Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 07:46 PM EDT

PDB ID	:	3TBV
Title	:	CRYSTAL STRUCTURE OF THE MURINE CLASS I MAJOR HISTOCOMPATIBILITY COMPLEX H-2DB IN COMPLEX WITH THE LCMV-DERIVED GP33 ALTERED PEPTIDE ligand (A2G,V3P,Y4A)
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Deposited on	:	2011-08-08
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

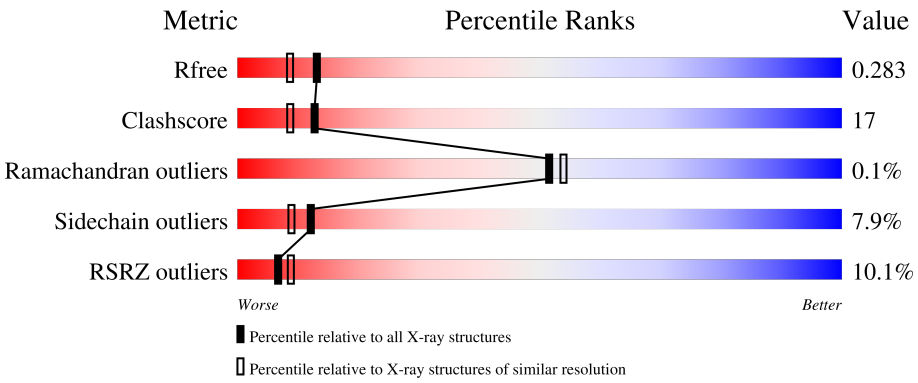
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	13% 70% 25% 5%
1	C	276	11% 71% 23% 5%
1	E	276	12% 73% 20% 5% •
1	G	276	16% 72% 23% • •

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Mol	Chain	Length	Quality of chain
2	B	99	3% 75% 20% 5%
2	D	99	3% 70% 27%
2	F	99	2% 66% 30%
2	H	99	3% 65% 34%
3	I	9	56% 33% 11%
3	J	9	44% 44% 11%
3	K	9	56% 33% 11%
3	L	9	56% 33% 11%

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	SO4	F	100	-	-	X	-
5	GOL	E	341	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13548 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2264	1430	400	425	9	0	0	0
1	C	276	2264	1430	400	425	9	0	0	0
1	E	276	2264	1430	400	425	9	0	0	0
1	G	276	2264	1430	400	425	9	0	0	0

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	820	524	138	151	7	0	0	0
2	D	99	820	524	138	151	7	0	0	0
2	F	99	820	524	138	151	7	0	0	0
2	H	99	820	524	138	151	7	0	0	0

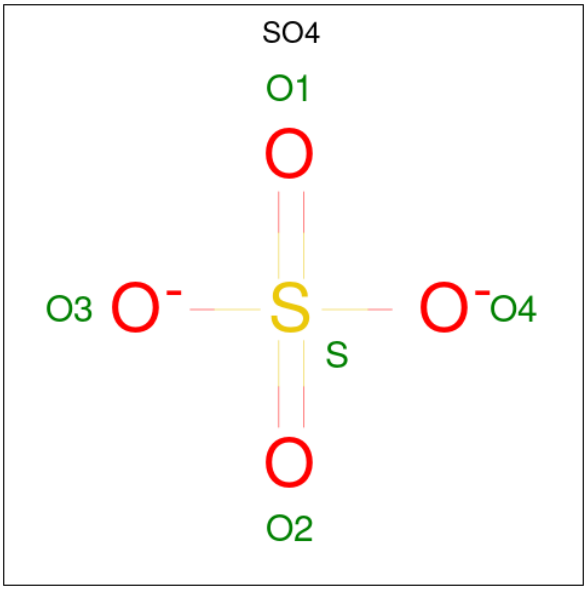
- Molecule 3 is a protein called Glycoprotein G1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	9	65	41	11	12	1	0	0	0
3	J	9	65	41	11	12	1	0	0	0
3	K	9	65	41	11	12	1	0	0	0
3	L	9	65	41	11	12	1	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	2	GLY	ALA	engineered mutation	UNP P07399
I	3	PRO	VAL	engineered mutation	UNP P07399
I	4	ALA	TYR	engineered mutation	UNP P07399
I	9	MET	CYS	engineered mutation	UNP P07399
J	2	GLY	ALA	engineered mutation	UNP P07399
J	3	PRO	VAL	engineered mutation	UNP P07399
J	4	ALA	TYR	engineered mutation	UNP P07399
J	9	MET	CYS	engineered mutation	UNP P07399
K	2	GLY	ALA	engineered mutation	UNP P07399
K	3	PRO	VAL	engineered mutation	UNP P07399
K	4	ALA	TYR	engineered mutation	UNP P07399
K	9	MET	CYS	engineered mutation	UNP P07399
L	2	GLY	ALA	engineered mutation	UNP P07399
L	3	PRO	VAL	engineered mutation	UNP P07399
L	4	ALA	TYR	engineered mutation	UNP P07399
L	9	MET	CYS	engineered mutation	UNP P07399

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
4	A	1	5	4	1		0	0
			Total	O	S			
4	C	1	5	4	1		0	0
			Total	O	S			
4	E	1	5	4	1		0	0

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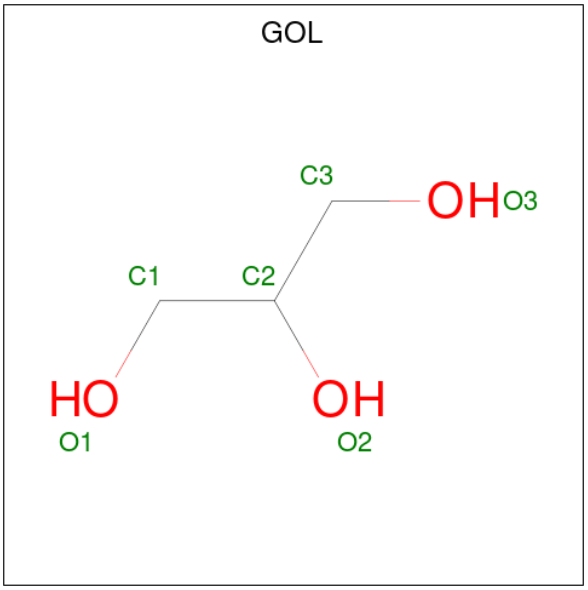
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	F	1	5	4	1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0
			Total	C	O		
5	A	1	6	3	3	0	0
			Total	C	O		
5	B	1	6	3	3	0	0
			Total	C	O		
5	E	1	6	3	3	0	0
			Total	C	O		
5	E	1	6	3	3	0	0
			Total	C	O		
5	H	1	6	3	3	0	0
			Total	C	O		
5	H	1	6	3	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	132	132	132	0	0

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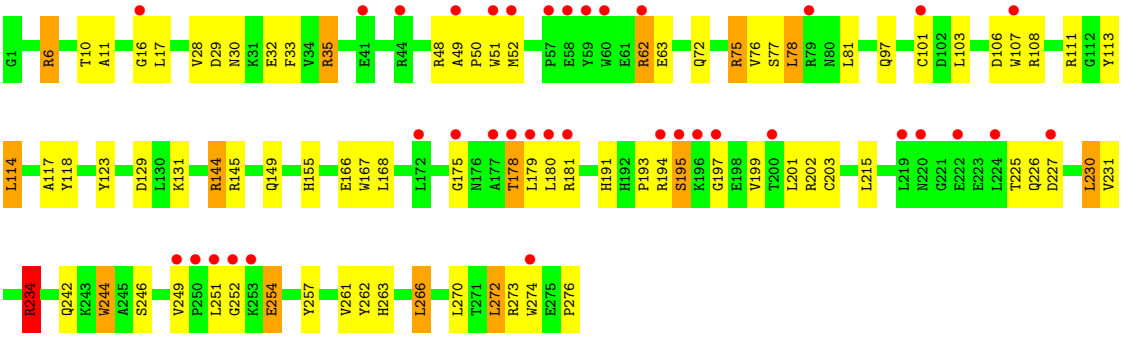
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	B	67	67	67	0	0
			Total	O		
6	C	164	164	164	0	0
			Total	O		
6	D	77	77	77	0	0
			Total	O		
6	E	154	154	154	0	0
			Total	O		
6	F	69	69	69	0	0
			Total	O		
6	G	128	128	128	0	0
			Total	O		
6	H	74	74	74	0	0
			Total	O		
6	I	4	4	4	0	0
			Total	O		
6	J	9	9	9	0	0
			Total	O		
6	K	10	10	10	0	0
			Total	O		
6	L	2	2	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

