



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:03 PM UTC

PDB ID : 3A0K / pdb_00003a0k
Title : Crystal structure of an antinflamatory legume lectin from Cymbosema roseum seeds
Authors : Rocha, B.A.M.; Delatorre, P.; Marinho, E.S.; Benevides, R.G.; Moura, T.R.; Souza, L.A.G.; Nascimento, K.S.; Sampaio, A.H.; Cavada, B.S.
Deposited on : 2009-03-20
Resolution : 1.80 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

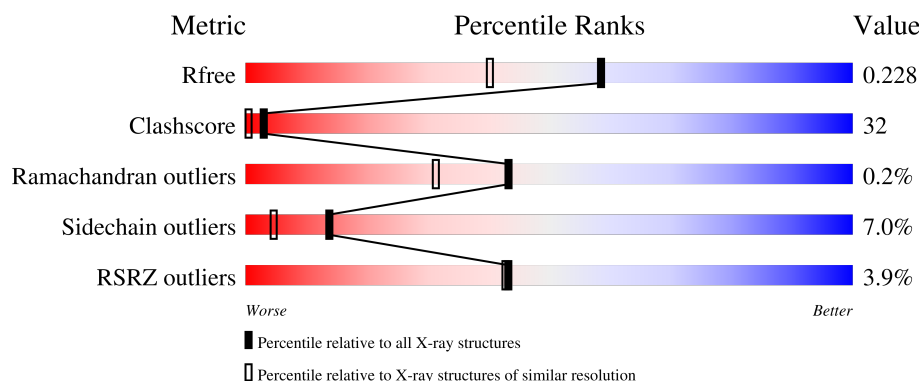
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

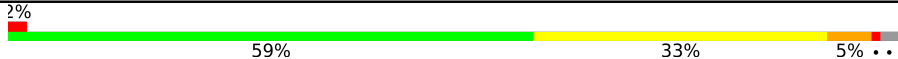
The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	237	
1	C	237	
1	E	237	
1	G	237	

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	ABA	E	240	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7804 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 *Cymbosema roseum* mannose-specific lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1752	1105	288	358	1			
1	C	232	Total	C	N	O	S	0	0	0
			1752	1105	288	358	1			
1	E	237	Total	C	N	O	S	0	0	0
			1787	1125	294	367	1			
1	G	237	Total	C	N	O	S	0	0	0
			1787	1125	294	367	1			

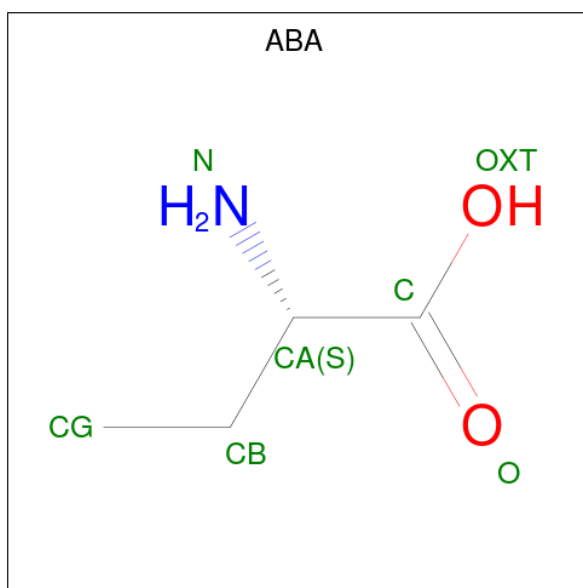
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	G	1	Total	Mn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ALPHA-AMINOBUTYRIC ACID (CCD ID: ABA) (formula: $C_4H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			6	4	1	1		
4	G	1	Total	C	N	O	0	0
			6	4	1	1		

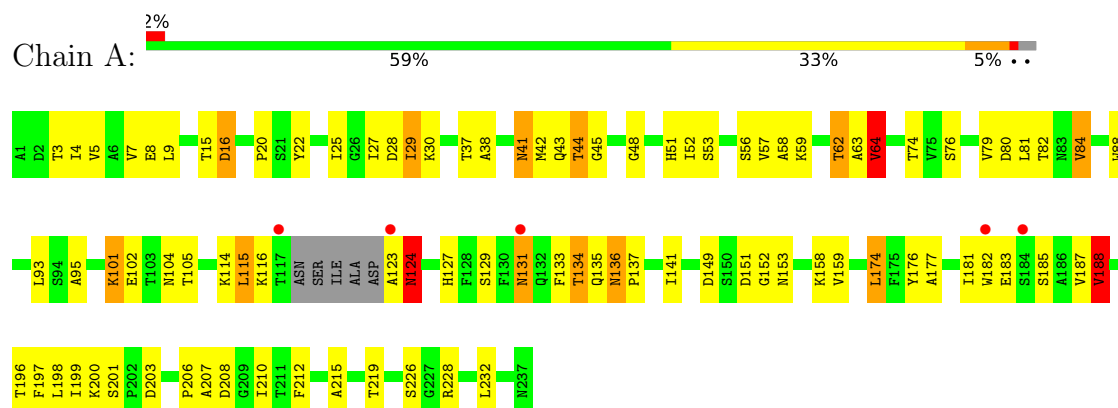
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	190	Total	O	0	0
			190	190		
5	C	150	Total	O	0	0
			150	150		
5	E	167	Total	O	0	0
			167	167		
5	G	199	Total	O	0	0
			199	199		

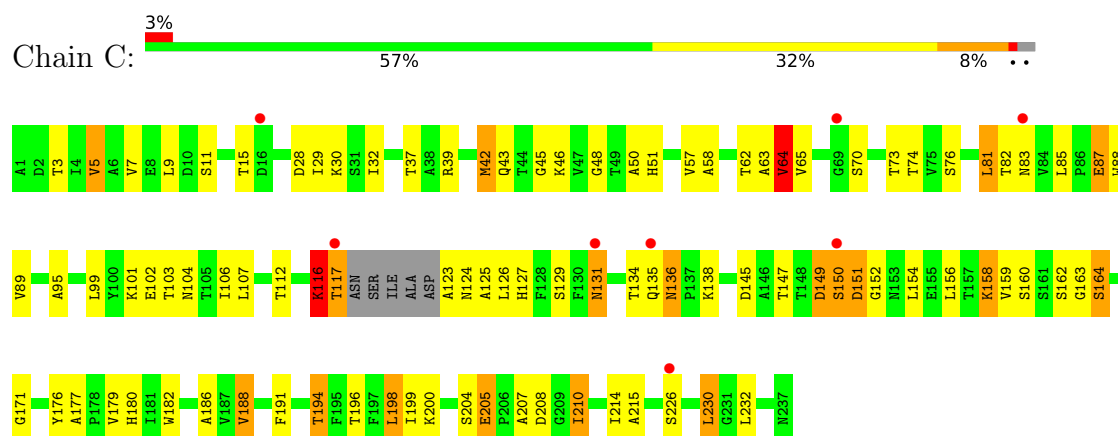
3 Residue-property plots

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

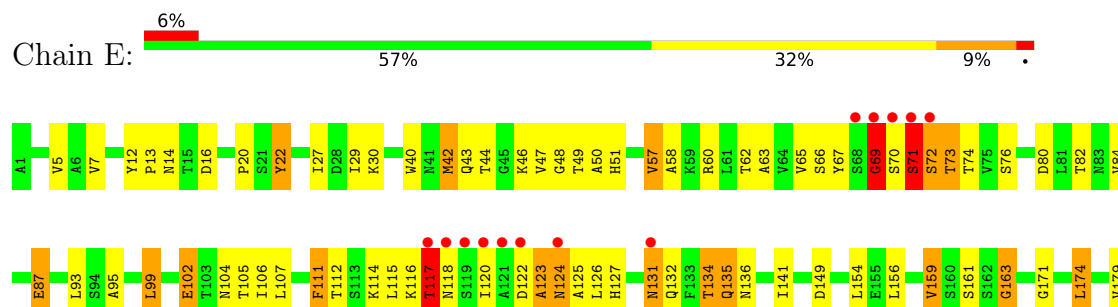
- Molecule 1: *Cymbosema roseum* mannose-specific lectin



