Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 09:46 AM EDT

PDB ID	:	6E8D
Title	:	Crystal structure of the Bacillus subtilis sliding clamp-MutL complex.
Authors	:	Guarne, A.; Almawi, A.W.
Deposited on	:	2018-07-28
Resolution	:	2.34 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:

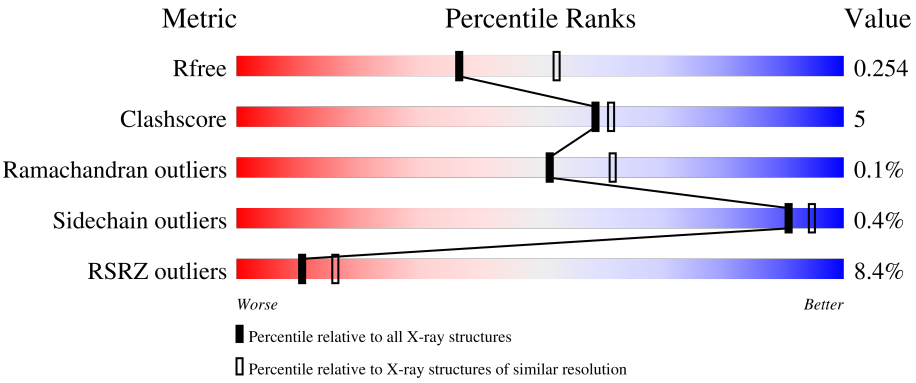
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	512	9% 84% 7% 9%
1	B	512	8% 83% 6% 11%
1	C	512	6% 80% 9% 11%
1	D	512	6% 78% 8% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13668 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,DNA mismatch repair protein MutL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	1	0
			3457	2204	577	668	8			
1	B	458	Total	C	N	O	S	0	1	0
			3419	2178	568	665	8			
1	C	454	Total	C	N	O	S	0	1	0
			3402	2179	556	659	8			
1	D	439	Total	C	N	O	S	0	0	0
			3202	2049	526	620	7			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP A0A085C685
A	-4	GLY	-	expression tag	UNP A0A085C685
A	-3	SER	-	expression tag	UNP A0A085C685
A	-2	SER	-	expression tag	UNP A0A085C685
A	-1	HIS	-	expression tag	UNP A0A085C685
A	0	HIS	-	expression tag	UNP A0A085C685
A	1	HIS	-	expression tag	UNP A0A085C685
A	2	HIS	-	expression tag	UNP A0A085C685
A	3	HIS	-	expression tag	UNP A0A085C685
A	4	HIS	-	expression tag	UNP A0A085C685
A	5	GLY	-	expression tag	UNP A0A085C685
A	6	SER	-	expression tag	UNP A0A085C685
A	7	GLY	-	expression tag	UNP A0A085C685
A	8	GLY	-	expression tag	UNP A0A085C685
A	9	GLY	-	expression tag	UNP A0A085C685
A	10	ASN	-	expression tag	UNP A0A085C685
A	11	ASN	-	expression tag	UNP A0A085C685
A	12	ASN	-	expression tag	UNP A0A085C685
A	13	ASN	-	expression tag	UNP A0A085C685
A	14	ASN	-	expression tag	UNP A0A085C685
A	15	ASN	-	expression tag	UNP A0A085C685

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Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ASN	-	expression tag	UNP A0A085C685
A	17	ASN	-	expression tag	UNP A0A085C685
A	18	ASN	-	expression tag	UNP A0A085C685
A	19	ASN	-	expression tag	UNP A0A085C685
A	20	LEU	-	expression tag	UNP A0A085C685
A	21	GLY	-	expression tag	UNP A0A085C685
A	22	ILE	-	expression tag	UNP A0A085C685
A	23	GLU	-	expression tag	UNP A0A085C685
A	24	GLU	-	expression tag	UNP A0A085C685
A	25	ASN	-	expression tag	UNP A0A085C685
A	26	LEU	-	expression tag	UNP A0A085C685
A	27	TYR	-	expression tag	UNP A0A085C685
A	28	PHE	-	expression tag	UNP A0A085C685
A	29	GLN	-	expression tag	UNP A0A085C685
A	30	SER	-	expression tag	UNP A0A085C685
A	31	HIS	-	expression tag	UNP A0A085C685
A	32	MET	-	expression tag	UNP A0A085C685
A	412	ASP	GLY	linker	UNP A0A164SDM9
A	413	SER	GLU	linker	UNP A0A164SDM9
B	-5	MET	-	initiating methionine	UNP A0A085C685
B	-4	GLY	-	expression tag	UNP A0A085C685
B	-3	SER	-	expression tag	UNP A0A085C685
B	-2	SER	-	expression tag	UNP A0A085C685
B	-1	HIS	-	expression tag	UNP A0A085C685
B	0	HIS	-	expression tag	UNP A0A085C685
B	1	HIS	-	expression tag	UNP A0A085C685
B	2	HIS	-	expression tag	UNP A0A085C685
B	3	HIS	-	expression tag	UNP A0A085C685
B	4	HIS	-	expression tag	UNP A0A085C685
B	5	GLY	-	expression tag	UNP A0A085C685
B	6	SER	-	expression tag	UNP A0A085C685
B	7	GLY	-	expression tag	UNP A0A085C685
B	8	GLY	-	expression tag	UNP A0A085C685
B	9	GLY	-	expression tag	UNP A0A085C685
B	10	ASN	-	expression tag	UNP A0A085C685
B	11	ASN	-	expression tag	UNP A0A085C685
B	12	ASN	-	expression tag	UNP A0A085C685
B	13	ASN	-	expression tag	UNP A0A085C685
B	14	ASN	-	expression tag	UNP A0A085C685
B	15	ASN	-	expression tag	UNP A0A085C685
B	16	ASN	-	expression tag	UNP A0A085C685
B	17	ASN	-	expression tag	UNP A0A085C685

