Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2016 – 04:21 PM EDT

PDB ID	:	5LP7
Title	:	Crystal structure of 3-Ketoacyl-CoA Thiolase (MmgA) from Bacillus subtilis.
Authors	:	Baker, G.E.; Race, P.R.
Deposited on	:	2016-08-11
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:

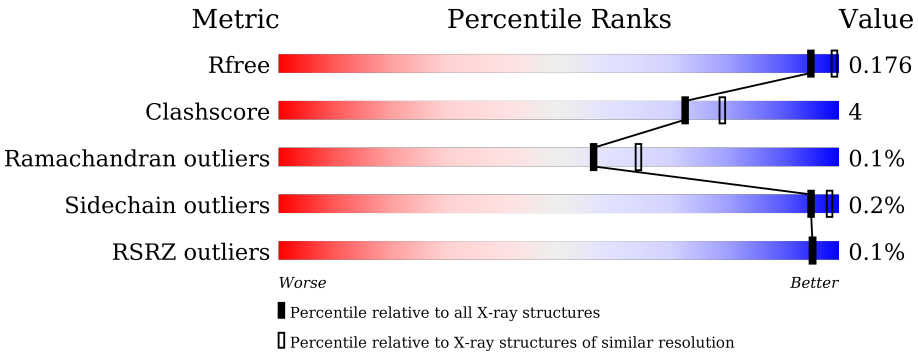
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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	393	79% 15%
1	B	393	82% 14%
1	C	393	80% 17%
1	D	393	81% 15%
1	E	393	80% 17%
1	F	393	% 79% 16%

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Mol	Chain	Length	Quality of chain
1	G	393	
1	H	393	

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
2	GOL	A	401	-	-	-	X
2	GOL	B	401	-	-	-	X
2	GOL	B	402	-	-	-	X
2	GOL	C	401	-	-	-	X
2	GOL	D	401	-	-	-	X
2	GOL	E	401	-	-	-	X
2	GOL	F	401	-	-	-	X

2 Entry composition (i)

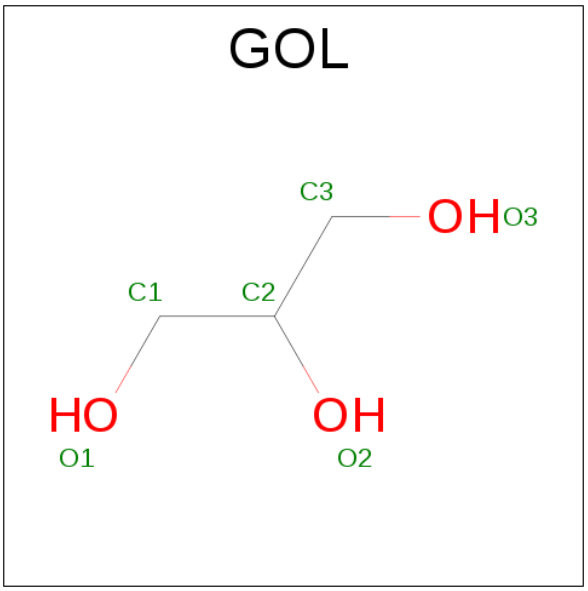
There are 3 unique types of molecules in this entry. The entry contains 22740 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	386	Total	C	N	O	S	0	0	0
			2733	1707	484	524	18			
1	E	386	Total	C	N	O	S	0	0	0
			2740	1702	490	531	17			
1	A	386	Total	C	N	O	S	0	0	0
			2730	1703	486	523	18			
1	B	388	Total	C	N	O	S	0	0	0
			2753	1716	491	528	18			
1	C	387	Total	C	N	O	S	0	0	0
			2749	1713	497	522	17			
1	F	380	Total	C	N	O	S	0	0	0
			2641	1648	468	507	18			
1	G	385	Total	C	N	O	S	0	0	0
			2728	1702	482	528	16			
1	D	386	Total	C	N	O	S	0	0	0
			2740	1710	491	521	18			

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	82	Total O 82 82	0	0
3	E	80	Total O 80 80	0	0
3	A	110	Total O 110 110	0	0
3	B	146	Total O 146 146	0	0

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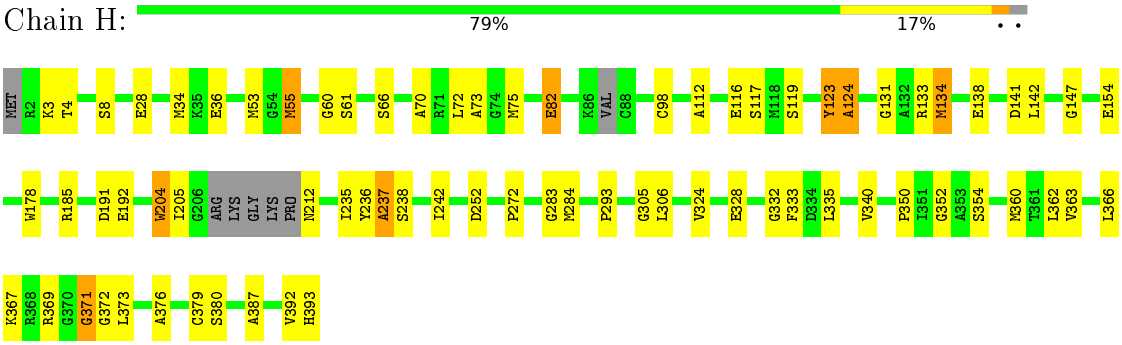
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	136	Total O 136 136	0	0
3	F	80	Total O 80 80	0	0
3	G	119	Total O 119 119	0	0
3	D	125	Total O 125 125	0	0

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.

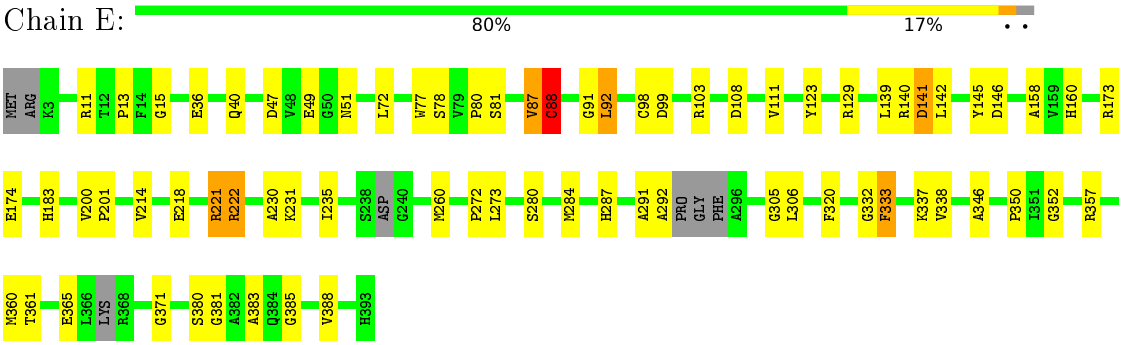
- Molecule 1: Acetyl-CoA acetyltransferase

Chain H:



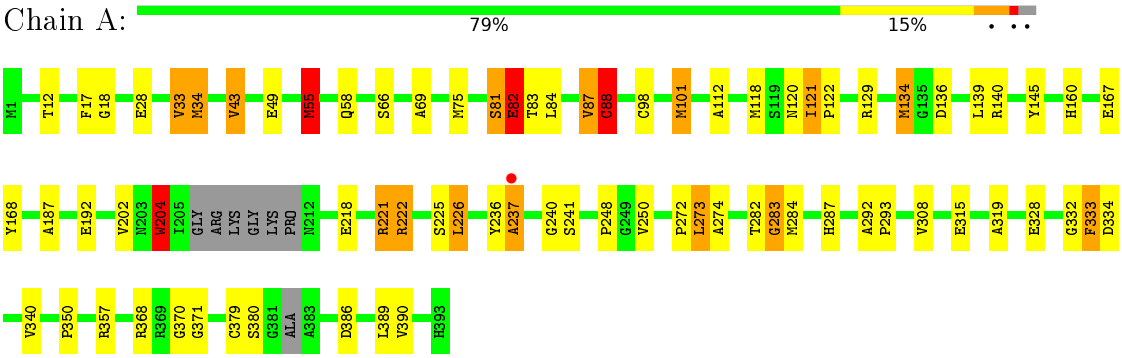
- Molecule 1: Acetyl-CoA acetyltransferase

Chain E:



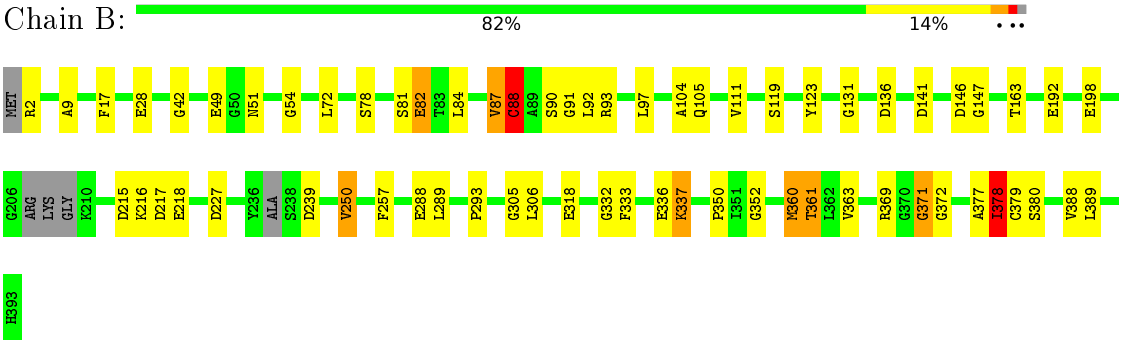
- Molecule 1: Acetyl-CoA acetyltransferase

Chain A:



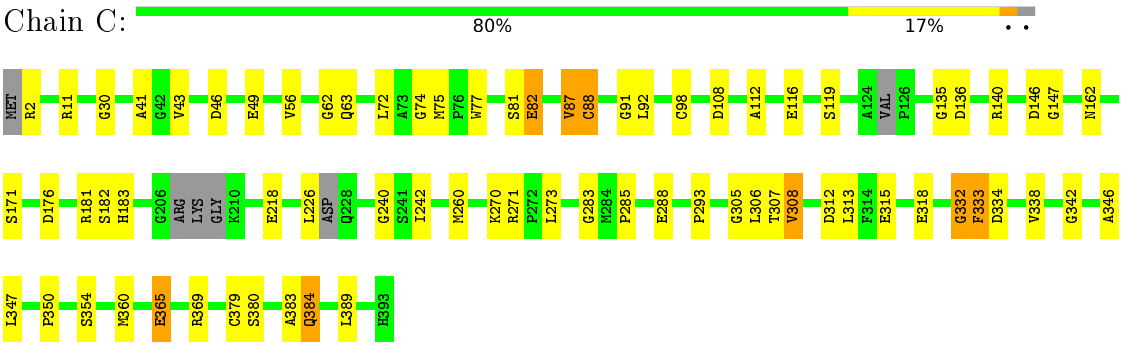
- Molecule 1: Acetyl-CoA acetyltransferase