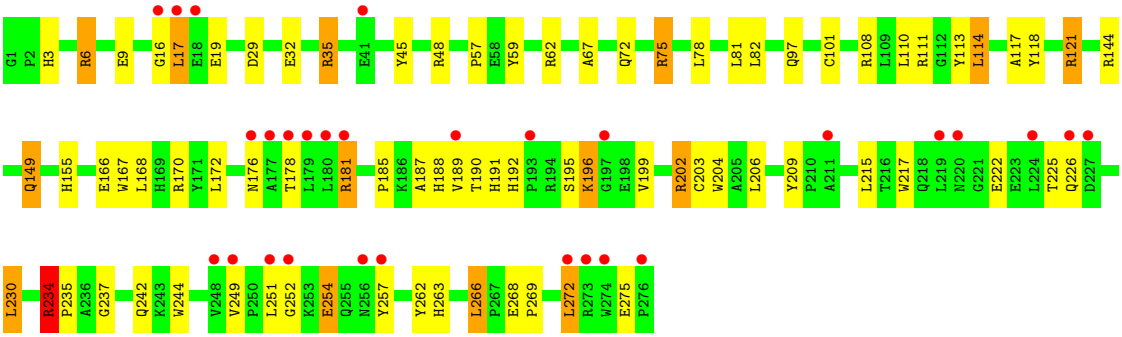
• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain A:



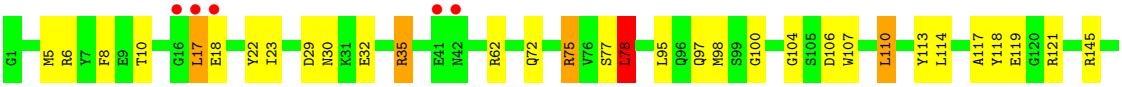
• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

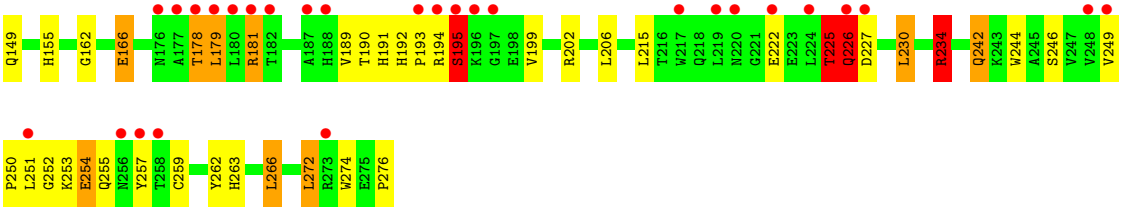
Chain C:



• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

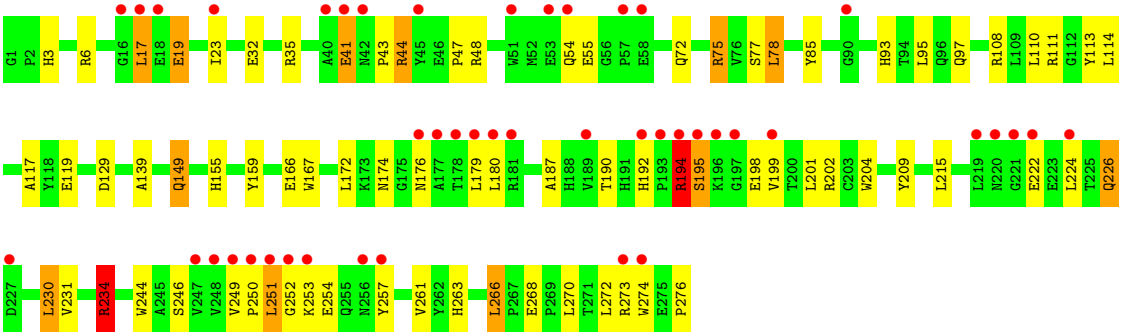
Chain E:





- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain G:



- Molecule 2: Beta-2-microglobulin

Chain B:

- Molecule 2: Beta-2-microglobulin

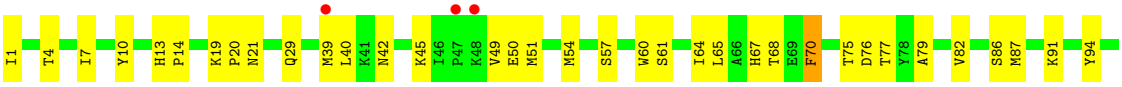
Chain D:

- Molecule 2: Beta-2-microglobulin

Chain F:

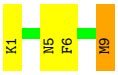
- Molecule 2: Beta-2-microglobulin

Chain H:



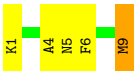
• Molecule 3: Glycoprotein G1

Chain I:



• Molecule 3: Glycoprotein G1

Chain J:

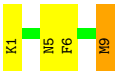


• Molecule 3: Glycoprotein G1

Chain K:

• Molecule 3: Glycoprotein G1

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.58Å 126.47Å 102.11Å 90.00° 106.71° 90.00°	Depositor
Resolution (Å)	49.51 – 2.10 63.24 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.51-2.10) 99.1 (63.24-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.225 , 0.278 0.232 , 0.283	Depositor DCC
R_{free} test set	6806 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	33.1	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13548	wwPDB-VP
Average B, all atoms (Å^2)	53.0	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 48.04 % 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 9.1085e-05. 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.91	3/2331 (0.1%)	1.02	7/3166 (0.2%)
1	C	0.91	2/2331 (0.1%)	0.96	10/3166 (0.3%)
1	E	0.96	0/2331	1.06	11/3166 (0.3%)
1	G	0.88	0/2331	0.96	4/3166 (0.1%)
2	B	0.99	1/846 (0.1%)	0.97	0/1148
2	D	0.90	1/846 (0.1%)	0.96	1/1148 (0.1%)
2	F	0.98	1/846 (0.1%)	0.95	2/1148 (0.2%)
2	H	0.92	0/846	0.94	2/1148 (0.2%)
3	I	3.52	1/66 (1.5%)	1.19	0/86
3	J	3.30	2/66 (3.0%)	1.27	0/86
3	K	3.26	1/66 (1.5%)	1.05	0/86
3	L	1.94	1/66 (1.5%)	1.13	0/86
All	All	1.01	13/12972 (0.1%)	0.99	37/17600 (0.2%)

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	1
1	G	0	1
All	All	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	9	MET	C-OXT	27.14	1.75	1.23
3	K	9	MET	C-OXT	24.50	1.69	1.23
3	J	9	MET	C-OXT	23.53	1.68	1.23
3	L	9	MET	C-OXT	12.89	1.47	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	4	ALA	CA-CB	7.34	1.67	1.52
2	B	93	VAL	CB-CG1	-7.05	1.38	1.52
1	A	123	TYR	CD2-CE2	5.48	1.47	1.39
2	D	56	PHE	CB-CG	5.42	1.60	1.51
1	A	76	VAL	CB-CG2	5.34	1.64	1.52
1	C	59	TYR	CD1-CE1	5.22	1.47	1.39
1	A	244	TRP	CB-CG	5.18	1.59	1.50
2	F	62	PHE	CE1-CZ	5.11	1.47	1.37
1	C	9	GLU	CG-CD	5.02	1.59	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	ARG	NE-CZ-NH2	-19.77	110.42	120.30
1	A	234	ARG	NE-CZ-NH1	18.44	129.52	120.30
1	E	234	ARG	NE-CZ-NH1	17.34	128.97	120.30
1	E	234	ARG	NE-CZ-NH2	-15.07	112.76	120.30
1	G	234	ARG	NE-CZ-NH1	14.79	127.69	120.30
1	G	234	ARG	NE-CZ-NH2	-14.04	113.28	120.30
1	E	35	ARG	NE-CZ-NH2	-11.61	114.49	120.30
1	E	35	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	E	225	THR	CB-CA-C	-10.24	83.94	111.60
1	C	121	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	178	THR	CB-CA-C	7.87	132.85	111.60
1	C	16	GLY	N-CA-C	7.72	132.40	113.10
1	C	234	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	C	121	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	E	121	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	E	78	LEU	CA-CB-CG	6.93	131.25	115.30
1	C	62	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	35	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	F	59	ASP	CB-CG-OD1	6.30	123.97	118.30
2	D	64	ILE	CB-CA-C	-6.18	99.23	111.60
1	G	195	SER	CB-CA-C	6.11	121.71	110.10
1	E	226	GLN	N-CA-C	5.78	126.60	111.00
1	A	234	ARG	CD-NE-CZ	5.76	131.67	123.60
1	C	35	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	82	LEU	CA-CB-CG	5.76	128.54	115.30
1	E	195	SER	CB-CA-C	-5.65	99.37	110.10
1	C	234	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	35	ARG	NE-CZ-NH2	-5.48	117.56	120.30
2	H	51	MET	CG-SD-CE	5.28	108.65	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	6	ARG	NE-CZ-NH2	-5.19	117.70	120.30
2	H	76	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	6	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	35	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	G	129	ASP	CB-CG-OD1	5.05	122.85	118.30
2	F	51	MET	CG-SD-CE	5.04	108.26	100.20
1	E	121	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	E	234	ARG	CD-NE-CZ	5.03	130.64	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	GLY	Peptide
1	G	194	ARG	Peptide

