



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:17 AM UTC

PDB ID : 3C5I / pdb_00003c5i
Title : Crystal structure of Plasmodium knowlesi choline kinase, PKH_134520
Authors : Wernimont, A.K.; Hills, T.; Lew, J.; Wasney, G.; Senesterra, G.; Kozieradzki, I.; Cossar, D.; Vedadi, M.; Schapira, M.; Bochkarev, A.; Arrowsmith, C.H.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Hui, R.; Artz, J.D.; Xiao, T.; Structural Genomics Consortium (SGC)
Deposited on : 2008-01-31
Resolution : 2.20 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:

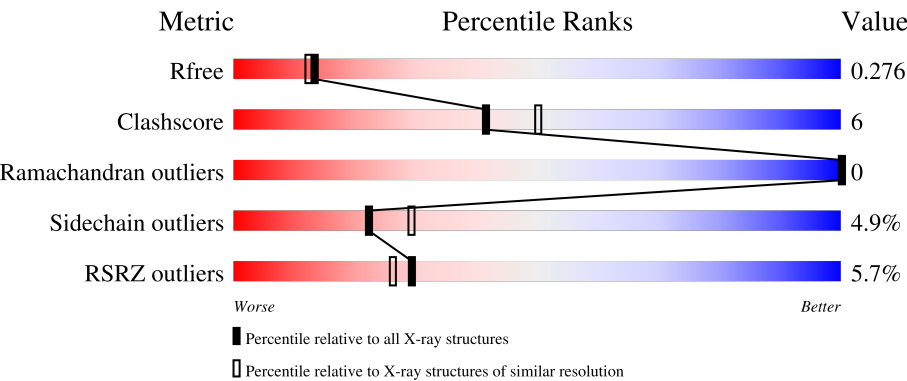
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	369	3% 76% 15% 7%
1	B	369	12% 76% 15% 7%
1	C	369	% 80% 15% ..
1	D	369	6% 82% 13% ..

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Mol	Chain	Length	Quality of chain
2	E	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	D	374	-	-	X	-
6	GOL	D	375	-	-	X	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12122 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 Choline kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	5	0
			2836	1856	451	519	10			
1	B	345	Total	C	N	O	S	0	4	0
			2863	1872	456	526	9			
1	C	353	Total	C	N	O	S	0	5	0
			2953	1928	472	543	10			
1	D	355	Total	C	N	O	S	0	3	0
			2933	1919	466	538	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	PDB 3C5I
B	1	GLY	-	expression tag	PDB 3C5I
C	1	GLY	-	expression tag	PDB 3C5I
D	1	GLY	-	expression tag	PDB 3C5I

- Molecule 2 is a protein called Cleaved fragment of N-terminal expression tag.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			48	33	7	8			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

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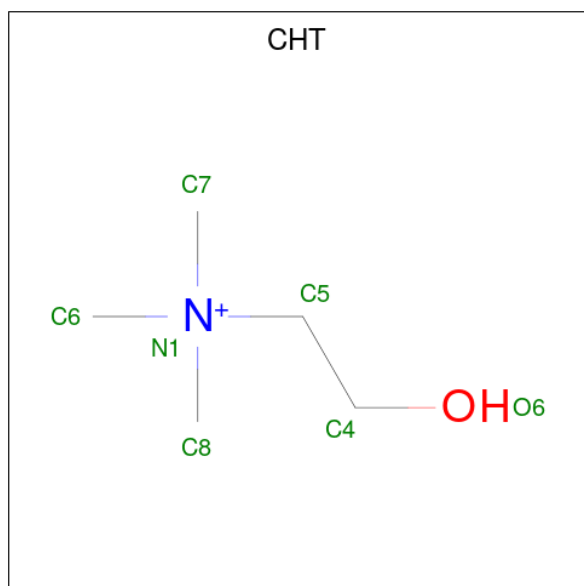
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

- Molecule 5 is CHOLINE ION (CCD ID: CHT) (formula: C₅H₁₄NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			7	5	1	1		
5	B	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	U	0	0
			1	1		
7	C	1	Total	U	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	U	0	0
			1	1		

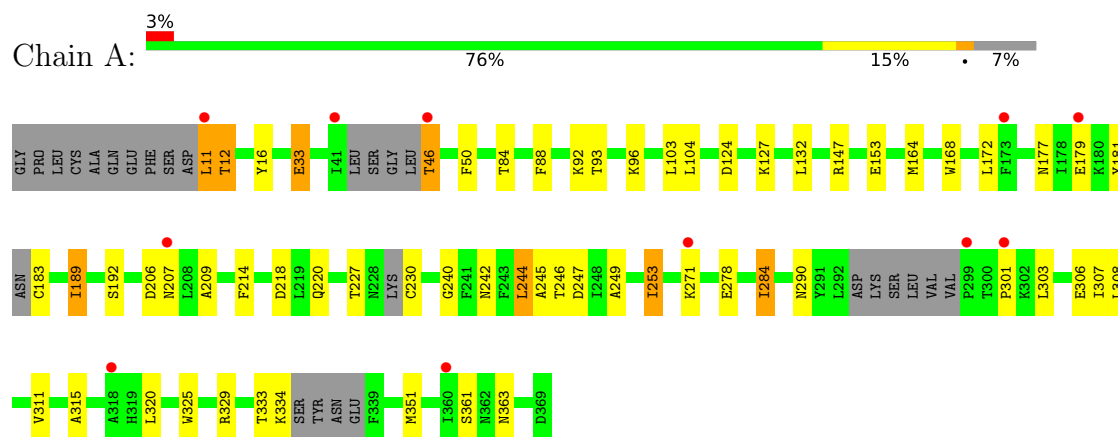
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	105	Total	O	0	0
			105	105		
8	B	83	Total	O	0	0
			83	83		
8	C	122	Total	O	0	0
			122	122		
8	D	93	Total	O	0	0
			93	93		
8	E	1	Total	O	0	0
			1	1		