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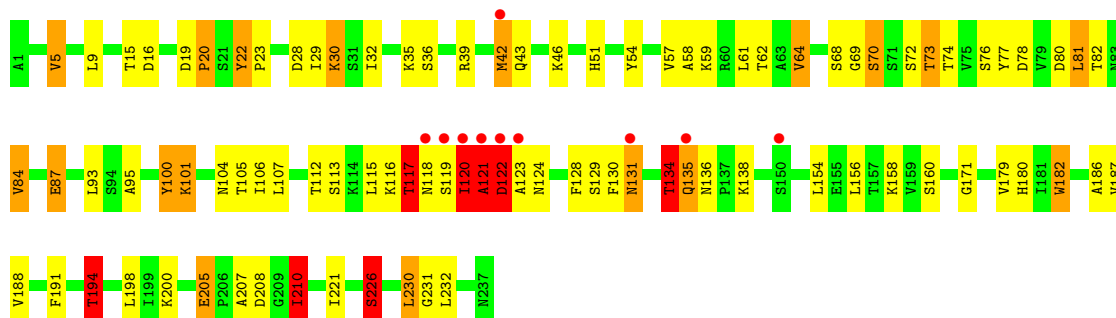


- Molecule 1: *Cymbosema roseum* mannose-specific lectin





- Molecule 1: *Cymbosema roseum* mannose-specific lectin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.03Å 103.07Å 122.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.12 – 1.80 33.12 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (33.12-1.80) 98.2 (33.12-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 1.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.182 , 0.235 0.177 , 0.228	Depositor DCC
R_{free} test set	3952 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7804	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ABA, MN, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.55	9/1791 (0.5%)	1.57	15/2443 (0.6%)
1	C	1.46	8/1791 (0.4%)	1.56	20/2443 (0.8%)
1	E	1.55	9/1827 (0.5%)	1.61	21/2494 (0.8%)
1	G	1.66	20/1827 (1.1%)	1.91	28/2494 (1.1%)
All	All	1.56	46/7236 (0.6%)	1.67	84/9874 (0.9%)

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	C	0	1
1	E	0	2
1	G	0	5
All	All	0	8

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	120	ILE	C-N	16.19	1.55	1.33
1	G	134	THR	C-N	11.68	1.51	1.33
1	E	12	TYR	CA-C	-7.76	1.46	1.52
1	G	123	ALA	CA-C	-7.72	1.41	1.52
1	G	194	THR	CA-C	-7.06	1.44	1.52
1	G	123	ALA	C-N	6.37	1.42	1.33
1	A	16	ASP	CB-CG	-6.23	1.36	1.52
1	A	181	ILE	CA-CB	-6.23	1.47	1.54
1	G	124	ASN	C-O	-6.22	1.16	1.23
1	G	105	THR	C-O	-6.16	1.16	1.24
1	A	115	LEU	CB-CG	-6.11	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	122	ASP	C-O	-5.98	1.16	1.24
1	G	179	VAL	N-CA	-5.93	1.39	1.46
1	G	123	ALA	C-O	-5.87	1.16	1.23
1	E	49	THR	CA-C	-5.85	1.45	1.52
1	G	221	ILE	CA-CB	-5.81	1.46	1.54
1	E	111	PHE	N-CA	-5.78	1.39	1.46
1	C	116	LYS	CB-CG	5.71	1.69	1.52
1	C	136	ASN	C-O	-5.64	1.18	1.24
1	E	159	VAL	C-O	-5.60	1.18	1.24
1	C	180	HIS	C-O	-5.57	1.16	1.23
1	E	22	TYR	N-CA	-5.55	1.40	1.46
1	E	221	ILE	CA-CB	-5.54	1.47	1.54
1	G	210	ILE	CB-CG1	-5.46	1.42	1.53
1	C	188	VAL	CA-CB	-5.45	1.46	1.54
1	E	14	ASN	CA-C	-5.34	1.46	1.53
1	A	62	THR	CA-C	-5.30	1.46	1.52
1	A	53	SER	CA-C	-5.26	1.46	1.52
1	C	5	VAL	N-CA	-5.24	1.40	1.46
1	C	125	ALA	CA-C	-5.24	1.46	1.52
1	C	186	ALA	C-O	-5.21	1.17	1.23
1	A	3	THR	CA-C	-5.19	1.46	1.52
1	G	121	ALA	CA-CB	-5.18	1.45	1.53
1	G	226	SER	CA-CB	5.15	1.60	1.53
1	G	64	VAL	CA-C	-5.12	1.46	1.52
1	G	19	ASP	CA-C	-5.10	1.47	1.53
1	G	20	PRO	N-CA	-5.08	1.40	1.47
1	A	38	ALA	CA-CB	5.06	1.62	1.53
1	A	188	VAL	CA-C	-5.05	1.46	1.52
1	E	180	HIS	N-CA	-5.05	1.40	1.46
1	C	37	THR	CA-C	-5.05	1.46	1.52
1	E	102	GLU	CA-C	-5.04	1.46	1.52
1	G	70	SER	C-O	-5.01	1.17	1.23
1	A	84	VAL	C-O	-5.00	1.17	1.24
1	G	100	TYR	CA-CB	-5.00	1.46	1.53
1	G	182	TRP	CA-C	-5.00	1.46	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	135	GLN	CA-C-N	-23.19	93.90	122.42
1	G	135	GLN	C-N-CA	-23.19	93.90	122.42
1	G	122	ASP	CA-C-N	19.48	152.23	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	122	ASP	C-N-CA	19.48	152.23	121.26
1	E	71	SER	CB-CA-C	-15.83	90.33	109.80
1	G	135	GLN	O-C-N	15.72	144.15	122.46
1	G	122	ASP	O-C-N	-13.59	104.52	122.59
1	G	69	GLY	N-CA-C	-13.53	95.51	115.00
1	A	188	VAL	CB-CA-C	-11.72	93.75	111.80
1	E	210	ILE	CG1-CB-CG2	-10.97	77.78	110.70
1	E	72	SER	N-CA-C	10.33	126.52	110.20
1	C	149	ASP	CA-C-N	-8.92	104.54	121.66
1	C	149	ASP	C-N-CA	-8.92	104.54	121.66
1	G	134	THR	O-C-N	-8.85	110.50	122.36
1	C	150	SER	CA-CB-OG	-8.69	93.73	111.10
1	C	64	VAL	CB-CA-C	-8.66	96.83	110.69
1	A	64	VAL	CB-CA-C	-8.48	96.03	110.71
1	G	16	ASP	N-CA-CB	-8.01	98.04	110.06
1	C	150	SER	N-CA-CB	8.01	121.43	110.38
1	E	188	VAL	CB-CA-C	-7.89	96.69	111.30
1	E	117	THR	N-CA-C	-7.77	97.51	108.23
1	G	134	THR	CA-C-N	7.69	134.59	121.14
1	G	134	THR	C-N-CA	7.69	134.59	121.14
1	G	64	VAL	CG1-CB-CG2	7.57	127.46	110.80
1	A	16	ASP	CB-CG-OD1	-7.41	101.37	118.40
1	G	64	VAL	CB-CA-C	-7.34	99.20	110.50
1	A	115	LEU	CB-CA-C	-7.07	99.95	110.62
1	G	123	ALA	CB-CA-C	-6.84	100.56	110.06
1	A	64	VAL	CA-CB-CG2	6.70	121.79	110.40
1	G	121	ALA	O-C-N	6.68	131.12	122.23
1	A	15	THR	N-CA-C	-6.61	104.47	112.54
1	E	57	VAL	N-CA-C	-6.59	105.32	111.45
1	G	131	ASN	N-CA-C	-6.56	105.31	113.38
1	C	131	ASN	N-CA-C	-6.54	105.33	113.38
1	G	15	THR	CA-C-N	6.46	129.23	120.38
1	G	15	THR	C-N-CA	6.46	129.23	120.38
1	C	204	SER	N-CA-C	-6.44	105.39	113.18
1	E	42	MET	CB-CG-SD	-6.40	93.51	112.70
1	E	123	ALA	N-CA-C	-6.37	104.43	111.82
1	G	117	THR	N-CA-CB	-6.18	101.33	110.85
1	A	44	THR	CB-CA-C	6.12	119.56	109.70
1	G	123	ALA	O-C-N	6.08	131.39	123.07
1	G	84	VAL	CB-CA-C	-5.99	105.75	111.44
1	C	15	THR	N-CA-C	-5.97	105.25	112.54
1	G	5	VAL	N-CA-C	-5.92	99.96	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	99	LEU	N-CA-C	-5.90	104.43	111.69
1	C	64	VAL	CG1-CB-CG2	5.88	123.75	110.80
1	A	131	ASN	N-CA-C	-5.84	105.47	113.30
1	C	7	VAL	N-CA-C	-5.82	99.37	107.80
1	C	83	ASN	CA-C-N	-5.77	117.04	123.16
1	C	83	ASN	C-N-CA	-5.77	117.04	123.16
1	G	124	ASN	N-CA-C	-5.77	102.74	110.24
1	G	231	GLY	N-CA-C	-5.75	106.22	115.08
1	E	131	ASN	N-CA-C	-5.66	106.04	113.17
1	A	93	LEU	N-CA-C	-5.61	100.64	109.50
1	E	69	GLY	O-C-N	-5.60	115.41	122.70
1	A	16	ASP	CA-CB-CG	-5.59	107.01	112.60
1	G	30	LYS	CD-CE-NZ	-5.52	94.23	111.90
1	G	73	THR	N-CA-C	-5.51	100.42	109.40
1	E	212	PHE	N-CA-C	-5.49	100.75	109.59
1	A	136	ASN	CA-C-N	-5.48	112.98	119.84
1	A	136	ASN	C-N-CA	-5.48	112.98	119.84
1	A	124	ASN	N-CA-C	-5.44	103.17	110.24
1	E	115	LEU	CB-CA-C	-5.40	102.47	110.62
1	E	124	ASN	CB-CA-C	5.37	118.63	109.99
1	C	188	VAL	CB-CA-C	-5.32	101.50	110.71
1	E	87	GLU	CB-CG-CD	-5.30	103.59	112.60
1	A	187	VAL	N-CA-C	-5.24	104.97	112.35
1	G	22	TYR	N-CA-C	-5.22	102.13	108.14
1	E	224	GLY	N-CA-C	-5.22	108.07	115.43
1	E	47	VAL	CA-C-N	-5.22	117.05	122.69
1	E	47	VAL	C-N-CA	-5.22	117.05	122.69
1	C	205	GLU	CB-CA-C	-5.19	101.33	111.29
1	C	9	LEU	N-CA-C	-5.17	97.43	107.62
1	A	212	PHE	N-CA-C	-5.17	101.27	109.59
1	E	135	GLN	CA-C-N	-5.16	116.81	123.16
1	E	135	GLN	C-N-CA	-5.16	116.81	123.16
1	C	103	THR	N-CA-C	-5.16	102.84	110.48
1	G	205	GLU	CB-CG-CD	-5.14	103.87	112.60
1	C	87	GLU	N-CA-CB	5.10	118.19	110.28
1	C	64	VAL	CA-CB-CG2	5.09	119.06	110.40
1	C	65	VAL	N-CA-C	-5.08	100.80	108.12
1	C	151	ASP	N-CA-C	-5.04	105.37	113.28
1	E	163	GLY	N-CA-C	-5.02	108.31	115.64

