Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:47 AM GMT

PDB ID	:	3C5I
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

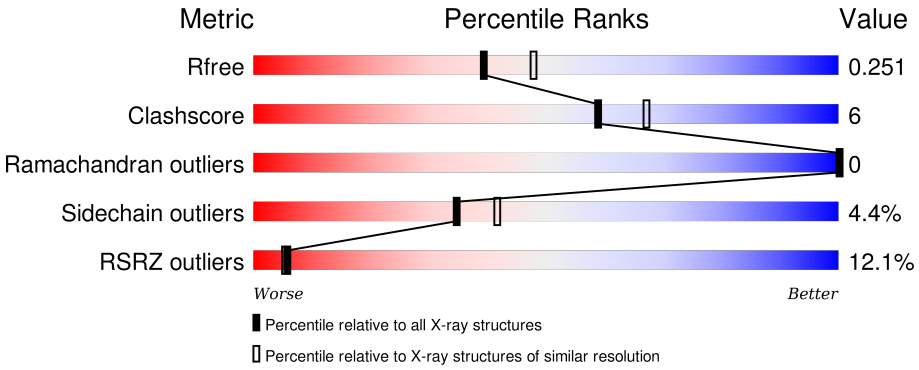
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	9% 77% 15% • 7%
1	B	369	12% 76% 15% •• 7%
1	C	369	14% 83% 13% •
1	D	369	11% 83% 12% ••
2	E	6	50% 33% 50% 17%

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
4	CA	C	371	-	-	-	X
4	CA	D	371	-	-	-	X
6	UNL	C	372	-	-	-	X
7	GOL	B	1003	-	-	-	X
7	GOL	B	1004	-	-	-	X
7	GOL	C	373	-	-	-	X
7	GOL	C	374	-	-	-	X
7	GOL	D	373	-	-	-	X
7	GOL	D	374	-	-	X	-
7	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 (three-letter code: MG) (formula: Mg).

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

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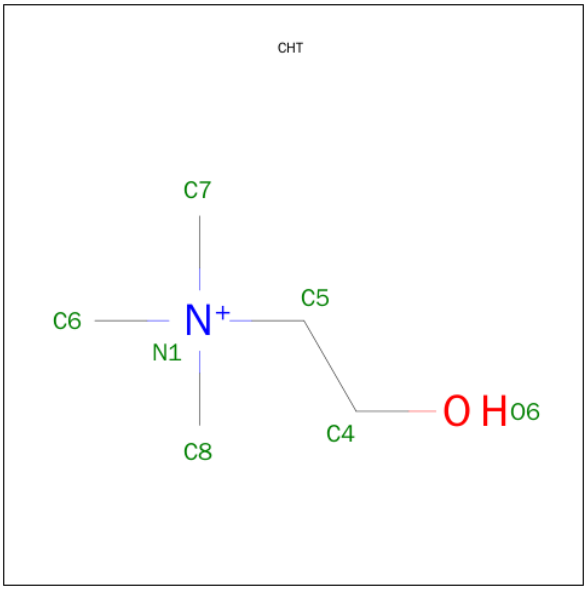
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is CHOLINE ION (three-letter code: CHT) (formula: $C_5H_{14}NO$).

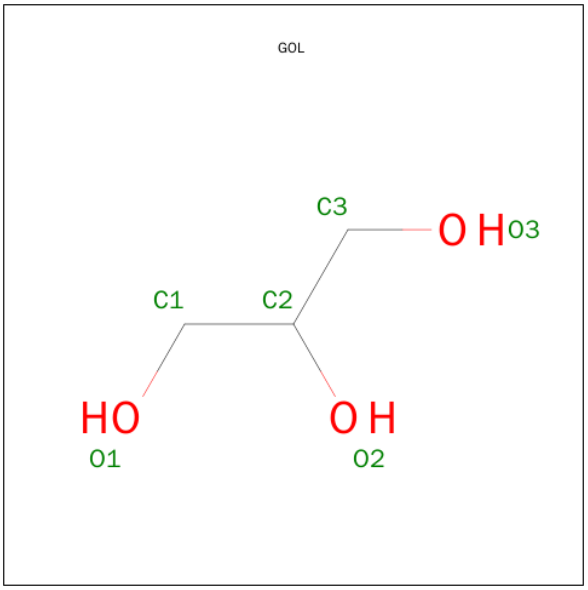


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 7 5 1 1	0	0
5	B	1	Total C N O 7 5 1 1	0	0

- Molecule 6 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 8 is water.