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	2264	0	2136	68	0
1	C	2264	0	2136	72	0
1	E	2264	0	2136	83	0
1	G	2264	0	2136	68	0
2	B	820	0	796	31	0
2	D	820	0	796	43	0
2	F	820	0	796	31	0
2	H	820	0	796	36	0
3	I	65	0	66	7	0
3	J	65	0	66	9	0
3	K	65	0	66	11	0
3	L	65	0	66	6	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	3	0
5	A	12	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	8	3	0
5	E	12	0	16	9	0
5	H	12	0	16	3	0
6	A	132	0	0	5	0
6	B	67	0	0	6	0
6	C	164	0	0	8	0
6	D	77	0	0	2	0
6	E	154	0	0	1	0
6	F	69	0	0	4	0
6	G	128	0	0	4	0
6	H	74	0	0	1	0
6	I	4	0	0	0	0
6	J	9	0	0	0	0
6	K	10	0	0	0	0
6	L	2	0	0	0	0
All	All	13548	0	12048	411	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 17.

All (411) 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)
3:J:9:MET:OXT	3:J:9:MET:C	1.68	1.30
3:K:9:MET:C	3:K:9:MET:OXT	1.69	1.29
3:I:9:MET:OXT	3:I:9:MET:C	1.74	1.23
1:E:226:GLN:CD	1:E:226:GLN:O	1.75	1.22
1:E:226:GLN:O	1:E:226:GLN:NE2	1.94	0.98
2:D:49:VAL:HG23	2:D:67:HIS:O	1.63	0.97
2:B:87:MET:HE1	2:B:91:LYS:HB2	1.51	0.91
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.07	0.89
2:D:47:PRO:O	2:D:48:LYS:HD2	1.74	0.86
1:C:234:ARG:HD3	2:D:10:TYR:CZ	2.11	0.85
2:H:39:MET:HE1	2:H:68:THR:HB	1.58	0.85
1:E:226:GLN:CD	1:E:226:GLN:C	2.36	0.83
1:C:167:TRP:CZ2	3:J:1:LYS:HE3	2.13	0.83
2:D:47:PRO:O	2:D:48:LYS:CD	2.28	0.82
2:B:57:SER:OG	5:B:100:GOL:H31	1.83	0.78
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.19	0.78
2:F:74:GLU:OE2	2:F:74:GLU:HA	1.81	0.78
5:E:340:GOL:O3	5:E:340:GOL:O1	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:C	1:A:230:LEU:HD12	2.05	0.77
1:E:97:GLN:HE22	3:K:5:ASN:HD21	1.34	0.76
1:E:202:ARG:HD2	1:E:244:TRP:CD2	2.21	0.76
1:E:145:ARG:HD3	5:E:341:GOL:H12	1.69	0.75
2:H:39:MET:HE3	2:H:68:THR:CG2	2.17	0.74
1:G:167:TRP:CE2	3:L:1:LYS:HD2	2.22	0.74
2:D:39:MET:HE1	2:D:68:THR:HB	1.69	0.74
2:B:52:SER:HA	6:B:483:HOH:O	1.86	0.73
1:G:97:GLN:HE22	3:L:5:ASN:HD21	1.36	0.72
2:D:39:MET:CE	2:D:68:THR:CG2	2.68	0.72
1:G:249:VAL:HG22	1:G:257:TYR:CE2	2.25	0.71
2:D:39:MET:HE3	2:D:68:THR:CG2	2.20	0.71
2:D:64:ILE:HG22	2:D:65:LEU:N	2.05	0.70
2:H:39:MET:CE	2:H:68:THR:HB	2.20	0.70
1:C:226:GLN:O	1:C:226:GLN:NE2	2.24	0.70
2:H:39:MET:HE2	2:H:49:VAL:CG2	2.22	0.70
1:E:234:ARG:HD3	2:F:10:TYR:CZ	2.28	0.69
1:E:77:SER:HB3	3:K:9:MET:CG	2.23	0.69
2:H:1:ILE:N	6:H:104:HOH:O	2.27	0.68
2:D:49:VAL:CG2	2:D:67:HIS:O	2.40	0.68
1:G:202:ARG:NH2	6:G:726:HOH:O	2.26	0.68
2:F:46:ILE:HG23	2:F:47:PRO:HD2	1.75	0.67
2:H:57:SER:OG	5:H:101:GOL:C1	2.43	0.67
1:E:32:GLU:OE2	1:E:35:ARG:HD2	1.95	0.67
1:G:32:GLU:OE2	1:G:48:ARG:HD2	1.95	0.67
1:C:263:HIS:HB3	1:C:266:LEU:HD22	1.76	0.66
1:C:222:GLU:OE2	1:C:222:GLU:HA	1.95	0.66
1:G:6:ARG:NH2	1:G:113:TYR:CE1	2.65	0.65
2:D:64:ILE:CG2	2:D:65:LEU:N	2.60	0.65
2:H:39:MET:HE2	2:H:49:VAL:HG22	1.79	0.64
1:C:202:ARG:HD2	1:C:244:TRP:CD2	2.32	0.64
2:D:39:MET:HE3	2:D:68:THR:HG21	1.79	0.64
1:A:263:HIS:HB3	1:A:266:LEU:HD22	1.77	0.64
1:G:194:ARG:HB2	1:G:199:VAL:HA	1.80	0.64
1:G:249:VAL:HG22	1:G:257:TYR:CZ	2.33	0.64
2:D:49:VAL:HG23	2:D:67:HIS:C	2.18	0.63
1:C:32:GLU:OE2	1:C:48:ARG:HD2	1.99	0.63
1:E:226:GLN:OE1	1:E:227:ASP:HB2	1.98	0.63
1:A:32:GLU:OE2	1:A:48:ARG:HD2	1.99	0.63
2:D:39:MET:HE1	2:D:68:THR:CB	2.28	0.63
1:E:226:GLN:O	1:E:226:GLN:OE1	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:ASN:O	1:G:180:LEU:HD22	2.00	0.62
2:H:39:MET:CE	2:H:68:THR:CG2	2.78	0.62
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.35	0.62
2:D:39:MET:CE	2:D:49:VAL:HG21	2.29	0.62
2:B:39:MET:HE2	2:B:49:VAL:HG22	1.82	0.62
2:H:57:SER:OG	5:H:101:GOL:H12	1.99	0.62
1:E:117:ALA:HB2	2:F:60:TRP:CE2	2.35	0.61
2:H:39:MET:HE1	2:H:68:THR:CB	2.30	0.61
1:C:230:LEU:HD12	1:C:230:LEU:C	2.21	0.61
2:H:39:MET:HE3	2:H:68:THR:HG21	1.81	0.61
1:E:181:ARG:HD3	1:E:181:ARG:H	1.64	0.61
1:E:97:GLN:NE2	3:K:5:ASN:HD21	1.98	0.61
2:F:87:MET:HE3	2:F:91:LYS:HD2	1.82	0.60
1:G:230:LEU:C	1:G:230:LEU:HD12	2.21	0.60
1:C:111:ARG:HD3	1:C:113:TYR:CZ	2.36	0.60
1:A:175:GLY:O	1:A:179:LEU:HG	2.01	0.60
1:E:145:ARG:CD	5:E:341:GOL:H12	2.31	0.60
1:G:234:ARG:HD3	2:H:10:TYR:CZ	2.36	0.60
1:E:251:LEU:HD23	1:E:252:GLY:N	2.16	0.60
2:B:40:LEU:HD23	2:B:45:LYS:HA	1.83	0.60
2:F:87:MET:HE1	2:F:91:LYS:HB2	1.83	0.60
1:E:145:ARG:HD3	5:E:341:GOL:C1	2.32	0.60
1:G:97:GLN:NE2	3:L:5:ASN:HD21	1.99	0.60
1:G:110:LEU:HD13	6:G:657:HOH:O	2.02	0.59
1:E:251:LEU:HD23	1:E:252:GLY:H	1.67	0.59
2:B:39:MET:HE3	2:B:68:THR:CG2	2.32	0.59
2:D:39:MET:HE1	2:D:68:THR:CG2	2.33	0.59
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.38	0.59
1:E:145:ARG:CD	5:E:341:GOL:C1	2.80	0.58
1:G:17:LEU:HD23	1:G:17:LEU:H	1.68	0.58
1:C:195:SER:N	6:C:866:HOH:O	2.35	0.58
1:C:97:GLN:HE22	3:J:5:ASN:HD21	1.52	0.58
1:E:234:ARG:HD3	2:F:10:TYR:CE2	2.39	0.58
2:B:39:MET:HE2	2:B:49:VAL:HG13	1.86	0.58
2:D:39:MET:CE	2:D:49:VAL:CG2	2.82	0.58
1:A:72:GLN:OE1	1:A:75:ARG:NH1	2.36	0.58
1:C:226:GLN:O	1:C:226:GLN:CD	2.41	0.57
2:D:39:MET:CE	2:D:68:THR:HG22	2.34	0.57
1:C:234:ARG:HD3	2:D:10:TYR:CE2	2.38	0.57
1:E:226:GLN:C	1:E:226:GLN:OE1	2.42	0.57
1:C:57:PRO:HD2	6:C:669:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ARG:NH2	6:C:689:HOH:O	2.38	0.57
1:E:104:GLY:N	1:E:110:LEU:HD22	2.20	0.57
1:E:191:HIS:HB2	1:E:274:TRP:CZ3	2.40	0.57
1:E:17:LEU:H	1:E:17:LEU:HD23	1.70	0.56
1:G:155:HIS:HB3	3:L:6:PHE:CZ	2.40	0.56
3:J:9:MET:OXT	3:J:9:MET:O	2.22	0.56
2:H:7:ILE:CD1	2:H:82:VAL:HG21	2.36	0.56
1:A:230:LEU:C	1:A:230:LEU:CD1	2.73	0.56
1:C:167:TRP:CE2	3:J:1:LYS:HE3	2.39	0.56
1:G:201:LEU:O	1:G:246:SER:HA	2.05	0.56
2:F:4:THR:HG23	4:F:100:SO4:O4	2.05	0.56
1:G:263:HIS:HB3	1:G:266:LEU:HD22	1.89	0.55
2:F:87:MET:CE	2:F:91:LYS:HB2	2.36	0.55
1:E:230:LEU:HD12	1:E:230:LEU:C	2.26	0.55
2:D:39:MET:CE	2:D:68:THR:HB	2.36	0.55
1:G:111:ARG:HD3	1:G:113:TYR:OH	2.07	0.55
1:E:77:SER:HB3	3:K:9:MET:HG3	1.88	0.54
2:F:58:LYS:HE2	6:F:195:HOH:O	2.06	0.54
1:E:202:ARG:HD2	1:E:244:TRP:CE3	2.42	0.54
2:F:50:GLU:HB2	2:F:67:HIS:CE1	2.42	0.54
1:E:222:GLU:HA	1:E:222:GLU:OE2	2.08	0.54
1:E:77:SER:HB3	3:K:9:MET:HG2	1.88	0.54
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.43	0.54
1:E:8:PHE:CE2	5:E:340:GOL:H11	2.43	0.54
2:H:4:THR:HG22	2:H:86:SER:HB2	1.90	0.54
1:C:251:LEU:HD23	1:C:252:GLY:N	2.22	0.53
1:G:194:ARG:CB	1:G:198:GLU:O	2.56	0.53
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.42	0.53
2:F:47:PRO:O	2:F:48:LYS:HD3	2.07	0.53
1:E:206:LEU:HD23	1:E:242:GLN:HB3	1.90	0.53