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	116	LYS	Peptide
1	E	69	GLY	Peptide
1	E	71	SER	Peptide
1	G	120	ILE	Peptide
1	G	121	ALA	Peptide
1	G	122	ASP	Peptide
1	G	134	THR	Mainchain
1	G	68	SER	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	1752	0	1701	114	2
1	C	1752	0	1703	146	0
1	E	1787	0	1735	133	3
1	G	1787	0	1732	136	1
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	E	6	0	8	10	0
4	G	6	0	8	2	0
5	A	190	0	0	11	3
5	C	150	0	0	9	1
5	E	167	0	0	16	2
5	G	199	0	0	20	8
All	All	7804	0	6887	447	10

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 32.

All (447) 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:E:123:ALA:HA	1:G:131:ASN:ND2	1.20	1.42
1:A:95:ALA:CB	1:A:210:ILE:HG22	1.52	1.39
1:A:131:ASN:OD1	1:C:123:ALA:CA	1.68	1.39
4:E:240:ABA:HA	5:E:540:HOH:O	1.16	1.32
1:E:67:TYR:HD2	1:E:71:SER:OG	1.01	1.31
1:E:71:SER:HB2	5:E:327:HOH:O	1.19	1.29
1:E:226:SER:HB3	5:E:585:HOH:O	1.34	1.28
1:C:95:ALA:CB	1:C:210:ILE:HG22	1.65	1.26
1:A:123:ALA:N	1:C:131:ASN:HD22	1.31	1.26
1:E:43:GLN:NE2	1:E:70:SER:HB2	1.48	1.25
1:A:226:SER:HB2	5:A:264:HOH:O	1.35	1.24
1:C:134:THR:HG22	1:C:136:ASN:H	1.06	1.20
1:G:87:GLU:OE1	1:G:182:TRP:HB3	1.39	1.20
1:E:123:ALA:CA	1:G:131:ASN:ND2	2.03	1.19
1:C:42:MET:CE	5:C:665:HOH:O	1.65	1.19
1:C:42:MET:HE3	5:C:665:HOH:O	1.18	1.17
1:E:124:ASN:OD1	1:G:130:PHE:HA	1.38	1.17
1:A:64:VAL:HG21	1:G:188:VAL:HG21	1.27	1.16
1:A:134:THR:HG22	5:A:317:HOH:O	1.45	1.14
1:E:117:THR:HG23	1:E:118:ASN:H	1.10	1.13
1:G:198:LEU:CD1	1:G:200:LYS:HG3	1.78	1.13
1:C:116:LYS:HD2	1:C:117:THR:OG1	1.46	1.11
1:C:226:SER:OG	5:C:690:HOH:O	1.69	1.10
1:G:134:THR:HG22	1:G:136:ASN:H	1.05	1.10
1:A:131:ASN:OD1	1:C:123:ALA:HA	0.89	1.06
1:E:62:THR:HG22	1:E:76:SER:OG	1.55	1.06
1:A:123:ALA:N	1:C:131:ASN:ND2	2.04	1.05
1:C:131:ASN:OD1	1:E:120:ILE:HD11	1.56	1.05
1:E:71:SER:CB	5:E:327:HOH:O	1.82	1.05
1:A:123:ALA:HB3	1:C:131:ASN:HD21	1.16	1.03
1:G:198:LEU:HD11	1:G:200:LYS:HG3	1.42	1.02
1:A:134:THR:HG21	1:C:88:TRP:HZ2	1.21	1.02
1:E:117:THR:HG23	1:E:118:ASN:N	1.69	1.02
1:A:95:ALA:HB2	1:A:210:ILE:CG2	1.90	1.01
1:A:131:ASN:CG	1:C:123:ALA:HA	1.85	1.01
1:C:95:ALA:HB2	1:C:210:ILE:HG22	1.03	1.01
1:C:150:SER:O	1:C:151:ASP:HB2	1.59	1.00
1:A:176:TYR:CE1	1:C:176:TYR:CE1	2.50	1.00
1:E:67:TYR:CD2	1:E:71:SER:OG	1.89	1.00
1:E:123:ALA:O	1:E:124:ASN:CG	2.06	0.99
1:A:95:ALA:HB2	1:A:210:ILE:HG22	1.00	0.98
1:A:64:VAL:HG21	1:G:188:VAL:CG2	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:THR:HG23	5:A:250:HOH:O	1.62	0.98
1:E:205:GLU:HG2	5:E:263:HOH:O	1.63	0.98
1:G:134:THR:HG22	1:G:136:ASN:N	1.77	0.98
1:C:95:ALA:HB2	1:C:210:ILE:CG2	1.95	0.97
1:G:187:VAL:HG12	1:G:188:VAL:HG23	1.47	0.97
1:A:95:ALA:CB	1:A:210:ILE:CG2	2.43	0.97
1:C:135:GLN:H	1:C:135:GLN:NE2	1.66	0.93
1:C:159:VAL:CG1	1:C:163:GLY:HA2	1.97	0.93
5:E:442:HOH:O	1:G:138:LYS:HE2	1.68	0.93
1:G:82:THR:HG1	1:G:182:TRP:CG	1.85	0.93
1:E:123:ALA:HA	1:G:131:ASN:HD22	1.32	0.92
1:C:135:GLN:H	1:C:135:GLN:CD	1.75	0.92
1:A:104:ASN:OD1	1:A:210:ILE:HG23	1.70	0.92
1:C:64:VAL:HG13	1:C:74:THR:HG22	1.51	0.91
1:E:123:ALA:HA	1:G:131:ASN:HD21	1.33	0.91
1:C:51:HIS:HD2	1:C:194:THR:CG2	1.83	0.91
1:E:43:GLN:NE2	1:E:70:SER:CB	2.33	0.91
1:G:28:ASP:O	1:G:29:ILE:HD13	1.71	0.91
1:G:198:LEU:HD11	1:G:200:LYS:CG	2.02	0.90
1:A:64:VAL:CG2	1:G:188:VAL:HG21	2.02	0.89
1:G:198:LEU:HD13	1:G:200:LYS:HG3	1.53	0.89
1:A:57:VAL:HG23	1:A:188:VAL:HG13	1.52	0.89
1:A:95:ALA:HB1	1:A:210:ILE:HG22	1.54	0.89
1:A:64:VAL:HG13	1:A:74:THR:HG22	1.54	0.88
1:G:120:ILE:HG22	1:G:121:ALA:O	1.73	0.88
1:G:87:GLU:CD	5:G:563:HOH:O	2.15	0.88
1:C:150:SER:OG	1:C:151:ASP:N	1.85	0.87
1:G:42:MET:HB2	5:G:599:HOH:O	1.72	0.87
1:G:134:THR:CG2	1:G:136:ASN:H	1.87	0.87
1:A:176:TYR:HE1	1:C:176:TYR:CE1	1.93	0.87
1:A:123:ALA:HB3	1:C:131:ASN:ND2	1.90	0.86
1:E:159:VAL:CG1	1:E:163:GLY:HA2	2.05	0.86
1:C:134:THR:HG22	1:C:136:ASN:N	1.91	0.86
1:C:104:ASN:OD1	1:C:210:ILE:HG23	1.76	0.85
1:G:80:ASP:OD1	1:G:82:THR:HG22	1.77	0.85
1:C:159:VAL:CG1	1:C:163:GLY:C	2.50	0.85
1:G:51:HIS:HD2	1:G:194:THR:CG2	1.88	0.85
1:E:57:VAL:HG23	1:E:188:VAL:HG13	1.60	0.84
1:C:159:VAL:HG13	1:C:163:GLY:C	2.02	0.83
1:G:62:THR:HG22	1:G:76:SER:OG	1.78	0.83
1:A:176:TYR:CE1	1:C:176:TYR:HE1	1.95	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ASP:O	1:C:29:ILE:HD13	1.78	0.83
1:E:43:GLN:HE21	1:E:70:SER:HB2	1.44	0.83
1:G:28:ASP:C	1:G:29:ILE:HD13	2.04	0.83
1:E:117:THR:CG2	1:E:118:ASN:N	2.41	0.82
1:E:124:ASN:HB3	4:E:240:ABA:N	1.94	0.82
1:E:43:GLN:HE22	1:E:70:SER:N	1.78	0.81
1:G:42:MET:HG2	5:G:541:HOH:O	1.80	0.81
1:A:123:ALA:CB	1:C:131:ASN:HD21	1.92	0.81
1:G:82:THR:HG1	1:G:182:TRP:CD1	1.99	0.81
1:C:159:VAL:HG12	1:C:163:GLY:HA2	1.63	0.81
1:C:95:ALA:CB	1:C:210:ILE:CG2	2.55	0.79
1:C:159:VAL:CG1	1:C:163:GLY:CA	2.60	0.79
1:A:123:ALA:CA	1:C:131:ASN:ND2	2.44	0.79
1:A:134:THR:HG21	1:C:88:TRP:CZ2	2.12	0.78
1:E:131:ASN:HD22	1:G:122:ASP:C	1.91	0.78
1:A:41:ASN:H	1:A:41:ASN:HD22	1.31	0.77
1:A:123:ALA:CB	1:C:131:ASN:ND2	2.47	0.77
1:A:82:THR:HG21	1:A:182:TRP:CD2	2.20	0.77
1:E:40:TRP:HA	1:E:73:THR:HG21	1.66	0.77