Chain B:



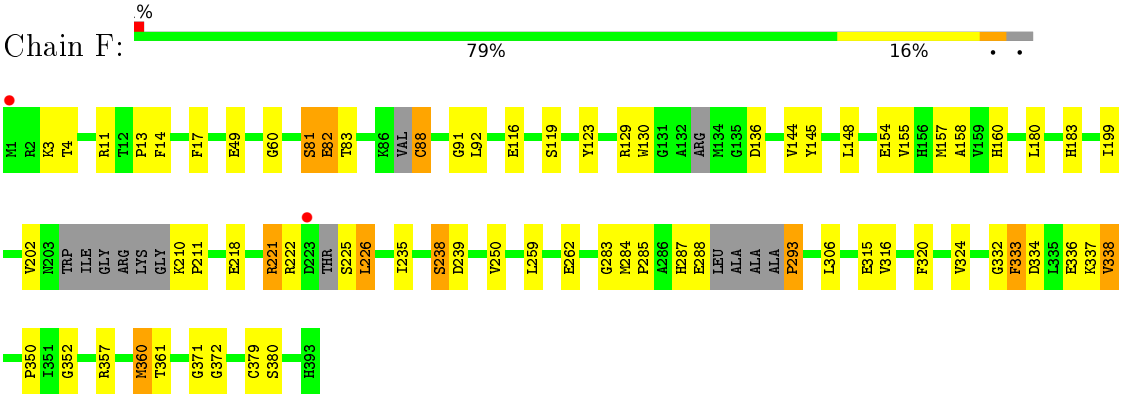
- Molecule 1: Acetyl-CoA acetyltransferase

Chain C:



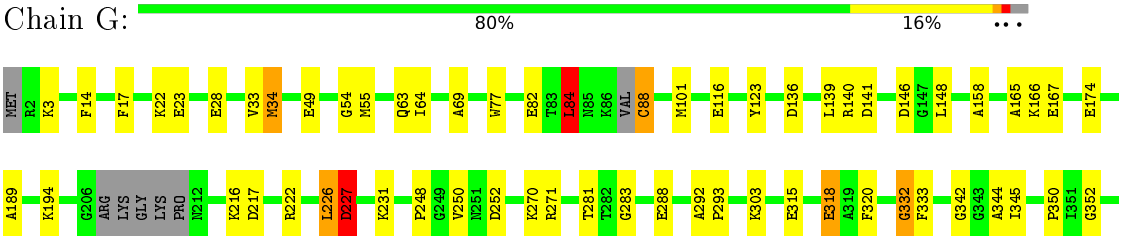
- Molecule 1: Acetyl-CoA acetyltransferase

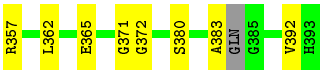
Chain F:



- Molecule 1: Acetyl-CoA acetyltransferase

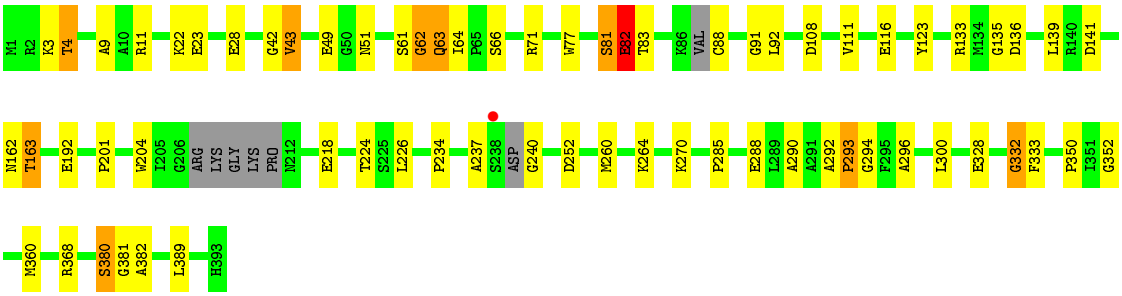
Chain G:





• Molecule 1: Acetyl-CoA acetyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.18Å 141.12Å 211.46Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	31.92 – 2.20 33.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (31.92-2.20) 98.3 (33.91-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.150 , 0.205 0.170 , 0.176	Depositor DCC
R_{free} test set	7962 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 10.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.426 for h,-k,-l	Xtriage
Reported twinning fraction	0.425 for H, K, L 0.575 for -H, -K, L	Depositor
Outliers	5 of 161152 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	22740	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.91	39/2769 (1.4%)	1.49	52/3742 (1.4%)
1	B	1.88	34/2792 (1.2%)	1.34	39/3773 (1.0%)
1	C	1.86	43/2787 (1.5%)	1.33	38/3762 (1.0%)
1	D	1.86	31/2778 (1.1%)	1.31	30/3753 (0.8%)
1	E	1.81	28/2777 (1.0%)	1.42	35/3756 (0.9%)
1	F	1.80	30/2675 (1.1%)	1.33	34/3614 (0.9%)
1	G	1.82	35/2766 (1.3%)	1.33	39/3733 (1.0%)
1	H	1.77	33/2772 (1.2%)	1.35	40/3741 (1.1%)
All	All	1.84	273/22116 (1.2%)	1.36	307/29874 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	6
1	C	0	4
1	D	0	6
1	E	0	4
1	F	0	4
1	G	0	3
1	H	0	2
All	All	0	38

