



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:33 PM UTC

PDB ID : 6E8D / pdb_00006e8d
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

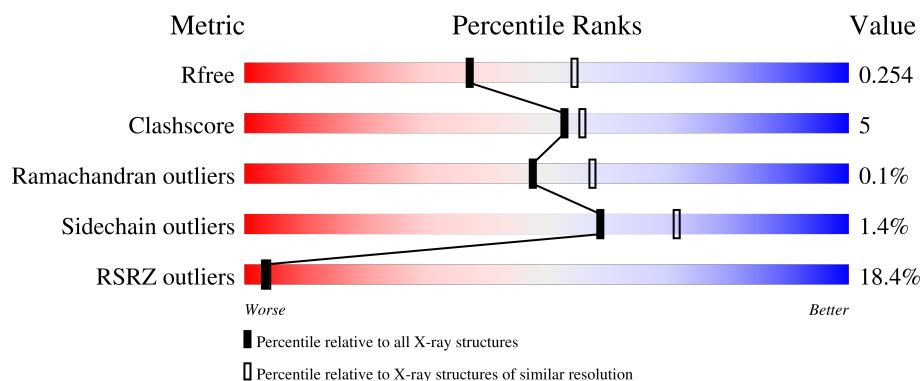
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (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 $\leq 5\%$. 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	512	16% 83% 7% 9%
1	B	512	17% 82% 7% 11%
1	C	512	16% 77% 10% 11%
1	D	512	16% 77% 8% 14%

2 Entry composition

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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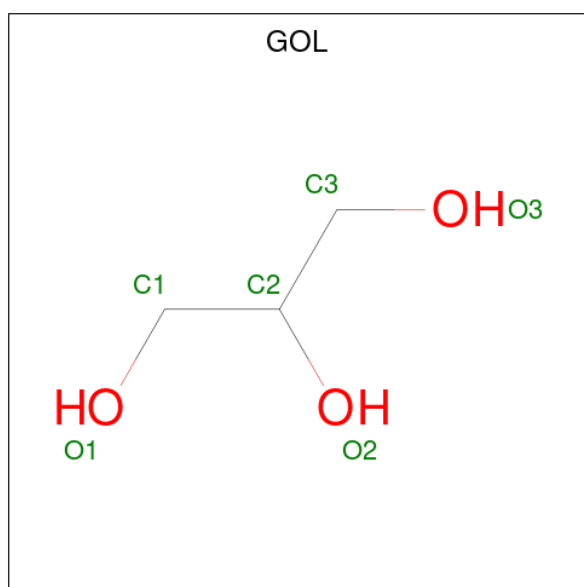
Chain	Residue	Modelled	Actual	Comment	Reference
C	20	LEU	-	expression tag	UNP A0A085C685
C	21	GLY	-	expression tag	UNP A0A085C685
C	22	ILE	-	expression tag	UNP A0A085C685
C	23	GLU	-	expression tag	UNP A0A085C685
C	24	GLU	-	expression tag	UNP A0A085C685
C	25	ASN	-	expression tag	UNP A0A085C685
C	26	LEU	-	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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

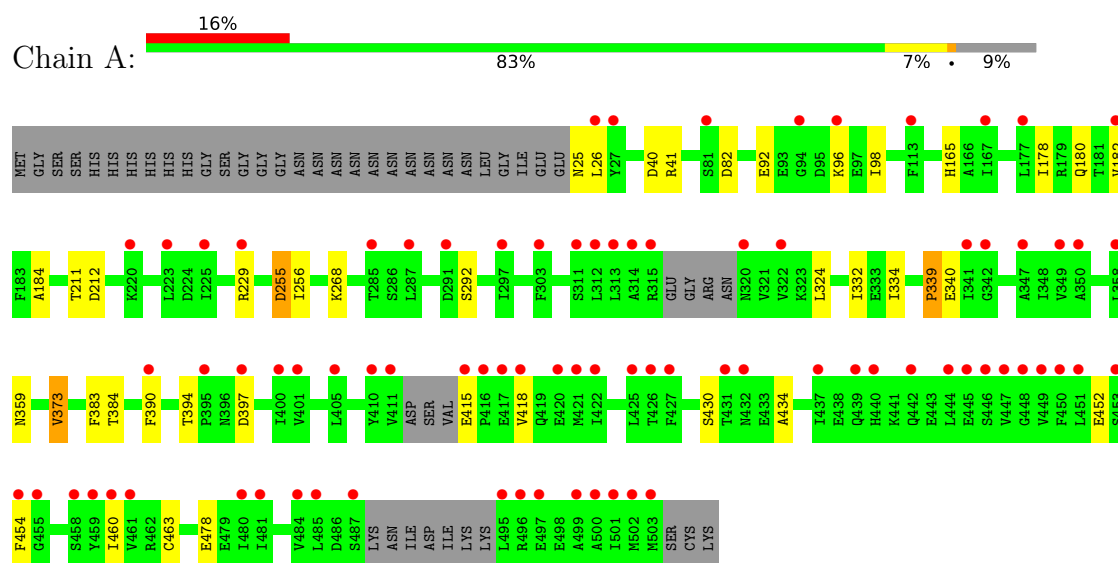
- Molecule 3 is water.