1:A:123:ALA:CA	1:C:131:ASN:HD22	1.98	0.76
1:C:116:LYS:HE3	1:E:51:HIS:HE1	1.50	0.76
1:E:159:VAL:HG13	1:E:163:GLY:C	2.11	0.76
1:G:43:GLN:OE1	1:G:46:LYS:CD	2.33	0.75
1:E:123:ALA:CA	1:G:131:ASN:HD22	1.88	0.75
1:C:62:THR:HG21	1:E:58:ALA:HB2	1.69	0.75
1:C:51:HIS:HD2	1:C:194:THR:HG21	1.52	0.74
4:E:240:ABA:C	5:E:558:HOH:O	2.35	0.74
1:A:131:ASN:OD1	1:C:123:ALA:C	2.32	0.73
1:G:51:HIS:CD2	1:G:194:THR:HB	2.23	0.73
1:C:159:VAL:HG11	1:C:163:GLY:HA2	1.70	0.73
1:A:41:ASN:H	1:A:41:ASN:ND2	1.85	0.73
1:A:104:ASN:OD1	1:A:210:ILE:CG2	2.36	0.73
1:G:87:GLU:CG	5:G:563:HOH:O	2.37	0.73
1:G:23:PRO:HG2	1:G:42:MET:HE2	1.71	0.72
1:E:114:LYS:HG2	1:E:122:ASP:OD2	1.89	0.72
1:G:198:LEU:HD11	1:G:200:LYS:CD	2.20	0.71
1:C:149:ASP:OD2	1:C:150:SER:O	2.09	0.71
1:G:30:LYS:HD3	1:G:84:VAL:HG13	1.71	0.71
1:A:101:LYS:NZ	1:A:203:ASP:OD1	2.24	0.71
1:G:205:GLU:OE2	5:G:623:HOH:O	2.08	0.71
1:G:226:SER:HB3	5:G:347:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ASN:HB3	1:C:210:ILE:HG21	1.73	0.70
1:E:123:ALA:O	1:E:124:ASN:OD1	2.09	0.70
1:E:123:ALA:C	1:G:131:ASN:HD22	1.99	0.70
1:E:124:ASN:HB3	4:E:240:ABA:CA	2.21	0.70
1:G:51:HIS:HD2	1:G:194:THR:HG21	1.56	0.70
1:G:87:GLU:HG3	5:G:563:HOH:O	1.92	0.70
1:G:113:SER:OG	4:G:240:ABA:HG2	1.92	0.70
1:C:135:GLN:CD	1:C:135:GLN:N	2.46	0.69
1:E:66:SER:HA	1:E:71:SER:O	1.93	0.69
1:C:62:THR:HG22	1:C:76:SER:OG	1.92	0.69
1:G:42:MET:CB	5:G:541:HOH:O	2.40	0.69
1:G:43:GLN:OE1	1:G:46:LYS:HD3	1.91	0.68
1:C:116:LYS:CD	1:C:117:THR:OG1	2.35	0.68
1:G:226:SER:CB	5:G:347:HOH:O	2.41	0.68
1:E:43:GLN:HE22	1:E:70:SER:HB2	1.53	0.68
1:C:51:HIS:CD2	1:C:194:THR:HB	2.29	0.68
1:E:226:SER:CB	5:E:585:HOH:O	2.07	0.67
1:C:116:LYS:CD	1:C:117:THR:HA	2.23	0.67
1:C:95:ALA:HB1	1:C:210:ILE:HG22	1.71	0.67
1:C:126:LEU:CD2	1:C:179:VAL:HG22	2.24	0.67
4:E:240:ABA:HG1	1:G:128:PHE:HB2	1.77	0.67
1:C:58:ALA:HA	1:E:62:THR:HG21	1.75	0.67
1:A:151:ASP:HB2	5:A:692:HOH:O	1.94	0.67
1:A:29:ILE:HD12	1:A:79:VAL:HG21	1.76	0.66
1:C:150:SER:O	1:C:151:ASP:CB	2.34	0.66
1:G:187:VAL:C	1:G:188:VAL:HG23	2.20	0.66
1:G:32:ILE:HD11	1:G:230:LEU:HD22	1.76	0.66
1:C:51:HIS:CD2	1:C:194:THR:CG2	2.74	0.66
1:A:62:THR:HG22	1:A:76:SER:OG	1.96	0.66
1:A:95:ALA:HB1	1:A:210:ILE:CG2	2.18	0.65
1:E:82:THR:HG22	1:E:182:TRP:CG	2.31	0.65
1:C:158:LYS:CB	1:C:158:LYS:HZ2	2.09	0.65
1:C:107:LEU:HD12	1:C:107:LEU:N	2.11	0.65
1:C:58:ALA:CA	1:E:62:THR:HG21	2.27	0.65
1:E:159:VAL:CG1	1:E:163:GLY:CA	2.75	0.64
1:C:32:ILE:HD11	1:C:230:LEU:HD22	1.79	0.64
1:C:51:HIS:CD2	1:C:194:THR:HG21	2.31	0.64
1:C:62:THR:HG21	1:E:58:ALA:CA	2.28	0.64
1:C:57:VAL:HG13	1:E:74:THR:HG23	1.80	0.64
1:C:87:GLU:HB3	1:C:182:TRP:O	1.98	0.64
1:G:156:LEU:O	1:G:171:GLY:HA3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:THR:HG22	1:C:182:TRP:HB2	1.79	0.64
1:E:123:ALA:CA	1:G:131:ASN:HD21	1.96	0.63
1:E:123:ALA:HA	1:G:131:ASN:CG	2.14	0.63
1:C:62:THR:HG21	1:E:58:ALA:CB	2.29	0.62
1:A:88:TRP:CG	1:C:138:LYS:HD2	2.35	0.62
1:E:159:VAL:HG11	1:E:163:GLY:HA2	1.82	0.61
1:A:58:ALA:CA	1:G:62:THR:HG21	2.30	0.61
1:C:158:LYS:HD3	5:C:389:HOH:O	2.00	0.61
1:E:124:ASN:OD1	1:G:130:PHE:CA	2.32	0.61
1:E:43:GLN:HE22	1:E:70:SER:CA	2.14	0.61
1:E:131:ASN:ND2	1:G:122:ASP:C	2.57	0.61
1:E:82:THR:HG22	1:E:182:TRP:CB	2.31	0.61
1:A:20:PRO:HB2	1:A:22:TYR:CZ	2.36	0.60
1:C:28:ASP:C	1:C:29:ILE:HD13	2.26	0.60
1:A:176:TYR:CD1	1:C:176:TYR:CE1	2.88	0.60
1:E:116:LYS:HG2	1:E:122:ASP:OD1	2.02	0.60
1:C:104:ASN:HB3	1:C:210:ILE:CG2	2.33	0.59
1:E:43:GLN:HE22	1:E:70:SER:H	1.48	0.59
1:C:158:LYS:CB	1:C:158:LYS:NZ	2.64	0.58
1:A:41:ASN:ND2	1:A:41:ASN:N	2.50	0.58
1:G:64:VAL:HG13	1:G:74:THR:HG22	1.85	0.58
1:G:82:THR:HG21	5:G:634:HOH:O	2.02	0.58
1:E:132:GLN:HE22	1:G:117:THR:HB	1.68	0.58
1:C:207:ALA:HB1	1:C:208:ASP:HA	1.85	0.58
1:A:58:ALA:HA	1:G:62:THR:HG21	1.87	0.57
1:E:132:GLN:CD	1:G:120:ILE:HG13	2.30	0.57
1:A:82:THR:CG2	1:A:182:TRP:CD2	2.86	0.57
1:C:116:LYS:HD2	1:C:117:THR:CA	2.34	0.57
1:E:126:LEU:HD22	1:E:179:VAL:HG22	1.86	0.57
1:E:159:VAL:HG12	1:E:163:GLY:HA2	1.87	0.57
1:G:51:HIS:CD2	1:G:194:THR:CG2	2.80	0.57
1:E:62:THR:CG2	1:E:76:SER:OG	2.42	0.56
1:A:30:LYS:HA	5:A:323:HOH:O	2.04	0.56
1:A:176:TYR:CD1	1:C:176:TYR:CD1	2.93	0.56
1:C:116:LYS:HD2	1:C:117:THR:CB	2.33	0.56
1:E:131:ASN:HB3	1:G:120:ILE:HG21	1.87	0.56
1:C:106:ILE:HB	1:C:154:LEU:HB3	1.86	0.56
1:C:116:LYS:HD2	1:C:117:THR:HA	1.86	0.56
1:C:158:LYS:HZ2	1:C:158:LYS:HB2	1.69	0.56
1:G:43:GLN:OE1	1:G:46:LYS:HD2	2.05	0.56
1:A:102:GLU:HB2	1:A:199:ILE:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD21	1:A:219:THR:HG23	1.88	0.56
1:G:51:HIS:CD2	1:G:194:THR:HG21	2.39	0.56
1:A:136:ASN:HB3	5:A:582:HOH:O	2.04	0.55
1:C:159:VAL:HG12	1:C:163:GLY:CA	2.30	0.55
1:C:156:LEU:O	1:C:171:GLY:HA3	2.05	0.55
1:E:134:THR:HG22	1:E:136:ASN:H	1.69	0.55
4:E:240:ABA:HB3	1:G:130:PHE:CE1	2.41	0.55
1:G:82:THR:OG1	1:G:182:TRP:CG	2.58	0.55
1:C:81:LEU:HG	1:C:85:LEU:HD12	1.88	0.55
1:C:82:THR:HG22	1:C:182:TRP:CB	2.37	0.55
1:G:39:ARG:O	1:G:73:THR:HG23	2.06	0.55
1:A:104:ASN:CG	1:A:210:ILE:CG2	2.79	0.55
1:E:125:ALA:O	4:E:240:ABA:HB2	2.06	0.55
1:G:180:HIS:H	4:G:240:ABA:HN2	1.52	0.55