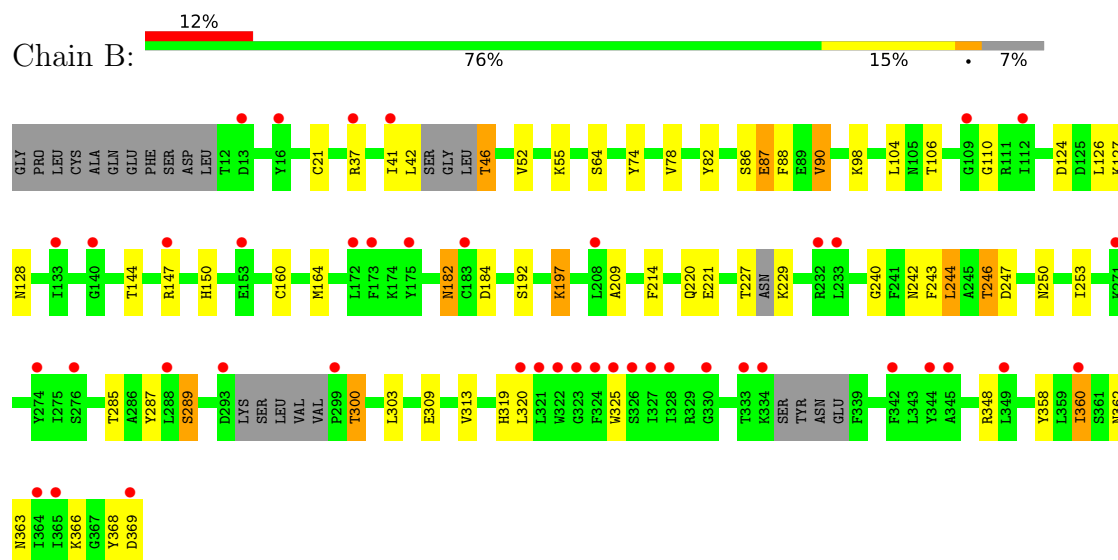
3 Residue-property plots

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.