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

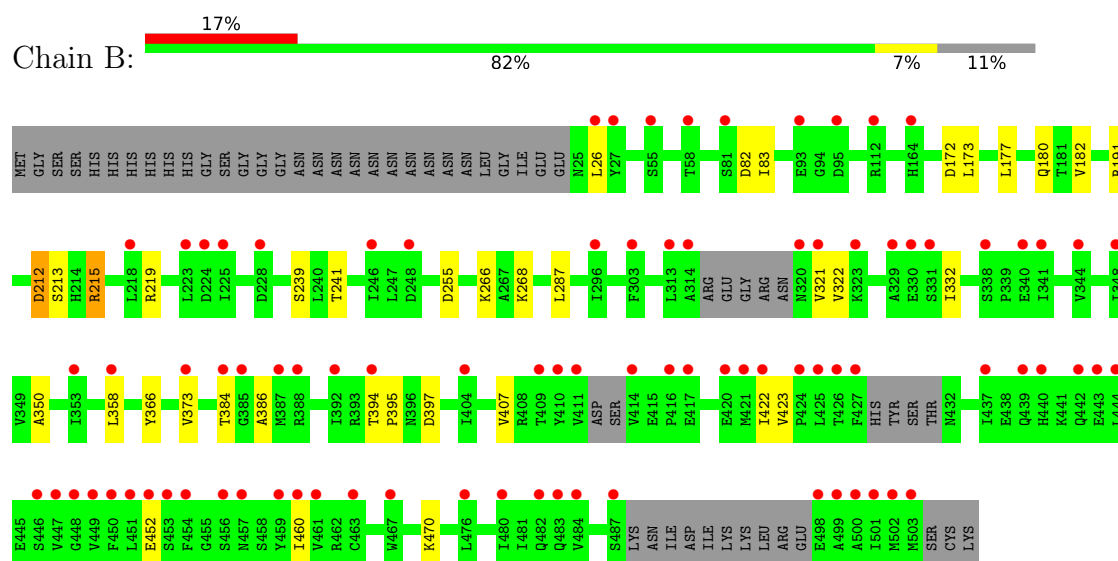
3 Residue-property plots

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.

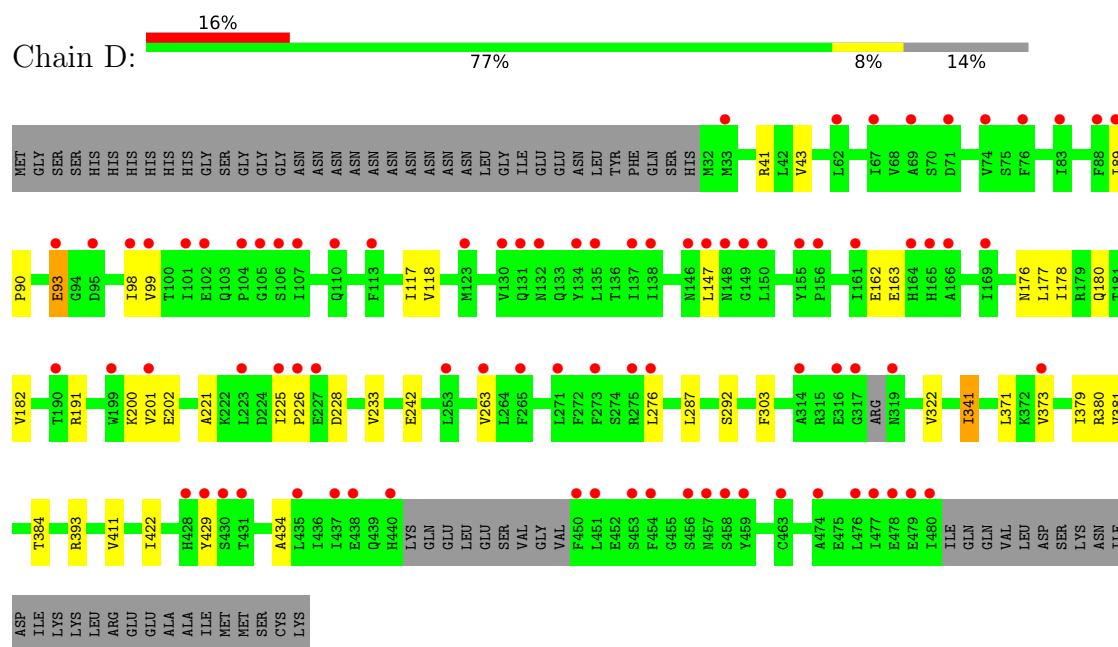
- Molecule 1: Beta sliding clamp,DNA mismatch repair protein MutL



