/13	-
3	1PE	B	402	-	-	3/13/13/13	-
3	1PE	C	401	-	-	5/13/13/13	-
3	1PE	B	405	-	-	2/4/4/13	-
3	1PE	D	401	-	-	1/7/7/13	-
3	1PE	A	401	-	-	2/10/10/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	409	GOL	C1-C2-C3-O3
3	B	402	1PE	C12-C22-OH3-C23
4	B	409	GOL	O2-C2-C3-O3
3	C	402	1PE	C13-C23-OH3-C22
3	K	101	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
3	I	101	1PE	C15-C25-OH5-C14
3	C	401	1PE	C16-C26-OH6-C15
3	B	407	1PE	C25-C15-OH6-C26
3	B	405	1PE	C14-C24-OH4-C13
3	B	404	1PE	C24-C14-OH5-C25
3	D	402	1PE	C15-C25-OH5-C14
3	I	101	1PE	C25-C15-OH6-C26
3	B	407	1PE	C15-C25-OH5-C14
3	C	401	1PE	C12-C22-OH3-C23
3	A	401	1PE	C24-C14-OH5-C25
3	B	406	1PE	C24-C14-OH5-C25
3	A	402	1PE	C24-C14-OH5-C25
3	C	403	1PE	C16-C26-OH6-C15
3	I	101	1PE	C12-C22-OH3-C23
3	K	101	1PE	C15-C25-OH5-C14
3	I	101	1PE	C13-C23-OH3-C22
3	B	402	1PE	C15-C25-OH5-C14
3	B	405	1PE	C23-C13-OH4-C24
3	D	401	1PE	C15-C25-OH5-C14
3	I	101	1PE	C23-C13-OH4-C24
3	C	401	1PE	C23-C13-OH4-C24
3	B	403	1PE	C13-C23-OH3-C22
3	B	402	1PE	C23-C13-OH4-C24
3	C	401	1PE	C24-C14-OH5-C25
3	C	402	1PE	C12-C22-OH3-C23
3	B	406	1PE	C16-C26-OH6-C15
3	A	402	1PE	C15-C25-OH5-C14
3	C	401	1PE	OH6-C15-C25-OH5
3	B	406	1PE	OH6-C15-C25-OH5
3	K	101	1PE	C25-C15-OH6-C26
3	C	403	1PE	OH6-C15-C25-OH5
3	A	401	1PE	C13-C23-OH3-C22
3	I	101	1PE	OH7-C16-C26-OH6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	409	GOL	2	0
3	C	403	1PE	2	0
3	B	402	1PE	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	368/368 (100%)	0.10	8 (2%) 62 63	22, 38, 67, 116	0
1	B	364/368 (98%)	-0.03	4 (1%) 80 82	22, 35, 57, 76	0
1	C	366/368 (99%)	0.08	9 (2%) 57 59	23, 39, 61, 107	0
1	D	365/368 (99%)	0.11	10 (2%) 54 56	23, 42, 63, 94	0
2	H	4/6 (66%)	-0.03	0 100 100	34, 39, 48, 50	0
2	I	4/6 (66%)	-0.27	0 100 100	26, 29, 33, 36	0
2	J	4/6 (66%)	-0.06	0 100 100	35, 41, 44, 48	0
2	K	4/6 (66%)	-0.38	0 100 100	29, 36, 36, 37	0
All	All	1479/1496 (98%)	0.06	31 (2%) 63 65	22, 38, 63, 116	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	120	ASP	6.7
1	C	119	LEU	6.4
1	A	366	LEU	6.3
1	C	26	THR	6.3
1	C	22	GLY	5.9
1	D	25	PRO	4.8
1	B	366	LEU	4.7
1	D	26	THR	4.5
1	D	366	LEU	4.4
1	A	22	GLY	4.0
1	A	24	ARG	4.0
1	C	27	LEU	3.8
1	B	26	THR	3.6
1	C	209	GLY	3.5
1	D	122	TRP	3.5
1	B	119	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	22	GLY	3.1
1	C	366	LEU	3.1
1	B	284	TYR	2.9
1	D	0	HIS	2.9
1	A	27	LEU	2.9
1	D	119	LEU	2.7
1	D	118	ASN	2.5
1	A	117	PRO	2.4
1	C	121	ASP	2.3
1	A	118	ASN	2.3
1	D	-1	SER	2.3
1	A	209	GLY	2.2
1	C	210	GLY	2.2
1	D	311	SER	2.0
1	A	23	GLY	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, 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	B-factors(Å^2)	Q<0.9
2	ALC	H	3	11/12	0.95	0.08	32,39,45,46	0
2	ALC	I	3	11/12	0.95	0.11	22,27,32,34	0
2	ALC	K	3	11/12	0.96	0.11	26,32,40,41	0
2	ALC	J	3	11/12	0.97	0.09	32,36,40,45	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, 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	B-factors(Å^2)	Q<0.9
4	GOL	H	101	6/6	0.45	0.18	78,81,83,83	0
4	GOL	D	403	6/6	0.57	0.26	72,74,75,75	0
4	GOL	A	404	6/6	0.65	0.24	67,69,72,72	0
4	GOL	I	102	6/6	0.68	0.28	49,65,69,69	0
3	1PE	C	403	8/16	0.78	0.18	61,66,69,70	0
4	GOL	B	409	6/6	0.81	0.18	41,57,59,62	0
3	1PE	C	402	7/16	0.81	0.14	64,65,68,69	0
3	1PE	B	406	10/16	0.82	0.14	64,69,76,78	0
3	1PE	D	401	10/16	0.83	0.12	55,57,60,61	0
4	GOL	A	405	6/6	0.83	0.10	59,61,63,65	0
3	1PE	C	401	16/16	0.86	0.12	48,54,62,63	0
3	1PE	B	402	16/16	0.86	0.20	60,65,73,76	0
4	GOL	B	408	6/6	0.87	0.16	47,60,67,69	0
3	1PE	B	407	13/16	0.89	0.14	57,63,70,72	0
3	1PE	B	404	10/16	0.89	0.14	61,65,73,75	0
3	1PE	A	402	7/16	0.89	0.12	45,49,61,62	0
3	1PE	D	402	7/16	0.90	0.14	58,61,67,71	0
3	1PE	B	405	7/16	0.91	0.10	45,49,51,54	0
3	1PE	A	401	13/16	0.92	0.14	39,57,73,73	0
3	1PE	K	101	16/16	0.93	0.10	41,49,66,69	0
3	1PE	B	403	7/16	0.93	0.11	52,57,63,66	0
3	1PE	A	403	13/16	0.93	0.12	47,54,73,74	0
3	1PE	I	101	16/16	0.93	0.14	38,49,59,62	0
3	1PE	B	401	10/16	0.97	0.14	39,51,64,69	0

6.5 Other polymers (i)

There are no such residues in this entry.