All (273) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	22	LYS	C-N	-20.02	0.88	1.34
1	B	336	GLU	C-N	-19.16	0.90	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	307	THR	C-N	-18.98	0.90	1.34
1	B	87	VAL	C-N	-18.74	0.91	1.34
1	B	91	GLY	C-N	-18.54	0.91	1.34
1	A	240	GLY	C-N	-18.15	0.92	1.34
1	G	101	MET	C-N	-17.96	0.92	1.34
1	E	99	ASP	C-N	-17.87	0.93	1.34
1	A	87	VAL	C-N	-17.54	0.93	1.34
1	F	225	SER	C-N	-17.23	0.94	1.34
1	B	2	ARG	C-N	-17.11	0.94	1.34
1	C	270	LYS	C-N	-17.00	0.94	1.34
1	D	23	GLU	C-N	-16.64	0.95	1.34
1	F	91	GLY	C-N	-16.21	0.96	1.34
1	H	360	MET	C-N	-15.99	0.97	1.34
1	E	87	VAL	C-N	-15.75	0.97	1.34
1	D	62	GLY	C-N	15.61	1.70	1.34
1	F	155	VAL	C-N	-15.21	0.99	1.34
1	G	165	ALA	C-N	-15.15	0.99	1.34
1	F	360	MET	C-N	-15.01	0.99	1.34
1	C	360	MET	C-N	-14.68	1.00	1.34
1	D	162	ASN	C-N	-14.56	1.00	1.34
1	E	91	GLY	C-N	-14.27	1.01	1.34
1	H	205	ILE	C-N	-14.09	1.07	1.33
1	G	23	GLU	C-N	-14.04	1.01	1.34
1	A	225	SER	C-N	-13.56	1.02	1.34
1	E	273	LEU	C-N	-13.48	1.03	1.34
1	A	120	ASN	C-N	-12.39	1.05	1.34
1	E	230	ALA	C-N	-12.19	1.06	1.34
1	D	270	LYS	C-N	-12.02	1.06	1.34
1	F	211	PRO	C-N	-11.90	1.06	1.34
1	A	222	ARG	C-N	-11.71	1.07	1.34
1	A	272	PRO	C-N	-11.71	1.07	1.34
1	A	221	ARG	C-N	-11.60	1.07	1.34
1	A	82	GLU	C-N	-11.57	1.07	1.34
1	G	166	LYS	C-N	-11.55	1.07	1.34
1	A	241	SER	C-N	-11.52	1.07	1.34
1	D	63	GLN	C-N	-11.47	1.07	1.34
1	E	221	ARG	C-N	-11.38	1.07	1.34
1	F	154	GLU	C-N	11.31	1.60	1.34
1	A	389	LEU	C-N	-10.99	1.08	1.34
1	G	34	MET	C-N	-10.73	1.09	1.34
1	C	273	LEU	C-N	-10.54	1.09	1.34
1	D	42	GLY	C-N	-10.53	1.09	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	284	MET	C-N	10.45	1.54	1.34
1	F	226	LEU	C-N	-10.31	1.10	1.34
1	C	389	LEU	C-N	-10.25	1.10	1.34
1	H	305	GLY	C-N	-10.24	1.10	1.34
1	E	337	LYS	C-N	-10.10	1.10	1.34
1	D	201	PRO	N-CD	10.09	1.61	1.47
1	E	222	ARG	C-N	-10.01	1.11	1.34
1	C	334	ASP	C-N	-9.79	1.11	1.34
1	D	224	THR	C-N	-9.53	1.12	1.34
1	A	75	MET	C-N	9.52	1.52	1.34
1	F	145	TYR	C-N	9.52	1.55	1.34
1	G	270	LYS	C-N	-9.45	1.12	1.34
1	A	273	LEU	C-N	-9.11	1.13	1.34
1	E	360	MET	C-N	-9.06	1.13	1.34
1	A	121	ILE	C-N	-9.04	1.17	1.34
1	G	63	GLN	C-N	-8.94	1.13	1.34
1	D	226	LEU	C-N	-8.92	1.13	1.34
1	A	83	THR	C-N	-8.89	1.13	1.34
1	A	33	VAL	C-N	8.87	1.54	1.34
1	B	389	LEU	C-N	-8.78	1.13	1.34
1	A	333	PHE	C-N	8.76	1.54	1.34
1	A	84	LEU	C-N	-8.74	1.14	1.34
1	A	226	LEU	C-N	-8.63	1.14	1.34
1	H	124	ALA	C-N	-8.57	1.14	1.34
1	E	98	CYS	C-N	-8.56	1.14	1.34
1	B	216	LYS	C-N	-8.50	1.14	1.34
1	F	338	VAL	C-N	-8.36	1.14	1.34
1	D	92	LEU	C-N	-8.27	1.15	1.34
1	E	174	GLU	C-N	-8.26	1.15	1.34
1	F	337	LYS	C-N	-8.08	1.15	1.34
1	G	33	VAL	C-N	-8.08	1.15	1.34
1	G	167	GLU	C-N	-8.04	1.15	1.34
1	G	54	GLY	C-N	-8.02	1.15	1.34
1	C	306	LEU	C-N	-7.98	1.15	1.34
1	B	42	GLY	C-N	-7.98	1.15	1.34
1	G	49	GLU	CD-OE2	-7.98	1.16	1.25
1	F	222	ARG	C-N	7.92	1.52	1.34
1	G	283	GLY	C-N	-7.92	1.15	1.34
1	D	82	GLU	C-N	-7.82	1.16	1.34
1	E	231	LYS	C-N	-7.70	1.16	1.34
1	C	271	ARG	C-N	-7.67	1.19	1.34
1	E	142	LEU	C-N	-7.55	1.16	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	367	LYS	C-N	-7.49	1.16	1.34
1	H	82	GLU	CD-OE2	-7.39	1.17	1.25
1	E	92	LEU	C-N	-7.29	1.17	1.34
1	A	82	GLU	CD-OE1	-7.25	1.17	1.25
1	D	4	THR	C-N	-7.20	1.17	1.34
1	D	163	THR	C-N	-7.16	1.17	1.34
1	D	49	GLU	CD-OE1	-7.13	1.17	1.25
1	E	141	ASP	C-N	-7.11	1.17	1.34
1	G	22	LYS	C-N	-7.10	1.17	1.34
1	H	283	GLY	C-N	-7.10	1.17	1.34
1	F	144	VAL	C-N	-7.08	1.17	1.34
1	A	237	ALA	C-N	-7.08	1.17	1.34
1	H	82	GLU	CD-OE1	-7.08	1.17	1.25
1	F	361	THR	C-N	-7.07	1.17	1.34
1	H	272	PRO	C-N	-7.04	1.17	1.34
1	C	74	GLY	C-N	-7.04	1.17	1.34
1	H	55	MET	C-O	-6.99	1.10	1.23
1	E	272	PRO	C-N	-6.97	1.18	1.34
1	C	182	SER	CB-OG	-6.97	1.33	1.42
1	H	354	SER	CB-OG	-6.93	1.33	1.42
1	H	306	LEU	C-N	-6.91	1.18	1.34
1	H	4	THR	C-N	-6.90	1.18	1.34
1	C	119	SER	CB-OG	-6.88	1.33	1.42
1	A	328	GLU	CD-OE2	-6.86	1.18	1.25
1	D	49	GLU	CD-OE2	-6.82	1.18	1.25
1	A	82	GLU	CD-OE2	-6.81	1.18	1.25
1	D	82	GLU	CD-OE2	-6.80	1.18	1.25
1	F	202	VAL	C-N	-6.79	1.18	1.34
1	C	49	GLU	CD-OE1	-6.78	1.18	1.25
1	C	332	GLY	C-N	6.74	1.49	1.34
1	B	378	ILE	C-N	-6.74	1.18	1.34
1	A	334	ASP	C-N	-6.67	1.18	1.34
1	F	116	GLU	CD-OE1	-6.58	1.18	1.25
1	F	221	ARG	C-N	-6.55	1.19	1.34
1	B	217	ASP	C-N	-6.55	1.19	1.34
1	C	46	ASP	C-N	-6.51	1.19	1.34
1	G	49	GLU	CD-OE1	-6.50	1.18	1.25
1	C	315	GLU	CD-OE1	-6.46	1.18	1.25
1	G	77	TRP	CB-CG	-6.43	1.38	1.50
1	B	227	ASP	C-N	6.38	1.48	1.34
1	C	116	GLU	CD-OE1	-6.37	1.18	1.25
1	C	365	GLU	CD-OE1	-6.36	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	250	VAL	C-N	-6.35	1.19	1.34
1	C	315	GLU	CD-OE2	-6.33	1.18	1.25
1	H	363	VAL	C-N	-6.32	1.19	1.34
1	G	88	CYS	C-N	-6.32	1.19	1.34
1	H	352	GLY	C-O	-6.30	1.13	1.23
1	C	365	GLU	CD-OE2	-6.30	1.18	1.25
1	B	49	GLU	CD-OE1	-6.29	1.18	1.25
1	C	288	GLU	CD-OE2	-6.25	1.18	1.25
1	B	218	GLU	CD-OE2	-6.24	1.18	1.25
1	B	306	LEU	C-N	-6.23	1.19	1.34
1	C	383	ALA	C-N	-6.19	1.19	1.34
1	C	147	GLY	C-O	-6.15	1.13	1.23
1	G	82	GLU	CD-OE2	-6.11	1.19	1.25
1	H	204	TRP	C-N	-6.06	1.20	1.34
1	C	333	PHE	C-N	6.05	1.48	1.34
1	H	8	SER	CB-OG	-6.05	1.34	1.42
1	C	347	LEU	C-O	-6.04	1.11	1.23
1	B	288	GLU	CD-OE1	-6.04	1.19	1.25
1	C	72	LEU	C-O	-6.04	1.11	1.23
1	B	192	GLU	CD-OE1	-6.03	1.19	1.25
1	D	352	GLY	C-O	-6.02	1.14	1.23
1	E	15	GLY	C-O	-6.01	1.14	1.23
1	G	365	GLU	CD-OE1	-6.00	1.19	1.25
1	F	82	GLU	C-N	-5.99	1.20	1.34
1	D	380	SER	CB-OG	-5.97	1.34	1.42
1	D	328	GLU	CD-OE2	-5.93	1.19	1.25
1	E	218	GLU	CD-OE2	-5.92	1.19	1.25
1	G	318	GLU	CD-OE1	-5.90	1.19	1.25
1	E	381	GLY	C-O	-5.89	1.14	1.23
1	B	198	GLU	C-O	-5.87	1.12	1.23
1	F	352	GLY	C-O	-5.85	1.14	1.23
1	G	271	ARG	C-N	-5.84	1.23	1.34
1	E	173	ARG	C-N	-5.83	1.20	1.34
1	B	333	PHE	C-N	-5.82	1.20	1.34
1	G	28	GLU	CD-OE1	-5.80	1.19	1.25
1	F	129	ARG	C-O	-5.78	1.12	1.23
1	G	82	GLU	CD-OE1	-5.77	1.19	1.25
1	H	362	LEU	C-N	-5.75	1.20	1.34
1	B	352	GLY	C-O	-5.74	1.14	1.23
1	G	315	GLU	CD-OE1	-5.73	1.19	1.25
1	A	129	ARG	C-O	-5.72	1.12	1.23
1	C	318	GLU	CD-OE2	-5.72	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	135	GLY	C-O	-5.72	1.14	1.23
1	D	218	GLU	CD-OE1	-5.71	1.19	1.25
1	H	133	ARG	C-N	-5.69	1.21	1.34
1	F	49	GLU	CD-OE2	-5.68	1.19	1.25
1	H	36	GLU	CD-OE2	-5.67	1.19	1.25
1	G	227	ASP	C-N	-5.66	1.21	1.34
1	B	147	GLY	C-O	-5.66	1.14	1.23
1	B	377	ALA	C-N	-5.64	1.21	1.34
1	B	192	GLU	CD-OE2	-5.64	1.19	1.25
1	D	192	GLU	CD-OE2	-5.62	1.19	1.25
1	C	91	GLY	C-O	-5.61	1.14	1.23
1	C	181	ARG	CZ-NH2	-5.61	1.25	1.33
1	D	61	SER	CB-OG	-5.61	1.34	1.42
1	H	380	SER	CB-OG	-5.60	1.34	1.42
1	D	91	GLY	C-N	-5.60	1.21	1.34
1	C	49	GLU	CD-OE2	-5.59	1.19	1.25
1	E	352	GLY	C-O	-5.58	1.14	1.23
1	A	28	GLU	CD-OE1	-5.56	1.19	1.25
1	H	61	SER	CB-OG	-5.56	1.35	1.42
1	C	283	GLY	C-N	-5.56	1.21	1.34
1	H	119	SER	CB-OG	-5.54	1.35	1.42
1	G	342	GLY	C-O	-5.53	1.14	1.23
1	H	131	GLY	C-O	-5.51	1.14	1.23
1	C	62	GLY	C-O	-5.50	1.14	1.23
1	E	49	GLU	CD-OE1	-5.50	1.19	1.25
1	A	49	GLU	CD-OE1	-5.49	1.19	1.25
1	B	163	THR	C-O	-5.49	1.12	1.23
1	A	192	GLU	CD-OE1	-5.49	1.19	1.25
1	B	91	GLY	C-O	-5.48	1.14	1.23
1	F	60	GLY	C-O	-5.47	1.14	1.23
1	H	154	GLU	CD-OE1	-5.47	1.19	1.25
1	A	43	VAL	C-N	-5.45	1.21	1.34
1	H	147	GLY	C-O	-5.43	1.15	1.23
1	F	218	GLU	CD-OE1	-5.42	1.19	1.25
1	B	388	VAL	C-N	-5.42	1.21	1.34
1	D	293	PRO	C-O	-5.41	1.12	1.23
1	B	131	GLY	C-O	-5.40	1.15	1.23
1	F	262	GLU	CD-OE1	-5.39	1.19	1.25
1	G	288	GLU	CD-OE1	-5.39	1.19	1.25
1	B	119	SER	CB-OG	-5.37	1.35	1.42
1	G	23	GLU	CD-OE2	-5.37	1.19	1.25
1	C	171	SER	CB-OG	-5.37	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	352	GLY	C-O	-5.37	1.15	1.23
1	E	280	SER	CB-OG	-5.36	1.35	1.42
1	G	64	ILE	C-N	-5.36	1.24	1.34
1	C	342	GLY	C-O	-5.34	1.15	1.23
1	F	315	GLU	CD-OE1	-5.32	1.19	1.25
1	G	365	GLU	CD-OE2	-5.32	1.19	1.25
1	F	49	GLU	CD-OE1	-5.31	1.19	1.25
1	B	82	GLU	CD-OE2	-5.31	1.19	1.25
1	B	332	GLY	C-N	5.30	1.46	1.34
1	E	81	SER	CB-OG	-5.30	1.35	1.42
1	C	242	ILE	C-O	-5.29	1.13	1.23
1	A	315	GLU	CD-OE2	-5.29	1.19	1.25
1	A	55	MET	C-O	-5.26	1.13	1.23
1	E	129	ARG	C-O	-5.25	1.13	1.23
1	E	365	GLU	CD-OE1	-5.24	1.19	1.25
1	A	340	VAL	C-O	-5.23	1.13	1.23
1	F	333	PHE	C-N	-5.23	1.22	1.34
1	B	88	CYS	C-N	5.22	1.46	1.34
1	C	305	GLY	C-N	-5.21	1.22	1.34
1	G	174	GLU	CD-OE2	-5.21	1.20	1.25
1	D	3	LYS	C-N	-5.20	1.22	1.34
1	C	81	SER	CB-OG	-5.19	1.35	1.42
1	A	28	GLU	CD-OE2	-5.18	1.20	1.25
1	G	116	GLU	CD-OE1	-5.18	1.20	1.25
1	C	288	GLU	CD-OE1	-5.17	1.20	1.25
1	H	116	GLU	CD-OE1	-5.17	1.20	1.25
1	D	116	GLU	CD-OE1	-5.16	1.20	1.25
1	A	18	GLY	C-O	-5.16	1.15	1.23
1	A	167	GLU	CD-OE2	-5.16	1.20	1.25
1	F	92	LEU	C-N	-5.16	1.22	1.34
1	E	218	GLU	CD-OE1	-5.15	1.20	1.25
1	A	282	THR	C-O	-5.15	1.13	1.23
1	H	123	TYR	CZ-OH	-5.14	1.29	1.37
1	H	138	GLU	CD-OE2	-5.14	1.20	1.25
1	A	218	GLU	CD-OE2	-5.14	1.20	1.25
1	C	218	GLU	CD-OE2	-5.14	1.20	1.25
1	D	28	GLU	CD-OE2	-5.13	1.20	1.25
1	E	305	GLY	C-N	-5.13	1.22	1.34
1	B	49	GLU	CD-OE2	-5.11	1.20	1.25
1	A	134	MET	C-O	-5.11	1.13	1.23
1	F	119	SER	CB-OG	-5.11	1.35	1.42
1	H	60	GLY	C-O	-5.10	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	30	GLY	C-O	-5.10	1.15	1.23
1	H	192	GLU	CD-OE2	-5.09	1.20	1.25
1	H	3	LYS	C-N	-5.08	1.22	1.34
1	C	82	GLU	CD-OE2	-5.08	1.20	1.25
1	G	362	LEU	C-N	-5.08	1.22	1.34
1	B	82	GLU	CD-OE1	-5.08	1.20	1.25
1	A	192	GLU	CD-OE2	-5.07	1.20	1.25
1	B	318	GLU	CD-OE2	-5.07	1.20	1.25
1	G	332	GLY	C-N	5.07	1.45	1.34
1	F	130	TRP	CG-CD1	-5.06	1.29	1.36
1	C	318	GLU	CD-OE1	-5.05	1.20	1.25
1	D	290	ALA	C-O	-5.05	1.13	1.23
1	C	354	SER	CB-OG	-5.05	1.35	1.42
1	B	28	GLU	CD-OE1	-5.04	1.20	1.25
1	A	168	TYR	CZ-OH	-5.04	1.29	1.37
1	C	135	GLY	C-O	-5.04	1.15	1.23
1	D	288	GLU	CD-OE2	-5.03	1.20	1.25
1	F	123	TYR	CZ-OH	-5.02	1.29	1.37
1	G	281	THR	C-N	-5.01	1.22	1.34

