



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:13 PM UTC

PDB ID : 2J55 / pdb_00002j55
Title : X-ray reduced Paraccocus denitrificans methylamine dehydrogenase O-quinone in complex with amicyanin.
Authors : Pearson, A.R.; Pahl, R.; Davidson, V.L.; Wilmot, C.M.
Deposited on : 2006-09-12
Resolution : 2.15 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

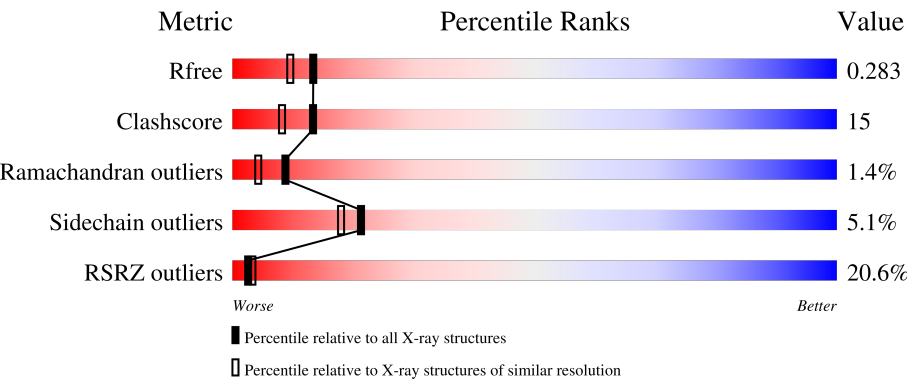
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	105	64% 56%32%10%
1	B	105	6% 76%22%
2	H	386	3% 75%19%
2	J	386	33% 64%29%5%
3	L	131	23% 54%34%8%5%

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Mol	Chain	Length	Quality of chain
3	M	131	

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
3	TRQ	M	57	-	-	X	-
5	GOL	H	1389	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10411 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 AMICYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			806	516	132	152	6			
1	B	105	Total	C	N	O	S	0	0	0
			806	516	132	152	6			

- Molecule 2 is a protein called METHYLAMINE DEHYDROGENASE HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	382	Total	C	N	O	S	0	3	0
			2988	1891	510	579	8			
2	J	381	Total	C	N	O	S	0	1	0
			2963	1876	508	571	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	312	PHE	LEU	SEE REMARK 999	UNP P29894
H	313	VAL	LEU	SEE REMARK 999	UNP P29894
J	312	PHE	LEU	SEE REMARK 999	UNP P29894
J	313	VAL	LEU	SEE REMARK 999	UNP P29894

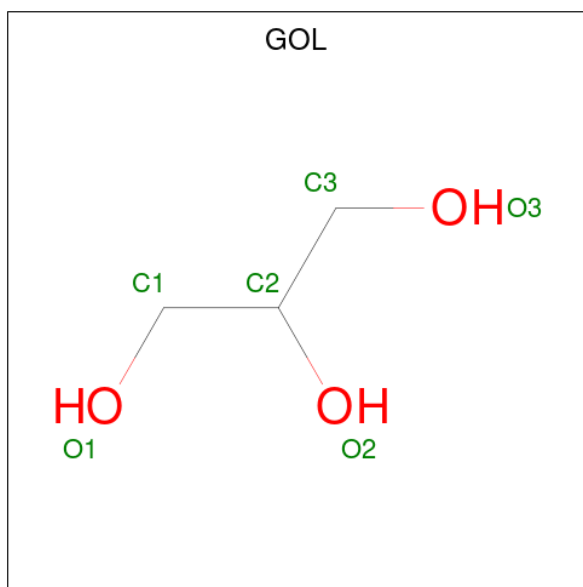
- Molecule 3 is a protein called METHYLAMINE DEHYDROGENASE LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			
3	M	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cu 1 1	0	0
4	B	1	Total Cu 1 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0
5	L	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	29	Total O 29 29	0	0
6	B	109	Total O 109 109	0	0
6	H	406	Total O 406 406	0	0
6	J	205	Total O 205 205	0	0

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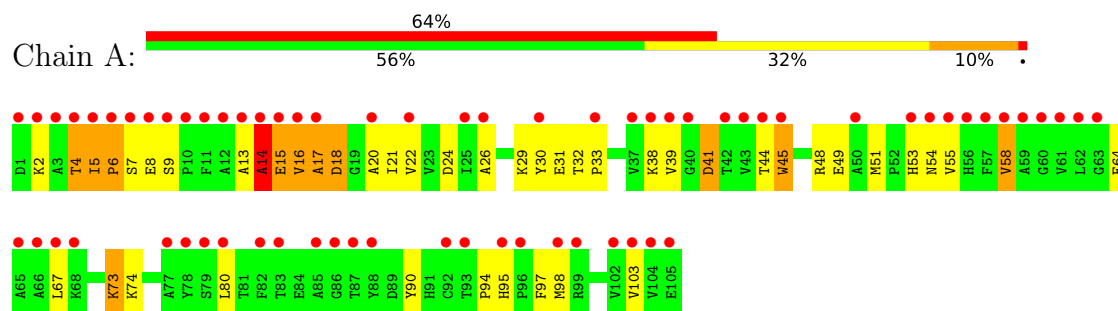
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	75	Total 75	O 75	0	0
6	M	86	Total 86	O 86	0	0