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Chain	Residue	Modelled	Actual	Comment	Reference
B	18	ASN	-	expression tag	UNP A0A085C685
B	19	ASN	-	expression tag	UNP A0A085C685
B	20	LEU	-	expression tag	UNP A0A085C685
B	21	GLY	-	expression tag	UNP A0A085C685
B	22	ILE	-	expression tag	UNP A0A085C685
B	23	GLU	-	expression tag	UNP A0A085C685
B	24	GLU	-	expression tag	UNP A0A085C685
B	25	ASN	-	expression tag	UNP A0A085C685
B	26	LEU	-	expression tag	UNP A0A085C685
B	27	TYR	-	expression tag	UNP A0A085C685
B	28	PHE	-	expression tag	UNP A0A085C685
B	29	GLN	-	expression tag	UNP A0A085C685
B	30	SER	-	expression tag	UNP A0A085C685
B	31	HIS	-	expression tag	UNP A0A085C685
B	32	MET	-	expression tag	UNP A0A085C685
B	412	ASP	GLY	linker	UNP A0A164SDM9
B	413	SER	GLU	linker	UNP A0A164SDM9
C	-5	MET	-	initiating methionine	UNP A0A085C685
C	-4	GLY	-	expression tag	UNP A0A085C685
C	-3	SER	-	expression tag	UNP A0A085C685
C	-2	SER	-	expression tag	UNP A0A085C685
C	-1	HIS	-	expression tag	UNP A0A085C685
C	0	HIS	-	expression tag	UNP A0A085C685
C	1	HIS	-	expression tag	UNP A0A085C685
C	2	HIS	-	expression tag	UNP A0A085C685
C	3	HIS	-	expression tag	UNP A0A085C685
C	4	HIS	-	expression tag	UNP A0A085C685
C	5	GLY	-	expression tag	UNP A0A085C685
C	6	SER	-	expression tag	UNP A0A085C685
C	7	GLY	-	expression tag	UNP A0A085C685
C	8	GLY	-	expression tag	UNP A0A085C685
C	9	GLY	-	expression tag	UNP A0A085C685
C	10	ASN	-	expression tag	UNP A0A085C685
C	11	ASN	-	expression tag	UNP A0A085C685
C	12	ASN	-	expression tag	UNP A0A085C685
C	13	ASN	-	expression tag	UNP A0A085C685
C	14	ASN	-	expression tag	UNP A0A085C685
C	15	ASN	-	expression tag	UNP A0A085C685
C	16	ASN	-	expression tag	UNP A0A085C685
C	17	ASN	-	expression tag	UNP A0A085C685
C	18	ASN	-	expression tag	UNP A0A085C685
C	19	ASN	-	expression tag	UNP A0A085C685

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	LEU	-	expression tag	UNP A0A085C685
C	21	GLY	-	expression tag	UNP A0A085C685
C	22	ILE	-	expression tag	UNP A0A085C685
C	23	GLU	-	expression tag	UNP A0A085C685
C	24	GLU	-	expression tag	UNP A0A085C685
C	25	ASN	-	expression tag	UNP A0A085C685
C	26	LEU	-	expression tag	UNP A0A085C685
C	27	TYR	-	expression tag	UNP A0A085C685
C	28	PHE	-	expression tag	UNP A0A085C685
C	29	GLN	-	expression tag	UNP A0A085C685
C	30	SER	-	expression tag	UNP A0A085C685
C	31	HIS	-	expression tag	UNP A0A085C685
C	32	MET	-	expression tag	UNP A0A085C685
C	412	ASP	GLY	linker	UNP A0A164SDM9
C	413	SER	GLU	linker	UNP A0A164SDM9
D	-5	MET	-	initiating methionine	UNP A0A085C685
D	-4	GLY	-	expression tag	UNP A0A085C685
D	-3	SER	-	expression tag	UNP A0A085C685
D	-2	SER	-	expression tag	UNP A0A085C685
D	-1	HIS	-	expression tag	UNP A0A085C685
D	0	HIS	-	expression tag	UNP A0A085C685
D	1	HIS	-	expression tag	UNP A0A085C685
D	2	HIS	-	expression tag	UNP A0A085C685
D	3	HIS	-	expression tag	UNP A0A085C685
D	4	HIS	-	expression tag	UNP A0A085C685
D	5	GLY	-	expression tag	UNP A0A085C685
D	6	SER	-	expression tag	UNP A0A085C685
D	7	GLY	-	expression tag	UNP A0A085C685
D	8	GLY	-	expression tag	UNP A0A085C685
D	9	GLY	-	expression tag	UNP A0A085C685
D	10	ASN	-	expression tag	UNP A0A085C685
D	11	ASN	-	expression tag	UNP A0A085C685
D	12	ASN	-	expression tag	UNP A0A085C685
D	13	ASN	-	expression tag	UNP A0A085C685
D	14	ASN	-	expression tag	UNP A0A085C685
D	15	ASN	-	expression tag	UNP A0A085C685
D	16	ASN	-	expression tag	UNP A0A085C685
D	17	ASN	-	expression tag	UNP A0A085C685
D	18	ASN	-	expression tag	UNP A0A085C685
D	19	ASN	-	expression tag	UNP A0A085C685
D	20	LEU	-	expression tag	UNP A0A085C685
D	21	GLY	-	expression tag	UNP A0A085C685