All (307) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	222	ARG	O-C-N	-28.82	76.58	122.70
1	E	222	ARG	CA-C-N	23.47	168.84	117.20
1	H	237	ALA	CB-CA-C	17.79	136.79	110.10
1	A	333	PHE	O-C-N	15.26	147.12	122.70
1	D	82	GLU	O-C-N	-15.00	98.70	122.70
1	F	82	GLU	CB-CA-C	14.64	139.68	110.40
1	G	332	GLY	O-C-N	-13.76	100.68	122.70
1	D	332	GLY	O-C-N	-13.67	100.83	122.70
1	B	215	ASP	C-N-CA	13.50	155.45	121.70
1	B	215	ASP	O-C-N	-13.15	101.67	122.70
1	G	227	ASP	O-C-N	-13.10	101.74	122.70
1	A	55	MET	O-C-N	-13.03	101.85	122.70
1	D	294	GLY	N-CA-C	-12.62	81.56	113.10
1	F	81	SER	O-C-N	-12.45	102.78	122.70
1	B	378	ILE	O-C-N	-12.31	103.00	122.70
1	F	238	SER	N-CA-C	-12.21	78.02	111.00
1	H	305	GLY	O-C-N	-12.12	103.31	122.70
1	A	237	ALA	CB-CA-C	11.94	128.01	110.10
1	H	305	GLY	C-N-CA	11.70	150.96	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	238	SER	N-CA-C	-11.58	79.72	111.00
1	E	337	LYS	C-N-CA	11.52	150.49	121.70
1	A	333	PHE	CA-C-N	-11.44	92.02	117.20
1	A	241	SER	O-C-N	-11.44	104.40	122.70
1	B	332	GLY	O-C-N	-11.34	104.55	122.70
1	E	230	ALA	O-C-N	-11.28	104.65	122.70
1	G	333	PHE	O-C-N	10.98	140.27	122.70
1	A	82	GLU	O-C-N	-10.94	105.19	122.70
1	A	87	VAL	C-N-CA	10.82	148.76	121.70
1	A	84	LEU	O-C-N	-10.82	105.38	122.70
1	E	333	PHE	O-C-N	10.77	139.94	122.70
1	G	226	LEU	O-C-N	-10.63	105.70	122.70
1	F	332	GLY	O-C-N	-10.43	106.02	122.70
1	F	333	PHE	O-C-N	10.42	139.37	122.70
1	A	389	LEU	C-N-CA	10.39	147.69	121.70
1	G	101	MET	CA-C-O	-10.29	98.49	120.10
1	D	332	GLY	C-N-CA	10.27	147.36	121.70
1	A	120	ASN	O-C-N	-10.20	106.39	122.70
1	D	82	GLU	C-N-CA	10.12	147.00	121.70
1	A	120	ASN	C-N-CA	10.02	146.75	121.70
1	E	222	ARG	N-CA-C	9.94	137.84	111.00
1	C	270	LYS	C-N-CA	9.93	146.52	121.70
1	C	333	PHE	O-C-N	9.91	138.55	122.70
1	A	34	MET	O-C-N	-9.87	106.92	122.70
1	A	82	GLU	CB-CA-C	9.85	130.10	110.40
1	H	204	TRP	O-C-N	-9.78	107.05	122.70
1	B	337	LYS	O-C-N	-9.73	107.14	122.70
1	D	3	LYS	C-N-CA	9.71	145.97	121.70
1	B	305	GLY	C-N-CA	9.59	145.68	121.70
1	C	308	VAL	O-C-N	-9.54	107.43	122.70
1	A	81	SER	O-C-N	-9.54	107.44	122.70
1	H	3	LYS	C-N-CA	9.52	145.49	121.70
1	B	215	ASP	CA-C-N	9.50	138.09	117.20
1	A	371	GLY	N-CA-C	9.49	136.83	113.10
1	B	305	GLY	O-C-N	-9.43	107.61	122.70
1	A	55	MET	CA-C-O	9.31	139.65	120.10
1	H	134	MET	O-C-N	-9.28	107.42	123.20
1	G	372	GLY	N-CA-C	9.25	136.22	113.10
1	H	305	GLY	CA-C-N	9.14	137.30	117.20
1	G	34	MET	CA-C-O	-9.13	100.94	120.10
1	F	136	ASP	CB-CG-OD1	9.12	126.50	118.30
1	H	55	MET	O-C-N	-9.02	108.27	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	82	GLU	CA-C-N	9.01	137.02	117.20
1	D	332	GLY	CA-C-N	8.98	136.95	117.20
1	A	241	SER	CA-C-N	8.97	136.93	117.20
1	E	337	LYS	O-C-N	-8.96	108.37	122.70
1	G	332	GLY	CA-C-N	8.93	136.84	117.20
1	A	389	LEU	O-C-N	-8.84	108.56	122.70
1	G	227	ASP	CA-C-N	8.84	136.64	117.20
1	E	333	PHE	CA-C-N	-8.83	97.77	117.20
1	E	305	GLY	C-N-CA	8.80	143.71	121.70
1	D	83	THR	N-CA-CB	8.78	126.99	110.30
1	F	333	PHE	CA-C-N	-8.76	97.93	117.20
1	F	222	ARG	O-C-N	8.74	136.68	122.70
1	A	101	MET	O-C-N	-8.65	108.86	122.70
1	C	11	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	E	332	GLY	O-C-N	-8.47	109.15	122.70
1	F	154	GLU	O-C-N	-8.35	109.35	122.70
1	C	181	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	E	230	ALA	C-N-CA	8.24	142.31	121.70
1	B	360	MET	O-C-N	8.23	135.88	122.70
1	H	82	GLU	O-C-N	8.14	135.73	122.70
1	G	333	PHE	CA-C-N	-8.12	99.34	117.20
1	A	273	LEU	O-C-N	-8.04	109.84	122.70
1	C	383	ALA	O-C-N	-8.02	109.86	122.70
1	B	217	ASP	O-C-N	-8.00	109.89	122.70
1	E	371	GLY	N-CA-C	7.97	133.02	113.10
1	F	338	VAL	O-C-N	-7.96	109.97	122.70
1	F	332	GLY	CA-C-N	7.86	134.50	117.20
1	H	3	LYS	O-C-N	-7.82	110.19	122.70
1	C	333	PHE	CA-C-N	-7.79	100.06	117.20
1	E	272	PRO	O-C-N	7.78	135.15	122.70
1	A	134	MET	O-C-N	-7.76	110.01	123.20
1	A	43	VAL	O-C-N	-7.73	110.33	122.70
1	C	383	ALA	C-N-CA	7.71	140.98	121.70
1	H	55	MET	CA-C-O	7.70	136.27	120.10
1	A	272	PRO	O-C-N	-7.68	110.41	122.70
1	H	371	GLY	N-CA-C	7.67	132.28	113.10
1	E	305	GLY	O-C-N	-7.65	110.46	122.70
1	D	293	PRO	C-N-CA	7.64	138.36	122.30
1	C	181	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	88	CYS	CA-C-N	-7.55	100.59	117.20
1	H	332	GLY	O-C-N	-7.55	110.62	122.70
1	E	230	ALA	CA-C-N	7.53	133.76	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	145	TYR	O-C-N	7.52	134.74	122.70
1	B	332	GLY	CA-C-N	7.51	133.73	117.20
1	G	281	THR	O-C-N	-7.51	110.69	122.70
1	F	211	PRO	O-C-N	7.49	134.68	122.70
1	B	87	VAL	C-N-CA	7.48	140.40	121.70
1	C	333	PHE	CB-CA-C	-7.46	95.48	110.40
1	G	136	ASP	CB-CG-OD1	7.41	124.97	118.30
1	H	82	GLU	CA-C-N	-7.40	100.92	117.20
1	C	384	GLN	O-C-N	7.40	135.78	123.20
1	E	174	GLU	O-C-N	-7.38	110.90	122.70
1	G	55	MET	O-C-N	-7.37	110.91	122.70
1	B	333	PHE	CA-C-N	-7.36	101.01	117.20
1	B	333	PHE	O-C-N	7.36	134.48	122.70
1	D	226	LEU	O-C-N	-7.33	110.97	122.70
1	A	120	ASN	CA-C-N	7.30	133.26	117.20
1	H	333	PHE	O-C-N	7.27	134.33	122.70
1	E	88	CYS	CA-C-N	-7.26	101.22	117.20
1	F	332	GLY	C-N-CA	7.24	139.81	121.70
1	C	270	LYS	O-C-N	-7.23	111.13	122.70
1	C	74	GLY	O-C-N	-7.22	111.14	122.70
1	A	332	GLY	O-C-N	-7.22	111.15	122.70
1	A	225	SER	O-C-N	-7.21	111.16	122.70
1	H	204	TRP	C-N-CA	7.19	139.66	121.70
1	D	3	LYS	O-C-N	-7.19	111.20	122.70
1	H	191	ASP	CB-CG-OD1	7.18	124.76	118.30
1	G	217	ASP	CB-CG-OD2	7.17	124.76	118.30
1	B	146	ASP	CB-CG-OD1	7.17	124.76	118.30
1	F	222	ARG	CA-C-N	-7.12	101.54	117.20
1	B	136	ASP	CB-CG-OD1	7.08	124.67	118.30
1	H	205	ILE	O-C-N	-7.06	111.19	123.20
1	E	99	ASP	O-C-N	-7.04	111.44	122.70
1	D	23	GLU	O-C-N	-7.02	111.46	122.70
1	C	271	ARG	O-C-N	-7.02	107.77	121.10
1	A	272	PRO	C-N-CA	7.00	139.21	121.70
1	C	140	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	87	VAL	O-C-N	-6.99	111.52	122.70
1	E	87	VAL	C-N-CA	6.96	139.10	121.70
1	G	252	ASP	CB-CG-OD1	6.95	124.56	118.30
1	B	372	GLY	N-CA-C	6.92	130.41	113.10
1	F	3	LYS	C-N-CA	6.92	139.00	121.70
1	B	42	GLY	C-N-CA	6.91	138.97	121.70
1	A	389	LEU	CA-C-N	6.88	132.34	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	63	GLN	C-N-CA	6.87	138.88	121.70
1	C	75	MET	CA-C-N	-6.86	97.90	117.10
1	A	84	LEU	CA-C-N	6.86	132.28	117.20
1	F	235	ILE	N-CA-C	6.85	129.50	111.00
1	G	22	LYS	C-N-CA	-6.83	104.63	121.70
1	C	332	GLY	O-C-N	-6.79	111.84	122.70
1	H	372	GLY	N-CA-C	6.75	129.97	113.10
1	C	384	GLN	CA-C-N	-6.74	102.71	116.20
1	H	369	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	D	293	PRO	CA-C-N	6.70	129.60	116.20
1	E	47	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	75	MET	CA-C-N	-6.67	98.42	117.10