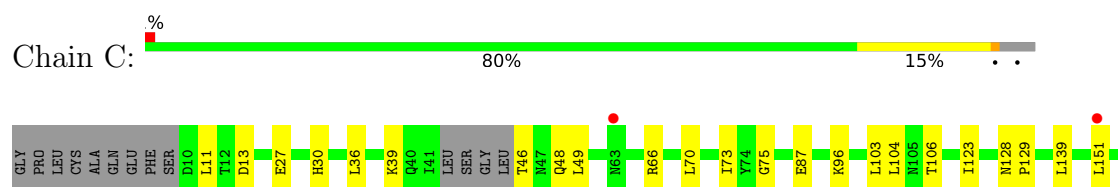
• Molecule 1: Choline kinase

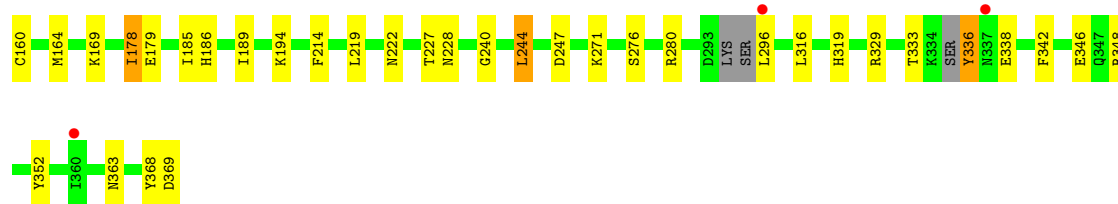


• Molecule 1: Choline kinase

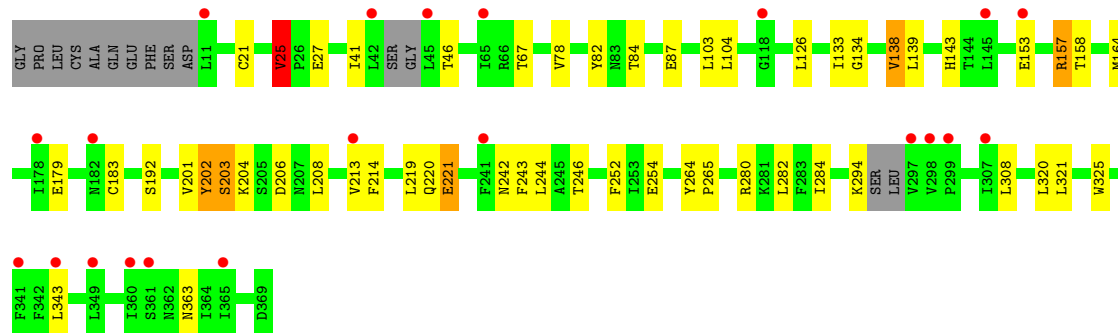
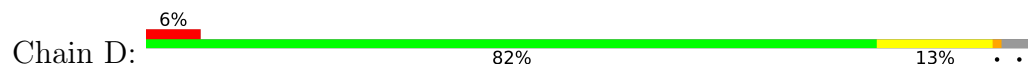


• Molecule 1: Choline kinase

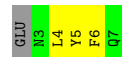




● Molecule 1: Choline kinase



● Molecule 2: Cleaved fragment of N-terminal expression tag



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.98Å 71.99Å 116.39Å 90.00° 97.72° 90.00°	Depositor
Resolution (Å)	24.79 – 2.20 24.79 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.79-2.20) 99.9 (24.79-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	36.68 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.212 , 0.260 0.245 , 0.276	Depositor DCC
R_{free} test set	4735 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12122	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5163e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, CA, CHT, GOL, MG

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	1.10	12/2919 (0.4%)	0.93	2/3947 (0.1%)
1	B	0.98	11/2944 (0.4%)	0.99	0/3985
1	C	0.74	2/3040 (0.1%)	0.92	3/4113 (0.1%)
1	D	1.12	16/3015 (0.5%)	0.99	6/4088 (0.1%)
2	E	0.60	0/49	0.67	0/65
All	All	0.99	41/11967 (0.3%)	0.95	11/16198 (0.1%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	THR	N-CA	29.05	2.01	1.46
1	D	204	LYS	C-O	23.18	1.51	1.24
1	D	153	GLU	CD-OE1	18.27	1.60	1.25
1	D	294	LYS	C-O	16.27	1.56	1.23
1	A	278	GLU	CD-OE1	15.45	1.54	1.25
1	A	363	ASN	CG-ND2	11.35	1.57	1.33
1	D	203	SER	CB-OG	11.01	1.64	1.42
1	B	197	LYS	CE-NZ	10.26	1.80	1.49
1	D	157	ARG	C-O	9.52	1.36	1.24
1	A	363	ASN	CG-OD1	8.73	1.40	1.23
1	A	179	GLU	CD-OE1	8.58	1.41	1.25
1	B	289[A]	SER	CB-OG	7.77	1.57	1.42
1	B	289[B]	SER	CB-OG	7.77	1.57	1.42
1	B	360	ILE	CB-CG2	7.73	1.78	1.52
1	D	206	ASP	CG-OD2	7.69	1.40	1.25
1	B	366	LYS	C-N	7.53	1.43	1.33
1	A	177	ASN	C-O	7.53	1.33	1.24
1	D	203	SER	C-N	7.38	1.43	1.33
1	D	363	ASN	CG-OD1	7.36	1.37	1.23
1	A	361	SER	CB-OG	7.24	1.56	1.42
1	A	179	GLU	CD-OE2	6.94	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	366	LYS	CA-C	6.92	1.61	1.52
1	D	203	SER	N-CA	6.75	1.55	1.46
1	D	153	GLU	CD-OE2	6.67	1.38	1.25
1	D	206	ASP	CG-OD1	6.56	1.37	1.25
1	C	368	TYR	C-N	6.51	1.42	1.33
1	D	25	VAL	CA-CB	6.49	1.60	1.53
1	B	147	ARG	CZ-NH1	6.42	1.41	1.32
1	A	46	THR	CA-C	6.39	1.66	1.52
1	C	368	TYR	C-O	6.03	1.30	1.24
1	D	204	LYS	C-N	5.98	1.41	1.33
1	A	147	ARG	CZ-NH1	5.97	1.41	1.32
1	B	46	THR	CB-OG1	5.86	1.53	1.43
1	B	285	THR	CB-OG1	5.83	1.53	1.43
1	D	153	GLU	CG-CD	5.79	1.66	1.52
1	B	363	ASN	CG-ND2	5.53	1.44	1.33
1	D	204	LYS	CA-C	5.50	1.60	1.52
1	A	290	ASN	CG-OD1	5.39	1.33	1.23
1	A	278	GLU	CD-OE2	5.34	1.35	1.25
1	D	202	TYR	C-O	5.22	1.30	1.24
1	B	144	THR	CA-CB	5.10	1.62	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	THR	N-CA-C	-9.77	83.66	111.00
1	D	25	VAL	CA-C-N	6.55	128.03	119.84
1	D	25	VAL	C-N-CA	6.55	128.03	119.84
1	C	123	ILE	N-CA-C	5.81	116.46	110.36
1	D	203	SER	N-CA-C	5.58	119.19	112.38
1	A	253	ILE	CB-CA-C	-5.49	104.73	112.14
1	D	204	LYS	O-C-N	5.32	127.75	122.12
1	D	203	SER	CA-C-O	-5.21	113.19	119.49
1	D	203	SER	O-C-N	5.16	129.09	122.39
1	C	13	ASP	CA-C-N	5.04	124.64	119.05
1	C	13	ASP	C-N-CA	5.04	124.64	119.05