1:C:155:HIS:HB3	3:J:6:PHE:CZ	2.43	0.53
1:E:250:PRO:HB2	1:E:253:LYS:HB2	1.90	0.53
1:G:202:ARG:HD3	1:G:246:SER:HB3	1.90	0.53
1:A:226:GLN:OE1	1:A:227:ASP:HB2	2.08	0.53
2:B:87:MET:HE3	2:B:91:LYS:HD2	1.90	0.53
3:I:9:MET:OXT	3:I:9:MET:O	2.23	0.53
1:E:194:ARG:HG2	1:E:195:SER:H	1.73	0.53
2:H:87:MET:HE1	2:H:91:LYS:HD2	1.90	0.53
1:A:111:ARG:HD3	1:A:113:TYR:OH	2.08	0.53
1:A:178:THR:HG22	6:A:723:HOH:O	2.08	0.53
2:B:57:SER:OG	5:B:100:GOL:C3	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ARG:HD3	1:C:113:TYR:OH	2.09	0.53
1:A:28:VAL:HB	6:A:664:HOH:O	2.08	0.52
1:G:274:TRP:NE1	1:G:276:PRO:HG3	2.24	0.52
1:A:197:GLY:O	1:A:251:LEU:HB2	2.10	0.52
1:E:202:ARG:CD	1:E:244:TRP:CE3	2.93	0.52
1:A:144:ARG:NH2	6:A:628:HOH:O	2.41	0.52
1:A:249:VAL:HG22	1:A:257:TYR:CE2	2.44	0.52
2:H:64:ILE:HG22	2:H:65:LEU:N	2.25	0.52
1:C:190:THR:OG1	1:C:192:HIS:HE1	1.92	0.52
1:C:226:GLN:O	1:C:226:GLN:CG	2.57	0.52
1:A:10:THR:HG22	1:A:11:ALA:N	2.24	0.52
1:A:77:SER:HB3	3:I:9:MET:HG2	1.92	0.51
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.45	0.51
1:E:181:ARG:HD3	1:E:181:ARG:N	2.24	0.51
1:A:234:ARG:HD2	1:A:242:GLN:OE1	2.10	0.51
1:A:251:LEU:HD23	1:A:252:GLY:N	2.26	0.51
1:E:249:VAL:HG22	1:E:257:TYR:CZ	2.45	0.51
1:C:234:ARG:HD3	2:D:10:TYR:CE1	2.45	0.51
1:E:225:THR:HG22	1:E:225:THR:O	2.11	0.51
1:G:202:ARG:HD2	1:G:244:TRP:CE3	2.46	0.51
2:D:46:ILE:HG23	2:D:47:PRO:HD2	1.93	0.50
1:E:194:ARG:CG	1:E:195:SER:H	2.23	0.50
1:C:111:ARG:HG2	1:C:113:TYR:CE1	2.45	0.50
1:G:194:ARG:HB3	1:G:198:GLU:O	2.10	0.50
1:A:262:TYR:CD2	1:C:108:ARG:HD3	2.46	0.50
2:F:46:ILE:CG2	2:F:47:PRO:HD2	2.41	0.50
1:A:262:TYR:CD1	1:A:262:TYR:N	2.80	0.50
2:B:39:MET:CE	2:B:68:THR:CG2	2.89	0.50
2:B:39:MET:CE	2:B:68:THR:HG22	2.42	0.50
1:E:178:THR:O	1:E:178:THR:CG2	2.60	0.50
1:E:262:TYR:CG	1:G:108:ARG:HD3	2.47	0.50
2:F:4:THR:HG23	4:F:100:SO4:O3	2.11	0.50
2:H:21:ASN:HB3	2:H:70:PHE:CE1	2.46	0.50
1:A:78:LEU:HD12	6:A:350:HOH:O	2.10	0.50
2:B:46:ILE:HG23	2:B:47:PRO:HD2	1.93	0.50
1:G:176:ASN:OD1	1:G:180:LEU:HD21	2.12	0.50
1:E:202:ARG:HD3	1:E:246:SER:HB3	1.94	0.49
1:E:23:ILE:HD12	2:F:54:MET:SD	2.52	0.49
1:G:224:LEU:HD12	1:G:226:GLN:HE22	1.77	0.49
1:C:167:TRP:CZ3	1:C:170:ARG:HD3	2.47	0.49
2:H:39:MET:CE	2:H:68:THR:CB	2.89	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.49
1:E:72:GLN:OE1	1:E:75:ARG:HD3	2.12	0.49
1:E:191:HIS:HB2	1:E:274:TRP:CH2	2.46	0.49
1:G:17:LEU:HD23	1:G:17:LEU:N	2.27	0.49
2:B:44:LYS:HB3	6:B:228:HOH:O	2.12	0.49
1:E:155:HIS:HB3	3:K:6:PHE:CZ	2.47	0.49
2:B:52:SER:N	6:B:483:HOH:O	2.46	0.49
1:E:29:ASP:O	1:E:30:ASN:HB2	2.13	0.49
2:F:4:THR:HG23	4:F:100:SO4:S	2.52	0.49
1:A:6:ARG:NH2	1:A:113:TYR:CE1	2.81	0.49
1:C:237:GLY:HA3	6:D:288:HOH:O	2.13	0.49
2:D:91:LYS:NZ	6:D:887:HOH:O	2.44	0.49
2:B:1:ILE:HB	6:B:396:HOH:O	2.13	0.49
2:H:29:GLN:HA	2:H:61:SER:HB2	1.94	0.49
1:A:193:PRO:HA	1:A:199:VAL:HG12	1.95	0.48
1:C:185:PRO:HG2	1:C:266:LEU:HD21	1.93	0.48
1:C:263:HIS:HB3	1:C:266:LEU:CD2	2.41	0.48
1:G:159:TYR:CD2	1:G:159:TYR:C	2.86	0.48
2:H:19:LYS:HE3	2:H:19:LYS:HB3	1.55	0.48
1:C:176:ASN:ND2	6:C:558:HOH:O	2.45	0.48
2:B:57:SER:HG	5:B:100:GOL:H31	1.79	0.48
1:C:97:GLN:NE2	3:J:5:ASN:HD21	2.11	0.48
1:C:191:HIS:CE1	1:C:199:VAL:HG21	2.49	0.48
2:D:39:MET:HE2	2:D:49:VAL:HB	1.95	0.48
2:F:47:PRO:HG2	6:F:281:HOH:O	2.12	0.48
1:G:41:GLU:O	1:G:43:PRO:HD3	2.13	0.48
1:A:191:HIS:HB2	1:A:274:TRP:CZ3	2.48	0.48
1:A:234:ARG:HD3	2:B:10:TYR:CD2	2.48	0.48
1:A:145:ARG:HD3	5:A:341:GOL:H32	1.96	0.48
1:C:45:TYR:CE2	1:C:67:ALA:HB2	2.48	0.48
2:D:47:PRO:O	2:D:48:LYS:HD3	2.13	0.48
1:G:230:LEU:C	1:G:230:LEU:CD1	2.82	0.48
2:B:52:SER:CA	6:B:483:HOH:O	2.56	0.47
1:G:149:GLN:HE21	1:G:149:GLN:HA	1.79	0.47
2:B:39:MET:CE	2:B:68:THR:HB	2.44	0.47
1:G:190:THR:OG1	1:G:192:HIS:HE1	1.96	0.47
1:A:167:TRP:CE2	3:I:1:LYS:HD2	2.49	0.47
1:E:72:GLN:OE1	1:E:75:ARG:NH1	2.47	0.47
1:C:206:LEU:HD23	1:C:242:GLN:HG2	1.96	0.47
1:G:261:VAL:HB	1:G:270:LEU:HB2	1.96	0.47
1:C:187:ALA:C	1:C:272:LEU:HD11	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:NE	6:A:347:HOH:O	2.47	0.47
1:E:230:LEU:C	1:E:230:LEU:CD1	2.83	0.47
1:A:194:ARG:HG2	1:A:195:SER:H	1.80	0.47
2:H:13:HIS:O	2:H:14:PRO:C	2.52	0.47
1:C:230:LEU:C	1:C:230:LEU:CD1	2.82	0.47
2:D:59:ASP:O	2:D:60:TRP:HB2	2.15	0.47
1:G:72:GLN:OE1	1:G:75:ARG:NH1	2.48	0.47
1:A:33:PHE:C	1:A:48:ARG:HB2	2.36	0.47
1:A:29:ASP:O	1:A:30:ASN:HB2	2.16	0.46
1:C:168:LEU:O	1:C:172:LEU:HG	2.14	0.46
1:C:187:ALA:HB1	1:C:272:LEU:HD12	1.96	0.46
2:F:96:ASP:C	2:F:96:ASP:OD1	2.52	0.46
1:C:178:THR:CG2	1:C:178:THR:O	2.63	0.46
1:E:104:GLY:CA	1:E:110:LEU:HD22	2.46	0.46
1:A:17:LEU:HD12	1:A:17:LEU:N	2.30	0.46
1:A:191:HIS:HE1	1:A:254:GLU:OE1	1.97	0.46
1:E:262:TYR:CD2	1:G:108:ARG:HG2	2.50	0.46
1:A:251:LEU:HD23	1:A:251:LEU:C	2.36	0.46
5:A:340:GOL:O2	2:B:54:MET:O	2.34	0.46
1:G:44:ARG:HD2	6:G:533:HOH:O	2.16	0.46
1:A:178:THR:O	1:A:181:ARG:HB3	2.16	0.46
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.51	0.46
1:E:234:ARG:HD3	2:F:10:TYR:CE1	2.51	0.46
2:H:57:SER:OG	5:H:101:GOL:H11	2.15	0.46
1:C:192:HIS:CD2	2:D:98:ASP:CG	2.89	0.46
1:C:209:TYR:C	1:C:209:TYR:CD2	2.88	0.46
1:G:187:ALA:HA	1:G:204:TRP:O	2.15	0.46
1:G:251:LEU:HD23	1:G:252:GLY:H	1.81	0.46
2:D:39:MET:HE1	2:D:68:THR:HG22	1.96	0.46
1:E:95:LEU:HD11	3:K:9:MET:CE	2.46	0.46
2:F:16:GLU:OE1	2:F:19:LYS:HD3	2.16	0.46
2:F:31:HIS:CD2	2:F:32:PRO:HA	2.51	0.46
2:B:39:MET:HE1	2:B:68:THR:HB	1.98	0.45
2:H:87:MET:CE	2:H:91:LYS:HB2	2.45	0.45
1:C:144:ARG:NH2	6:C:394:HOH:O	2.49	0.45
1:C:178:THR:O	1:C:178:THR:HG22	2.17	0.45
1:E:263:HIS:HB3	1:E:266:LEU:HD22	1.98	0.45
1:A:274:TRP:NE1	1:A:276:PRO:HG3	2.31	0.45
1:E:72:GLN:OE1	1:E:75:ARG:CD	2.64	0.45
1:A:244:TRP:HZ3	1:A:246:SER:HG	1.64	0.45
1:E:35:ARG:NH2	2:F:53:ASP:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:HIS:HB2	1:A:274:TRP:CH2	2.52	0.45
1:A:251:LEU:C	1:A:251:LEU:CD2	2.85	0.45
2:D:87:MET:HE3	2:D:91:LYS:HD2	1.99	0.45
1:E:202:ARG:HD2	1:E:244:TRP:CE2	2.51	0.45
1:E:262:TYR:CD1	1:G:108:ARG:HD3	2.51	0.45
1:G:174:ASN:ND2	6:G:387:HOH:O	2.50	0.45
2:H:7:ILE:HD11	2:H:82:VAL:HG21	1.99	0.45
1:C:17:LEU:CD1	6:C:385:HOH:O	2.64	0.45
2:D:39:MET:HE1	2:D:49:VAL:CG2	2.45	0.45
1:A:201:LEU:O	1:A:246:SER:HA	2.16	0.45
2:B:87:MET:CE	2:B:91:LYS:HB2	2.35	0.45
1:E:162:GLY:O	1:E:166:GLU:HB2	2.16	0.45
1:E:181:ARG:O	1:E:181:ARG:HG2	2.17	0.45
2:H:40:LEU:HD23	2:H:45:LYS:HA	1.99	0.45
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.52	0.45