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



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



4 Data and refinement statistics

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 48.26 – 2.34	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.26-2.34) 97.1 (48.26-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.33 , 81.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.46	1/3510 (0.0%)	0.76	5/4784 (0.1%)
1	B	0.46	0/3469	0.72	2/4724 (0.0%)
1	C	0.45	0/3459	0.76	7/4715 (0.1%)
1	D	0.40	0/3250	0.68	4/4440 (0.1%)
All	All	0.44	1/13688 (0.0%)	0.73	18/18663 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	ASP	C-O	-5.43	1.17	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	ASP	N-CA-C	-10.06	100.75	113.43
1	C	135	LEU	N-CA-C	9.15	123.33	108.32
1	D	228	ASP	N-CA-C	9.00	121.09	111.28
1	A	82	ASP	N-CA-C	-8.96	102.26	113.55
1	A	339	PRO	CB-CA-C	-8.32	100.90	111.71
1	C	28	PHE	N-CA-C	8.20	120.22	111.28
1	C	29	GLN	N-CA-C	6.91	123.22	114.31
1	D	341	ILE	N-CA-C	6.58	117.47	111.81
1	A	339	PRO	N-CA-C	6.06	120.76	110.95
1	C	220	LYS	N-CA-C	5.94	118.50	107.99
1	A	454	PHE	N-CA-C	5.56	117.42	111.36
1	C	220	LYS	CB-CA-C	-5.52	101.78	110.79
1	C	448	GLY	CA-C-N	5.52	130.66	122.71
1	C	448	GLY	C-N-CA	5.52	130.66	122.71
1	D	191	ARG	CA-C-N	5.40	126.58	119.84
1	D	191	ARG	C-N-CA	5.40	126.58	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	ASP	O-C-N	-5.17	116.84	122.84
1	A	256	ILE	N-CA-C	5.04	115.11	107.75

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	29	0
1	C	3402	0	3321	48	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
3	D	37	0	0	0	0
All	All	13668	0	13143	132	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 (132) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:201:VAL:C	1:D:202:GLU:HG2	2.12	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: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:C:32:MET:HA	1:C:32:MET:HE2	1.78	0.65
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
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	0.57
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	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:28:PHE:C	1:C:28:PHE:CD1	2.92	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:C:454:PHE:CD1	1:C:454:PHE:C	2.92	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:C:137:ILE:HG22	1:C:146:ASN:CG	2.43	0.44
1:A:324:LEU:HD13	1:A:334:ILE:HG13	1.99	0.44
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:C:456:SER:O	1:C:457:ASN:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:212:ASP:CG	1:C:213:SER:H	2.26	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: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
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:B:268:LYS:NZ	1:C:378:GLU:OE2	2.53	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:216:LEU:C	1:C:216:LEU:HD12	2.46	0.40
1:C:127:GLU:CD	1:C:139:ARG:NH1	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	43	50
1	D	433/512 (85%)	418 (96%)	15 (4%)	0	100	100
All	All	1791/2048 (88%)	1729 (96%)	61 (3%)	1 (0%)	48	57

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%)	357 (99%)	5 (1%)	59	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	363/461 (79%)	361 (99%)	2 (1%)	78	86
1	C	361/461 (78%)	353 (98%)	8 (2%)	45	58
1	D	331/461 (72%)	326 (98%)	5 (2%)	57	69
All	All	1417/1844 (77%)	1397 (99%)	20 (1%)	59	71