1	F	136	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	D	368	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	H	204	TRP	CA-C-N	6.57	131.66	117.20
1	B	336	GLU	C-N-CA	6.57	138.13	121.70
1	C	305	GLY	C-N-CA	6.54	138.05	121.70
1	G	350	PRO	N-CA-C	-6.53	95.13	112.10
1	B	305	GLY	CA-C-N	6.51	131.52	117.20
1	D	333	PHE	O-C-N	6.50	133.10	122.70
1	E	273	LEU	O-C-N	-6.50	112.30	122.70
1	B	360	MET	C-N-CA	-6.47	105.52	121.70
1	D	71	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	H	124	ALA	C-N-CA	6.43	137.77	121.70
1	C	82	GLU	O-C-N	-6.41	112.44	122.70
1	C	11	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	G	34	MET	CA-C-N	6.39	131.25	117.20
1	B	378	ILE	CA-C-N	6.35	131.18	117.20
1	E	337	LYS	CA-C-N	6.35	131.17	117.20
1	A	83	THR	C-N-CA	6.33	137.53	121.70
1	H	252	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	G	146	ASP	CB-CG-OD1	6.30	123.97	118.30
1	F	83	THR	N-CA-CB	6.28	122.23	110.30
1	B	216	LYS	O-C-N	6.23	132.67	122.70
1	E	221	ARG	O-C-N	-6.23	112.74	122.70
1	H	252	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	350	PRO	N-CA-C	-6.20	95.98	112.10
1	G	226	LEU	CA-C-N	6.18	130.79	117.20
1	A	83	THR	N-CA-CB	6.18	122.04	110.30
1	G	136	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	C	75	MET	CA-C-O	6.16	133.03	120.10
1	H	238	SER	N-CA-CB	6.13	119.70	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	146	ASP	CB-CG-OD1	6.12	123.81	118.30
1	C	226	LEU	CA-CB-CG	6.12	129.37	115.30
1	G	84	LEU	CA-CB-CG	6.10	129.32	115.30
1	C	350	PRO	N-CA-C	-6.09	96.28	112.10
1	B	337	LYS	CA-C-N	6.08	130.59	117.20
1	C	383	ALA	CA-C-N	6.08	130.59	117.20
1	A	386	ASP	CB-CG-OD2	6.06	123.76	118.30
1	G	252	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	G	22	LYS	O-C-N	6.01	132.32	122.70
1	F	210	LYS	O-C-N	-6.00	109.70	121.10
1	G	101	MET	CA-C-N	5.97	130.34	117.20
1	G	332	GLY	C-N-CA	5.97	136.63	121.70
1	E	272	PRO	CA-C-N	-5.96	104.10	117.20
1	D	92	LEU	O-C-N	-5.94	113.20	122.70
1	C	334	ASP	CB-CG-OD1	5.93	123.64	118.30
1	B	332	GLY	C-N-CA	5.92	136.51	121.70
1	B	336	GLU	O-C-N	-5.92	113.22	122.70
1	H	283	GLY	O-C-N	5.92	132.17	122.70
1	A	136	ASP	CB-CG-OD1	5.90	123.61	118.30
1	E	332	GLY	CA-C-N	5.88	130.14	117.20
1	A	221	ARG	CA-C-N	-5.85	104.34	117.20
1	A	284	MET	N-CA-C	5.84	126.77	111.00
1	A	84	LEU	C-N-CA	5.84	136.30	121.70
1	F	92	LEU	O-C-N	-5.84	113.36	122.70
1	A	134	MET	CA-C-O	5.83	132.35	120.10
1	D	42	GLY	C-N-CA	5.83	136.26	121.70
1	E	235	ILE	N-CA-C	5.82	126.71	111.00
1	D	368	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	D	136	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	273	LEU	CA-C-N	5.79	129.93	117.20
1	F	360	MET	CA-CB-CG	5.77	123.11	113.30
1	H	333	PHE	CA-C-N	-5.76	104.52	117.20
1	C	146	ASP	CB-CG-OD1	5.75	123.47	118.30
1	G	3	LYS	C-N-CA	5.75	136.06	121.70
1	H	134	MET	CA-C-O	5.73	132.14	120.10
1	F	81	SER	CA-C-N	5.71	129.76	117.20
1	E	174	GLU	CA-C-N	5.69	129.72	117.20
1	F	259	LEU	CA-CB-CG	5.68	128.36	115.30
1	H	369	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	A	204	TRP	O-C-N	-5.65	113.66	122.70
1	G	140	ARG	NE-CZ-NH1	-5.65	117.48	120.30
1	F	288	GLU	CB-CA-C	5.64	121.69	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	139	LEU	CB-CG-CD2	5.62	120.56	111.00
1	C	308	VAL	CA-C-N	5.62	129.56	117.20
1	G	22	LYS	CA-C-N	-5.61	104.86	117.20
1	H	373	LEU	CA-CB-CG	5.58	128.14	115.30
1	C	270	LYS	CA-C-N	5.57	129.46	117.20
1	D	252	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	371	GLY	N-CA-C	5.56	127.01	113.10
1	F	371	GLY	N-CA-C	5.54	126.95	113.10
1	G	216	LYS	O-C-N	-5.53	113.86	122.70
1	E	350	PRO	N-CA-C	-5.52	97.74	112.10
1	E	361	THR	N-CA-CB	5.52	120.78	110.30
1	G	222	ARG	N-CA-C	-5.51	96.11	111.00
1	G	55	MET	CA-C-N	5.51	129.32	117.20
1	F	350	PRO	N-CA-C	-5.50	97.79	112.10
1	B	91	GLY	C-N-CA	5.49	135.42	121.70
1	C	2	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	E	72	LEU	CB-CG-CD1	5.46	120.29	111.00
1	A	390	VAL	CB-CA-C	-5.46	101.03	111.40
1	B	289	LEU	CA-CB-CG	5.45	127.84	115.30
1	D	350	PRO	N-CA-C	-5.44	97.95	112.10
1	B	378	ILE	C-N-CA	5.44	135.30	121.70
1	H	117	SER	N-CA-CB	5.43	118.65	110.50
1	C	140	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	H	134	MET	C-N-CA	5.42	133.69	122.30
1	F	82	GLU	N-CA-C	-5.41	96.39	111.00
1	F	372	GLY	N-CA-C	5.41	126.62	113.10
1	C	226	LEU	N-CA-C	-5.39	96.46	111.00
1	C	136	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	81	SER	C-N-CA	-5.37	108.27	121.70
1	F	338	VAL	CA-C-N	5.37	129.00	117.20
1	B	361	THR	C-N-CA	5.36	135.10	121.70
1	C	176	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	74	GLY	CA-C-N	5.36	128.98	117.20
1	H	362	LEU	CB-CG-CD2	5.35	120.10	111.00
1	B	350	PRO	N-CA-C	-5.34	98.22	112.10
1	D	43	VAL	O-C-N	-5.32	114.18	122.70
1	H	237	ALA	N-CA-C	-5.31	96.65	111.00
1	C	63	GLN	CA-CB-CG	5.30	125.06	113.40
1	A	370	GLY	C-N-CA	5.30	133.43	122.30
1	B	388	VAL	O-C-N	-5.29	114.23	122.70
1	D	293	PRO	N-CA-C	5.28	125.83	112.10
1	C	333	PHE	N-CA-C	5.28	125.25	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	139	LEU	CB-CG-CD1	5.27	119.96	111.00
1	D	23	GLU	CA-C-N	5.26	128.77	117.20
1	G	281	THR	CA-C-N	5.25	128.76	117.20
1	H	3	LYS	CA-C-N	5.25	128.75	117.20
1	H	124	ALA	O-C-N	-5.25	114.30	122.70
1	F	306	LEU	CA-CB-CG	5.24	127.36	115.30
1	G	101	MET	O-C-N	5.23	131.06	122.70
1	B	2	ARG	C-N-CA	5.22	134.75	121.70
1	B	227	ASP	O-C-N	5.22	131.05	122.70
1	A	332	GLY	CA-C-N	5.21	128.66	117.20
1	E	98	CYS	O-C-N	-5.20	114.39	122.70
1	A	225	SER	CA-C-N	5.18	128.60	117.20
1	A	75	MET	CA-C-O	5.18	130.98	120.10
1	G	383	ALA	N-CA-C	5.17	124.95	111.00
1	A	282	THR	CA-C-N	5.15	126.51	116.20
1	H	393	HIS	N-CA-C	5.15	124.91	111.00
1	B	217	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	217	ASP	CA-C-N	5.15	128.52	117.20
1	E	103	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	G	148	LEU	CA-CB-CG	5.13	127.10	115.30
1	F	81	SER	N-CA-CB	-5.13	102.81	110.50
1	F	293	PRO	CA-N-CD	-5.12	104.33	111.50
1	B	2	ARG	O-C-N	-5.12	114.51	122.70
1	H	350	PRO	N-CA-C	-5.11	98.81	112.10
1	D	11	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	92	LEU	CB-CG-CD2	5.10	119.67	111.00
1	H	205	ILE	C-N-CA	5.10	133.00	122.30
1	E	221	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	G	140	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	D	333	PHE	CA-C-N	-5.08	106.02	117.20
1	G	139	LEU	N-CA-C	-5.08	97.28	111.00
1	F	154	GLU	C-N-CA	5.08	134.40	121.70
1	A	226	LEU	C-N-CA	-5.07	109.02	121.70
1	B	97	LEU	CA-CB-CG	5.04	126.90	115.30
1	E	139	LEU	N-CA-C	-5.04	97.40	111.00
1	A	283	GLY	N-CA-C	5.01	125.64	113.10