2:H:64:ILE:CG2	2:H:65:LEU:N	2.80	0.45
1:C:6:ARG:NH2	1:C:113:TYR:CE1	2.85	0.45
1:C:235:PRO:HD2	2:D:26:TYR:CE2	2.51	0.45
2:D:46:ILE:CG2	2:D:47:PRO:HD2	2.47	0.45
1:A:49:ALA:O	1:A:50:PRO:C	2.54	0.44
2:H:39:MET:CE	2:H:68:THR:HG22	2.46	0.44
1:C:181:ARG:H	1:C:181:ARG:HD3	1.82	0.44
3:K:8:THR:O	3:K:9:MET:C	2.55	0.44
1:A:194:ARG:CG	1:A:195:SER:H	2.30	0.44
1:C:72:GLN:OE1	1:C:75:ARG:HD3	2.17	0.44
2:D:87:MET:HE1	2:D:91:LYS:HB2	1.99	0.44
1:E:178:THR:O	1:E:178:THR:HG23	2.18	0.44
1:E:190:THR:OG1	1:E:192:HIS:HE1	2.00	0.44
5:E:340:GOL:H32	6:F:847:HOH:O	2.17	0.44
1:G:43:PRO:C	1:G:44:ARG:HG2	2.38	0.44
1:G:93:HIS:HA	1:G:119:GLU:OE1	2.17	0.44
1:G:250:PRO:HB2	1:G:253:LYS:HB2	1.99	0.44
1:E:8:PHE:CD1	1:E:98:MET:HG2	2.52	0.44
1:G:85:TYR:CZ	1:G:139:ALA:HB3	2.52	0.44
1:C:81:LEU:HD13	1:C:118:TYR:CD1	2.53	0.44
1:C:188:HIS:N	1:C:272:LEU:HD11	2.33	0.44
1:E:18:GLU:N	6:E:456:HOH:O	2.50	0.44
1:G:23:ILE:HD12	2:H:54:MET:SD	2.58	0.44
1:G:194:ARG:HB2	1:G:198:GLU:O	2.17	0.44
1:C:203:CYS:HB2	1:C:217:TRP:CZ2	2.53	0.44
2:D:9:VAL:HG23	2:D:93:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:ARG:NH2	1:E:113:TYR:CE1	2.86	0.44
1:E:17:LEU:H	1:E:17:LEU:CD2	2.29	0.44
1:E:274:TRP:NE1	1:E:276:PRO:HG3	2.33	0.44
1:G:179:LEU:HD12	1:G:179:LEU:O	2.18	0.44
1:A:225:THR:O	1:A:227:ASP:N	2.51	0.43
2:F:47:PRO:O	2:F:48:LYS:CD	2.66	0.43
1:E:230:LEU:HD12	1:E:230:LEU:O	2.18	0.43
1:A:155:HIS:HB3	3:I:6:PHE:CZ	2.53	0.43
1:E:17:LEU:CD2	1:E:17:LEU:N	2.81	0.43
2:F:32:PRO:HB2	2:F:33:PRO:HD2	2.00	0.43
1:A:97:GLN:HE22	3:I:5:ASN:HD21	1.67	0.43
2:D:39:MET:HE3	2:D:68:THR:HG22	1.96	0.43
1:E:145:ARG:HE	5:E:341:GOL:C1	2.32	0.43
1:G:226:GLN:O	1:G:226:GLN:CG	2.66	0.43
1:A:63:GLU:OE2	1:A:63:GLU:HA	2.19	0.43
1:C:3:HIS:HA	1:C:29:ASP:OD1	2.19	0.43
1:C:249:VAL:HG22	1:C:257:TYR:CE2	2.54	0.43
1:A:49:ALA:O	1:A:51:TRP:N	2.52	0.43
1:A:203:CYS:O	1:A:244:TRP:HA	2.19	0.43
1:C:187:ALA:HA	1:C:204:TRP:O	2.18	0.43
1:C:190:THR:OG1	1:C:202:ARG:HB3	2.19	0.43
2:H:19:LYS:O	2:H:20:PRO:C	2.57	0.43
1:A:225:THR:O	1:A:226:GLN:C	2.55	0.43
2:B:16:GLU:OE2	2:B:19:LYS:HE2	2.19	0.43
1:C:155:HIS:HB3	3:J:6:PHE:CE2	2.53	0.43
2:D:39:MET:SD	2:D:49:VAL:HG21	2.58	0.43
1:G:231:VAL:HG13	1:G:244:TRP:CZ2	2.54	0.43
1:C:181:ARG:O	1:C:181:ARG:HG2	2.18	0.42
2:D:41:LYS:HG3	2:D:78:TYR:CE2	2.54	0.42
2:F:48:LYS:HD3	2:F:48:LYS:HA	1.60	0.42
1:G:19:GLU:OE2	1:G:75:ARG:HD2	2.19	0.42
1:G:167:TRP:CZ2	3:L:1:LYS:HD2	2.54	0.42
1:E:178:THR:HG22	1:E:179:LEU:HD23	2.01	0.42
1:A:32:GLU:OE2	1:A:35:ARG:HD2	2.19	0.42
1:C:48:ARG:NH2	6:C:729:HOH:O	2.51	0.42
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.54	0.42
2:D:17:ASN:HA	2:D:72:PRO:O	2.19	0.42
2:D:39:MET:HE2	2:D:49:VAL:CG2	2.50	0.42
1:E:10:THR:O	1:E:22:TYR:HA	2.20	0.42
1:E:77:SER:CB	3:K:9:MET:HG2	2.49	0.42
1:E:189:VAL:HG23	1:E:272:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:GLN:HA	2:F:61:SER:HB2	2.00	0.42
1:G:234:ARG:HD3	2:H:10:TYR:CD2	2.52	0.42
1:C:234:ARG:CD	2:D:10:TYR:CE2	3.02	0.42
1:E:262:TYR:CD2	1:G:108:ARG:HD3	2.55	0.42
1:G:3:HIS:CG	1:G:172:LEU:HD11	2.54	0.42
2:B:85:ASP:HB2	6:B:109:HOH:O	2.20	0.42
1:E:95:LEU:HD11	3:K:9:MET:HE3	2.00	0.42
1:E:106:ASP:O	1:E:107:TRP:HB2	2.20	0.42
1:A:97:GLN:NE2	3:I:5:ASN:HD21	2.17	0.42
2:B:87:MET:CE	2:B:91:LYS:HD2	2.49	0.42
1:E:78:LEU:HD13	1:E:95:LEU:HB2	2.01	0.42
1:G:172:LEU:HD23	1:G:179:LEU:HD11	2.01	0.42
1:A:103:LEU:HD11	1:A:168:LEU:HD23	2.01	0.42
2:D:9:VAL:CG2	2:D:93:VAL:HG22	2.49	0.42
2:F:32:PRO:CB	2:F:33:PRO:HD2	2.50	0.42
1:A:272:LEU:HD23	1:A:272:LEU:HA	1.85	0.42
2:B:19:LYS:HB3	2:B:19:LYS:HE3	1.63	0.42
1:C:202:ARG:HG2	1:C:204:TRP:NE1	2.35	0.42
2:F:13:HIS:HA	6:F:366:HOH:O	2.20	0.42
1:E:145:ARG:CD	5:E:341:GOL:H11	2.49	0.42
1:G:266:LEU:HB3	1:G:268:GLU:O	2.20	0.42
1:C:189:VAL:HG23	1:C:272:LEU:HD13	2.01	0.41
2:D:32:PRO:CB	2:D:33:PRO:CD	2.98	0.41
1:G:77:SER:HB3	3:L:9:MET:HG2	2.02	0.41
2:H:39:MET:HE2	2:H:49:VAL:HG21	2.02	0.41
2:H:87:MET:HE2	2:H:91:LYS:HB2	2.01	0.41
1:A:231:VAL:HG13	1:A:244:TRP:CZ2	2.55	0.41
5:A:340:GOL:O2	2:B:55:SER:HA	2.21	0.41
1:C:195:SER:O	1:C:196:LYS:C	2.57	0.41
1:C:199:VAL:HG21	1:C:254:GLU:OE1	2.20	0.41
1:E:118:TYR:CD2	1:E:119:GLU:HG2	2.55	0.41
1:G:78:LEU:HD13	1:G:95:LEU:HB2	2.02	0.41
1:G:226:GLN:O	1:G:226:GLN:HG2	2.19	0.41
1:C:149:GLN:NE2	6:C:831:HOH:O	2.54	0.41
1:C:167:TRP:CE3	1:C:170:ARG:HD3	2.55	0.41
1:E:193:PRO:HA	1:E:199:VAL:HG12	2.03	0.41
2:F:75:THR:HG22	2:F:76:ASP:N	2.36	0.41
1:G:54:GLN:O	1:G:55:GLU:C	2.58	0.41
1:A:17:LEU:N	1:A:17:LEU:CD1	2.84	0.41
1:A:129:ASP:O	1:A:131:LYS:HG3	2.20	0.41
1:A:108:ARG:HD3	1:C:262:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:LEU:HD23	1:E:272:LEU:HA	1.85	0.41
1:E:5:MET:O	1:E:100:GLY:HA3	2.21	0.41
1:A:51:TRP:CZ3	1:A:52:MET:SD	3.14	0.41
1:C:114:LEU:HD23	1:C:114:LEU:HA	1.82	0.41
1:A:262:TYR:CG	1:C:108:ARG:HD3	2.55	0.41
1:C:268:GLU:HB2	1:C:269:PRO:CD	2.51	0.41
2:F:13:HIS:O	2:F:14:PRO:C	2.57	0.41
1:A:230:LEU:HD12	1:A:230:LEU:O	2.20	0.41
1:A:261:VAL:HB	1:A:270:LEU:HB2	2.03	0.41
1:C:167:TRP:CH2	3:J:1:LYS:HE3	2.53	0.40
1:E:254:GLU:O	1:E:255:GLN:HG2	2.21	0.40
2:F:23:LEU:HB2	2:F:70:PHE:CD1	2.56	0.40
1:G:190:THR:OG1	1:G:192:HIS:CE1	2.74	0.40
1:G:274:TRP:CE2	1:G:276:PRO:HG3	2.56	0.40
2:H:79:ALA:HB2	2:H:94:TYR:CD1	2.57	0.40
1:A:106:ASP:O	1:A:107:TRP:HB2	2.21	0.40
1:C:266:LEU:HB3	1:C:268:GLU:O	2.21	0.40
1:G:222:GLU:HA	1:G:222:GLU:OE2	2.22	0.40
2:H:50:GLU:HB2	2:H:67:HIS:CE1	2.56	0.40
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.86	0.40
2:D:19:LYS:HB3	2:D:19:LYS:HE3	1.85	0.40
1:G:230:LEU:HD12	1:G:230:LEU:O	2.20	0.40
1:C:251:LEU:HD23	1:C:252:GLY:H	1.87	0.40
1:G:209:TYR:CD2	1:G:209:TYR:C	2.95	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	274/276 (99%)	257 (94%)	17 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	274/276 (99%)	260 (95%)	14 (5%)	0	100	100
1	E	274/276 (99%)	259 (94%)	15 (6%)	0	100	100
1	G	274/276 (99%)	261 (95%)	13 (5%)	0	100	100
2	B	97/99 (98%)	94 (97%)	2 (2%)	1 (1%)	15	11
2	D	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	F	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
2	H	97/99 (98%)	91 (94%)	5 (5%)	1 (1%)	15	11
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	J	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	K	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1512/1536 (98%)	1433 (95%)	77 (5%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	42	ASN
2	B	47	PRO