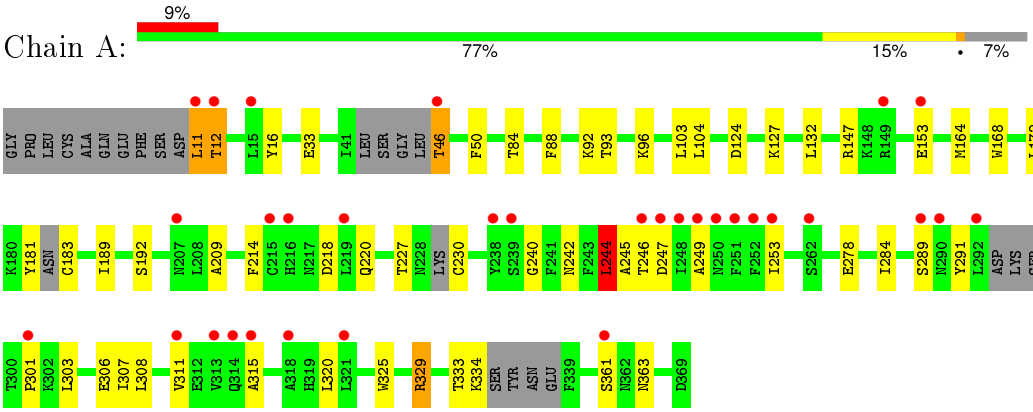
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	105	Total	O	0	0
			105	105		
8	B	83	Total	O	0	0
			83	83		
8	C	122	Total	O	0	0
			122	122		
8	D	93	Total	O	0	0
			93	93		
8	E	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

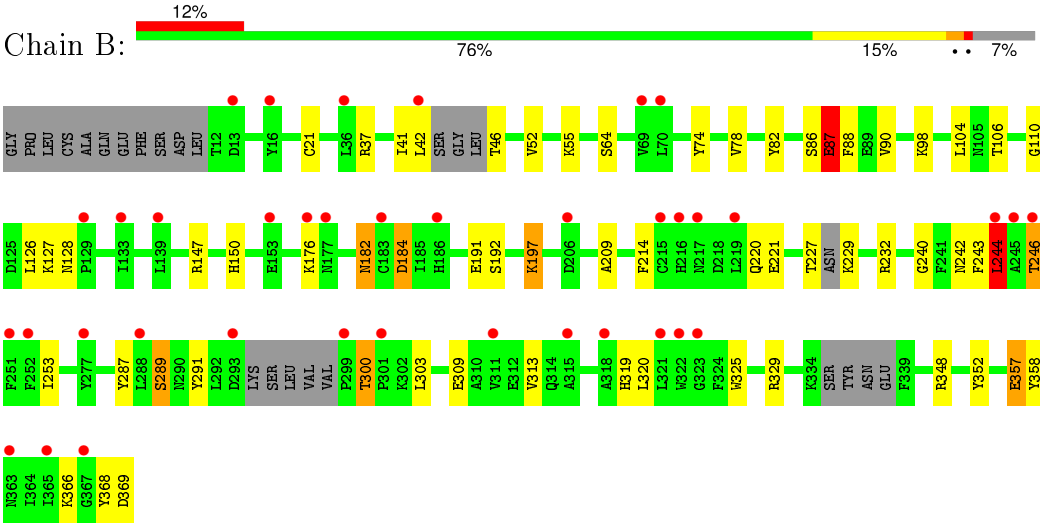
- Molecule 1: Choline kinase

Chain A:



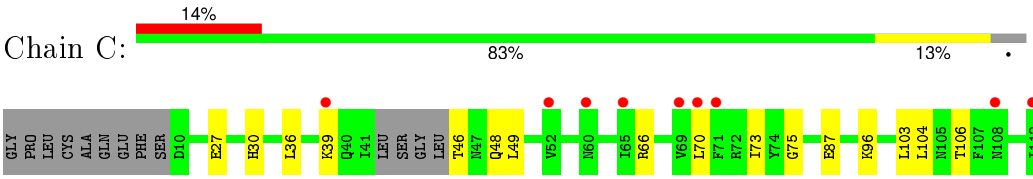
- Molecule 1: Choline kinase

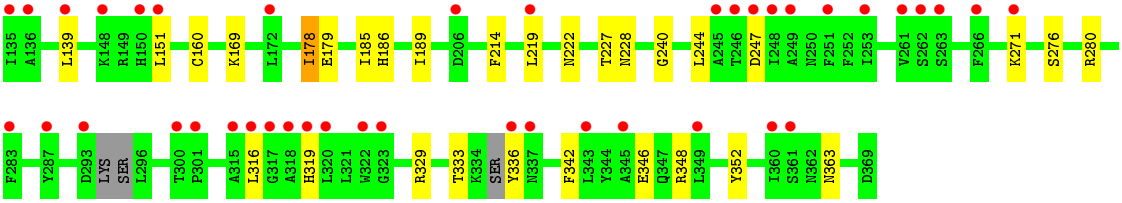
Chain B:



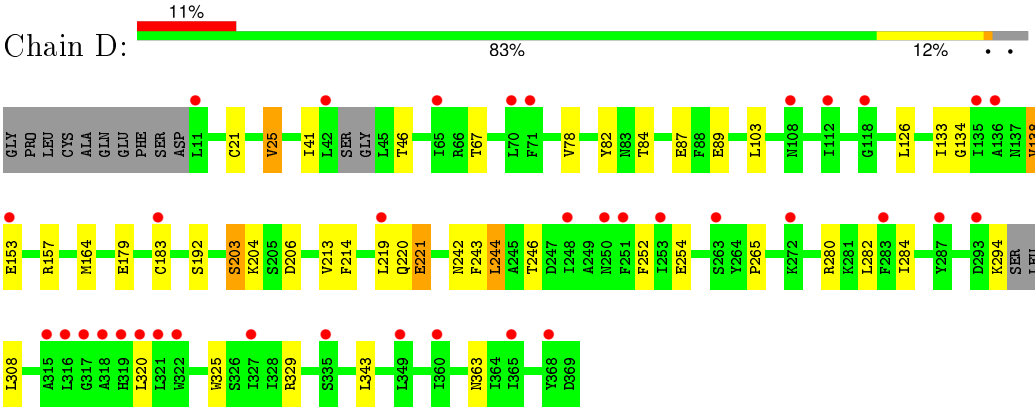
- Molecule 1: Choline kinase

Chain C:





- Molecule 1: Choline kinase



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

4 Data and refinement statistics (i)

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) 100.0 (24.79-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	36.68 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.212 , 0.260 0.207 , 0.251	Depositor DCC
R_{free} test set	4735 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.3	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 94289 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.91	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, GOL, MG, CHT, CA