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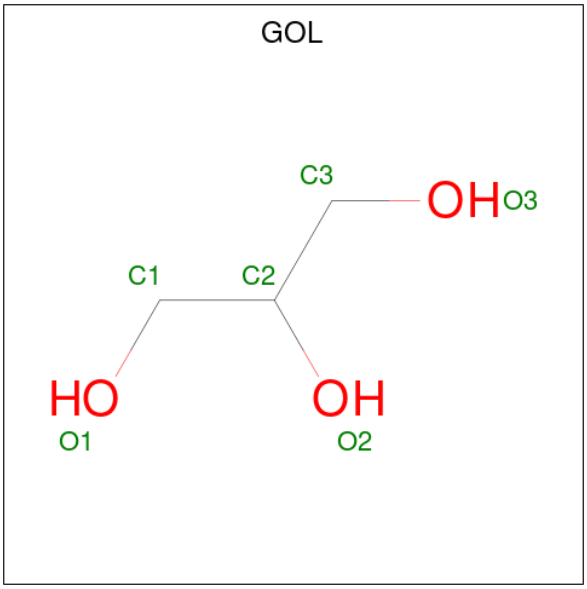
Chain	Residue	Modelled	Actual	Comment	Reference
D	22	ILE	-	expression tag	UNP A0A085C685
D	23	GLU	-	expression tag	UNP A0A085C685
D	24	GLU	-	expression tag	UNP A0A085C685
D	25	ASN	-	expression tag	UNP A0A085C685
D	26	LEU	-	expression tag	UNP A0A085C685
D	27	TYR	-	expression tag	UNP A0A085C685
D	28	PHE	-	expression tag	UNP A0A085C685
D	29	GLN	-	expression tag	UNP A0A085C685
D	30	SER	-	expression tag	UNP A0A085C685
D	31	HIS	-	expression tag	UNP A0A085C685
D	32	MET	-	expression tag	UNP A0A085C685
D	412	ASP	GLY	linker	UNP A0A164SDM9
D	413	SER	GLU	linker	UNP A0A164SDM9

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is water.

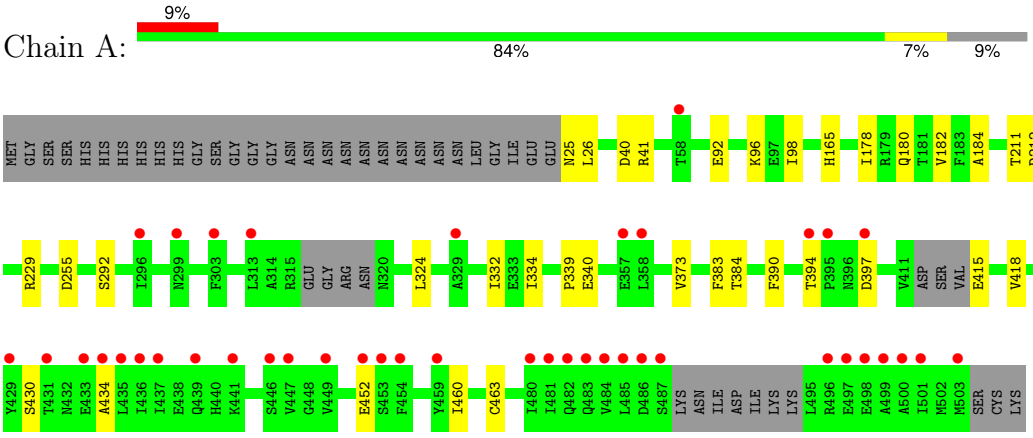
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	46	Total O 46 46	0	0
3	B	44	Total O 44 44	0	0
3	C	43	Total O 43 43	0	0
3	D	37	Total O 37 37	0	0

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.