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	234/234 (100%)	217 (93%)	17 (7%)	14	11
1	C	234/234 (100%)	212 (91%)	22 (9%)	8	5
1	E	234/234 (100%)	212 (91%)	22 (9%)	8	5
1	G	234/234 (100%)	212 (91%)	22 (9%)	8	5
2	B	94/94 (100%)	88 (94%)	6 (6%)	17	14
2	D	94/94 (100%)	88 (94%)	6 (6%)	17	14
2	F	94/94 (100%)	87 (93%)	7 (7%)	13	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	94/94 (100%)	91 (97%)	3 (3%)	39 41
3	I	6/6 (100%)	6 (100%)	0	100 100
3	J	6/6 (100%)	6 (100%)	0	100 100
3	K	6/6 (100%)	6 (100%)	0	100 100
3	L	6/6 (100%)	6 (100%)	0	100 100
All	All	1336/1336 (100%)	1231 (92%)	105 (8%)	12 9

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ARG
1	A	75	ARG
1	A	78	LEU
1	A	101	CYS
1	A	114	LEU
1	A	144	ARG
1	A	149	GLN
1	A	166	GLU
1	A	180	LEU
1	A	195	SER
1	A	215	LEU
1	A	230	LEU
1	A	234	ARG
1	A	254	GLU
1	A	266	LEU
1	A	272	LEU
1	A	273	ARG
2	B	1	ILE
2	B	19	LYS
2	B	70	PHE
2	B	75	THR
2	B	93	VAL
2	B	97	ARG
1	C	17	LEU
1	C	19	GLU
1	C	35	ARG
1	C	75	ARG
1	C	78	LEU
1	C	101	CYS
1	C	110	LEU