1:E:159:VAL:CG1	1:E:163:GLY:C	2.79	0.55
1:E:60:ARG:HG2	1:E:62:THR:CG2	2.37	0.54
1:A:51:HIS:HB2	1:A:64:VAL:HG23	1.90	0.54
1:G:70:SER:OG	5:G:568:HOH:O	2.02	0.54
1:C:39:ARG:O	1:C:73:THR:HG23	2.07	0.54
1:G:198:LEU:HD11	1:G:200:LYS:HD3	1.87	0.54
1:A:114:LYS:HD3	1:A:116:LYS:NZ	2.23	0.54
1:C:62:THR:CG2	1:E:58:ALA:HB2	2.37	0.54
1:A:104:ASN:HB3	1:A:210:ILE:HG21	1.90	0.54
1:C:64:VAL:HG21	1:E:188:VAL:HG22	1.90	0.54
1:C:207:ALA:CB	1:C:208:ASP:HA	2.38	0.54
1:A:95:ALA:HB1	1:A:104:ASN:CG	2.33	0.54
1:A:134:THR:CG2	1:C:88:TRP:HZ2	2.08	0.53
1:G:187:VAL:O	1:G:188:VAL:CG2	2.56	0.53
1:E:205:GLU:CG	5:E:263:HOH:O	2.34	0.53
1:E:82:THR:HG23	5:E:278:HOH:O	2.09	0.53
1:G:5:VAL:HG13	1:G:29:ILE:HD12	1.89	0.53
1:G:187:VAL:C	1:G:188:VAL:CG2	2.81	0.53
1:A:62:THR:HG21	1:G:58:ALA:CA	2.38	0.53
1:E:106:ILE:HB	1:E:154:LEU:HB3	1.91	0.53
1:C:198:LEU:HD22	1:C:200:LYS:HG3	1.89	0.53
1:E:60:ARG:HG2	1:E:62:THR:HG23	1.90	0.53
1:A:82:THR:HG21	1:A:182:TRP:CE3	2.43	0.53
1:G:23:PRO:HB2	1:G:42:MET:HG3	1.89	0.53
1:E:43:GLN:HE22	1:E:70:SER:CB	2.13	0.52
1:C:57:VAL:CG1	1:E:74:THR:HG23	2.40	0.52
1:C:158:LYS:HE3	5:C:389:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:LEU:HB2	4:E:240:ABA:HG3	1.92	0.51
1:C:5:VAL:HG13	1:C:29:ILE:CD1	2.39	0.51
1:C:64:VAL:HG13	1:C:74:THR:CG2	2.32	0.51
1:E:126:LEU:HG	1:E:127:HIS:N	2.20	0.51
1:E:123:ALA:C	1:G:131:ASN:ND2	2.59	0.51
1:G:23:PRO:CB	1:G:42:MET:HG3	2.41	0.51
1:E:71:SER:OG	1:E:71:SER:O	2.26	0.51
1:E:131:ASN:HD21	1:G:122:ASP:CB	2.24	0.51
1:G:82:THR:CG2	5:G:634:HOH:O	2.57	0.51
1:A:127:HIS:HB3	1:C:127:HIS:HB3	1.92	0.51
1:A:42:MET:HE1	1:A:206:PRO:HG2	1.93	0.50
1:A:105:THR:O	1:A:197:PHE:HA	2.11	0.50
1:C:104:ASN:CG	1:C:210:ILE:HG23	2.35	0.50
1:A:51:HIS:NE2	1:G:116:LYS:HG2	2.27	0.50
1:C:82:THR:HG22	1:C:182:TRP:CG	2.46	0.50
1:C:159:VAL:HG13	1:C:163:GLY:O	2.11	0.50
1:C:95:ALA:HB1	1:C:210:ILE:CG2	2.37	0.50
1:C:45:GLY:HA2	1:C:200:LYS:HG2	1.93	0.50
1:G:106:ILE:HB	1:G:154:LEU:HB3	1.94	0.50
1:E:132:GLN:NE2	1:G:120:ILE:HG13	2.27	0.50
1:A:62:THR:HG21	1:G:58:ALA:HB2	1.93	0.50
1:E:124:ASN:HA	1:G:129:SER:O	2.11	0.50
1:C:51:HIS:CD2	1:C:194:THR:CB	2.94	0.49
1:E:134:THR:HB	5:E:598:HOH:O	2.11	0.49
1:A:64:VAL:HG13	1:A:74:THR:CG2	2.36	0.49
1:C:104:ASN:OD1	1:C:210:ILE:CG2	2.57	0.49
1:C:126:LEU:HD23	1:C:179:VAL:HG22	1.93	0.49
1:C:57:VAL:HG13	1:E:74:THR:CG2	2.42	0.49
1:A:134:THR:OG1	1:A:135:GLN:N	2.45	0.49
1:A:134:THR:HG23	1:A:137:PRO:HA	1.94	0.49
1:G:107:LEU:HD12	1:G:107:LEU:N	2.28	0.49
1:G:64:VAL:HG12	1:G:72:SER:HB2	1.95	0.48
1:E:180:HIS:CE1	1:G:134:THR:OG1	2.66	0.48
1:G:51:HIS:HD2	1:G:194:THR:CB	2.24	0.48
1:C:62:THR:HG21	1:E:58:ALA:HA	1.95	0.48
1:E:131:ASN:HB3	1:G:120:ILE:CG2	2.44	0.48
1:G:118:ASN:OD1	1:G:119:SER:N	2.46	0.48
1:A:59:LYS:HE3	1:A:80:ASP:OD2	2.13	0.48
1:A:123:ALA:O	1:A:124:ASN:C	2.56	0.48
1:E:42:MET:CE	1:E:206:PRO:HG2	2.43	0.48
1:G:62:THR:HG22	1:G:76:SER:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:ASN:ND2	1:G:122:ASP:CA	2.77	0.48
1:A:134:THR:CG2	1:A:137:PRO:HA	2.44	0.48
1:G:23:PRO:HG2	1:G:42:MET:CE	2.43	0.48
1:G:95:ALA:HB1	1:G:104:ASN:CG	2.39	0.48
1:E:141:ILE:HB	1:E:174:LEU:HB2	1.96	0.48
1:A:129:SER:O	1:C:124:ASN:HA	2.14	0.48
1:A:176:TYR:HD1	1:C:176:TYR:CD1	2.31	0.48
1:A:9:LEU:HD12	1:A:9:LEU:N	2.29	0.48
1:A:176:TYR:HD1	1:C:176:TYR:HD1	1.62	0.47
1:C:42:MET:HE1	5:C:665:HOH:O	1.63	0.47
1:E:123:ALA:CB	1:G:131:ASN:HD21	2.27	0.47
1:G:54:TYR:CD1	1:G:81:LEU:HD22	2.49	0.47
1:E:134:THR:HG22	1:E:136:ASN:N	2.30	0.47
1:A:114:LYS:HD3	1:A:116:LYS:HZ1	1.79	0.47
1:C:51:HIS:HB2	1:C:64:VAL:HG23	1.96	0.47
1:E:67:TYR:N	1:E:71:SER:O	2.47	0.47
1:E:112:THR:O	1:E:191:PHE:HA	2.15	0.47
1:G:51:HIS:CD2	1:G:194:THR:CB	2.96	0.47
1:E:50:ALA:O	1:E:194:THR:HA	2.14	0.47
1:A:58:ALA:HB2	1:G:62:THR:HG21	1.97	0.47
1:E:217:THR:HG21	1:G:138:LYS:HE3	1.97	0.47
1:E:122:ASP:OD2	1:E:125:ALA:HB2	2.15	0.46
1:A:176:TYR:CE1	1:C:176:TYR:CD1	3.01	0.46
1:E:71:SER:HB3	5:E:290:HOH:O	2.15	0.46
1:G:5:VAL:HG13	1:G:29:ILE:CD1	2.46	0.46
1:G:100:TYR:HB2	1:G:207:ALA:HB3	1.97	0.46
1:G:134:THR:CG2	1:G:135:GLN:N	2.78	0.46
1:E:65:VAL:O	1:E:72:SER:HA	2.16	0.46
1:G:200:LYS:HE3	5:G:458:HOH:O	2.16	0.46
1:A:101:LYS:HZ3	1:A:101:LYS:HG2	1.55	0.46
1:C:57:VAL:HG23	1:C:188:VAL:HG13	1.96	0.46
1:G:51:HIS:HD2	1:G:194:THR:HB	1.70	0.46
1:A:62:THR:HG21	1:G:58:ALA:HA	1.97	0.46
1:C:43:GLN:HE22	1:C:70:SER:CB	2.28	0.46
1:G:42:MET:HB2	5:G:541:HOH:O	2.12	0.46
1:C:3:THR:O	1:C:215:ALA:HA	2.16	0.45
1:G:9:LEU:HB2	1:G:210:ILE:HG22	1.98	0.45
1:E:180:HIS:HE1	1:G:134:THR:OG1	1.98	0.45
1:A:25:ILE:O	1:A:37:THR:HA	2.15	0.45
1:C:116:LYS:HD3	1:C:117:THR:HA	1.96	0.45
1:G:210:ILE:HG21	1:G:210:ILE:HD13	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:HIS:HD2	1:C:194:THR:CB	2.24	0.45
1:C:149:ASP:CG	1:C:150:SER:O	2.59	0.45
1:G:39:ARG:O	1:G:73:THR:CG2	2.65	0.45
1:A:134:THR:HG23	1:A:137:PRO:CA	2.47	0.45
1:G:187:VAL:O	1:G:188:VAL:HG23	2.17	0.45
1:C:46:LYS:HA	1:C:46:LYS:HD3	1.69	0.45
1:E:149:ASP:OD1	1:E:149:ASP:C	2.60	0.45
1:A:159:VAL:CG2	5:A:256:HOH:O	2.66	0.44
1:E:117:THR:CG2	1:E:118:ASN:H	1.93	0.44
1:G:93:LEU:HD13	1:G:106:ILE:HG13	1.99	0.44