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	2836	0	2714	37	0
1	B	2863	0	2727	40	0
1	C	2953	0	2855	26	0
1	D	2933	0	2798	40	0
2	E	48	0	42	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	7	0	14	4	0
5	B	7	0	14	3	0
6	A	12	0	16	2	0
6	B	12	0	16	0	0
6	C	18	0	24	5	0
6	D	18	0	23	16	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	105	0	0	1	0
8	B	83	0	0	3	0
8	C	122	0	0	2	0
8	D	93	0	0	5	0
8	E	1	0	0	0	0
All	All	12122	0	11243	146	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 (146) 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:B:360:ILE:CB	1:B:360:ILE:CG2	1.78	1.54
1:D:203:SER:CB	1:D:203:SER:OG	1.64	1.44
1:B:197:LYS:CE	1:B:197:LYS:NZ	1.80	1.43
1:B:289[B]:SER:OG	1:B:289[B]:SER:CB	1.66	1.43
1:A:46:THR:N	1:A:46:THR:CA	2.01	1.24
1:B:220:GLN:HE22	5:B:1001:CHT:H83	1.28	0.96
1:A:220:GLN:OE1	5:A:1001:CHT:H83	1.70	0.92
1:B:37:ARG:HG3	1:B:55:LYS:HG2	1.54	0.86
1:B:220:GLN:NE2	5:B:1001:CHT:H83	1.93	0.83
1:C:160:CYS:SG	6:C:374:GOL:H11	2.19	0.83
1:D:164:MET:SD	6:D:375:GOL:H31	2.21	0.81
1:D:220:GLN:NE2	6:D:374:GOL:H2	1.96	0.80
1:B:360:ILE:CG2	1:B:360:ILE:CA	2.64	0.76
1:D:220:GLN:HE22	6:D:374:GOL:H2	1.50	0.75
1:D:164:MET:HG2	6:D:375:GOL:C3	2.18	0.73
1:A:46:THR:N	1:A:46:THR:C	2.46	0.72
1:C:276:SER:O	1:C:280:ARG:HG3	1.90	0.72
1:C:30:HIS:O	6:C:373:GOL:H11	1.90	0.72
1:A:284:ILE:HD13	1:A:308:LEU:HD21	1.73	0.71
1:D:126:LEU:HD11	1:D:221:GLU:HG3	1.72	0.70
1:D:164:MET:CG	6:D:375:GOL:C3	2.70	0.70
1:D:243:PHE:O	1:D:246:THR:HG22	1.91	0.70
1:A:253:ILE:HD12	6:A:1003:GOL:H31	1.73	0.68
1:B:253:ILE:HD12	1:B:319:HIS:NE2	2.09	0.67
1:A:88:PHE:CE2	1:A:92:LYS:HD2	2.32	0.65
1:B:368:TYR:O	1:B:369:ASP:HB2	1.96	0.65
1:D:164:MET:HG2	6:D:375:GOL:H32	1.76	0.65
1:C:48:GLN:HG2	1:C:73:ILE:HB	1.78	0.65
1:D:164:MET:CG	6:D:375:GOL:H32	2.25	0.64
1:B:197:LYS:NZ	1:B:197:LYS:CD	2.59	0.64
1:A:164:MET:HE2	1:A:168:TRP:CH2	2.33	0.64
1:C:46:THR:O	1:C:75:GLY:HA3	1.98	0.63
1:D:164:MET:CG	6:D:375:GOL:H31	2.28	0.62
1:D:143:HIS:O	1:D:213:VAL:HG21	2.00	0.62
1:B:192:SER:HA	1:B:320:LEU:HD13	1.82	0.61
1:B:87:GLU:HG3	1:B:88:PHE:N	2.16	0.61
1:D:164:MET:HG2	6:D:375:GOL:H31	1.83	0.60
1:D:265:PRO:HB3	1:D:343:LEU:HD23	1.82	0.60
1:B:244:LEU:HG	1:B:287:TYR:OH	2.02	0.60
1:D:203:SER:CB	1:D:203:SER:HG	2.07	0.60
1:A:209:ALA:HA	1:A:244:LEU:HD22	1.83	0.60
1:C:169:LYS:HD2	1:C:189:ILE:HG23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:MET:HE2	6:A:1003:GOL:H2	1.85	0.58
1:D:143:HIS:O	1:D:213:VAL:CG2	2.51	0.58
1:C:227:THR:O	1:C:228:ASN:HB2	2.02	0.58
1:B:209:ALA:HA	1:B:244:LEU:HD22	1.87	0.57
1:A:284:ILE:HD13	1:A:308:LEU:CD2	2.34	0.57
1:A:220:GLN:OE1	5:A:1001:CHT:C8	2.50	0.57
1:D:220:GLN:HE22	6:D:374:GOL:C2	2.18	0.57
1:C:27:GLU:HG2	8:C:422:HOH:O	2.05	0.56
1:D:78:VAL:HG13	1:D:82:TYR:CZ	2.40	0.56
6:D:375:GOL:H2	8:D:384:HOH:O	2.04	0.56
1:D:252:PHE:CE2	1:D:280:ARG:HG2	2.42	0.55
1:C:342:PHE:O	1:C:346:GLU:HG2	2.08	0.53
1:A:124:ASP:OD2	1:A:127:LYS:NZ	2.40	0.53
1:B:242:ASN:CG	1:B:246:THR:HG21	2.34	0.53
1:B:78:VAL:HG22	1:B:82:TYR:CZ	2.44	0.53
1:B:124:ASP:HA	1:B:127:LYS:HE3	1.89	0.53
1:A:11:LEU:HD13	1:A:16:TYR:CE2	2.44	0.53
1:D:192:SER:HA	1:D:320:LEU:HD13	1.91	0.53
1:B:289[B]:SER:CB	1:B:289[B]:SER:HG	2.09	0.52
1:C:160:CYS:HB3	1:C:164:MET:HE2	1.92	0.52
1:C:240:GLY:HA3	6:C:374:GOL:H2	1.90	0.52
1:B:160:CYS:HB3	1:B:164:MET:HE2	1.92	0.52
1:D:164:MET:SD	6:D:375:GOL:C3	2.98	0.51
1:A:333:THR:O	1:A:334:LYS:CD	2.58	0.51
1:C:329:ARG:O	1:C:333:THR:HG23	2.10	0.51
1:A:307:ILE:O	1:A:311:VAL:HG23	2.10	0.51
1:B:227:THR:O	1:B:229:LYS:N	2.44	0.51
1:C:319:HIS:HD2	1:C:348:ARG:HE	1.59	0.50
1:B:300:THR:HG22	1:B:303:LEU:H	1.76	0.50
1:C:178:ILE:HD12	1:C:185:ILE:HG21	1.93	0.50
1:C:66:ARG:NH2	8:C:392:HOH:O	2.41	0.50
1:B:128:ASN:ND2	8:B:1085:HOH:O	2.29	0.50