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Mol	Chain	Res	Type
1	C	114	LEU
1	C	121	ARG
1	C	149	GLN
1	C	166	GLU
1	C	181	ARG
1	C	196	LYS
1	C	202	ARG
1	C	215	LEU
1	C	225	THR
1	C	230	LEU
1	C	234	ARG
1	C	254	GLU
1	C	266	LEU
1	C	272	LEU
1	C	275	GLU
2	D	48	LYS
2	D	70	PHE
2	D	74	GLU
2	D	75	THR
2	D	77	THR
2	D	93	VAL
1	E	17	LEU
1	E	62	ARG
1	E	75	ARG
1	E	78	LEU
1	E	110	LEU
1	E	114	LEU
1	E	149	GLN
1	E	166	GLU
1	E	178	THR
1	E	179	LEU
1	E	181	ARG
1	E	195	SER
1	E	215	LEU
1	E	225	THR
1	E	226	GLN
1	E	230	LEU
1	E	234	ARG
1	E	242	GLN
1	E	254	GLU
1	E	259	CYS
1	E	266	LEU

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Mol	Chain	Res	Type
1	E	272	LEU
2	F	2	GLN
2	F	4	THR
2	F	48	LYS
2	F	74	GLU
2	F	75	THR
2	F	77	THR
2	F	97	ARG
1	G	17	LEU
1	G	19	GLU
1	G	35	ARG
1	G	41	GLU
1	G	44	ARG
1	G	47	PRO
1	G	75	ARG
1	G	78	LEU
1	G	114	LEU
1	G	149	GLN
1	G	166	GLU
1	G	194	ARG
1	G	195	SER
1	G	215	LEU
1	G	226	GLN
1	G	230	LEU
1	G	234	ARG
1	G	251	LEU
1	G	254	GLU
1	G	266	LEU
1	G	272	LEU
1	G	273	ARG
2	H	70	PHE
2	H	75	THR
2	H	77	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	97	GLN
1	A	192	HIS
2	B	2	GLN
1	C	54	GLN

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Mol	Chain	Res	Type
1	C	97	GLN
1	C	155	HIS
1	C	176	ASN
1	C	192	HIS
2	D	34	HIS
1	E	97	GLN
1	E	115	GLN
1	E	149	GLN
1	E	192	HIS
1	G	97	GLN
1	G	149	GLN
1	G	174	ASN
1	G	192	HIS
1	G	226	GLN
2	H	2	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
4	SO4	E	339	-	4,4,4	0.13	0	6,6,6	0.38	0
4	SO4	C	339	-	4,4,4	0.25	0	6,6,6	1.01	0
5	GOL	B	100	-	5,5,5	0.58	0	5,5,5	0.96	1 (20%)
5	GOL	E	341	-	5,5,5	0.39	0	5,5,5	0.42	0
5	GOL	E	340	-	5,5,5	0.66	0	5,5,5	1.58	2 (40%)
4	SO4	A	339	-	4,4,4	0.18	0	6,6,6	0.28	0
5	GOL	H	100	-	5,5,5	0.50	0	5,5,5	1.03	0
5	GOL	H	101	-	5,5,5	0.56	0	5,5,5	0.72	0
4	SO4	F	100	-	4,4,4	0.34	0	6,6,6	0.42	0
5	GOL	A	340	-	5,5,5	0.72	0	5,5,5	0.85	0
5	GOL	A	341	-	5,5,5	0.65	0	5,5,5	0.32	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	GOL	B	100	-	-	0/4/4/4	-
5	GOL	E	341	-	-	4/4/4/4	-
5	GOL	E	340	-	-	0/4/4/4	-
5	GOL	H	100	-	-	3/4/4/4	-
5	GOL	H	101	-	-	0/4/4/4	-
5	GOL	A	340	-	-	2/4/4/4	-
5	GOL	A	341	-	-	4/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	340	GOL	C3-C2-C1	-2.54	101.83	111.70
5	E	340	GOL	O2-C2-C3	2.11	118.40	109.12
5	B	100	GOL	O3-C3-C2	2.01	119.83	110.20