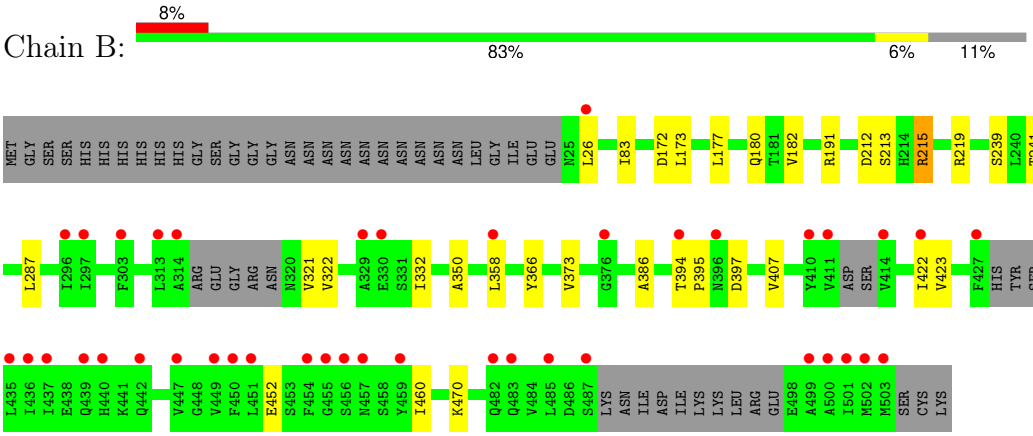
• Molecule 1: Beta sliding clamp,DNA mismatch repair protein MutL

Chain A:



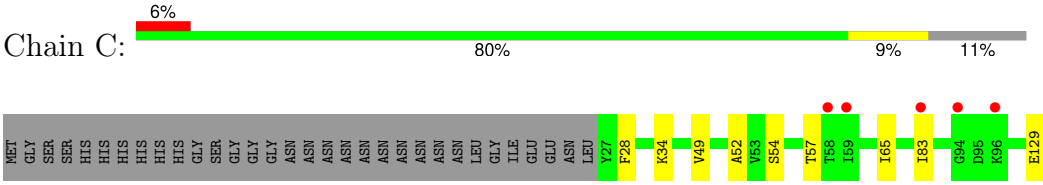
• Molecule 1: Beta sliding clamp,DNA mismatch repair protein MutL

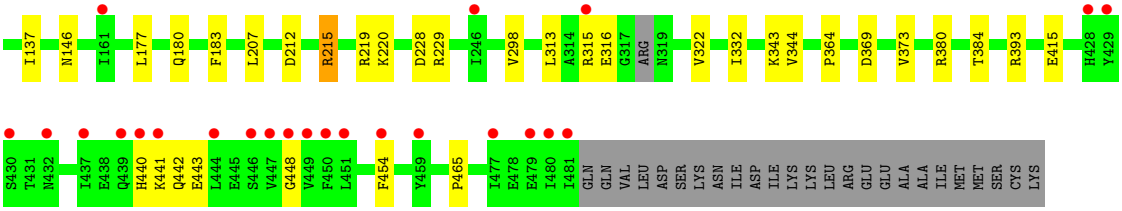
Chain B:



• Molecule 1: Beta sliding clamp,DNA mismatch repair protein MutL

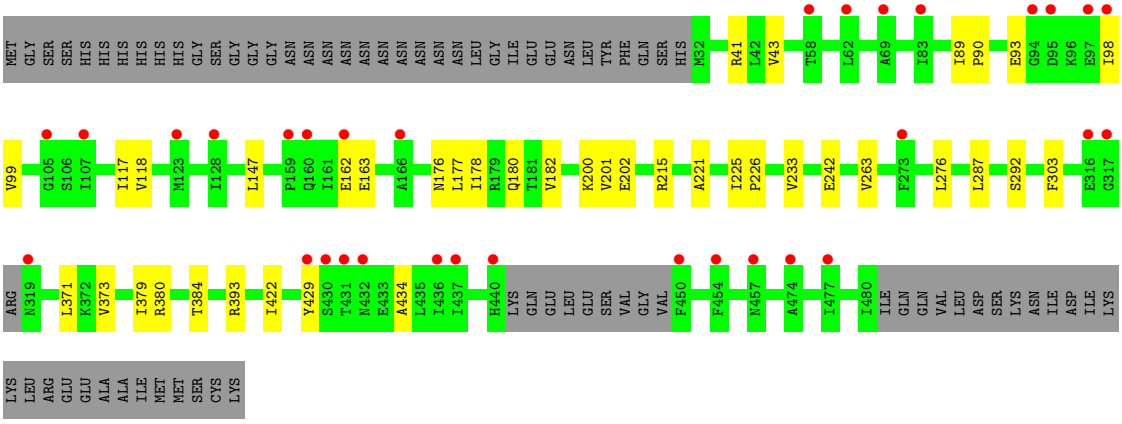
Chain C:





• Molecule 1: Beta sliding clamp,DNA mismatch repair protein MutL

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.02Å 83.89Å 128.26Å 80.30° 83.57° 89.96°	Depositor
Resolution (Å)	48.26 – 2.34 48.25 – 1.86	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.26-2.34) 72.0 (48.25-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.216 , 0.250 0.229 , 0.254	Depositor DCC
R_{free} test set	2000 reflections (1.37%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 68.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13668	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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: GOL

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	0.33	0/3510	0.50	0/4784
1	B	0.33	0/3469	0.49	0/4724
1	C	0.34	0/3459	0.52	0/4715
1	D	0.29	0/3250	0.44	0/4440
All	All	0.32	0/13688	0.49	0/18663

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	3457	0	3358	26	0
1	B	3419	0	3340	28	0
1	C	3402	0	3321	41	0
1	D	3202	0	3100	30	0
2	A	6	0	8	0	0
2	C	12	0	16	0	0
3	A	46	0	0	1	0
3	B	44	0	0	0	0
3	C	43	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	37	0	0	0	0
All	All	13668	0	13143	125	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 5.

All (125) 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:180:GLN:HA	1:C:373:VAL:HG11	1.47	0.94
1:C:180:GLN:HA	1:C:373:VAL:CG1	1.98	0.92
1:A:394:THR:OG1	1:A:397:ASP:HB2	1.69	0.92
1:B:394:THR:OG1	1:B:397:ASP:HB3	1.72	0.90
1:C:133:GLN:O	1:C:134:TYR:HB2	1.75	0.84
1:A:418:VAL:CG1	1:A:463:CYS:HB3	2.09	0.83
1:B:83:ILE:HD11	1:B:239:SER:OG	1.79	0.83
1:D:292:SER:HA	1:D:384:THR:CG2	2.09	0.82
1:C:315:ARG:HD2	1:C:315:ARG:H	1.46	0.81
1:D:201:VAL:O	1:D:202:GLU:HG2	1.81	0.81
1:C:315:ARG:HD2	1:C:315:ARG:N	2.02	0.73
1:C:180:GLN:HG2	1:C:373:VAL:HG12	1.72	0.72
1:D:292:SER:HA	1:D:384:THR:HG22	1.72	0.71
1:A:339:PRO:O	1:A:340:GLU:HG2	1.91	0.69
1:A:96:LYS:HE3	1:A:98:ILE:HD11	1.74	0.69
1:C:49:VAL:HG21	1:C:65:ILE:HD11	1.75	0.68
1:A:418:VAL:HG11	1:A:463:CYS:HB3	1.74	0.67
1:C:442:GLN:HG3	1:C:442:GLN:O	1.94	0.67
1:D:201:VAL:C	1:D:202:GLU:HG2	2.12	0.66
1:C:448:GLY:O	1:C:465:PRO:CG	2.43	0.66
1:A:180:GLN:HG2	1:A:373:VAL:HG13	1.78	0.66
1:A:324:LEU:HD11	1:A:332:ILE:CG2	2.27	0.65
1:C:180:GLN:HG2	1:C:373:VAL:CG1	2.26	0.64
1:B:180:GLN:HA	1:B:373:VAL:HG11	1.80	0.64
1:C:52:ALA:HA	1:C:83:ILE:HD11	1.79	0.63
1:C:315:ARG:H	1:C:315:ARG:CD	2.11	0.62
1:D:371:LEU:HD22	1:D:379:ILE:HD13	1.81	0.62
1:B:191:ARG:NH1	1:B:423:VAL:HG12	2.14	0.62
1:D:371:LEU:CD2	1:D:379:ILE:HD13	2.29	0.62
1:A:415:GLU:N	1:A:415:GLU:OE1	2.32	0.61
1:A:452:GLU:HB3	1:A:460:ILE:CG1	2.30	0.61
1:A:165:HIS:HA	1:A:229:ARG:CZ	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ASP:OD1	1:C:229:ARG:N	2.33	0.61
1:B:83:ILE:HD11	1:B:239:SER:CB	2.31	0.60
1:A:178:ILE:HG23	1:A:182:VAL:CG2	2.33	0.59
1:D:163:GLU:O	1:D:163:GLU:HG2	2.04	0.58
1:B:452:GLU:HB2	1:B:460:ILE:CG1	2.36	0.56
1:A:211:THR:OG1	1:A:212:ASP:O	2.25	0.54
1:B:191:ARG:HH12	1:B:423:VAL:HG12	1.72	0.54
1:D:380:ARG:NH1	1:D:393:ARG:NH1	2.57	0.53
1:B:177:LEU:CD2	1:B:219:ARG:HG3	2.39	0.53
1:A:452:GLU:HB3	1:A:460:ILE:HG13	1.89	0.53
1:C:34:LYS:HD2	1:C:129:GLU:OE2	2.08	0.53
1:C:54:SER:OG	1:C:57:THR:HB	2.09	0.53
1:C:180:GLN:HA	1:C:373:VAL:HG13	1.90	0.53
1:B:394:THR:HB	1:B:395:PRO:HD2	1.91	0.52
1:C:49:VAL:HG21	1:C:65:ILE:CD1	2.38	0.52
1:C:137:ILE:HG22	1:C:146:ASN:HA	1.91	0.51
1:C:212:ASP:CB	1:C:215:ARG:HD2	2.41	0.51
1:D:303:PHE:CD2	1:D:379:ILE:HD11	2.45	0.51
1:B:358:LEU:HD11	1:B:386:ALA:HB2	1.93	0.50
1:C:440:HIS:O	1:C:443:GLU:N	2.42	0.50