1:C:214:PHE:CE2	1:C:240:GLY:HA2	2.46	0.50
1:B:126:LEU:HD11	1:B:221:GLU:HG3	1.94	0.49
1:A:329:ARG:NH2	8:A:1063:HOH:O	2.45	0.49
1:D:280:ARG:HB3	1:D:308:LEU:HD21	1.93	0.49
1:A:218:ASP:OD1	5:A:1001:CHT:HC41	2.13	0.49
1:D:133:ILE:HG13	1:D:282:LEU:HD11	1.94	0.48
1:D:242:ASN:HB3	1:D:246:THR:HG21	1.95	0.48
1:B:86:SER:O	1:B:90:VAL:HG13	2.13	0.48
1:A:93:THR:HA	1:A:96[A]:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:VAL:CG1	1:D:82:TYR:CZ	2.97	0.47
1:D:221:GLU:H	1:D:221:GLU:CD	2.22	0.47
1:D:21:CYS:O	1:D:25:VAL:HG13	2.14	0.47
1:A:172:LEU:HD12	1:A:189:ILE:HD11	1.96	0.47
1:A:242:ASN:ND2	1:A:246[A]:THR:HG21	2.28	0.47
2:E:4:LEU:HD23	2:E:5:TYR:CE1	2.50	0.46
1:A:325:TRP:CH2	5:A:1001:CHT:HC51	2.51	0.46
1:A:209:ALA:HB1	1:A:245:ALA:HB2	1.97	0.46
1:D:134:GLY:O	1:D:138:VAL:HG12	2.15	0.46
1:D:213:VAL:HG22	8:D:381:HOH:O	2.15	0.46
1:B:74:TYR:CE1	1:B:110:GLY:HA2	2.51	0.46
1:D:243:PHE:O	1:D:246:THR:CG2	2.61	0.45
1:A:12:THR:HG22	1:A:50:PHE:HZ	1.82	0.45
1:C:27:GLU:OE2	1:C:66:ARG:HD2	2.16	0.45
1:A:253:ILE:HD11	1:A:315:ALA:HB1	1.99	0.45
1:C:194:LYS:NZ	1:C:369:ASP:OD1	2.44	0.45
1:A:33:GLU:H	1:A:33:GLU:CD	2.25	0.45
1:B:319:HIS:HD2	1:B:348:ARG:HE	1.65	0.45
6:D:375:GOL:H12	8:D:443:HOH:O	2.16	0.45
1:A:206:ASP:O	1:A:207:ASN:C	2.60	0.44
1:C:139:LEU:HD13	1:C:219:LEU:HD11	1.98	0.44
1:B:64:SER:HB2	1:C:186:HIS:CD2	2.52	0.44
1:C:316:LEU:HD22	1:C:352:TYR:CE1	2.53	0.44
1:D:220:GLN:HB3	1:D:254:GLU:HG3	1.99	0.44
1:B:182:ASN:HD22	1:B:184:ASP:H	1.64	0.44
1:C:49:LEU:HD22	1:C:70:LEU:HD11	2.00	0.44
1:A:181:TYR:O	1:A:183:CYS:N	2.51	0.43
1:D:325:TRP:CZ2	6:D:374:GOL:H11	2.53	0.43
1:A:192:SER:HA	1:A:320:LEU:HD13	2.00	0.43
1:B:368:TYR:O	1:B:369:ASP:CB	2.65	0.43
1:A:227:THR:HG1	1:A:230:CYS:N	2.16	0.43
1:D:201:VAL:O	1:D:202:TYR:C	2.61	0.43
1:D:220:GLN:HE22	6:D:374:GOL:C3	2.32	0.43
1:B:309:GLU:O	1:B:313:VAL:HG23	2.20	0.42
1:D:284:ILE:HD12	1:D:308:LEU:HG	2.00	0.42
1:A:124:ASP:HA	1:A:127:LYS:HE3	2.01	0.42
1:A:249:ALA:O	1:A:253:ILE:HG12	2.20	0.42
1:B:358:TYR:O	1:B:362:ASN:HB2	2.20	0.42
1:B:243:PHE:O	1:B:246:THR:HB	2.20	0.42
1:D:214:PHE:HB3	8:D:390:HOH:O	2.19	0.42
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LEU:O	1:A:306:GLU:HG2	2.20	0.41
1:C:336:TYR:CD2	1:C:336:TYR:C	2.98	0.41
6:D:374:GOL:H31	8:D:464:HOH:O	2.20	0.41
1:A:88:PHE:CD2	1:A:92:LYS:HD2	2.54	0.41
1:B:250:ASN:HB2	8:B:1005:HOH:O	2.20	0.41
1:D:164:MET:HE3	1:D:321:LEU:HD21	2.02	0.41
1:A:11:LEU:HD13	1:A:16:TYR:HE2	1.84	0.41
6:C:375:GOL:H11	2:E:6:PHE:HB2	2.01	0.41
1:B:21:CYS:SG	1:B:52:VAL:HG11	2.60	0.41
1:C:30:HIS:O	6:C:373:GOL:C1	2.64	0.41
1:A:214:PHE:CE2	1:A:240:GLY:HA2	2.55	0.41
1:B:98:LYS:HA	1:B:98:LYS:HD3	1.96	0.41
1:B:214:PHE:CE2	1:B:240:GLY:HA2	2.56	0.41
1:B:325:TRP:CZ2	5:B:1001:CHT:HC41	2.56	0.41
1:C:128:ASN:HA	1:C:129:PRO:HD3	1.96	0.41
1:D:157:ARG:O	1:D:158:THR:C	2.63	0.41
1:D:139:LEU:HD13	1:D:219:LEU:HD11	2.03	0.41
1:D:264:TYR:CD1	1:D:264:TYR:C	3.00	0.40
1:B:87:GLU:HG2	8:B:1065:HOH:O	2.22	0.40
1:C:244:LEU:HD23	1:C:244:LEU:C	2.47	0.40
1:A:301:PRO:HB3	1:B:150:HIS:CB	2.51	0.40
1:B:221:GLU:H	1:B:221:GLU:CD	2.30	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	336/369 (91%)	325 (97%)	11 (3%)	0	100	100
1	B	339/369 (92%)	329 (97%)	10 (3%)	0	100	100
1	C	350/369 (95%)	340 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	352/369 (95%)	339 (96%)	13 (4%)	0	100	100
2	E	3/6 (50%)	3 (100%)	0	0	100	100
All	All	1380/1482 (93%)	1336 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/343 (87%)	284 (95%)	14 (5%)	23	31
1	B	298/343 (87%)	286 (96%)	12 (4%)	28	38
1	C	316/343 (92%)	296 (94%)	20 (6%)	16	19
1	D	307/343 (90%)	291 (95%)	16 (5%)	21	26
2	E	5/6 (83%)	5 (100%)	0	100	100
All	All	1224/1378 (89%)	1162 (95%)	62 (5%)	22	27