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	1.14	17/2919 (0.6%)	0.73	3/3947 (0.1%)
1	B	0.94	15/2944 (0.5%)	0.75	4/3985 (0.1%)
1	C	0.63	0/3040	0.67	0/4113
1	D	1.10	10/3015 (0.3%)	0.73	3/4088 (0.1%)
2	E	0.63	0/49	0.45	0/65
All	All	0.97	42/11967 (0.4%)	0.72	10/16198 (0.1%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	153	GLU	CD-OE1	31.28	1.60	1.25
1	A	46	THR	N-CA	27.55	2.01	1.46
1	A	278	GLU	CD-OE1	26.41	1.54	1.25
1	D	294	LYS	C-O	17.23	1.56	1.23
1	D	203	SER	CB-OG	16.85	1.64	1.42
1	D	204	LYS	C-O	14.79	1.51	1.23
1	A	179	GLU	CD-OE1	14.54	1.41	1.25
1	B	197	LYS	CE-NZ	12.43	1.80	1.49
1	B	289[A]	SER	CB-OG	11.88	1.57	1.42
1	B	289[B]	SER	CB-OG	11.88	1.57	1.42
1	A	179	GLU	CD-OE2	11.72	1.38	1.25
1	D	153	GLU	CD-OE2	11.24	1.38	1.25
1	A	361	SER	CB-OG	11.05	1.56	1.42
1	D	153	GLU	CG-CD	9.72	1.66	1.51
1	A	363	ASN	CG-ND2	9.69	1.57	1.32
1	A	278	GLU	CD-OE2	8.95	1.35	1.25
1	B	291	TYR	CE1-CZ	8.36	1.49	1.38
1	B	360	ILE	CB-CG2	8.13	1.78	1.52
1	A	363	ASN	CG-OD1	7.36	1.40	1.24
1	D	157	ARG	C-O	6.97	1.36	1.23
1	B	147	ARG	CZ-NH1	6.68	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	206	ASP	CG-OD2	6.35	1.40	1.25
1	B	291	TYR	CG-CD1	6.27	1.47	1.39
1	A	147	ARG	CZ-NH1	6.20	1.41	1.33
1	D	363	ASN	CG-OD1	6.17	1.37	1.24
1	A	291	TYR	CE2-CZ	6.14	1.46	1.38
1	B	366	LYS	C-N	5.80	1.43	1.33
1	A	289[A]	SER	CB-OG	5.78	1.49	1.42
1	A	289[B]	SER	CB-OG	5.78	1.49	1.42
1	B	176	LYS	CD-CE	5.68	1.65	1.51
1	B	357[A]	GLU	CD-OE1	5.66	1.31	1.25
1	B	357[B]	GLU	CD-OE1	5.66	1.31	1.25
1	B	357[A]	GLU	CD-OE2	5.50	1.31	1.25
1	B	357[B]	GLU	CD-OE2	5.50	1.31	1.25
1	A	177	ASN	C-O	5.42	1.33	1.23
1	D	206	ASP	CG-OD1	5.42	1.37	1.25
1	A	291	TYR	CE1-CZ	5.31	1.45	1.38
1	B	362	ASN	CB-CG	5.31	1.63	1.51
1	A	291	TYR	CG-CD2	5.20	1.46	1.39
1	A	46	THR	CA-C	5.16	1.66	1.52
1	A	291	TYR	CG-CD1	5.10	1.45	1.39
1	B	87	GLU	CG-CD	-5.10	1.44	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	46	THR	N-CA-C	-10.13	83.66	111.00
1	D	153	GLU	OE1-CD-OE2	8.28	133.24	123.30
1	D	244	LEU	CA-CB-CG	7.99	133.68	115.30
1	A	244	LEU	CA-CB-CG	7.82	133.29	115.30
1	D	329	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	244	LEU	CA-CB-CG	6.92	131.21	115.30
1	B	329	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	B	197	LYS	CD-CE-NZ	-5.87	98.19	111.70
1	A	329	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	B	147	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	34	0
1	B	2863	0	2727	39	0
1	C	2953	0	2855	22	0
1	D	2933	0	2798	36	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	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	12	0	16	1	0
7	B	12	0	16	0	0
7	C	18	0	24	5	0
7	D	18	0	23	16	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	134	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 (134) 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:CA	1:A:46:THR:N	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	7:C:374:GOL:H11	2.19	0.83
1:D:164:MET:SD	7:D:375:GOL:H31	2.21	0.81
1:D:220:GLN:NE2	7:D:374:GOL:H2	1.96	0.80
1:B:360:ILE:CA	1:B:360:ILE:CG2	2.64	0.76
1:D:220:GLN:HE22	7:D:374:GOL:H2	1.50	0.75
1:D:164:MET:HG2	7:D:375:GOL:C3	2.18	0.73
1:C:276:SER:O	1:C:280:ARG:HG3	1.90	0.72
1:C:30:HIS:O	7: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	7: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	7:A:1003:GOL:H31	1.73	0.68
1:A:46:THR:C	1:A:46:THR:N	2.46	0.67
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:D:164:MET:HG2	7:D:375:GOL:H32	1.76	0.65
1:B:368:TYR:O	1:B:369:ASP:HB2	1.96	0.65