1:C:207:LEU:CD2	1:C:220:LYS:HG2	2.42	0.50
1:D:41:ARG:NH1	1:D:89:ILE:HG23	2.27	0.49
1:B:332:ILE:CD1	1:B:350:ALA:HB2	2.43	0.48
1:A:324:LEU:HD11	1:A:332:ILE:HG23	1.95	0.48
1:D:292:SER:HA	1:D:384:THR:HG23	1.91	0.48
1:C:448:GLY:O	1:C:465:PRO:HG3	2.13	0.47
1:B:255:ASP:HB3	1:B:266:LYS:HB2	1.96	0.46
1:B:321:VAL:HG21	1:B:407:VAL:HG11	1.97	0.46
1:D:233:VAL:HB	1:D:276:LEU:HD22	1.96	0.46
1:C:137:ILE:HG22	1:C:146:ASN:OD1	2.16	0.46
1:D:178:ILE:HG23	1:D:182:VAL:HG21	1.98	0.45
1:C:313:LEU:HD11	1:C:343:LYS:HA	1.98	0.45
1:D:263:VAL:CG2	1:D:276:LEU:HD21	2.46	0.45
1:D:371:LEU:CD2	1:D:379:ILE:CD1	2.95	0.45
1:B:177:LEU:HD22	1:B:219:ARG:HG3	1.98	0.45
1:C:315:ARG:O	1:C:316:GLU:HB2	2.17	0.45
1:A:292:SER:HA	1:A:384:THR:HG22	1.99	0.45
1:B:452:GLU:HB2	1:B:460:ILE:HG13	1.98	0.45
1:D:201:VAL:O	1:D:202:GLU:CG	2.58	0.45
1:A:178:ILE:HG23	1:A:182:VAL:HG23	1.97	0.44
1:A:324:LEU:HD13	1:A:334:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:ARG:NH1	1:C:393:ARG:NH1	2.66	0.44
1:A:92:GLU:HB2	3:A:745:HOH:O	2.17	0.44
1:B:332:ILE:HD11	1:B:350:ALA:HB2	1.99	0.44
1:D:98:ILE:HG22	1:D:99:VAL:HG23	1.98	0.44
1:A:339:PRO:O	1:A:340:GLU:CG	2.61	0.44
1:B:212:ASP:OD1	1:B:215:ARG:HG3	2.17	0.43
1:D:225:ILE:HB	1:D:226:PRO:CD	2.47	0.43
1:A:184:ALA:O	1:A:212:ASP:N	2.51	0.43
1:A:383:PHE:CD2	1:A:390:PHE:CB	3.02	0.43
1:D:200:LYS:HE3	1:D:202:GLU:HG3	2.01	0.43
1:C:313:LEU:CD1	1:C:344:VAL:HG23	2.49	0.43
1:C:322:VAL:HG23	1:C:364:PRO:HG3	1.99	0.43
1:D:287:LEU:HD22	1:D:422:ILE:HG23	2.00	0.43
1:B:173:LEU:O	1:B:177:LEU:HG	2.19	0.43
1:D:162:GLU:O	1:D:163:GLU:HB3	2.18	0.43
1:C:28:PHE:CD1	1:C:28:PHE:C	2.92	0.43
1:D:180:GLN:HG2	1:D:373:VAL:CG1	2.49	0.43
1:C:415:GLU:HG3	1:C:448:GLY:HA3	2.00	0.43
1:C:313:LEU:CD1	1:C:343:LYS:HA	2.49	0.43
1:A:178:ILE:HG23	1:A:182:VAL:HG21	2.01	0.43
1:B:321:VAL:HG12	1:B:322:VAL:N	2.33	0.43
1:A:40:ASP:OD1	1:A:41:ARG:N	2.51	0.42
1:B:182:VAL:HG21	1:B:241:THR:HG23	2.00	0.42
1:C:215:ARG:NH2	1:C:369:ASP:OD2	2.52	0.42
1:D:176:ASN:O	1:D:180:GLN:HG3	2.19	0.42
1:D:117:ILE:HD12	1:D:147:LEU:HD11	2.01	0.42
1:A:25:ASN:OD1	1:A:26:LEU:N	2.53	0.42
1:B:177:LEU:HD23	1:B:219:ARG:HG2	2.00	0.42
1:C:454:PHE:CD1	1:C:454:PHE:C	2.92	0.42
1:D:429:TYR:HB2	1:D:434:ALA:HB2	2.02	0.42
1:B:366:TYR:OH	1:B:470:LYS:HE3	2.20	0.42
1:D:163:GLU:O	1:D:163:GLU:CG	2.68	0.42
1:C:137:ILE:CG2	1:C:146:ASN:OD1	2.68	0.42
1:B:177:LEU:CD2	1:B:219:ARG:CG	2.98	0.41
1:D:90:PRO:HG2	1:D:93:GLU:HG3	2.00	0.41
1:B:26:LEU:N	1:B:26:LEU:HD12	2.35	0.41
1:C:298:VAL:HG11	1:C:332:ILE:HD12	2.02	0.41
1:D:43:VAL:HG22	1:D:118:VAL:HG12	2.02	0.41
1:B:172:ASP:OD1	1:B:173:LEU:N	2.53	0.41
1:C:177:LEU:HD12	1:C:219:ARG:HG2	2.01	0.41
1:D:242:GLU:OE2	1:D:242:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LEU:HD13	1:B:422:ILE:HG13	2.02	0.41
1:C:183:PHE:CE1	1:C:373:VAL:HG21	2.55	0.41
1:C:65:ILE:HG23	1:C:65:ILE:O	2.21	0.41
1:C:212:ASP:HB3	1:C:215:ARG:HD2	2.01	0.41
1:B:177:LEU:HD23	1:B:219:ARG:CG	2.51	0.41
1:A:180:GLN:HG2	1:A:373:VAL:CG1	2.48	0.41
1:D:177:LEU:HD21	1:D:221:ALA:HB2	2.01	0.41
1:A:430:SER:O	1:A:434:ALA:HB2	2.20	0.40
1:B:213:SER:O	1:B:422:ILE:N	2.53	0.40
1:C:180:GLN:CA	1:C:373:VAL:CG1	2.85	0.40
1:C:448:GLY:O	1:C:465:PRO:CD	2.69	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	458/512 (90%)	440 (96%)	18 (4%)	0	100	100
1	B	449/512 (88%)	436 (97%)	13 (3%)	0	100	100
1	C	451/512 (88%)	435 (96%)	15 (3%)	1 (0%)	47	55
1	D	433/512 (85%)	418 (96%)	15 (4%)	0	100	100
All	All	1791/2048 (88%)	1729 (96%)	61 (3%)	1 (0%)	51	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	441	LYS