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	MET	Mainchain

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Mol	Chain	Res	Type	Group
1	A	204	TRP	Mainchain
1	A	221	ARG	Mainchain
1	A	226	LEU	Mainchain
1	A	43	VAL	Mainchain
1	A	55	MET	Mainchain
1	A	81	SER	Mainchain
1	A	82	GLU	Mainchain
1	A	88	CYS	Mainchain
1	B	337	LYS	Mainchain
1	B	361	THR	Mainchain
1	B	378	ILE	Mainchain
1	B	81	SER	Mainchain
1	B	82	GLU	Mainchain
1	B	88	CYS	Mainchain
1	C	308	VAL	Mainchain
1	C	332	GLY	Mainchain
1	C	82	GLU	Mainchain
1	C	88	CYS	Mainchain
1	D	163	THR	Mainchain
1	D	332	GLY	Mainchain,Peptide
1	D	4	THR	Mainchain
1	D	82	GLU	Mainchain,Peptide
1	E	221	ARG	Mainchain
1	E	222	ARG	Mainchain
1	E	306	LEU	Mainchain
1	E	88	CYS	Mainchain
1	F	4	THR	Mainchain
1	F	81	SER	Mainchain
1	F	82	GLU	Mainchain
1	F	88	CYS	Mainchain
1	G	226	LEU	Mainchain
1	G	227	ASP	Mainchain
1	G	332	GLY	Mainchain
1	H	134	MET	Mainchain
1	H	55	MET	Mainchain

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	2730	0	2587	33	0
1	B	2753	0	2625	18	0
1	C	2749	0	2635	20	0
1	D	2740	0	2639	20	0
1	E	2740	0	2618	28	0
1	F	2641	0	2475	30	0
1	G	2728	0	2598	20	0
1	H	2733	0	2614	18	0
2	A	6	0	8	0	0
2	B	12	0	16	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
2	G	6	0	8	0	0
3	A	110	0	0	0	0
3	B	146	0	0	0	0
3	C	136	0	0	0	0
3	D	125	0	0	0	0
3	E	80	0	0	0	0
3	F	80	0	0	0	0
3	G	119	0	0	0	0
3	H	82	0	0	0	0
All	All	22740	0	20855	181	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 4.