1:C:102:GLU:HB2	1:C:199:ILE:HG23	1.98	0.44
1:E:156:LEU:O	1:E:171:GLY:HA3	2.17	0.44
1:G:59:LYS:HD3	1:G:80:ASP:HB2	1.99	0.44
1:A:82:THR:CG2	5:A:250:HOH:O	2.39	0.44
1:G:160:SER:HB2	5:G:291:HOH:O	2.17	0.44
1:A:133:PHE:O	1:A:152:GLY:HA2	2.18	0.44
1:A:201:SER:CB	1:A:206:PRO:HB3	2.46	0.44
1:C:57:VAL:HG12	1:E:62:THR:HB	2.00	0.44
1:E:102:GLU:HB2	1:E:199:ILE:HG23	1.97	0.44
1:C:194:THR:HG21	5:E:694:HOH:O	2.16	0.44
1:E:93:LEU:HA	1:E:211:THR:O	2.18	0.44
4:E:240:ABA:HB3	1:G:130:PHE:CD1	2.53	0.44
1:A:8:GLU:C	1:A:9:LEU:HD12	2.43	0.44
1:C:205:GLU:HB2	5:C:275:HOH:O	2.17	0.44
1:E:71:SER:HB3	5:E:327:HOH:O	1.82	0.44
1:A:4:ILE:HD13	1:A:215:ALA:HB2	2.00	0.44
1:C:58:ALA:CB	1:E:62:THR:HG21	2.48	0.44
1:E:93:LEU:HD23	1:E:212:PHE:HA	1.99	0.44
1:G:134:THR:HG22	1:G:135:GLN:N	2.31	0.44
1:C:48:GLY:O	1:C:196:THR:HA	2.18	0.43
1:A:101:LYS:NZ	1:A:203:ASP:CG	2.76	0.43
1:A:159:VAL:O	1:A:159:VAL:HG23	2.18	0.43
1:G:51:HIS:HB2	1:G:64:VAL:HG23	2.00	0.43
1:A:153:ASN:HB2	5:A:692:HOH:O	2.18	0.43
1:E:114:LYS:CG	1:E:122:ASP:OD2	2.63	0.43
1:E:210:ILE:HG21	1:E:210:ILE:HD13	1.05	0.43
1:A:29:ILE:HG23	1:A:84:VAL:HG11	1.99	0.43
1:A:58:ALA:CB	1:G:62:THR:HG21	2.49	0.43
1:A:131:ASN:OD1	1:C:123:ALA:N	2.43	0.43
1:C:104:ASN:CG	1:C:210:ILE:CG2	2.91	0.43
1:C:159:VAL:HG11	1:C:163:GLY:CA	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:PRO:HB2	1:E:22:TYR:CZ	2.54	0.43
1:A:5:VAL:HG21	1:A:81:LEU:HD22	2.01	0.43
1:A:62:THR:CG2	1:A:76:SER:OG	2.65	0.43
1:E:16:ASP:OD2	1:E:16:ASP:N	2.50	0.43
1:E:5:VAL:HG13	1:E:29:ILE:CD1	2.49	0.42
1:C:58:ALA:HB2	1:E:62:THR:HG21	2.01	0.42
1:G:78:ASP:HB3	5:G:290:HOH:O	2.19	0.42
1:A:43:GLN:O	1:A:44:THR:C	2.62	0.42
1:E:80:ASP:OD1	1:E:80:ASP:C	2.61	0.42
1:E:123:ALA:O	1:G:131:ASN:ND2	2.51	0.42
1:E:134:THR:CG2	1:E:136:ASN:H	2.32	0.42
1:E:224:GLY:O	1:E:229:LEU:HD12	2.19	0.42
1:E:123:ALA:C	1:E:124:ASN:CG	2.85	0.42
1:G:117:THR:HA	1:G:186:ALA:HA	2.02	0.42
1:C:39:ARG:O	1:C:73:THR:CG2	2.67	0.42
1:E:42:MET:HE3	1:E:206:PRO:HG2	2.02	0.42
1:G:30:LYS:HA	5:G:299:HOH:O	2.19	0.42
1:A:141:ILE:HB	1:A:174:LEU:HB2	2.02	0.42
1:A:207:ALA:HB1	1:A:208:ASP:HA	2.01	0.42
1:G:191:PHE:CD1	1:G:191:PHE:C	2.98	0.42
1:C:89:VAL:HG21	1:C:214:ILE:CG2	2.50	0.42
1:E:30:LYS:HD3	1:E:84:VAL:HG13	2.01	0.42
1:E:131:ASN:CG	5:E:328:HOH:O	2.62	0.42
1:E:107:LEU:HD12	1:E:107:LEU:N	2.35	0.42
1:G:57:VAL:HG23	1:G:188:VAL:HG13	2.01	0.42
1:A:177:ALA:HB2	1:C:177:ALA:HB2	2.01	0.42
1:C:134:THR:HG22	1:C:135:GLN:N	2.35	0.42
1:C:158:LYS:CE	5:C:389:HOH:O	2.67	0.42
1:E:43:GLN:NE2	1:E:70:SER:CA	2.77	0.42
1:A:62:THR:HG21	1:G:58:ALA:CB	2.49	0.41
1:A:183:GLU:O	1:A:185:SER:N	2.52	0.41
1:C:116:LYS:HE3	1:E:194:THR:HG21	2.02	0.41
1:A:7:VAL:HG21	1:A:52:ILE:HG12	2.02	0.41
1:A:16:ASP:OD2	1:A:228:ARG:NH1	2.48	0.41
1:A:48:GLY:O	1:A:196:THR:HA	2.20	0.41
1:C:158:LYS:HZ3	1:C:158:LYS:HG2	1.39	0.41
1:E:51:HIS:O	1:E:63:ALA:HA	2.20	0.41
1:E:105:THR:O	1:E:197:PHE:HA	2.20	0.41
1:A:124:ASN:HA	1:C:129:SER:O	2.20	0.41
1:C:51:HIS:O	1:C:63:ALA:HA	2.20	0.41
1:G:35:LYS:HB3	1:G:77:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:O	1:A:59:LYS:HG3	2.21	0.41
1:E:5:VAL:HG13	1:E:29:ILE:HD13	2.03	0.41
1:E:13:PRO:HB3	1:E:20:PRO:O	2.20	0.41
1:C:112:THR:O	1:C:191:PHE:HA	2.20	0.41
1:C:150:SER:C	1:C:152:GLY:H	2.29	0.41
1:C:145:ASP:O	1:C:147:THR:HG23	2.21	0.41
1:C:160:SER:N	1:C:164:SER:O	2.46	0.41
1:G:64:VAL:HG13	1:G:74:THR:CG2	2.50	0.41
1:G:207:ALA:HB1	1:G:208:ASP:HA	2.03	0.41
1:A:8:GLU:OE1	1:A:28:ASP:OD2	2.38	0.41
1:A:101:LYS:NZ	5:A:357:HOH:O	2.49	0.41
1:C:50:ALA:O	1:C:194:THR:HA	2.21	0.41
1:E:87:GLU:HB2	1:E:182:TRP:O	2.20	0.41
1:E:95:ALA:HB1	1:E:104:ASN:CG	2.45	0.41
4:E:240:ABA:HG2	5:G:319:HOH:O	2.20	0.41
1:G:112:THR:O	1:G:191:PHE:HA	2.21	0.41
1:G:136:ASN:C	1:G:136:ASN:HD22	2.29	0.41
1:A:51:HIS:O	1:A:63:ALA:HA	2.21	0.41
1:E:48:GLY:O	1:E:196:THR:HA	2.20	0.41
1:A:149:ASP:OD2	5:A:692:HOH:O	2.22	0.40
1:C:30:LYS:HA	5:C:266:HOH:O	2.21	0.40
1:E:111:PHE:O	1:E:127:HIS:HA	2.21	0.40
1:E:132:GLN:HE22	1:G:117:THR:CB	2.34	0.40
1:G:101:LYS:HE3	5:G:593:HOH:O	2.21	0.40
1:A:7:VAL:HG22	1:A:27:ILE:CD1	2.51	0.40
1:A:116:LYS:HB2	1:A:188:VAL:HG23	2.03	0.40
1:G:20:PRO:HB2	1:G:22:TYR:CZ	2.55	0.40
1:G:61:LEU:O	1:G:76:SER:HA	2.22	0.40
1:A:45:GLY:HA2	1:A:200:LYS:HG2	2.04	0.40
1:C:81:LEU:HD12	1:C:81:LEU:HA	1.94	0.40
1:E:7:VAL:HG22	1:E:27:ILE:CD1	2.51	0.40
1:C:194:THR:CG2	5:E:694:HOH:O	2.69	0.40
1:E:207:ALA:HA	1:E:208:ASP:HA	1.81	0.40
1:G:200:LYS:CE	5:G:267:HOH:O	2.69	0.40
1:C:95:ALA:HB1	1:C:104:ASN:CG	2.47	0.40
1:G:9:LEU:N	1:G:9:LEU:HD12	2.36	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:691:HOH:O	5:G:696:HOH:O[2_554]	0.35	1.85
1:A:151:ASP:OD1	5:G:291:HOH:O[2_554]	0.95	1.25
5:E:301:HOH:O	5:G:310:HOH:O[3_645]	1.11	1.09
5:A:692:HOH:O	5:G:345:HOH:O[2_554]	1.13	1.07
1:A:151:ASP:CG	5:G:291:HOH:O[2_554]	1.41	0.79
1:E:46:LYS:NZ	5:G:344:HOH:O[2_554]	1.41	0.79
1:E:204:SER:OG	5:C:631:HOH:O[4_545]	1.94	0.26
5:A:705:HOH:O	5:G:501:HOH:O[2_554]	2.12	0.08
1:G:205:GLU:CD	5:E:301:HOH:O[3_655]	2.12	0.08
1:E:46:LYS:CE	5:G:344:HOH:O[2_554]	2.13	0.07