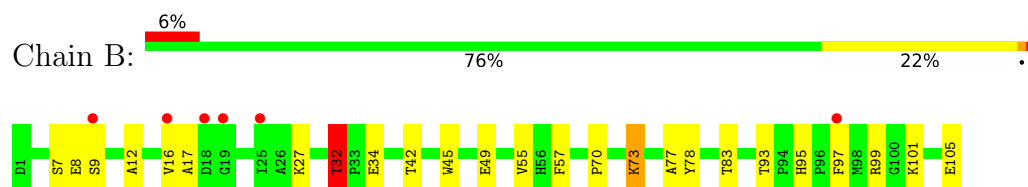
3 Residue-property plots [i](#)

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: AMICYANIN



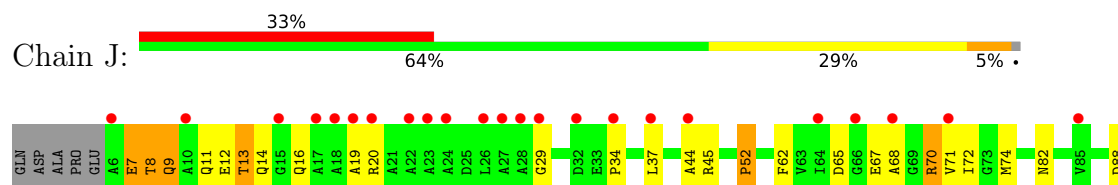
• Molecule 1: AMICYANIN

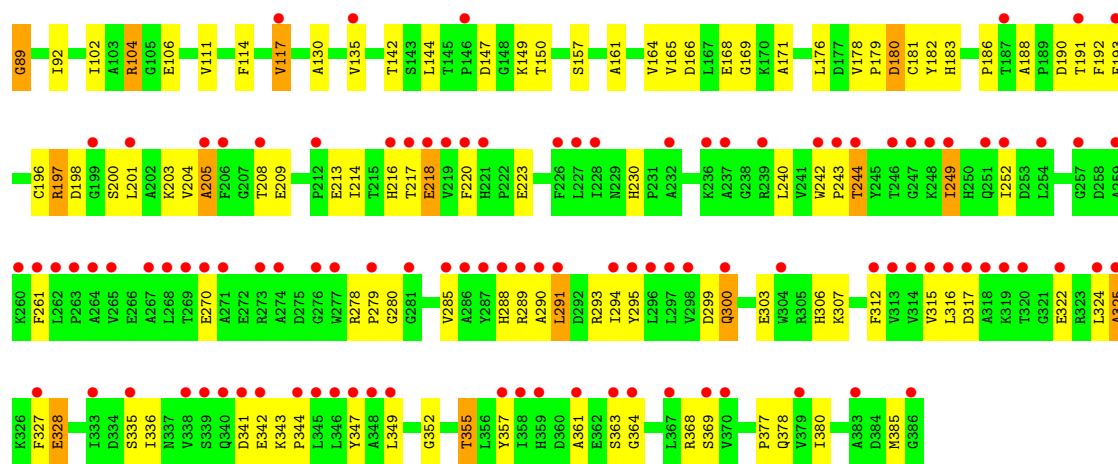


• Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

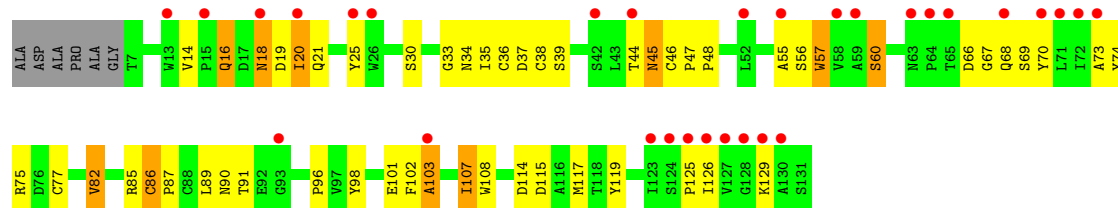


• Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

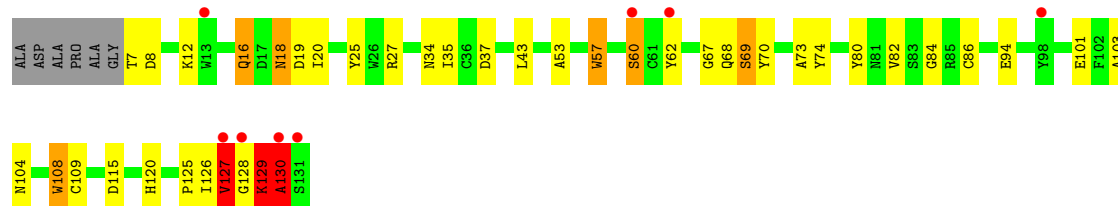




• Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN



• Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	122.73Å 122.73Å 246.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.70 – 2.15 21.70 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (21.70-2.15) 98.8 (21.70-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.189 , 0.245 0.231 , 0.283	Depositor DCC
R_{free} test set	5081 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10411	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: TRQ, GOL, CU