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	12	THR
1	A	33	GLU
1	A	84	THR
1	A	103	LEU
1	A	104	LEU
1	A	132	LEU
1	A	153	GLU
1	A	189	ILE
1	A	244	LEU
1	A	247	ASP
1	A	271[A]	LYS
1	A	271[B]	LYS

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Mol	Chain	Res	Type
1	A	284	ILE
1	B	41	ILE
1	B	42	LEU
1	B	46	THR
1	B	87	GLU
1	B	90	VAL
1	B	104	LEU
1	B	106	THR
1	B	182	ASN
1	B	244	LEU
1	B	246	THR
1	B	247	ASP
1	B	300	THR
1	C	11	LEU
1	C	36	LEU
1	C	39[A]	LYS
1	C	39[B]	LYS
1	C	87	GLU
1	C	96	LYS
1	C	103	LEU
1	C	104	LEU
1	C	106	THR
1	C	151	LEU
1	C	178	ILE
1	C	179	GLU
1	C	222	ASN
1	C	244	LEU
1	C	247	ASP
1	C	271	LYS
1	C	296	LEU
1	C	336	TYR
1	C	338	GLU
1	C	363	ASN
1	D	25	VAL
1	D	27	GLU
1	D	41	ILE
1	D	46	THR
1	D	67[A]	THR
1	D	67[B]	THR
1	D	84	THR
1	D	87	GLU
1	D	103	LEU