1:C:48:GLN:HG2	1:C:73:ILE:HB	1.78	0.65
1:D:164:MET:CG	7:D:375:GOL:H32	2.25	0.64
1:B:197:LYS:NZ	1:B:197:LYS:CD	2.59	0.64
1:C:46:THR:O	1:C:75:GLY:HA3	1.98	0.63
1:D:164:MET:CG	7: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	7: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:C:227:THR:O	1:C:228:ASN:HB2	2.02	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:D:143:HIS:O	1:D:213:VAL:CG2	2.51	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	7:D:374:GOL:C2	2.18	0.57
1:D:78:VAL:HG13	1:D:82:TYR:CZ	2.40	0.56
1:C:27:GLU:HG2	8:C:422:HOH:O	2.05	0.56
7: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:124:ASP:HA	1:B:127:LYS:HE3	1.89	0.53
1:B:78:VAL:HG22	1:B:82:TYR:CZ	2.44	0.53
1:D:192:SER:HA	1:D:320:LEU:HD13	1.91	0.53
1:A:11:LEU:HD13	1:A:16:TYR:CE2	2.44	0.53
1:B:289[B]:SER:HG	1:B:289[B]:SER:CB	2.09	0.52
1:C:240:GLY:HA3	7:C:374:GOL:H2	1.90	0.52
1:D:164:MET:SD	7: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:C:214:PHE:CE2	1:C:240:GLY:HA2	2.46	0.50
1:B:128:ASN:ND2	8:B:1085:HOH:O	2.29	0.50
1:B:126:LEU:HD11	1:B:221:GLU:HG3	1.94	0.49
1:D:280:ARG:HB3	1:D:308:LEU:HD21	1.93	0.49
1:A:329:ARG:NH2	8:A:1063:HOH:O	2.45	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:B:242:ASN:CG	1:B:246:THR:HG21	2.34	0.48
1:A:93:THR:HA	1:A:96[A]:LYS:HG2	1.96	0.47
1:D:78:VAL:CG1	1:D:82:TYR:CZ	2.97	0.47
1:D:21:CYS:O	1:D:25:VAL:HG13	2.14	0.47
1:B:191:GLU:OE1	1:B:352:TYR:OH	2.28	0.47
1:A:172:LEU:HD12	1:A:189:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:27:GLU:OE2	1:C:66:ARG:HD2	2.16	0.45
1:A:12:THR:HG22	1:A:50:PHE:HZ	1.82	0.45
1:A:253:ILE:HD11	1:A:315:ALA:HB1	1.99	0.45
7:D:375:GOL:H12	8:D:443:HOH:O	2.16	0.45
1:B:319:HIS:HD2	1:B:348:ARG:HE	1.65	0.45
1:C:139:LEU:HD13	1:C:219:LEU:HD11	1.98	0.44
1:C:316:LEU:HD22	1:C:352:TYR:CE1	2.53	0.44
1:B:64:SER:HB2	1:C:186:HIS:CD2	2.52	0.44
1:D:220:GLN:HB3	1:D:254:GLU:HG3	1.99	0.44
1:C:49:LEU:HD22	1:C:70:LEU:HD11	2.00	0.44
1:B:182:ASN:HD22	1:B:184:ASP:H	1.64	0.44
1:D:325:TRP:CZ2	7:D:374:GOL:H11	2.53	0.43
1:A:181:TYR:O	1:A:183:CYS:N	2.51	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:164:MET:HE2	1:A:168:TRP:CH2	2.54	0.43
1:D:220:GLN:HE22	7:D:374:GOL:C3	2.32	0.43
1:D:221:GLU:H	1:D:221:GLU:CD	2.22	0.43
1:A:227:THR:HG1	1:A:230:CYS:N	2.17	0.42
1:D:284:ILE:HD12	1:D:308:LEU:HG	2.00	0.42
1:B:309:GLU:O	1:B:313:VAL:HG23	2.20	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
7:D:374:GOL:H31	8:D:464:HOH:O	2.20	0.41
1:A:303:LEU:O	1:A:306:GLU:HG2	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:A:11:LEU:HD13	1:A:16:TYR:HE2	1.84	0.41
7:C:375:GOL:H11	2:E:6:PHE:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:HIS:O	7:C:373:GOL:C1	2.64	0.41
1:B:21:CYS:SG	1:B:52:VAL:HG11	2.60	0.41
1:B:325:TRP:CZ2	5:B:1001:CHT:HC41	2.56	0.41
1:B:214:PHE:CE2	1:B:240:GLY:HA2	2.56	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:C:128:ASN:HA	1:C:129:PRO:HD3	1.96	0.41
1:D:139:LEU:HD13	1:D:219:LEU:HD11	2.03	0.41
1:B:87:GLU:HG2	8:B:1065:HOH:O	2.22	0.40
1:A:301:PRO:HB3	1:B:150:HIS:CB	2.51	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
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 (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	298/343 (87%)	288 (97%)	10 (3%)	44	54
1	B	298/343 (87%)	283 (95%)	15 (5%)	30	35
1	C	316/343 (92%)	299 (95%)	17 (5%)	27	31
1	D	307/343 (90%)	293 (95%)	14 (5%)	33	40
2	E	5/6 (83%)	5 (100%)	0	100	100
All	All	1224/1378 (89%)	1168 (95%)	56 (5%)	35	40