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	1.37	5/827 (0.6%)	1.43	10/1122 (0.9%)
1	B	1.60	6/827 (0.7%)	1.31	2/1122 (0.2%)
2	H	1.76	36/3071 (1.2%)	1.38	22/4184 (0.5%)
2	J	1.50	25/3043 (0.8%)	1.32	14/4147 (0.3%)
3	L	1.61	9/964 (0.9%)	1.35	10/1315 (0.8%)
3	M	1.60	8/964 (0.8%)	1.37	9/1315 (0.7%)
All	All	1.61	89/9696 (0.9%)	1.36	67/13205 (0.5%)

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
2	H	0	1
3	M	0	1
All	All	0	3

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	135	VAL	CA-CB	10.07	1.65	1.55
2	H	70	ARG	CZ-NH1	9.45	1.46	1.32
3	L	103	ALA	N-CA	8.39	1.56	1.46
2	H	36	ILE	CA-CB	8.19	1.64	1.54
2	J	117	VAL	CA-CB	8.03	1.67	1.54
2	H	111	VAL	CA-CB	7.94	1.63	1.54
2	H	44	ALA	CA-C	7.83	1.63	1.52
3	M	35	ILE	CA-CB	7.74	1.63	1.54
2	H	379	VAL	CA-CB	7.59	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	157	SER	CA-C	7.21	1.59	1.52
2	H	90	SER	C-O	-7.14	1.14	1.24
2	H	80	LEU	CA-CB	7.13	1.59	1.52
2	H	85	VAL	CA-CB	7.12	1.63	1.54
2	H	130	ALA	N-CA	7.08	1.51	1.46
2	J	230	HIS	CA-C	6.91	1.61	1.52
2	H	294	ILE	CA-CB	6.83	1.63	1.54
2	J	52	PRO	CA-C	6.74	1.61	1.52
3	M	103	ALA	CA-C	6.65	1.60	1.52
1	A	5	ILE	CA-CB	6.61	1.60	1.53
2	J	164	VAL	CA-CB	6.57	1.62	1.54
1	A	58	VAL	CA-CB	6.52	1.63	1.54
2	J	279	PRO	CA-C	6.48	1.60	1.52
1	A	103	VAL	CA-CB	6.37	1.61	1.54
3	L	20	ILE	CA-C	6.33	1.59	1.52
2	J	363	SER	CA-C	6.29	1.61	1.52
2	H	249	ILE	CG1-CD1	-6.28	1.27	1.51
3	L	107	ILE	CA-C	6.20	1.59	1.52
3	L	82	VAL	CA-CB	6.19	1.61	1.54
2	H	26	LEU	CA-C	6.13	1.60	1.52
2	H	152	LEU	CA-C	-6.12	1.45	1.52
2	H	123	ALA	CA-CB	6.11	1.64	1.53
2	J	171	ALA	CA-CB	6.09	1.64	1.53
2	H	51	ASP	CA-C	6.07	1.60	1.52
2	J	165	VAL	CA-CB	6.06	1.61	1.54
2	H	285	VAL	CA-C	6.02	1.59	1.52
3	L	48	PRO	CA-C	6.01	1.59	1.52
2	J	244	THR	CA-CB	5.96	1.62	1.53
1	B	93	THR	C-O	-5.96	1.18	1.24
3	M	108	TRP	CA-C	5.91	1.59	1.53
2	J	106	GLU	C-O	-5.86	1.16	1.23
2	H	355	THR	C-O	-5.84	1.17	1.23
1	B	101	LYS	C-O	5.80	1.30	1.23
1	A	4	THR	CA-CB	5.80	1.65	1.54
3	L	30	SER	C-O	-5.79	1.18	1.24
2	H	131	PRO	CA-C	5.79	1.58	1.52
2	H	71	VAL	CB-CG1	5.76	1.71	1.52
2	J	130	ALA	CA-CB	5.72	1.56	1.52
2	J	150	THR	CA-C	5.63	1.59	1.52
2	J	72	ILE	CA-CB	5.63	1.62	1.54
2	J	352	GLY	C-O	-5.60	1.17	1.23
2	H	110	TYR	CA-CB	5.60	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	77	CYS	C-O	5.54	1.30	1.24
2	J	279	PRO	C-O	5.52	1.29	1.23
2	H	34	PRO	N-CA	5.51	1.53	1.47
2	H	20	ARG	N-CA	5.50	1.52	1.46
2	H	64	ILE	CA-CB	5.49	1.62	1.54
2	H	66	GLY	N-CA	5.48	1.53	1.45
2	J	65	ASP	N-CA	5.47	1.53	1.46
2	J	280	GLY	N-CA	5.47	1.51	1.45
2	H	356	LEU	N-CA	-5.44	1.39	1.46
2	H	93	ALA	CA-C	-5.44	1.46	1.52
1	B	42	THR	N-CA	5.43	1.52	1.46
2	H	228	ILE	CA-CB	5.40	1.59	1.54
2	H	178	VAL	CA-CB	5.38	1.61	1.54
3	L	86	CYS	N-CA	5.37	1.50	1.46
2	J	193	PHE	N-CA	5.37	1.52	1.45
2	H	70	ARG	NE-CZ	5.35	1.39	1.33
2	J	368	ARG	N-CA	5.34	1.53	1.46
2	J	355	THR	N-CA	5.31	1.52	1.46
1	A	97	PHE	CA-C	5.30	1.60	1.52
2	H	200	SER	CA-C	5.30	1.60	1.53
3	M	82	VAL	CA-CB	5.29	1.60	1.54
2	H	342	GLU	C-O	5.24	1.30	1.24
3	M	34	ASN	N-CA	5.17	1.52	1.46
3	L	117	MET	N-CA	5.16	1.52	1.46
3	M	126	ILE	CA-CB	5.16	1.60	1.54
1	B	12	ALA	CA-CB	5.14	1.61	1.53
2	J	71	VAL	CA-CB	5.13	1.59	1.53
2	J	70	ARG	CA-C	5.13	1.58	1.52
2	H	33	GLU	CA-C	5.10	1.58	1.52
2	H	39	ALA	CA-C	5.09	1.59	1.53
3	M	82	VAL	CA-C	5.08	1.59	1.52
1	B	9	SER	CB-OG	5.06	1.52	1.42
2	H	57	ALA	CA-C	5.05	1.59	1.52
3	M	130	ALA	CA-CB	5.03	1.61	1.53
1	B	16	VAL	CA-C	5.03	1.58	1.53
2	H	172	PHE	CA-C	5.02	1.59	1.52
2	H	80	LEU	N-CA	-5.00	1.41	1.46
2	J	111	VAL	CA-CB	5.00	1.60	1.54