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Mol	Chain	Res	Type
1	D	104	LEU
1	D	138	VAL
1	D	179	GLU
1	D	183	CYS
1	D	208	LEU
1	D	221	GLU
1	D	244	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	210	ASN
1	B	137	ASN
1	B	171	GLN
1	B	182	ASN
1	B	220	GLN
1	B	362	ASN
1	C	29	ASN
1	C	207	ASN
1	C	222	ASN
1	C	250	ASN
1	C	319	HIS
1	C	337	ASN
1	C	363	ASN
1	D	48	GLN
1	D	61	ASN
1	D	63	ASN
1	D	220	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 8 are monoatomic and 3 are unknown - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GOL	C	373	-	5,5,5	0.65	0	5,5,5	0.92	0
6	GOL	D	373	-	5,5,5	0.49	0	5,5,5	0.47	0
6	GOL	A	1002	-	5,5,5	0.38	0	5,5,5	0.74	0
6	GOL	D	375	-	5,5,5	0.67	0	5,5,5	0.93	0
6	GOL	C	374	-	5,5,5	0.75	0	5,5,5	1.01	0
6	GOL	A	1003	-	5,5,5	0.51	0	5,5,5	0.92	0
6	GOL	B	1004	-	5,5,5	0.42	0	5,5,5	0.76	0
6	GOL	D	374	-	5,5,5	0.39	0	5,5,5	0.62	0
5	CHT	A	1001	-	6,6,6	0.83	0	8,8,8	0.47	0
5	CHT	B	1001	-	6,6,6	0.82	0	8,8,8	1.00	0
6	GOL	C	375	-	5,5,5	0.44	0	5,5,5	0.44	0
6	GOL	B	1003	-	5,5,5	0.56	0	5,5,5	0.37	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
6	GOL	C	373	-	-	3/4/4/4	-
6	GOL	D	373	-	-	0/4/4/4	-
6	GOL	A	1002	-	-	4/4/4/4	-
6	GOL	D	375	-	-	4/4/4/4	-
6	GOL	C	374	-	-	1/4/4/4	-
6	GOL	A	1003	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	1004	-	-	2/4/4/4	-
6	GOL	D	374	-	-	3/4/4/4	-
5	CHT	A	1001	-	-	3/4/4/4	-
5	CHT	B	1001	-	-	3/4/4/4	-
6	GOL	C	375	-	-	1/4/4/4	-
6	GOL	B	1003	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1002	GOL	O1-C1-C2-C3
6	A	1002	GOL	C1-C2-C3-O3
6	A	1003	GOL	O1-C1-C2-O2
6	A	1003	GOL	O1-C1-C2-C3
6	A	1003	GOL	C1-C2-C3-O3
6	B	1004	GOL	O1-C1-C2-O2
6	B	1004	GOL	O1-C1-C2-C3
6	C	373	GOL	C1-C2-C3-O3
6	D	375	GOL	C1-C2-C3-O3
6	D	375	GOL	O2-C2-C3-O3
5	A	1001	CHT	C4-C5-N1-C8
5	A	1001	CHT	C4-C5-N1-C7
5	B	1001	CHT	C4-C5-N1-C7
6	B	1003	GOL	O1-C1-C2-C3
6	D	374	GOL	O1-C1-C2-C3
6	D	375	GOL	O1-C1-C2-C3
6	A	1002	GOL	O1-C1-C2-O2
6	A	1002	GOL	O2-C2-C3-O3
6	B	1003	GOL	O1-C1-C2-O2
6	C	373	GOL	O2-C2-C3-O3
6	D	374	GOL	O1-C1-C2-O2
5	A	1001	CHT	C4-C5-N1-C6
6	A	1003	GOL	O2-C2-C3-O3
6	D	375	GOL	O1-C1-C2-O2
6	C	374	GOL	O2-C2-C3-O3
6	C	375	GOL	O1-C1-C2-O2
6	D	374	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	B	1001	CHT	C4-C5-N1-C6
5	B	1001	CHT	C4-C5-N1-C8
6	C	373	GOL	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	373	GOL	2	0
6	D	375	GOL	10	0
6	C	374	GOL	2	0
6	A	1003	GOL	2	0
6	D	374	GOL	6	0
5	A	1001	CHT	4	0
5	B	1001	CHT	3	0
6	C	375	GOL	1	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, 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	343/369 (92%)	0.81	11 (3%) 50 47	23, 39, 46, 55	6 (1%)
1	B	345/369 (93%)	1.13	43 (12%) 8 6	22, 39, 47, 56	6 (1%)
1	C	353/369 (95%)	0.71	5 (1%) 73 71	23, 39, 46, 52	5 (1%)