All (181) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:GLY:C	1:D:63:GLN:N	1.70	1.45
1:A:66:SER:OG	1:A:82:GLU:O	1.62	1.15
1:F:333:PHE:CD1	1:F:338:VAL:HG21	1.90	1.05
1:F:333:PHE:CE1	1:F:338:VAL:HG21	1.93	1.03
1:E:333:PHE:CD1	1:E:338:VAL:HG21	1.95	1.01
1:E:333:PHE:CE1	1:E:338:VAL:HG21	2.02	0.95
1:F:283:GLY:O	1:F:284:MET:HG2	1.72	0.88
1:E:88:CYS:HB2	1:E:380:SER:HA	1.59	0.84
1:A:88:CYS:HB2	1:A:380:SER:HA	1.62	0.82
1:F:333:PHE:CD1	1:F:338:VAL:CG2	2.64	0.80
1:A:66:SER:CB	1:A:82:GLU:O	2.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:PHE:CD1	1:E:338:VAL:CG2	2.68	0.76
1:G:88:CYS:HB2	1:G:380:SER:HA	1.69	0.74
1:G:189:ALA:HB1	1:G:194:LYS:HB2	1.70	0.73
1:C:293:PRO:HG3	1:C:379:CYS:HB3	1.71	0.73
1:B:360:MET:HA	1:B:363:VAL:HG22	1.70	0.71
1:F:88:CYS:HB2	1:F:380:SER:HA	1.74	0.69
1:C:333:PHE:CE1	1:C:338:VAL:HG21	2.27	0.69
1:F:88:CYS:HB2	1:F:380:SER:CB	2.23	0.69
1:A:293:PRO:HG3	1:A:379:CYS:HB3	1.74	0.68
1:G:34:MET:CE	1:G:69:ALA:HB1	2.24	0.67
1:A:118:MET:HA	1:A:121:ILE:HD12	1.75	0.67
1:C:333:PHE:CD1	1:C:338:VAL:HG21	2.32	0.64
1:E:88:CYS:HB2	1:E:380:SER:CB	2.28	0.64
1:F:160:HIS:CE1	1:F:287:HIS:HA	2.35	0.62
1:E:88:CYS:HB2	1:E:380:SER:CA	2.29	0.62
1:B:88:CYS:HB2	1:B:380:SER:CB	2.29	0.61
1:H:371:GLY:O	1:H:392:VAL:O	2.17	0.61
1:G:34:MET:HE1	1:G:69:ALA:CB	2.31	0.60
1:F:316:VAL:HG12	1:F:324:VAL:HG12	1.84	0.60
1:C:162:ASN:HD21	1:C:240:GLY:HA2	1.65	0.60
1:F:11:ARG:HB3	1:F:360:MET:SD	2.42	0.59
1:F:333:PHE:HD1	1:F:338:VAL:HG21	1.65	0.59
1:E:140:ARG:HD3	1:E:145:TYR:CG	2.38	0.57
1:F:283:GLY:C	1:F:284:MET:HG2	2.23	0.57
1:E:284:MET:O	1:E:383:ALA:HB3	2.04	0.57
1:F:88:CYS:HB2	1:F:380:SER:CA	2.33	0.57
1:C:312:ASP:O	1:C:313:LEU:HD23	2.05	0.56
1:F:238:SER:O	1:F:239:ASP:CB	2.53	0.56
1:C:333:PHE:CD1	1:C:333:PHE:O	2.59	0.55
1:A:88:CYS:HB2	1:A:380:SER:CA	2.35	0.55
1:C:88:CYS:HB2	1:C:380:SER:CB	2.36	0.55
1:E:291:ALA:O	1:E:292:ALA:HB2	2.07	0.54
1:A:292:ALA:N	1:A:293:PRO:HD2	2.21	0.54
1:C:56:VAL:HG13	1:C:87:VAL:HA	1.90	0.53
1:G:14:PHE:CE2	1:G:357:ARG:HD3	2.43	0.53
1:D:9:ALA:HB1	1:D:360:MET:HG3	1.91	0.53
1:E:291:ALA:O	1:E:292:ALA:CB	2.57	0.53
1:C:384:GLN:NE2	1:D:81:SER:H	2.07	0.52
1:E:13:PRO:HG2	1:E:214:VAL:HG12	1.90	0.52
1:C:98:CYS:SG	1:C:112:ALA:HB2	2.50	0.52
1:D:123:TYR:CE2	1:D:141:ASP:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:PHE:CD1	1:B:250:VAL:HG23	2.44	0.52
1:A:88:CYS:CB	1:A:380:SER:HA	2.38	0.51
1:D:63:GLN:O	1:D:64:ILE:C	2.46	0.51
1:H:366:LEU:O	1:H:371:GLY:HA3	2.10	0.51
1:A:98:CYS:HA	1:A:101:MET:HE3	1.92	0.51
1:C:88:CYS:HB2	1:C:380:SER:HB2	1.93	0.51
1:A:98:CYS:HA	1:A:101:MET:CE	2.41	0.51
1:G:34:MET:CE	1:G:69:ALA:CB	2.89	0.51
1:D:88:CYS:SG	1:D:380:SER:HA	2.52	0.50
1:A:34:MET:CE	1:A:69:ALA:HB1	2.41	0.50
1:D:204:TRP:N	1:D:204:TRP:CD1	2.79	0.50
1:C:333:PHE:CD1	1:C:338:VAL:CG2	2.94	0.50
1:H:236:TYR:O	1:H:237:ALA:HB2	2.11	0.50
1:B:293:PRO:HG3	1:B:379:CYS:HB3	1.93	0.50
1:G:248:PRO:HB3	1:G:344:ALA:O	2.13	0.49
1:A:283:GLY:HA2	1:B:78:SER:HA	1.94	0.49
1:D:234:PRO:HB3	1:D:240:GLY:O	2.12	0.49
1:H:98:CYS:SG	1:H:112:ALA:HB2	2.52	0.49
1:A:118:MET:HA	1:A:121:ILE:CD1	2.42	0.49
1:C:88:CYS:HB2	1:C:380:SER:HA	1.95	0.49
1:F:333:PHE:CE1	1:F:338:VAL:CG2	2.81	0.49
1:F:160:HIS:ND1	1:F:287:HIS:HA	2.27	0.48
1:H:82:GLU:HG3	1:G:84:LEU:HD21	1.93	0.48
1:A:202:VAL:HG12	1:A:204:TRP:HD1	1.79	0.48
1:D:62:GLY:C	1:D:63:GLN:CA	2.73	0.48
1:A:88:CYS:HB2	1:A:380:SER:CB	2.42	0.48
1:H:34:MET:HB2	1:H:73:ALA:HB2	1.95	0.48
1:C:56:VAL:HG22	1:C:87:VAL:O	2.13	0.48
1:E:333:PHE:CE1	1:E:338:VAL:CG2	2.89	0.48
1:G:17:PHE:HB2	1:G:250:VAL:HG23	1.95	0.48
1:G:371:GLY:O	1:G:392:VAL:O	2.31	0.48
1:B:104:ALA:C	1:B:105:GLN:HG2	2.34	0.47
1:A:17:PHE:HB2	1:A:250:VAL:O	2.15	0.47
1:E:36:GLU:O	1:E:40:GLN:HG3	2.15	0.47
1:F:13:PRO:HD3	1:F:199:ILE:HG23	1.95	0.47
1:B:88:CYS:HB2	1:B:380:SER:HB2	1.97	0.47
1:H:328:GLU:HG3	1:H:335:LEU:HD11	1.97	0.47
1:E:88:CYS:CB	1:E:380:SER:HA	2.39	0.46
1:A:187:ALA:HB1	1:A:222:ARG:NH1	2.31	0.46
1:D:293:PRO:O	1:D:296:ALA:HB3	2.15	0.46
1:G:303:LYS:HB3	1:G:303:LYS:HE3	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:TYR:CE2	1:G:141:ASP:HB2	2.49	0.46
1:C:77:TRP:CD2	1:D:285:PRO:HA	2.50	0.46
1:A:98:CYS:SG	1:A:112:ALA:HB2	2.56	0.46
1:E:123:TYR:CE2	1:E:141:ASP:HB2	2.50	0.46
1:E:78:SER:O	1:E:80:PRO:HD3	2.16	0.46
1:F:316:VAL:CG1	1:F:324:VAL:HG12	2.46	0.46
1:H:53:MET:HB2	1:H:66:SER:HB3	1.98	0.46
1:H:123:TYR:CE2	1:H:141:ASP:HB2	2.51	0.46
1:B:72:LEU:HA	1:B:72:LEU:HD23	1.69	0.46
1:F:283:GLY:C	1:F:284:MET:CG	2.84	0.46
1:A:248:PRO:HD2	1:A:319:ALA:O	2.15	0.46
1:A:121:ILE:HA	1:A:122:PRO:HD3	1.68	0.45
1:B:84:LEU:HD21	1:B:93:ARG:HG3	1.98	0.45
1:F:14:PHE:CE2	1:F:357:ARG:HD3	2.51	0.45
1:F:183:HIS:CE1	1:F:221:ARG:HG2	2.51	0.45
1:E:200:VAL:CG2	1:E:201:PRO:HD2	2.47	0.45
1:F:333:PHE:HE1	1:F:338:VAL:HG21	1.71	0.45
1:G:318:GLU:HB3	1:G:345:ILE:HG13	1.98	0.45
1:H:178:TRP:CZ2	1:H:324:VAL:HG11	2.52	0.45
1:B:369:ARG:C	1:B:371:GLY:H	2.19	0.45
1:G:227:ASP:O	1:G:231:LYS:HD2	2.16	0.45
1:E:160:HIS:ND1	1:E:287:HIS:HA	2.32	0.45
1:B:369:ARG:C	1:B:371:GLY:N	2.70	0.44
1:D:292:ALA:N	1:D:293:PRO:CD	2.80	0.44
1:B:51:ASN:HA	1:B:111:VAL:O	2.17	0.44
1:H:235:ILE:HD11	1:H:242:ILE:HG22	1.98	0.44
1:H:204:TRP:O	1:H:212:ASN:N	2.50	0.44
1:A:34:MET:HE1	1:A:69:ALA:CB	2.48	0.44
1:A:273:LEU:O	1:A:274:ALA:HB2	2.18	0.44
1:B:88:CYS:HB2	1:B:380:SER:HA	2.00	0.44
1:E:292:ALA:HB1	1:E:385:GLY:HA3	1.99	0.44
1:G:34:MET:HE2	1:G:69:ALA:HB1	1.98	0.44
1:H:28:GLU:HA	1:H:72:LEU:HD13	2.00	0.44
1:A:34:MET:CE	1:A:69:ALA:CB	2.95	0.44
1:E:11:ARG:HD3	1:E:357:ARG:HG3	2.00	0.44
1:E:140:ARG:HD3	1:E:145:TYR:CD1	2.53	0.44
1:B:9:ALA:HB2	1:B:257:PHE:CD1	2.53	0.43
1:D:51:ASN:HA	1:D:111:VAL:O	2.18	0.43
1:G:158:ALA:HA	1:G:320:PHE:CZ	2.53	0.43
1:G:88:CYS:HB2	1:G:380:SER:CB	2.48	0.43
1:G:88:CYS:HB2	1:G:380:SER:CA	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:TYR:O	1:A:237:ALA:HB2	2.18	0.43
1:H:124:ALA:HB2	1:H:142:LEU:HD11	1.99	0.43
1:B:92:LEU:HD23	1:B:378:ILE:HG22	1.98	0.43
1:C:183:HIS:CE1	1:C:346:ALA:HA	2.53	0.43
1:E:183:HIS:CE1	1:E:346:ALA:HA	2.54	0.43
1:E:158:ALA:HA	1:E:320:PHE:CZ	2.53	0.43
1:F:334:ASP:OD2	1:F:336:GLU:HB2	2.18	0.43
1:A:160:HIS:ND1	1:A:287:HIS:HA	2.33	0.43
1:D:108:ASP:HB3	1:D:264:LYS:HB2	1.99	0.43
1:F:158:ALA:HA	1:F:320:PHE:CZ	2.54	0.43
1:A:140:ARG:HD3	1:A:145:TYR:CG	2.54	0.43
1:D:234:PRO:HB2	1:D:237:ALA:O	2.19	0.43
1:D:300:LEU:HD21	1:D:389:LEU:N	2.34	0.43
1:H:376:ALA:O	1:H:387:ALA:HA	2.18	0.43
1:H:70:ALA:O	1:H:75:MET:HB2	2.19	0.43
1:G:34:MET:HE1	1:G:69:ALA:HB3	2.00	0.43
1:F:180:LEU:HD22	1:F:226:LEU:HG	2.01	0.42
1:F:88:CYS:HB2	1:F:380:SER:HB2	2.01	0.42
1:G:292:ALA:N	1:G:293:PRO:HD2	2.35	0.42
1:A:202:VAL:HG12	1:A:204:TRP:CD1	2.54	0.42
1:C:365:GLU:O	1:C:369:ARG:HG3	2.19	0.42
1:D:66:SER:CB	1:D:82:GLU:O	2.68	0.42
1:F:17:PHE:CD1	1:F:250:VAL:HG23	2.54	0.42
1:A:308:VAL:HG11	1:A:333:PHE:HA	2.00	0.42
1:A:34:MET:HE1	1:A:69:ALA:HB3	2.02	0.42
1:A:12:THR:HG23	1:A:33:VAL:HG13	2.01	0.42
1:E:108:ASP:O	1:E:260:MET:HA	2.20	0.42
1:E:92:LEU:HD11	1:E:388:VAL:HG21	2.02	0.42
1:H:185:ARG:HD3	1:H:340:VAL:O	2.20	0.42
1:E:77:TRP:CD2	1:F:285:PRO:HA	2.54	0.41
1:F:11:ARG:HD3	1:F:357:ARG:HG3	2.02	0.41
1:H:293:PRO:HD3	1:H:379:CYS:HB3	2.03	0.41
1:D:381:GLY:O	1:D:382:ALA:HB3	2.21	0.41
1:F:148:LEU:O	1:F:157:MET:HG2	2.21	0.41
1:A:55:MET:HE2	1:A:58:GLN:HA	2.03	0.41
1:D:43:VAL:HG21	1:D:260:MET:CE	2.51	0.41
1:F:293:PRO:HD3	1:F:379:CYS:HB3	2.01	0.41
1:A:34:MET:HE2	1:A:69:ALA:HB1	2.02	0.41
1:B:92:LEU:HD23	1:B:378:ILE:CG2	2.51	0.41
1:B:123:TYR:CE2	1:B:141:ASP:HB2	2.55	0.41
1:B:54:GLY:HA3	1:B:90:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:PRO:HA	1:D:77:TRP:CD2	2.56	0.40
1:A:357:ARG:HG2	1:A:357:ARG:HH11	1.86	0.40
1:C:41:ALA:HB1	1:C:43:VAL:HG13	2.04	0.40
1:E:51:ASN:HA	1:E:111:VAL:O	2.22	0.40
1:E:11:ARG:CD	1:E:357:ARG:HG3	2.51	0.40
1:C:108:ASP:O	1:C:260:MET:HA	2.21	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	380/393 (97%)	375 (99%)	4 (1%)	1 (0%)	46	50
1	B	382/393 (97%)	374 (98%)	7 (2%)	1 (0%)	46	50
1	C	379/393 (96%)	373 (98%)	5 (1%)	1 (0%)	46	50
1	D	378/393 (96%)	370 (98%)	8 (2%)	0	100	100
1	E	378/393 (96%)	370 (98%)	7 (2%)	1 (0%)	46	50
1	F	368/393 (94%)	361 (98%)	7 (2%)	0	100	100
1	G	377/393 (96%)	370 (98%)	7 (2%)	0	100	100
1	H	380/393 (97%)	374 (98%)	6 (2%)	0	100	100
All	All	3022/3144 (96%)	2967 (98%)	51 (2%)	4 (0%)	56	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	87	VAL
1	B	87	VAL
1	C	87	VAL
1	A	87	VAL