All (67) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	70	ARG	NE-CZ-NH2	-16.58	104.28	119.20
2	H	70	ARG	NE-CZ-NH1	16.05	137.55	121.50
2	H	320	THR	N-CA-C	11.20	127.11	113.23
1	A	16	VAL	N-CA-C	10.09	119.92	110.74
2	H	70	ARG	CD-NE-CZ	10.04	138.46	124.40
1	A	14	ALA	N-CA-C	-9.79	89.94	110.80
1	B	32	THR	CB-CA-C	-8.62	99.30	109.47
3	M	129	LYS	N-CA-C	8.44	123.19	109.94
2	H	289	ARG	NE-CZ-NH1	-8.16	113.34	121.50
1	A	16	VAL	CB-CA-C	-7.80	101.64	111.94
1	A	9	SER	CA-C-N	7.76	127.66	120.21
1	A	9	SER	C-N-CA	7.76	127.66	120.21
2	H	197	ARG	NE-CZ-NH2	7.58	126.02	119.20
2	H	211	THR	CA-C-N	-7.49	112.97	120.31
2	H	211	THR	C-N-CA	-7.49	112.97	120.31
2	J	197	ARG	NE-CZ-NH1	-7.31	114.19	121.50
2	J	104	ARG	CG-CD-NE	-6.79	97.05	112.00
2	J	178	VAL	CA-C-N	-6.64	111.54	119.84
2	J	178	VAL	C-N-CA	-6.64	111.54	119.84
2	J	197	ARG	NE-CZ-NH2	6.53	125.08	119.20
2	H	226	PHE	N-CA-C	6.52	118.78	108.67
2	J	8	THR	CA-C-N	6.51	133.42	121.70
2	J	8	THR	C-N-CA	6.51	133.42	121.70
3	M	86	CYS	O-C-N	6.51	124.52	121.53
3	L	90	ASN	N-CA-C	-6.34	99.48	109.50
3	L	14	VAL	CA-C-N	6.33	126.30	119.78
3	L	14	VAL	C-N-CA	6.33	126.30	119.78
2	H	117	VAL	N-CA-C	6.17	117.12	111.81
3	M	60	SER	N-CA-CB	6.14	119.47	109.95
2	H	13	THR	CB-CA-C	6.12	121.26	110.85
2	J	306	HIS	N-CA-C	6.12	120.60	113.20
3	M	8	ASP	CA-C-N	6.04	125.93	119.28
3	M	8	ASP	C-N-CA	6.04	125.93	119.28
2	H	342	GLU	N-CA-C	6.03	118.35	111.11
2	H	7	GLU	N-CA-C	5.99	119.14	110.28
2	H	275	ASP	N-CA-C	5.94	120.26	113.19
3	M	84	GLY	N-CA-C	-5.93	106.76	115.30
2	J	89	GLY	N-CA-C	5.92	123.42	114.61
3	M	104	ASN	N-CA-C	5.88	120.46	112.88
2	H	289	ARG	N-CA-C	5.84	117.33	110.97
1	A	45	TRP	CA-C-N	-5.82	115.52	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	TRP	C-N-CA	-5.82	115.52	123.14
2	J	8	THR	N-CA-C	-5.81	101.09	110.32
2	J	205	ALA	N-CA-C	-5.76	98.89	108.34
3	L	36	CYS	N-CA-C	5.60	119.21	112.38
1	A	5	ILE	N-CA-C	5.59	113.58	107.60
2	H	303	GLU	N-CA-C	5.58	119.35	112.54
1	B	16	VAL	N-CA-C	5.48	115.46	108.12
3	L	46	CYS	N-CA-C	5.37	116.65	109.83
3	M	86	CYS	CB-CA-C	-5.35	107.40	111.20
2	J	197	ARG	CG-CD-NE	-5.29	100.35	112.00
3	L	47	PRO	O-C-N	5.27	123.73	121.31
1	A	5	ILE	CA-C-N	5.25	126.40	119.84
1	A	5	ILE	C-N-CA	5.25	126.40	119.84
3	L	18	ASN	N-CA-C	5.25	122.00	114.39
2	J	7	GLU	N-CA-C	5.24	118.22	110.46
3	L	45	ASN	N-CA-C	5.22	117.91	109.40
3	M	74	TYR	N-CA-C	5.19	117.64	109.39
2	H	278	ARG	O-C-N	5.16	125.46	121.85
2	H	197	ARG	NE-CZ-NH1	-5.16	116.34	121.50
2	H	221	HIS	CA-C-N	5.11	125.12	120.21
2	H	221	HIS	C-N-CA	5.11	125.12	120.21
2	H	196	CYS	N-CA-C	5.10	118.33	110.42
3	L	60	SER	N-CA-C	5.08	117.04	108.96
2	H	255	SER	N-CA-C	5.07	118.57	112.38
3	L	39	SER	N-CA-C	5.03	118.95	112.41
2	J	196	CYS	N-CA-C	5.02	117.93	109.95