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	ASP
1	A	268	LYS
1	A	359	ASN
1	A	373	VAL
1	A	478	GLU
1	B	215	ARG
1	B	384	THR
1	C	99	VAL
1	C	135	LEU
1	C	215	ARG
1	C	263	VAL
1	C	344	VAL
1	C	381	VAL
1	C	384	THR
1	C	411	VAL
1	D	93	GLU
1	D	322	VAL
1	D	341	ILE
1	D	381	VAL
1	D	411	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	47	GLN
1	A	131	GLN
1	A	164	HIS
1	A	176	ASN
1	A	419	GLN
1	B	29	GLN
1	C	110	GLN

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Mol	Chain	Res	Type
1	C	148	ASN
1	C	320	ASN
1	D	198	ASN
1	D	232	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 oligosaccharides 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
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, 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	465/512 (90%)	1.03	83 (17%)	4 4	27, 80, 179, 243	1 (0%)
1	B	458/512 (89%)	1.12	88 (19%)	3 3	31, 81, 173, 264	1 (0%)
1	C	454/512 (88%)	1.10	80 (17%)	4 4	33, 79, 157, 225	1 (0%)
1	D	439/512 (85%)	1.09	84 (19%)	3 3	37, 84, 160, 214	0
All	All	1816/2048 (88%)	1.08	335 (18%)	3 4	27, 81, 169, 264	3 (0%)