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	256/291 (88%)	255 (100%)	1 (0%)	93 97
1	B	259/291 (89%)	258 (100%)	1 (0%)	93 97
1	C	255/291 (88%)	255 (100%)	0	100 100
1	D	255/291 (88%)	254 (100%)	1 (0%)	93 97
1	E	259/291 (89%)	259 (100%)	0	100 100
1	F	239/291 (82%)	239 (100%)	0	100 100
1	G	256/291 (88%)	255 (100%)	1 (0%)	93 97
1	H	257/291 (88%)	257 (100%)	0	100 100
All	All	2036/2328 (88%)	2032 (100%)	4 (0%)	95 98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	ARG
1	B	239	ASP
1	G	84	LEU
1	D	133	ARG

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

Mol	Chain	Res	Type
1	C	384	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	A	401	-	5,5,5	0.58	0	5,5,5	0.93	0
2	GOL	B	401	-	5,5,5	0.44	0	5,5,5	1.65	2 (40%)
2	GOL	B	402	-	5,5,5	0.38	0	5,5,5	0.43	0
2	GOL	C	401	-	5,5,5	0.33	0	5,5,5	0.77	0
2	GOL	D	401	-	5,5,5	0.44	0	5,5,5	0.79	0
2	GOL	E	401	-	5,5,5	0.79	0	5,5,5	0.67	0
2	GOL	F	401	-	5,5,5	0.20	0	5,5,5	0.51	0
2	GOL	G	401	-	5,5,5	0.49	0	5,5,5	0.93	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	A	401	-	-	0/4/4/4	0/0/0/0
2	GOL	B	401	-	-	0/4/4/4	0/0/0/0
2	GOL	B	402	-	-	0/4/4/4	0/0/0/0
2	GOL	C	401	-	-	0/4/4/4	0/0/0/0
2	GOL	D	401	-	-	0/4/4/4	0/0/0/0
2	GOL	E	401	-	-	0/4/4/4	0/0/0/0
2	GOL	F	401	-	-	0/4/4/4	0/0/0/0
2	GOL	G	401	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	GOL	O2-C2-C3	2.10	118.54	108.47
2	B	401	GOL	O3-C3-C2	2.87	124.53	109.97

There are no chirality outliers.

There are no torsion outliers.

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	17
1	E	16
1	G	13
1	D	13
1	F	13
1	H	11
1	B	11
1	C	11

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	62:GLY	C	63:GLN	N	1.70
1	H	204:TRP	C	205:ILE	N	1.20
1	F	82:GLU	C	83:THR	N	1.20
1	H	363:VAL	C	364:TYR	N	1.19
1	B	217:ASP	C	218:GLU	N	1.19
1	B	250:VAL	C	251:ASN	N	1.19
1	B	306:LEU	C	307:THR	N	1.19
1	C	46:ASP	C	47:ASP	N	1.19
1	C	271:ARG	C	272:PRO	N	1.19
1	C	383:ALA	C	384:GLN	N	1.19
1	F	221:ARG	C	222:ARG	N	1.19

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	88:CYS	C	89:ALA	N	1.19
1	H	4:THR	C	5:VAL	N	1.18
1	H	306:LEU	C	307:THR	N	1.18
1	E	272:PRO	C	273:LEU	N	1.18
1	A	334:ASP	C	335:LEU	N	1.18
1	B	378:ILE	C	379:CYS	N	1.18
1	F	202:VAL	C	203:ASN	N	1.18
1	H	272:PRO	C	273:LEU	N	1.17
1	H	283:GLY	C	284:MET	N	1.17
1	E	92:LEU	C	93:ARG	N	1.17
1	E	141:ASP	C	142:LEU	N	1.17
1	A	121:ILE	C	122:PRO	N	1.17
1	A	237:ALA	C	238:SER	N	1.17
1	C	74:GLY	C	75:MET	N	1.17
1	F	144:VAL	C	145:TYR	N	1.17
1	F	361:THR	C	362:LEU	N	1.17
1	G	22:LYS	C	23:GLU	N	1.17
1	D	4:THR	C	5:VAL	N	1.17
1	D	163:THR	C	164:ALA	N	1.17
1	H	367:LYS	C	368:ARG	N	1.16
1	E	142:LEU	C	143:MET	N	1.16
1	E	231:LYS	C	232:LEU	N	1.16
1	D	82:GLU	C	83:THR	N	1.16
1	E	174:GLU	C	175:GLN	N	1.15
1	B	42:GLY	C	43:VAL	N	1.15
1	C	306:LEU	C	307:THR	N	1.15
1	F	337:LYS	C	338:VAL	N	1.15
1	G	33:VAL	C	34:MET	N	1.15
1	G	54:GLY	C	55:MET	N	1.15
1	G	167:GLU	C	168:TYR	N	1.15
1	G	283:GLY	C	284:MET	N	1.15
1	D	92:LEU	C	93:ARG	N	1.15
1	H	124:ALA	C	125:VAL	N	1.14
1	E	98:CYS	C	99:ASP	N	1.14
1	A	84:LEU	C	85:ASN	N	1.14
1	A	226:LEU	C	227:ASP	N	1.14
1	B	216:LYS	C	217:ASP	N	1.14
1	F	338:VAL	C	339:ASN	N	1.14
1	E	360:MET	C	361:THR	N	1.13
1	A	83:THR	C	84:LEU	N	1.13
1	A	273:LEU	C	274:ALA	N	1.13
1	B	389:LEU	C	390:VAL	N	1.13

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	63:GLN	C	64:ILE	N	1.13
1	D	226:LEU	C	227:ASP	N	1.13
1	G	270:LYS	C	271:ARG	N	1.12
1	D	224:THR	C	225:SER	N	1.12
1	E	222:ARG	C	223:ASP	N	1.11
1	C	334:ASP	C	335:LEU	N	1.11
1	H	305:GLY	C	306:LEU	N	1.10
1	E	337:LYS	C	338:VAL	N	1.10
1	C	389:LEU	C	390:VAL	N	1.10
1	F	226:LEU	C	227:ASP	N	1.10
1	C	273:LEU	C	274:ALA	N	1.09
1	G	34:MET	C	35:LYS	N	1.09
1	D	42:GLY	C	43:VAL	N	1.09
1	A	389:LEU	C	390:VAL	N	1.08
1	H	205:ILE	C	206:GLY	N	1.07
1	E	221:ARG	C	222:ARG	N	1.07
1	A	82:GLU	C	83:THR	N	1.07
1	A	221:ARG	C	222:ARG	N	1.07
1	A	222:ARG	C	223:ASP	N	1.07
1	A	241:SER	C	242:ILE	N	1.07
1	A	272:PRO	C	273:LEU	N	1.07
1	G	166:LYS	C	167:GLU	N	1.07
1	D	63:GLN	C	64:ILE	N	1.07
1	E	230:ALA	C	231:LYS	N	1.06
1	F	211:PRO	C	212:ASN	N	1.06
1	D	270:LYS	C	271:ARG	N	1.06
1	A	120:ASN	C	121:ILE	N	1.05
1	E	273:LEU	C	274:ALA	N	1.03
1	A	225:SER	C	226:LEU	N	1.02
1	E	91:GLY	C	92:LEU	N	1.01
1	G	23:GLU	C	24:VAL	N	1.01
1	C	360:MET	C	361:THR	N	1.00
1	D	162:ASN	C	163:THR	N	1.00
1	F	155:VAL	C	156:HIS	N	0.99
1	F	360:MET	C	361:THR	N	0.99
1	G	165:ALA	C	166:LYS	N	0.99
1	H	360:MET	C	361:THR	N	0.97
1	E	87:VAL	C	88:CYS	N	0.97
1	F	91:GLY	C	92:LEU	N	0.96
1	C	270:LYS	C	271:ARG	N	0.95
1	D	23:GLU	C	24:VAL	N	0.95
1	B	2:ARG	C	3:LYS	N	0.94

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	225:SER	C	226:LEU	N	0.94
1	E	99:ASP	C	100:GLN	N	0.93
1	A	87:VAL	C	88:CYS	N	0.93
1	A	240:GLY	C	241:SER	N	0.92
1	G	101:MET	C	102:ILE	N	0.92
1	B	91:GLY	C	92:LEU	N	0.91
1	B	87:VAL	C	88:CYS	N	0.90
1	B	336:GLU	C	337:LYS	N	0.90
1	C	307:THR	C	308:VAL	N	0.90
1	D	22:LYS	C	23:GLU	N	0.88

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	386/393 (98%)	-0.77	1 (0%) 94 94	11, 21, 36, 58	0
1	B	388/393 (98%)	-0.86	0 100 100	10, 18, 32, 48	0
1	C	387/393 (98%)	-0.84	0 100 100	9, 17, 30, 62	0
1	D	386/393 (98%)	-0.80	1 (0%) 94 94	10, 19, 37, 53	0
1	E	386/393 (98%)	-0.80	0 100 100	11, 21, 37, 51	0
1	F	380/393 (96%)	-0.72	2 (0%) 91 91	12, 22, 40, 62	0
1	G	385/393 (97%)	-0.80	0 100 100	11, 19, 34, 58	0
1	H	386/393 (98%)	-0.81	0 100 100	10, 19, 33, 49	0
All	All	3084/3144 (98%)	-0.80	4 (0%) 95 95	9, 19, 35, 62	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	223	ASP	2.8
1	F	1	MET	2.5
1	A	237	ALA	2.5
1	D	238	SER	2.4

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

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

6.3 Carbohydrates

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
2	GOL	B	401	6/6	0.94	0.18	7.85	25,25,28,32	0
2	GOL	F	401	6/6	0.88	0.19	3.72	49,52,56,63	0
2	GOL	E	401	6/6	0.93	0.16	3.41	25,29,35,38	0
2	GOL	B	402	6/6	0.91	0.18	3.40	36,37,40,42	0
2	GOL	C	401	6/6	0.94	0.15	3.13	35,43,45,50	0
2	GOL	A	401	6/6	0.83	0.18	3.10	28,32,34,36	0
2	GOL	D	401	6/6	0.94	0.12	2.94	31,35,36,38	0
2	GOL	G	401	6/6	0.96	0.09	0.50	14,16,17,18	0

6.5 Other polymers (i)

There are no such residues in this entry.