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ALA	Peptide
2	H	320	THR	Peptide
3	M	129	LYS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	806	0	790	42	0
1	B	806	0	790	21	0
2	H	2988	0	2862	43	0
2	J	2963	0	2843	106	0
3	L	956	0	857	46	0
3	M	956	0	857	33	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	H	18	0	24	13	0
5	L	6	0	8	3	0
6	A	29	0	0	9	0
6	B	109	0	0	4	2
6	H	406	0	0	13	2
6	J	205	0	0	14	0
6	L	75	0	0	2	0
6	M	86	0	0	8	0
All	All	10411	0	9031	274	2

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 15.

All (274) 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:M:57:TRQ:CE3	3:M:108:TRP:HD1	0.86	1.49
2:H:70:ARG:NH2	5:H:1389:GOL:H2	1.27	1.43
2:H:70:ARG:NH2	5:H:1389:GOL:C2	1.98	1.27
1:A:14:ALA:O	1:A:16:VAL:N	1.70	1.20
2:H:289:ARG:NH1	2:H:384:ASP:OD2	1.81	1.13
2:H:70:ARG:CZ	5:H:1389:GOL:H2	1.88	1.03
3:L:68:GLN:HB2	6:L:2038:HOH:O	1.58	1.01
2:H:289:ARG:HH12	2:H:384:ASP:CG	1.68	1.00
2:J:217:THR:HG21	2:J:261:PHE:CZ	1.97	0.99
5:H:1389:GOL:H12	6:H:2012:HOH:O	1.62	0.97
2:J:8:THR:HA	2:J:9:GLN:HG3	1.44	0.96
3:M:57:TRQ:CZ3	3:M:108:TRP:HD1	1.79	0.95
3:M:127:VAL:HG22	3:M:128:GLY:H	1.31	0.93
1:A:16:VAL:HG13	1:A:17:ALA:N	1.87	0.89
1:A:21:ILE:HD11	1:A:41:ASP:OD1	1.72	0.88
2:J:34:PRO:HG2	3:L:75:ARG:NH1	1.88	0.88
2:J:217:THR:HG21	2:J:261:PHE:HZ	1.39	0.88
1:A:20:ALA:CB	6:A:2006:HOH:O	2.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:HB	6:A:2003:HOH:O	1.75	0.85
2:H:174:ARG:NH1	6:H:2216:HOH:O	2.09	0.85
3:M:127:VAL:HG22	3:M:128:GLY:N	1.93	0.84
2:H:218:GLU:HG3	6:H:2246:HOH:O	1.79	0.83
1:A:53:HIS:ND1	1:A:98:MET:HE1	1.94	0.82
3:L:16:GLN:NE2	3:L:18:ASN:H	1.78	0.82
2:J:270:GLU:HB2	6:J:2166:HOH:O	1.78	0.82
1:B:105:GLU:HG2	6:B:2107:HOH:O	1.80	0.81
2:H:70:ARG:HH21	5:H:1389:GOL:H2	1.39	0.81
1:A:16:VAL:HG13	1:A:17:ALA:H	1.46	0.81
3:M:68:GLN:HE21	3:M:129:LYS:NZ	1.78	0.81
2:J:197:ARG:NH1	3:M:101:GLU:OE1	2.13	0.80
2:J:291:LEU:HB3	2:J:293:ARG:HE	1.47	0.80
2:J:8:THR:HB	2:J:9:GLN:HB2	1.64	0.80
2:J:270:GLU:CB	6:J:2166:HOH:O	2.31	0.78
3:L:89:LEU:O	5:L:1132:GOL:O3	2.01	0.78
5:H:1389:GOL:H31	3:M:37:ASP:OD1	1.85	0.77
1:A:33:PRO:HD2	6:A:2009:HOH:O	1.83	0.77
1:B:73:LYS:HE2	6:M:2085:HOH:O	1.84	0.76
2:H:70:ARG:HH22	5:H:1389:GOL:C2	1.98	0.76
1:B:73:LYS:HD3	6:M:2085:HOH:O	1.87	0.75
3:M:127:VAL:CG2	3:M:128:GLY:N	2.49	0.75
2:J:8:THR:O	2:J:11:GLN:HB3	1.86	0.75
5:H:1389:GOL:C3	3:M:37:ASP:OD1	2.34	0.75