All (335) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	448	GLY	10.8
1	C	481	ILE	8.4
1	A	454	PHE	7.8
1	C	447	VAL	7.4
1	C	449	VAL	7.3
1	B	450	PHE	6.5
1	B	449	VAL	6.4
1	C	430	SER	6.3
1	A	451	LEU	6.2
1	D	480	ILE	6.2
1	B	444	LEU	6.2
1	C	134	TYR	6.1
1	C	480	ILE	6.1
1	A	447	VAL	5.9
1	C	429	TYR	5.9
1	B	313	LEU	5.8
1	C	450	PHE	5.7
1	C	444	LEU	5.5
1	B	460	ILE	5.3
1	C	441	LYS	5.3
1	B	501	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	313	LEU	5.2
1	A	450	PHE	5.2
1	A	417	GLU	5.1
1	B	448	GLY	5.1
1	B	411	VAL	5.1
1	D	155	TYR	5.0
1	B	425	LEU	4.9
1	B	447	VAL	4.9
1	B	451	LEU	4.8
1	B	414	VAL	4.8
1	D	319	ASN	4.8
1	A	358	LEU	4.7
1	B	112[A]	ARG	4.6
1	B	461	VAL	4.5
1	B	427	PHE	4.5
1	D	451	LEU	4.5
1	A	480	ILE	4.4
1	C	436	ILE	4.4
1	D	134	TYR	4.4
1	A	495	LEU	4.3
1	B	26	LEU	4.3
1	D	147	LEU	4.3
1	D	463	CYS	4.3
1	C	165[A]	HIS	4.2
1	B	459	TYR	4.2
1	C	435	LEU	4.2
1	B	422	ILE	4.2
1	A	26	LEU	4.2
1	C	463	CYS	4.2
1	B	330	GLU	4.1
1	B	442	GLN	4.1
1	C	128	ILE	4.1
1	C	133	GLN	4.1
1	B	358	LEU	4.0
1	B	409	THR	4.0
1	C	443	GLU	4.0
1	A	459	TYR	4.0
1	C	148	ASN	3.9
1	D	453	SER	3.9
1	C	437	ILE	3.9
1	D	459	TYR	3.9
1	C	442	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	451	LEU	3.9
1	C	455	GLY	3.9
1	A	499	ALA	3.9
1	A	496	ARG	3.9
1	B	440	HIS	3.9
1	A	416	PRO	3.8
1	D	161	ILE	3.8
1	D	102	GLU	3.8
1	C	454	PHE	3.8
1	D	107	ILE	3.8
1	B	410	TYR	3.7
1	A	502	MET	3.7
1	D	199	TRP	3.7
1	B	437	ILE	3.7
1	C	459	TYR	3.7
1	C	446	SER	3.7
1	C	339	PRO	3.6
1	D	149	GLY	3.6
1	A	440	HIS	3.6
1	B	314	ALA	3.6
1	B	487	SER	3.5
1	B	225	ILE	3.5
1	D	62	LEU	3.5
1	C	263	VAL	3.5
1	B	499	ALA	3.5
1	C	438	GLU	3.5
1	D	110	GLN	3.5
1	B	500	ALA	3.5
1	A	437	ILE	3.5
1	C	132	ASN	3.5
1	D	435	LEU	3.5
1	A	418	VAL	3.4
1	A	422	ILE	3.4
1	A	501	ILE	3.4
1	B	320	ASN	3.4
1	C	313	LEU	3.4
1	D	457	ASN	3.4
1	B	340	GLU	3.4
1	B	443	GLU	3.4
1	B	502	MET	3.4
1	C	163	GLU	3.3
1	C	118	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	54	SER	3.3
1	D	477	ILE	3.3
1	C	229	ARG	3.3
1	C	440	HIS	3.3
1	D	437	ILE	3.3
1	D	316	GLU	3.3
1	C	27	TYR	3.3
1	A	314	ALA	3.2
1	A	350	ALA	3.2
1	A	455	GLY	3.2
1	A	315	ARG	3.2
1	A	225	ILE	3.2
1	A	500	ALA	3.2
1	D	93	GLU	3.2
1	B	446	SER	3.1
1	D	479	GLU	3.1
1	A	411	VAL	3.1
1	B	416	PRO	3.1
1	D	450	PHE	3.1
1	C	248	ASP	3.1
1	D	317	GLY	3.1
1	A	27	TYR	3.1
1	A	503	MET	3.1
1	B	457	ASN	3.1
1	B	503	MET	3.1
1	A	446	SER	3.1
1	D	458	SER	3.1
1	A	448	GLY	3.1
1	A	223	LEU	3.1
1	B	394	THR	3.0
1	B	224	ASP	3.0
1	A	453	SER	3.0
1	D	430	SER	3.0
1	C	457	ASN	3.0
1	C	431	THR	3.0
1	C	439	GLN	3.0
1	A	96	LYS	3.0
1	A	481	ILE	3.0
1	C	246	ILE	3.0
1	D	225	ILE	3.0
1	A	229	ARG	3.0
1	D	429	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	338	SER	3.0
1	A	497	GLU	3.0
1	D	273	PHE	2.9
1	D	190	THR	2.9
1	C	445	GLU	2.9
1	C	152	ALA	2.9
1	C	434	ALA	2.9
1	D	428	HIS	2.9
1	A	449	VAL	2.9
1	C	161	ILE	2.9
1	A	415	GLU	2.9
1	B	453	SER	2.9
1	C	432	ASN	2.9
1	A	427	PHE	2.9
1	D	150	LEU	2.9
1	D	474	ALA	2.9
1	B	296	ILE	2.9
1	C	379	ILE	2.9
1	B	384	THR	2.9
1	B	417	GLU	2.9
1	B	498	GLU	2.9
1	D	156	PRO	2.9
1	C	428	HIS	2.9
1	A	425	LEU	2.9