All (56) 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	244	LEU
1	A	247	ASP
1	B	41	ILE
1	B	42	LEU
1	B	46	THR
1	B	87	GLU
1	B	104	LEU
1	B	106	THR
1	B	182	ASN
1	B	184	ASP
1	B	232	ARG
1	B	244	LEU
1	B	246	THR
1	B	247	ASP
1	B	300	THR
1	B	357[A]	GLU
1	B	357[B]	GLU
1	C	36	LEU
1	C	39[A]	LYS
1	C	39[B]	LYS

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Mol	Chain	Res	Type
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	336	TYR
1	C	363	ASN
1	D	25	VAL
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	89	GLU
1	D	103	LEU
1	D	138	VAL
1	D	179	GLU
1	D	183	CYS
1	D	221	GLU
1	D	244	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	137	ASN
1	B	182	ASN
1	B	220	GLN
1	B	279	ASN
1	C	29	ASN
1	C	222	ASN
1	C	319	HIS
1	C	363	ASN
1	D	29	ASN
1	D	63	ASN

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Mol	Chain	Res	Type
1	D	171	GLN
1	D	207	ASN
1	D	220	GLN
1	D	363	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 3 are unknown and 8 are monoatomic - 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	$\#\|Z\| > 2$
5	CHT	A	1001	-	6,6,6	0.78	0	8,8,8	0.51	0
7	GOL	A	1002	-	5,5,5	0.37	0	5,5,5	0.63	0
7	GOL	A	1003	-	5,5,5	0.44	0	5,5,5	0.87	0
5	CHT	B	1001	-	6,6,6	0.79	0	8,8,8	1.01	0
7	GOL	B	1003	-	5,5,5	0.54	0	5,5,5	0.35	0
7	GOL	B	1004	-	5,5,5	0.39	0	5,5,5	0.76	0
7	GOL	C	373	-	5,5,5	0.60	0	5,5,5	0.94	0
7	GOL	C	374	-	5,5,5	0.71	0	5,5,5	1.00	0
7	GOL	C	375	-	5,5,5	0.38	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GOL	D	373	-	5,5,5	0.49	0	5,5,5	0.38	0
7	GOL	D	374	-	5,5,5	0.35	0	5,5,5	0.61	0
7	GOL	D	375	-	5,5,5	0.65	0	5,5,5	0.87	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
5	CHT	A	1001	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1002	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1003	-	-	0/4/4/4	0/0/0/0
5	CHT	B	1001	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1003	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1004	-	-	0/4/4/4	0/0/0/0
7	GOL	C	373	-	-	0/4/4/4	0/0/0/0
7	GOL	C	374	-	-	0/4/4/4	0/0/0/0
7	GOL	C	375	-	-	0/4/4/4	0/0/0/0
7	GOL	D	373	-	-	0/4/4/4	0/0/0/0
7	GOL	D	374	-	-	0/4/4/4	0/0/0/0
7	GOL	D	375	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1001	CHT	4	0
7	A	1003	GOL	1	0
5	B	1001	CHT	3	0
7	C	373	GOL	2	0
7	C	374	GOL	2	0