1:A:20:ALA:HB1	6:A:2006:HOH:O	1.85	0.74
2:J:217:THR:HG21	2:J:261:PHE:CE2	2.22	0.74
2:J:369:SER:O	6:J:2197:HOH:O	2.06	0.73
1:B:49:GLU:OE1	6:B:2052:HOH:O	2.06	0.73
3:L:57:TRQ:HB2	3:L:108:TRP:NE1	2.04	0.73
2:H:179:PRO:HD3	2:H:214:ILE:HD12	1.71	0.72
2:J:312:PHE:CE1	2:J:328:GLU:HG3	2.25	0.71
2:J:317:ASP:HB2	2:J:324:LEU:HD21	1.72	0.71
2:H:317:ASP:O	2:H:321:GLY:HA2	1.90	0.71
1:A:53:HIS:HD1	1:A:98:MET:HE1	1.56	0.70
2:J:344:PRO:O	2:J:361:ALA:CB	2.39	0.70
3:L:16:GLN:HE22	3:L:19:ASP:H	1.40	0.69
2:H:70:ARG:NH2	5:H:1389:GOL:O2	2.25	0.69
2:J:166:ASP:OD2	6:J:2126:HOH:O	2.09	0.69
3:M:57:TRQ:HB2	3:M:108:TRP:NE1	2.08	0.68
3:L:19:ASP:O	3:L:25:TYR:HB2	1.94	0.68
1:A:20:ALA:HB2	6:A:2006:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ALA:HB3	1:A:20:ALA:HB2	1.75	0.67
3:M:68:GLN:HE21	3:M:129:LYS:HZ2	1.40	0.67
2:J:344:PRO:O	2:J:361:ALA:HB2	1.95	0.67
2:H:70:ARG:HH21	5:H:1389:GOL:C2	1.98	0.67
3:M:57:TRQ:CZ3	3:M:108:TRP:CD1	2.65	0.67
1:A:53:HIS:HD1	1:A:98:MET:CE	2.08	0.66
3:M:16:GLN:HE22	3:M:19:ASP:H	1.42	0.66
1:B:83:THR:O	6:B:2083:HOH:O	2.12	0.66
3:M:16:GLN:HE21	3:M:18:ASN:H	1.43	0.66
1:A:90:TYR:O	6:A:2026:HOH:O	2.15	0.65
5:L:1132:GOL:H31	6:L:2075:HOH:O	1.96	0.64
2:J:52:PRO:HG2	2:J:378:GLN:HE21	1.62	0.64
2:J:14:GLN:NE2	2:J:68:ALA:O	2.31	0.64
2:J:45:ARG:NH2	2:J:343:LYS:O	2.30	0.63
1:A:17:ALA:O	1:A:18:ASP:HB2	1.97	0.63
3:M:57:TRQ:HB2	3:M:108:TRP:HE1	1.63	0.63
5:H:1389:GOL:O1	6:H:2406:HOH:O	2.15	0.63
2:J:288:HIS:CE1	2:J:291:LEU:HD13	2.34	0.63
2:J:336:ILE:HA	2:J:347:TYR:O	1.99	0.62
3:L:16:GLN:HE21	3:L:18:ASN:H	1.46	0.62
2:J:182:TYR:O	2:J:183:HIS:HB2	1.97	0.62
2:J:11:GLN:HG2	3:L:21:GLN:OE1	1.99	0.62
3:L:20:ILE:HG22	3:L:25:TYR:CZ	2.34	0.62
2:J:315:VAL:HB	2:J:325:ALA:HB3	1.83	0.61
3:M:68:GLN:NE2	3:M:129:LYS:NZ	2.48	0.61
3:L:68:GLN:HG2	3:L:69:SER:N	2.16	0.61
2:H:273:ARG:HG2	6:H:2293:HOH:O	2.01	0.61
2:J:44:ALA:HB1	2:J:341:ASP:HB3	1.83	0.61
3:L:89:LEU:H	5:L:1132:GOL:H11	1.66	0.60
3:L:16:GLN:HE21	3:L:16:GLN:C	2.10	0.60
3:M:115:ASP:HB2	6:M:2077:HOH:O	2.01	0.60
2:J:16:GLN:HG3	2:J:20:ARG:NH2	2.17	0.60
1:B:99:ARG:NH2	2:J:180[B]:ASP:OD2	2.35	0.59
2:J:19:ALA:HB2	3:L:20:ILE:HG23	1.83	0.59
3:M:68:GLN:NE2	3:M:129:LYS:HZ1	2.01	0.59
2:H:62:PHE:CE2	2:H:74:MET:HE3	2.37	0.59
2:H:5:GLU:O	2:H:6:ALA:CB	2.51	0.58
2:H:211:THR:HG23	6:H:2237:HOH:O	2.03	0.58
2:J:8:THR:HA	2:J:9:GLN:CG	2.26	0.58
3:L:56:SER:HB2	3:L:74:TYR:O	2.03	0.58