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	228/237 (96%)	218 (96%)	10 (4%)	0	100	100
1	C	228/237 (96%)	219 (96%)	9 (4%)	0	100	100
1	E	235/237 (99%)	222 (94%)	12 (5%)	1 (0%)	30	19
1	G	235/237 (99%)	229 (97%)	5 (2%)	1 (0%)	30	19
All	All	926/948 (98%)	888 (96%)	36 (4%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	122	ASP
1	E	69	GLY

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	198/202 (98%)	186 (94%)	12 (6%)	17	6
1	C	198/202 (98%)	182 (92%)	16 (8%)	11	3
1	E	202/202 (100%)	189 (94%)	13 (6%)	16	6
1	G	202/202 (100%)	187 (93%)	15 (7%)	13	4
All	All	800/808 (99%)	744 (93%)	56 (7%)	14	4

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	41	ASN
1	A	64	VAL
1	A	101	LYS
1	A	115	LEU
1	A	124	ASN
1	A	134	THR
1	A	158	LYS
1	A	174	LEU
1	A	188	VAL
1	A	198	LEU
1	A	232	LEU
1	C	11	SER
1	C	42	MET
1	C	64	VAL
1	C	81	LEU
1	C	99	LEU
1	C	101	LYS
1	C	116	LYS
1	C	117	THR
1	C	158	LYS
1	C	162	SER
1	C	164	SER
1	C	194	THR
1	C	198	LEU
1	C	210	ILE
1	C	230	LEU
1	C	232	LEU
1	E	44	THR
1	E	73	THR