1	D	355/369 (96%)	0.88	21 (5%) 28 25	22, 39, 47, 58	4 (1%)
2	E	5/6 (83%)	1.12	0 100 100	46, 46, 47, 49	0
All	All	1401/1482 (94%)	0.88	80 (5%) 29 26	22, 39, 47, 58	21 (1%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	PRO	4.6
1	B	323	GLY	4.2
1	B	173	PHE	4.0
1	D	65	ILE	4.0
1	B	365	ILE	3.6
1	A	46	THR	3.4
1	B	293	ASP	3.4
1	D	241	PHE	3.3
1	B	288	LEU	3.3
1	B	274	TYR	3.3
1	A	11	LEU	3.2
1	B	349	LEU	3.1
1	B	334	LYS	3.1
1	B	140	GLY	3.0
1	D	360	ILE	3.0
1	C	337	ASN	2.9
1	B	37	ARG	2.9
1	B	153	GLU	2.9
1	A	360	ILE	2.8
1	D	11	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	233	LEU	2.7
1	B	326	SER	2.7
1	B	16	TYR	2.7
1	B	109	GLY	2.7
1	D	297	VAL	2.7
1	D	298	VAL	2.7
1	A	179	GLU	2.7
1	B	333	THR	2.7
1	B	147	ARG	2.7
1	B	345	ALA	2.6
1	A	207	ASN	2.6
1	D	118	GLY	2.6
1	B	344	TYR	2.6
1	B	327	ILE	2.6
1	B	342	PHE	2.5
1	B	13	ASP	2.5
1	B	183	CYS	2.5
1	B	133	ILE	2.5
1	B	360	ILE	2.5
1	B	299	PRO	2.5
1	C	296	LEU	2.5
1	D	349	LEU	2.5
1	B	328	ILE	2.4
1	D	178	ILE	2.4
1	B	232	ARG	2.4
1	D	365	ILE	2.4
1	D	45	LEU	2.4
1	D	343	LEU	2.4
1	B	320	LEU	2.4
1	B	321	LEU	2.4
1	D	42	LEU	2.4
1	D	299	PRO	2.3
1	D	213	VAL	2.3
1	D	307	ILE	2.3
1	A	271[A]	LYS	2.3
1	B	330	GLY	2.2
1	C	63	ASN	2.2
1	C	360	ILE	2.2
1	B	208	LEU	2.2
1	A	173	PHE	2.2
1	D	361	SER	2.2
1	B	322	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	172	LEU	2.2
1	D	145	LEU	2.2
1	D	153	GLU	2.2
1	B	175	TYR	2.1
1	C	151	LEU	2.1
1	B	324	PHE	2.1
1	D	341	PHE	2.1
1	B	276	SER	2.1
1	A	41	ILE	2.1
1	B	41	ILE	2.1
1	D	182	ASN	2.1
1	A	318	ALA	2.1
1	B	364	ILE	2.1
1	B	325	TRP	2.1
1	B	271	LYS	2.0
1	B	112	ILE	2.0
1	B	369	ASP	2.0
1	A	301	PRO	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($\text{\AA}^2$)	Q<0.9
6	GOL	D	375	6/6	0.43	0.40	22,23,27,27	6
6	GOL	C	375	6/6	0.69	0.19	52,55,55,58	0
6	GOL	B	1003	6/6	0.70	0.25	64,65,66,66	0
6	GOL	C	374	6/6	0.71	0.23	49,51,52,54	0
6	GOL	C	373	6/6	0.72	0.35	45,48,49,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	D	373	6/6	0.76	0.22	48,55,56,60	0
6	GOL	A	1003	6/6	0.76	0.19	48,51,53,55	0
6	GOL	D	374	6/6	0.77	0.19	43,51,53,54	0
6	GOL	A	1002	6/6	0.79	0.15	47,49,50,52	0
6	GOL	B	1004	6/6	0.81	0.12	59,60,61,61	0
5	CHT	A	1001	7/7	0.83	0.19	43,44,47,47	0
5	CHT	B	1001	7/7	0.86	0.16	44,48,50,50	0
4	CA	D	371	1/1	0.89	0.21	54,54,54,54	0
4	CA	A	371	1/1	0.91	0.13	48,48,48,48	0
4	CA	C	371	1/1	0.93	0.17	55,55,55,55	0
4	CA	B	371	1/1	0.93	0.17	48,48,48,48	0
7	UNL	D	372	1/-	0.96	0.64	30,30,30,30	0
3	MG	B	370	1/1	0.97	0.05	34,34,34,34	0
3	MG	D	370	1/1	0.98	0.04	31,31,31,31	0
3	MG	A	370	1/1	0.98	0.03	29,29,29,29	0
7	UNL	B	1002	1/-	0.98	0.58	30,30,30,30	0
7	UNL	C	372	1/-	0.98	0.59	30,30,30,30	0
3	MG	C	370	1/1	0.98	0.03	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.