3:M:16:GLN:NE2	3:M:18:ASN:H	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:144:LEU:O	2:J:186:PRO:HG2	2.04	0.57
1:B:95:HIS:HB3	1:B:97:PHE:CE2	2.39	0.57
2:J:217:THR:CG2	2:J:261:PHE:CE2	2.87	0.57
2:J:179:PRO:O	2:J:181:CYS:N	2.35	0.57
5:H:1389:GOL:H32	3:M:37:ASP:OD1	2.03	0.57
2:J:217:THR:CG2	2:J:261:PHE:CZ	2.81	0.57
1:A:21:ILE:CD1	1:A:41:ASP:OD1	2.51	0.57
2:J:82:ASN:HB3	2:J:142:THR:HB	1.86	0.56
2:J:34:PRO:HB3	3:L:44:THR:O	2.05	0.56
2:J:70:ARG:HH11	2:J:70:ARG:HG3	1.70	0.56
3:L:20:ILE:HG22	3:L:25:TYR:CE1	2.40	0.56
3:L:57:TRQ:HB2	3:L:108:TRP:HE1	1.68	0.56
2:J:349:LEU:HB2	2:J:380:ILE:HD11	1.87	0.56
2:J:216:HIS:CD2	6:J:2139:HOH:O	2.59	0.56
2:J:249:ILE:HD12	2:J:294:ILE:HG21	1.88	0.55
2:J:188:ALA:HB3	2:J:191:THR:HB	1.89	0.55
1:B:73:LYS:CD	6:M:2085:HOH:O	2.46	0.55
2:J:316:LEU:HA	2:J:324:LEU:HG	1.89	0.55
3:M:73:ALA:O	3:M:125:PRO:HD2	2.07	0.55
2:J:290:ALA:HB3	2:J:291:LEU:HD13	1.89	0.54
3:L:21:GLN:NE2	3:L:37:ASP:OD2	2.38	0.54
2:H:179:PRO:HD3	2:H:214:ILE:CD1	2.36	0.54
2:H:179:PRO:HB2	2:H:181:CYS:SG	2.48	0.54
3:L:38:CYS:HB3	3:L:85:ARG:NH1	2.22	0.54
2:H:222:PRO:HG2	2:H:225:GLU:HB2	1.88	0.54
1:A:16:VAL:O	1:A:17:ALA:CB	2.56	0.53
5:H:1387:GOL:H31	6:H:2277:HOH:O	2.07	0.53
2:J:92:ILE:HG13	2:J:114:PHE:HB2	1.89	0.53
2:J:217:THR:HG22	2:J:218:GLU:N	2.24	0.53
2:H:173:LYS:HE3	6:H:2214:HOH:O	2.08	0.53
3:L:68:GLN:HE22	3:L:129:LYS:HE2	1.74	0.53
1:A:18:ASP:C	1:A:20:ALA:H	2.16	0.53
6:H:2187:HOH:O	3:L:103:ALA:HB1	2.07	0.53
1:A:16:VAL:CG1	1:A:17:ALA:N	2.60	0.53
1:B:32:THR:HG22	1:B:34:GLU:H	1.73	0.53
2:H:9:GLN:HG2	6:H:2006:HOH:O	2.08	0.53
2:J:37:LEU:HD21	3:L:45:ASN:CB	2.39	0.52
2:J:349:LEU:HD11	2:J:377:PRO:HB2	1.91	0.52
2:J:249:ILE:CD1	2:J:294:ILE:HG21	2.39	0.52
1:B:73:LYS:CE	6:M:2085:HOH:O	2.47	0.52
2:H:240:LEU:HD13	2:H:252:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:147:ASP:OD2	2:J:149:LYS:HD2	2.09	0.52
2:J:62:PHE:CE2	2:J:74:MET:HE3	2.45	0.52
2:J:344:PRO:O	2:J:361:ALA:HB3	2.10	0.52
1:A:8:GLU:HB3	6:A:2002:HOH:O	2.10	0.51
2:H:173:LYS:CE	6:H:2214:HOH:O	2.58	0.51
1:A:53:HIS:ND1	1:A:98:MET:CE	2.62	0.51
2:H:82:ASN:HB3	2:H:142:THR:HB	1.93	0.51
3:L:55:ALA:O	3:L:56:SER:HB3	2.10	0.51
1:A:17:ALA:CB	1:A:20:ALA:HB2	2.41	0.51
2:H:5:GLU:O	2:H:6:ALA:HB2	2.10	0.51
2:J:34:PRO:HG2	3:L:75:ARG:HH12	1.71	0.51
1:A:8:GLU:O	6:A:2001:HOH:O	2.18	0.50
2:J:312:PHE:HE1	2:J:328:GLU:HG3	1.71	0.50
2:J:149:LYS:HD3	2:J:168:GLU:OE1	2.12	0.50