7	C	375	GOL	1	0
7	D	374	GOL	6	0
7	D	375	GOL	10	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	343/369 (92%)	0.64	33 (9%) 10 9	33, 39, 47, 55	1 (0%)
1	B	345/369 (93%)	0.78	43 (12%) 5 5	31, 39, 47, 56	2 (0%)
1	C	353/369 (95%)	0.78	50 (14%) 4 3	33, 39, 46, 52	0
1	D	355/369 (96%)	0.78	40 (11%) 7 6	31, 39, 47, 58	1 (0%)
2	E	5/6 (83%)	1.88	3 (60%) 0 0	46, 46, 47, 49	0
All	All	1401/1482 (94%)	0.75	169 (12%) 6 5	31, 39, 47, 58	4 (0%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	ILE	5.9
1	D	360	ILE	5.6
1	D	65	ILE	5.2
1	B	293	ASP	5.1
1	C	248	ILE	4.8
1	B	311	VAL	4.6
1	B	247	ASP	4.6
1	C	318	ALA	4.6
1	A	361	SER	4.4
1	B	139	LEU	4.4
1	C	139	LEU	4.4
1	D	318	ALA	4.4
1	D	248	ILE	4.3
1	D	297	VAL	4.3
1	A	46	THR	4.1
1	A	299	PRO	3.8
1	C	249	ALA	3.8
1	A	311	VAL	3.8
1	C	135	ILE	3.7
1	C	336	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	215	CYS	3.7
1	A	301	PRO	3.6
1	B	246	THR	3.6
1	A	318	ALA	3.6
1	D	319	HIS	3.6
1	D	320	LEU	3.5
1	C	69	VAL	3.5
1	A	249	ALA	3.4
1	C	360	ILE	3.4
1	B	251	PHE	3.3
1	A	246[A]	THR	3.3
1	C	253	ILE	3.2
1	B	318	ALA	3.2
1	D	251	PHE	3.2
1	C	251	PHE	3.2
1	C	112	ILE	3.2
1	C	301	PRO	3.2
1	B	245	ALA	3.1
1	C	287	TYR	3.1
1	C	263	SER	3.1
1	C	219	LEU	3.1
1	A	253	ILE	3.1
1	B	363	ASN	3.1
1	D	135	ILE	3.0
1	C	320	LEU	3.0
1	A	12	THR	3.0
1	B	206	ASP	3.0
1	D	153	GLU	3.0
1	D	219	LEU	3.0
1	D	317	GLY	3.0
1	D	298	VAL	2.9
1	B	16	TYR	2.9
1	B	249	ALA	2.9
1	D	139	LEU	2.9
1	A	219	LEU	2.9
1	C	151	LEU	2.9
1	A	216	HIS	2.9
1	B	365	ILE	2.9
1	C	319	HIS	2.9
1	A	248	ILE	2.8
1	B	177	ASN	2.8
1	C	65	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	219	LEU	2.8
1	A	321	LEU	2.8
1	B	215	CYS	2.8
1	C	39[A]	LYS	2.7
1	C	323	GLY	2.7
1	D	321	LEU	2.7
1	D	272	LYS	2.7
1	A	252	PHE	2.7
1	B	301	PRO	2.7
1	A	250	ASN	2.7
1	B	13	ASP	2.7
1	B	288	LEU	2.7
1	B	129	PRO	2.6
1	A	262	SER	2.6
1	D	316	LEU	2.6
1	D	315	ALA	2.6
1	C	108	ASN	2.6
1	D	299	PRO	2.6
1	C	271	LYS	2.6
1	A	15	LEU	2.6
1	B	36	LEU	2.6
1	C	293	ASP	2.6
1	D	287	TYR	2.6
1	C	70	LEU	2.6
1	B	252	PHE	2.6
1	B	299	PRO	2.6
1	D	112	ILE	2.6
1	C	349	LEU	2.5
1	B	183	CYS	2.5
1	A	149	ARG	2.5
1	D	322	TRP	2.5
1	A	247	ASP	2.5
1	C	300	THR	2.5
1	B	133	ILE	2.5
1	D	335	SER	2.5
1	D	365	ILE	2.5
1	C	206[A]	ASP	2.5
1	C	245	ALA	2.4
1	D	253	ILE	2.4
1	C	148	LYS	2.4
1	D	283	PHE	2.4