1	B	344	VAL	2.9
1	B	484	VAL	2.9
1	D	67	ILE	2.9
1	C	319	ASN	2.9
1	D	105	GLY	2.8
1	C	479	GLU	2.8
1	B	341	ILE	2.8
1	B	480	ILE	2.8
1	B	385	GLY	2.8
1	B	483	GLN	2.8
1	D	454	PHE	2.8
1	B	387	MET	2.8
1	D	148	ASN	2.8
1	C	213	SER	2.8
1	A	442	GLN	2.8
1	A	431	THR	2.8
1	D	227	GLU	2.8
1	A	397	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	71	ASP	2.7
1	A	405	LEU	2.7
1	B	164	HIS	2.7
1	C	67	ILE	2.7
1	C	95	ASP	2.7
1	C	107	ILE	2.7
1	C	314	ALA	2.7
1	B	439	GLN	2.7
1	A	460	ILE	2.7
1	B	476	LEU	2.7
1	C	433	GLU	2.6
1	A	303	PHE	2.6
1	B	424	PRO	2.6
1	C	225	ILE	2.6
1	C	119	LYS	2.6
1	A	287	LEU	2.6
1	A	113	PHE	2.6
1	D	165	HIS	2.6
1	D	476	LEU	2.5
1	A	291	ASP	2.5
1	A	421	MET	2.5
1	D	132	ASN	2.5
1	B	81	SER	2.5
1	A	458	SER	2.5
1	D	83	ILE	2.5
1	D	101	ILE	2.5
1	B	452	GLU	2.5
1	B	388	ARG	2.5
1	C	315	ARG	2.5
1	B	58	THR	2.5
1	B	426	THR	2.5
1	A	311	SER	2.5
1	A	341	ILE	2.5
1	A	349	VAL	2.5
1	D	106	SER	2.5
1	B	392	ILE	2.5
1	D	69	ALA	2.5
1	D	164	HIS	2.5
1	C	90	PRO	2.5
1	C	93	GLU	2.4
1	D	113	PHE	2.4
1	C	477	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	373	VAL	2.4
1	A	444	LEU	2.4
1	C	476	LEU	2.4
1	B	323	LYS	2.4
1	D	95	ASP	2.4
1	B	27	TYR	2.4
1	D	275	ARG	2.4
1	C	166	ALA	2.4
1	B	331	SER	2.4
1	B	348	ILE	2.4
1	D	98	ILE	2.4
1	D	131	GLN	2.4
1	A	445	GLU	2.4
1	A	484	VAL	2.4
1	C	411	VAL	2.4
1	D	123	MET	2.4
1	D	253	LEU	2.4
1	D	438	GLU	2.4
1	D	431	THR	2.3
1	B	353	ILE	2.3
1	D	76	PHE	2.3
1	B	223	LEU	2.3
1	C	227	GLU	2.3
1	A	182	VAL	2.3
1	B	454	PHE	2.3
1	B	482	GLN	2.3
1	B	463	CYS	2.3
1	D	276	LEU	2.3
1	C	412	ASP	2.3
1	A	487	SER	2.3
1	A	400	ILE	2.3
1	D	169	ILE	2.3
1	C	28	PHE	2.3
1	D	263	VAL	2.3
1	A	485	LEU	2.3
1	C	136	THR	2.3
1	B	55	SER	2.3
1	A	167	ILE	2.3
1	C	193	ILE	2.3
1	D	137	ILE	2.3
1	A	461	VAL	2.3
1	B	321	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	373	VAL	2.3
1	D	33	MET	2.2
1	D	440	HIS	2.2
1	D	478	GLU	2.2
1	D	99	VAL	2.2
1	D	135	LEU	2.2
1	A	432	ASN	2.2
1	A	410	TYR	2.2
1	A	297	ILE	2.2
1	B	404	ILE	2.2
1	A	322	VAL	2.2
1	D	201	VAL	2.2
1	A	342	GLY	2.2
1	D	89	ILE	2.2
1	A	320	ASN	2.2
1	A	401	VAL	2.2
1	A	390	PHE	2.2
1	C	114	PHE	2.2
1	D	265	PHE	2.2
1	A	220	LYS	2.2
1	C	31	HIS	2.2
1	A	285	THR	2.2
1	A	426	THR	2.2
1	A	312	LEU	2.1
1	B	218	LEU	2.1
1	C	258	ILE	2.1
1	D	138	ILE	2.1
1	D	104	PRO	2.1
1	A	439	GLN	2.1
1	A	347	ALA	2.1
1	B	456	SER	2.1
1	D	314	ALA	2.1
1	D	456	SER	2.1
1	B	246	ILE	2.1
1	C	400	ILE	2.1
1	D	223	LEU	2.1
1	B	95	ASP	2.1
1	B	228	ASP	2.1
1	D	130	VAL	2.1
1	D	88	PHE	2.1
1	A	94	GLY	2.1
1	C	474	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	166	ALA	2.1
1	D	271	LEU	2.1
1	B	248	ASP	2.1
1	B	303	PHE	2.1
1	A	81	SER	2.1
1	C	30	SER	2.1
1	B	329	ALA	2.1
1	B	421	MET	2.1
1	B	93	GLU	2.1
1	A	395	PRO	2.1
1	C	74	VAL	2.1
1	D	74	VAL	2.1
1	B	467	TRP	2.1
1	A	177[A]	LEU	2.0
1	D	146	ASN	2.0
1	D	226	PRO	2.0
1	C	199	TRP	2.0
1	A	420	GLU	2.0
1	B	420	GLU	2.0
1	C	57	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	601	6/6	0.77	0.17	71,73,76,84	0
2	GOL	C	601	6/6	0.82	0.15	65,78,83,84	0
2	GOL	C	602	6/6	0.87	0.15	50,80,84,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.