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Mol	Chain	Res	Type
1	E	99	LEU
1	E	117	THR
1	E	134	THR
1	E	135	GLN
1	E	161	SER
1	E	174	LEU
1	E	192	ASP
1	E	198	LEU
1	E	202	PRO
1	E	210	ILE
1	E	232	LEU
1	G	36	SER
1	G	42	MET
1	G	81	LEU
1	G	87	GLU
1	G	101	LYS
1	G	115	LEU
1	G	117	THR
1	G	122	ASP
1	G	134	THR
1	G	158	LYS
1	G	194	THR
1	G	210	ILE
1	G	226	SER
1	G	230	LEU
1	G	232	LEU

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

Mol	Chain	Res	Type
1	A	41	ASN
1	A	83	ASN
1	C	41	ASN
1	C	43	GLN
1	C	51	HIS
1	C	131	ASN
1	C	135	GLN
1	E	41	ASN
1	E	43	GLN
1	E	83	ASN
1	E	104	ASN
1	E	118	ASN

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Mol	Chain	Res	Type
1	E	132	GLN
1	E	135	GLN
1	G	41	ASN
1	G	51	HIS
1	G	131	ASN
1	G	136	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ABA	E	240	-	4,5,6	0.69	0	1,5,7	0.87	0
4	ABA	G	240	-	4,5,6	1.05	0	1,5,7	0.46	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
4	ABA	E	240	-	-	3/3/4/6	-
4	ABA	G	240	-	-	0/3/4/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	240	ABA	O-C-CA-CB
4	E	240	ABA	N-CA-CB-CG
4	E	240	ABA	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	240	ABA	10	0
4	G	240	ABA	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	232/237 (97%)	-0.36	5 (2%)	62	62	5, 12, 25, 40	6 (2%)
1	C	232/237 (97%)	-0.14	8 (3%)	48	48	7, 14, 28, 36	4 (1%)
1	E	237/237 (100%)	-0.09	14 (5%)	28	27	5, 12, 29, 40	6 (2%)
1	G	237/237 (100%)	-0.33	10 (4%)	40	40	5, 11, 25, 45	4 (1%)
All	All	938/948 (98%)	-0.23	37 (3%)	43	43	5, 12, 27, 45	20 (2%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	71	SER	12.9
1	A	123	ALA	5.4
1	G	119	SER	5.1
1	E	70	SER	4.7
1	E	122	ASP	4.5
1	G	123	ALA	4.4
1	G	121	ALA	4.0
1	C	83	ASN	3.6
1	G	120	ILE	3.6
1	C	117	THR	3.6
1	E	119	SER	3.4
1	C	131	ASN	3.2
1	C	150	SER	3.2
1	G	122	ASP	3.1
1	G	42	MET	3.0
1	E	131	ASN	2.9
1	A	182	TRP	2.9
1	E	124	ASN	2.8
1	G	131	ASN	2.6
1	E	120	ILE	2.5
1	A	117	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	182	TRP	2.5
1	E	68	SER	2.5
1	A	131	ASN	2.4
1	E	118	ASN	2.4
1	C	226	SER	2.4
1	E	117	THR	2.4
1	C	16	ASP	2.4
1	E	72	SER	2.3
1	A	184	SER	2.2
1	G	150	SER	2.1
1	E	69	GLY	2.1
1	C	69	GLY	2.1
1	E	121	ALA	2.1
1	G	118	ASN	2.0
1	G	135	GLN	2.0
1	C	135	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ABA	E	240	6/7	0.73	0.21	14,20,22,23	0
4	ABA	G	240	6/7	0.91	0.09	6,15,19,24	0
2	MN	A	238	1/1	0.99	0.02	11,11,11,11	0
2	MN	E	238	1/1	0.99	0.02	11,11,11,11	0
3	CA	A	239	1/1	1.00	0.01	10,10,10,10	0
3	CA	C	239	1/1	1.00	0.01	15,15,15,15	0
3	CA	E	239	1/1	1.00	0.03	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	G	239	1/1	1.00	0.01	10,10,10,10	0
2	MN	C	238	1/1	1.00	0.01	14,14,14,14	0
2	MN	G	238	1/1	1.00	0.03	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.