1	C	246	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	277	TYR	2.4
1	D	183	CYS	2.4
1	A	239	SER	2.4
1	C	361	SER	2.4
1	D	349	LEU	2.4
1	B	69	VAL	2.4
1	B	250	ASN	2.4
1	C	60	ASN	2.4
1	A	289[A]	SER	2.4
1	C	247	ASP	2.4
2	E	6	PHE	2.4
1	A	11	LEU	2.4
1	C	52	VAL	2.4
1	C	317	GLY	2.4
1	A	313	VAL	2.4
1	B	42	LEU	2.3
1	D	118	GLY	2.3
2	E	4	LEU	2.3
1	D	250	ASN	2.3
1	D	293	ASP	2.3
1	C	337	ASN	2.3
1	C	261	VAL	2.3
1	D	368	TYR	2.3
1	B	323	GLY	2.3
1	C	316	LEU	2.3
1	A	290	ASN	2.2
1	C	266	PHE	2.2
1	B	216	HIS	2.2
1	C	150	HIS	2.2
1	B	176	LYS	2.2
1	B	153	GLU	2.2
1	D	42	LEU	2.2
1	C	262	SER	2.2
1	B	322	TRP	2.2
1	A	153	GLU	2.2
2	E	5	TYR	2.2
1	B	315	ALA	2.2
1	D	327	ILE	2.2
1	B	217	ASN	2.1
1	D	70	LEU	2.1
1	C	315	ALA	2.1
1	A	314	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	112	ILE	2.1
1	C	283	PHE	2.1
1	B	321	LEU	2.1
1	B	186	HIS	2.1
1	C	322	TRP	2.1
1	A	207	ASN	2.1
1	D	263	SER	2.1
1	C	71	PHE	2.1
1	A	292	LEU	2.1
1	B	244	LEU	2.1
1	C	343	LEU	2.1
1	D	11	LEU	2.1
1	C	136	ALA	2.1
1	D	71	PHE	2.0
1	A	315	ALA	2.0
1	D	108	ASN	2.0
1	A	251	PHE	2.0
1	C	172	LEU	2.0
1	D	136	ALA	2.0
1	B	367	GLY	2.0
1	B	70	LEU	2.0
1	C	345	ALA	2.0
1	A	238	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
6	UNL	C	372	1/-	0.99	0.60	13.46	30,30,30,30	0
7	GOL	C	373	6/6	0.71	0.51	13.13	45,48,49,53	0
7	GOL	C	374	6/6	0.59	0.37	11.99	49,51,52,54	0
7	GOL	D	375	6/6	0.35	0.50	9.58	22,23,27,27	6
7	GOL	B	1004	6/6	0.80	0.30	8.40	59,60,61,61	0
4	CA	D	371	1/1	0.85	0.26	3.94	54,54,54,54	0
7	GOL	D	373	6/6	0.80	0.28	3.17	48,55,56,60	0
7	GOL	B	1003	6/6	0.66	0.26	3.05	64,65,66,66	0
4	CA	C	371	1/1	0.94	0.23	2.03	55,55,55,55	0
4	CA	B	371	1/1	0.95	0.20	1.89	48,48,48,48	0
5	CHT	B	1001	7/7	0.89	0.23	1.65	44,48,50,50	0
5	CHT	A	1001	7/7	0.84	0.25	1.49	43,44,47,47	0
7	GOL	D	374	6/6	0.84	0.23	1.16	43,51,53,54	0
7	GOL	A	1002	6/6	0.86	0.22	0.97	47,49,50,52	0
7	GOL	A	1003	6/6	0.83	0.24	0.55	48,51,53,55	0
4	CA	A	371	1/1	0.91	0.15	0.19	48,48,48,48	0
7	GOL	C	375	6/6	0.75	0.19	-0.20	52,55,55,58	0
3	MG	C	370	1/1	0.92	0.06	-	34,34,34,34	0
3	MG	D	370	1/1	0.94	0.04	-	31,31,31,31	0
3	MG	B	370	1/1	0.95	0.08	-	34,34,34,34	0
6	UNL	D	372	1/-	0.98	0.66	-	30,30,30,30	0
3	MG	A	370	1/1	0.94	0.04	-	29,29,29,29	0
6	UNL	B	1002	1/-	0.99	0.59	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.