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	340	GOL	C1-C2-C3-O3
5	A	341	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	E	341	GOL	C1-C2-C3-O3
5	H	100	GOL	O1-C1-C2-C3
5	A	341	GOL	C1-C2-C3-O3
5	E	341	GOL	O1-C1-C2-C3
5	A	340	GOL	O2-C2-C3-O3
5	A	341	GOL	O1-C1-C2-O2
5	E	341	GOL	O2-C2-C3-O3
5	E	341	GOL	O1-C1-C2-O2
5	H	100	GOL	O1-C1-C2-O2
5	A	341	GOL	O2-C2-C3-O3
5	H	100	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	100	GOL	3	0
5	E	341	GOL	6	0
5	E	340	GOL	3	0
5	H	101	GOL	3	0
4	F	100	SO4	3	0
5	A	340	GOL	2	0
5	A	341	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	276/276 (100%)	1.04	37 (13%)	3	4	20, 52, 113, 192	0
1	C	276/276 (100%)	0.85	29 (10%)	6	8	20, 47, 112, 203	0
1	E	276/276 (100%)	0.99	33 (11%)	4	5	20, 46, 129, 193	0
1	G	276/276 (100%)	1.03	45 (16%)	1	2	19, 51, 116, 190	0
2	B	99/99 (100%)	0.48	3 (3%)	50	56	25, 41, 72, 101	0
2	D	99/99 (100%)	0.65	3 (3%)	50	56	24, 47, 82, 95	0
2	F	99/99 (100%)	0.53	2 (2%)	65	69	25, 46, 73, 100	0
2	H	99/99 (100%)	0.58	3 (3%)	50	56	26, 44, 74, 95	0
3	I	9/9 (100%)	0.24	0	100	100	30, 35, 51, 54	0
3	J	9/9 (100%)	-0.03	0	100	100	22, 29, 33, 38	0
3	K	9/9 (100%)	0.11	0	100	100	20, 30, 36, 36	0
3	L	9/9 (100%)	0.22	0	100	100	25, 29, 45, 53	0
All	All	1536/1536 (100%)	0.85	155 (10%)	7	9	19, 47, 112, 203	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	178	THR	22.0
1	A	178	THR	18.7
1	E	177	ALA	17.6
1	G	178	THR	15.3
1	E	179	LEU	14.4
1	C	179	LEU	11.4
1	E	180	LEU	10.7
1	G	177	ALA	10.7
1	C	178	THR	10.4
1	A	179	LEU	9.1
1	G	179	LEU	8.1

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Mol	Chain	Res	Type	RSRZ
1	C	177	ALA	7.5
1	C	16	GLY	7.0
1	C	220	ASN	6.8
1	E	227	ASP	6.8
1	A	177	ALA	6.5
1	E	219	LEU	6.4
1	G	180	LEU	6.3
1	A	195	SER	6.3
1	C	17	LEU	6.2
1	E	257	TYR	5.7
2	D	47	PRO	5.7
1	E	224	LEU	5.7
1	C	180	LEU	5.3
1	A	180	LEU	5.2
1	E	196	LYS	5.1
1	A	227	ASP	4.9
1	G	220	ASN	4.9
1	E	251	LEU	4.8
1	E	226	GLN	4.6
1	G	197	GLY	4.5
1	G	253	LYS	4.5
1	G	51	TRP	4.5
1	G	17	LEU	4.4
1	A	220	ASN	4.4
1	G	199	VAL	4.4
1	A	196	LYS	4.4
1	E	249	VAL	4.3
1	C	219	LEU	4.3
1	C	189	VAL	4.3
1	C	256	ASN	4.3
1	G	249	VAL	4.3
1	A	252	GLY	4.2
1	A	57	PRO	4.2
1	E	193	PRO	4.0
1	A	251	LEU	4.0
1	G	250	PRO	4.0
1	C	227	ASP	3.9
1	E	41	GLU	3.8
1	A	222	GLU	3.8
1	G	251	LEU	3.8
1	G	196	LYS	3.7
1	E	256	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
2	F	1	ILE	3.7
2	F	47	PRO	3.6
1	E	222	GLU	3.6
1	G	195	SER	3.6
1	C	226	GLN	3.4
1	A	58	GLU	3.4
1	C	248	VAL	3.4
1	E	18	GLU	3.4
1	E	17	LEU	3.3
1	C	274	TRP	3.3
1	A	250	PRO	3.2
1	C	273	ARG	3.2
1	G	256	ASN	3.2
1	C	41	GLU	3.2
1	A	172	LEU	3.2
1	C	272	LEU	3.2
1	E	16	GLY	3.2
1	G	189	VAL	3.2
1	A	41	GLU	3.2
1	G	18	GLU	3.2
1	G	222	GLU	3.2
1	E	248	VAL	3.2
1	E	195	SER	3.2
1	C	252	GLY	3.1
1	G	193	PRO	3.1
1	G	274	TRP	3.1
1	G	227	ASP	3.1
1	E	187	ALA	3.1
1	A	175	GLY	3.1
1	C	181	ARG	3.1
1	E	220	ASN	3.1
1	A	274	TRP	3.1
1	E	181	ARG	3.1
1	G	252	GLY	3.0
1	C	193	PRO	3.0
1	A	249	VAL	3.0
1	G	90	GLY	3.0
1	E	188	HIS	2.9
1	A	16	GLY	2.9
1	G	40	ALA	2.9
1	C	251	LEU	2.9
1	C	249	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	224	LEU	2.9
1	C	276	PRO	2.9
1	G	45	TYR	2.8
1	E	176	ASN	2.8
1	E	182	THR	2.8
1	G	219	LEU	2.8
1	A	253	LYS	2.8
1	C	197	GLY	2.8
1	A	62	ARG	2.7
1	A	51	TRP	2.7
1	G	273	ARG	2.7
1	G	57	PRO	2.7
1	G	16	GLY	2.6
1	G	42	ASN	2.6
1	A	181	ARG	2.6
1	G	248	VAL	2.6
1	A	219	LEU	2.6
1	C	211	ALA	2.5
1	G	58	GLU	2.5
2	H	48	LYS	2.5
1	A	60	TRP	2.5
1	A	224	LEU	2.5
1	E	258	THR	2.5
1	C	224	LEU	2.4
2	H	39	MET	2.4
1	A	44	ARG	2.4
1	A	200	THR	2.4
1	G	54	GLN	2.4
1	G	41	GLU	2.3
1	G	194	ARG	2.3
1	G	192	HIS	2.3
1	G	176	ASN	2.3
2	B	44	LYS	2.3
1	A	101	CYS	2.2
1	A	59	TYR	2.2
1	G	181	ARG	2.2
1	A	49	ALA	2.2
1	A	52	MET	2.2
1	C	18	GLU	2.2
1	G	257	TYR	2.2
1	E	197	GLY	2.2
2	D	19	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	107	TRP	2.1
1	E	217	TRP	2.1
2	D	44	LYS	2.1
2	B	47	PRO	2.1
1	G	247	VAL	2.1
1	E	194	ARG	2.1
1	G	53	GLU	2.1
1	E	273	ARG	2.1
1	C	176	ASN	2.1
1	A	197	GLY	2.1
1	A	194	ARG	2.1
1	C	257	TYR	2.1
1	G	221	GLY	2.1
2	H	47	PRO	2.0
1	A	79	ARG	2.0
1	E	42	ASN	2.0
1	G	23	ILE	2.0
2	B	49	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	341	6/6	0.62	0.19	51,60,64,65	0
5	GOL	B	100	6/6	0.83	0.26	58,65,75,78	0
5	GOL	H	101	6/6	0.85	0.26	48,58,59,66	0
4	SO4	C	339	5/5	0.89	0.26	56,61,74,80	0
5	GOL	A	340	6/6	0.90	0.45	41,54,66,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	E	340	6/6	0.90	0.16	35,50,56,59	0
4	SO4	F	100	5/5	0.90	0.33	68,70,84,91	0
5	GOL	E	341	6/6	0.91	0.10	46,49,54,73	0
5	GOL	H	100	6/6	0.92	0.17	50,53,60,65	0
4	SO4	E	339	5/5	0.94	0.16	66,70,76,84	0
4	SO4	A	339	5/5	0.96	0.23	50,70,79,88	0

6.5 Other polymers (i)

There are no such residues in this entry.