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	362/461 (78%)	360 (99%)	2 (1%)	86	92
1	B	363/461 (79%)	362 (100%)	1 (0%)	92	96
1	C	361/461 (78%)	359 (99%)	2 (1%)	86	92
1	D	331/461 (72%)	330 (100%)	1 (0%)	92	96
All	All	1417/1844 (77%)	1411 (100%)	6 (0%)	91	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	ARG
1	A	255	ASP
1	B	215	ARG
1	C	215	ARG
1	C	384	THR
1	D	215	ARG

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

Mol	Chain	Res	Type
1	C	148	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	C	601	-	5,5,5	0.38	0	5,5,5	0.16	0
2	GOL	C	602	-	5,5,5	0.19	0	5,5,5	0.54	0
2	GOL	A	601	-	5,5,5	0.13	0	5,5,5	0.29	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	GOL	C	601	-	-	2/4/4/4	-
2	GOL	C	602	-	-	4/4/4/4	-
2	GOL	A	601	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-C3
2	A	601	GOL	C1-C2-C3-O3
2	C	601	GOL	C1-C2-C3-O3
2	C	601	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O2-C2-C3-O3
2	C	602	GOL	O1-C1-C2-C3
2	C	602	GOL	C1-C2-C3-O3
2	A	601	GOL	O1-C1-C2-O2
2	C	602	GOL	O2-C2-C3-O3
2	C	602	GOL	O1-C1-C2-O2

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 (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	465/512 (90%)	0.38	46 (9%)	7	12	27, 80, 179, 243	0
1	B	458/512 (89%)	0.41	43 (9%)	8	13	31, 81, 173, 264	0
1	C	454/512 (88%)	0.37	32 (7%)	16	24	33, 79, 157, 225	0
1	D	439/512 (85%)	0.28	32 (7%)	15	22	37, 84, 160, 214	0
All	All	1816/2048 (88%)	0.36	153 (8%)	11	16	27, 81, 169, 264	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	448	GLY	34.3
1	C	447	VAL	13.1
1	A	496	ARG	12.4
1	C	439	GLN	11.4
1	B	501	ILE	9.5
1	B	500	ALA	9.2
1	C	481	ILE	7.5
1	A	486	ASP	7.4
1	D	430	SER	7.2
1	D	429	TYR	6.8
1	B	459	TYR	6.8
1	B	503	MET	6.8
1	A	358	LEU	6.6
1	B	451	LEU	6.6
1	A	437	ILE	6.4
1	A	429	TYR	6.3
1	C	134	TYR	6.1
1	B	411	VAL	6.0
1	A	436	ILE	5.9
1	C	430	SER	5.9
1	C	428	HIS	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	454	PHE	5.7
1	D	431	THR	5.6
1	C	444	LEU	5.6
1	D	94	GLY	5.6
1	D	98	ILE	5.6
1	C	480	ILE	5.2
1	B	450	PHE	5.2
1	B	483	GLN	5.1
1	B	427	PHE	5.0
1	B	454	PHE	5.0
1	B	456	SER	5.0
1	A	439	GLN	4.9
1	D	437	ILE	4.9
1	D	454	PHE	4.9
1	C	429	TYR	4.8
1	B	449	VAL	4.8
1	B	329	ALA	4.8
1	A	497	GLU	4.7
1	B	432	ASN	4.7
1	D	474	ALA	4.6
1	B	410	TYR	4.6
1	C	449	VAL	4.5
1	D	95	ASP	4.5
1	A	449	VAL	4.3
1	A	498	GLU	4.3
1	A	427	PHE	4.3
1	A	435	LEU	4.3
1	C	161	ILE	4.2
1	D	316	GLU	4.2
1	A	503	MET	4.2
1	B	376	GLY	4.1
1	A	447	VAL	4.1
1	A	500	ALA	4.0
1	C	315	ARG	4.0
1	A	481	ILE	3.9
1	A	434	ALA	3.9
1	A	484	VAL	3.9
1	A	431	THR	3.8
1	B	440	HIS	3.8
1	A	329	ALA	3.7
1	C	450	PHE	3.7
1	C	94	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	485	LEU	3.6
1	B	482	GLN	3.6
1	A	501	ILE	3.5
1	C	441	LYS	3.5
1	D	159	PRO	3.5
1	B	485	LEU	3.4
1	D	97	GLU	3.4
1	A	482	GLN	3.4
1	C	459	TYR	3.4
1	D	440	HIS	3.4
1	D	83	ILE	3.3
1	C	451	LEU	3.3
1	B	499	ALA	3.2
1	D	436	ILE	3.2
1	D	62	LEU	3.2
1	C	446	SER	3.2
1	A	433	GLU	3.2
1	D	317	GLY	3.2
1	D	128	ILE	3.1
1	D	105	GLY	3.1
1	B	26	LEU	3.1
1	C	59	ILE	3.1
1	B	358	LEU	3.0
1	A	397	ASP	3.0
1	A	452	GLU	3.0
1	B	439	GLN	3.0
1	D	160	GLN	2.9
1	B	437	ILE	2.9
1	D	450	PHE	2.9
1	C	479	GLU	2.9
1	B	457	ASN	2.9
1	B	447	VAL	2.8
1	B	487	SER	2.8
1	B	442	GLN	2.8
1	B	303	PHE	2.8
1	A	453	SER	2.8
1	A	487	SER	2.7
1	A	223	LEU	2.7
1	D	162	GLU	2.7
1	C	477	ILE	2.7
1	C	440	HIS	2.7
1	C	432	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	455	GLY	2.6
1	B	313	LEU	2.6
1	B	296	ILE	2.6
1	D	457	ASN	2.6
1	A	499	ALA	2.6
1	C	454	PHE	2.5
1	B	297	ILE	2.5
1	A	303	PHE	2.5
1	B	422	ILE	2.5
1	D	166	ALA	2.5
1	A	483	GLN	2.5
1	A	313	LEU	2.5
1	C	96	LYS	2.4
1	B	330	GLU	2.4
1	D	273	PHE	2.4
1	D	319	ASN	2.4
1	A	296	ILE	2.4
1	B	435	LEU	2.4
1	C	58	THR	2.3
1	D	123	MET	2.3
1	A	459	TYR	2.3
1	A	426	THR	2.3
1	A	446	SER	2.3
1	A	394	THR	2.3
1	B	434	ALA	2.3
1	B	436	ILE	2.3
1	B	314	ALA	2.3
1	A	425	LEU	2.2
1	D	477	ILE	2.2
1	D	58	THR	2.2
1	A	299	ASN	2.2
1	B	396	ASN	2.2
1	C	437	ILE	2.2
1	D	432	ASN	2.2
1	A	441	LYS	2.2
1	C	83	ILE	2.2
1	C	132	ASN	2.2
1	A	480	ILE	2.2
1	D	107	ILE	2.1
1	C	246	ILE	2.1
1	B	414	VAL	2.1
1	A	395	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	133	GLN	2.1
1	D	69	ALA	2.1
1	A	58	THR	2.0
1	A	357	GLU	2.0
1	B	394	THR	2.0
1	B	502	MET	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 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
2	GOL	A	601	6/6	0.75	0.17	71,73,76,84	0
2	GOL	C	602	6/6	0.78	0.17	50,80,84,87	0
2	GOL	C	601	6/6	0.85	0.13	65,78,83,84	0

6.5 Other polymers (i)

There are no such residues in this entry.