2:J:244:THR:HB	6:J:2146:HOH:O	2.12	0.50
1:A:51:MET:O	1:A:53:HIS:CD2	2.65	0.49
1:A:16:VAL:O	1:A:17:ALA:HB2	2.12	0.49
1:A:38:LYS:O	1:A:41:ASP:HB2	2.12	0.49
2:J:52:PRO:CG	2:J:378:GLN:HE21	2.25	0.49
2:H:112:GLU:OE2	2:J:104:ARG:NH2	2.37	0.49
2:J:243:PRO:HG3	2:J:285:VAL:HB	1.94	0.49
1:A:14:ALA:C	1:A:16:VAL:H	2.11	0.49
2:J:70:ARG:NH1	6:J:2058:HOH:O	2.46	0.48
2:J:181:CYS:C	2:J:182:TYR:CD1	2.91	0.48
3:L:96:PRO:HB2	3:L:98:TYR:CE1	2.48	0.48
2:H:56:ALA:HA	3:L:82:VAL:HG12	1.96	0.48
2:H:307:LYS:HD2	3:L:91:THR:HG21	1.95	0.48
2:J:37:LEU:HD21	3:L:45:ASN:HB2	1.95	0.48
2:J:45:ARG:NH1	2:J:67:GLU:OE1	2.45	0.48
1:A:14:ALA:O	1:A:15:GLU:C	2.44	0.48
2:H:204:VAL:HG22	2:H:214:ILE:HD13	1.95	0.48
2:J:13:THR:HG21	6:J:2006:HOH:O	2.13	0.48
3:M:53:ALA:HB2	3:M:109:CYS:HA	1.94	0.48
2:J:13:THR:CG2	6:J:2007:HOH:O	2.61	0.48
1:B:45:TRP:CE2	1:B:55:VAL:HG11	2.49	0.48
2:J:8:THR:CA	2:J:9:GLN:HG3	2.31	0.48
2:J:8:THR:CB	2:J:9:GLN:HB2	2.39	0.48
2:J:278:ARG:HD2	2:J:303:GLU:HA	1.97	0.47
3:M:62:TYR:OH	3:M:67:GLY:HA2	2.14	0.47
3:L:35:ILE:HD12	3:L:86:CYS:HB3	1.97	0.47
1:B:97:PHE:HA	2:J:180[B]:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ARG:HH22	2:J:180[B]:ASP:CG	2.23	0.47
2:J:198:ASP:OD1	2:J:198:ASP:C	2.58	0.47
2:J:70:ARG:HG3	2:J:70:ARG:NH1	2.29	0.46
1:A:17:ALA:O	1:A:18:ASP:CB	2.62	0.46
2:J:29:GLY:O	6:J:2021:HOH:O	2.20	0.46
3:L:57:TRQ:HZ3	3:L:108:TRP:HB2	1.98	0.46
2:J:299:ASP:OD1	2:J:300:GLN:N	2.48	0.45
2:J:355:THR:HG21	2:J:357:TYR:CE1	2.51	0.45
3:L:57:TRQ:CZ3	3:L:108:TRP:HB2	2.45	0.45
1:A:26:ALA:HB3	1:A:31:GLU:OE2	2.16	0.45
1:A:95:HIS:HB2	1:A:98:MET:SD	2.56	0.45
2:J:328:GLU:O	6:J:2180:HOH:O	2.21	0.45
3:M:57:TRQ:CD2	3:M:108:TRP:CD1	2.78	0.45
2:J:223:GLU:HG3	6:J:2141:HOH:O	2.16	0.45
2:H:190:ASP:HB2	2:H:206:PHE:O	2.16	0.45
1:A:49:GLU:HA	1:A:74:LYS:HE2	1.99	0.45
2:H:270[A]:GLU:OE1	6:H:2286:HOH:O	2.21	0.45
2:J:217:THR:CG2	2:J:218:GLU:N	2.80	0.45
2:J:190:ASP:O	2:J:205:ALA:HA	2.16	0.45
3:M:18:ASN:C	3:M:18:ASN:HD22	2.24	0.45
2:J:270:GLU:HB3	6:J:2166:HOH:O	2.07	0.44
3:L:73:ALA:O	3:L:125:PRO:HD2	2.17	0.44
2:J:203:LYS:O	2:J:214:ILE:HA	2.17	0.44
2:J:204:VAL:HG22	2:J:214:ILE:HG12	2.00	0.44
1:A:22:VAL:HG22	1:A:44:THR:HB	1.99	0.44
1:A:2:LYS:HE2	6:A:2020:HOH:O	2.17	0.44
2:H:218:GLU:HG3	2:H:218:GLU:H	1.69	0.44
1:B:97:PHE:CZ	2:J:197:ARG:NH1	2.86	0.44
2:H:237:ALA:HB2	2:H:289:ARG:HG3	1.98	0.44
2:J:16:GLN:HB3	3:L:18:ASN:O	2.18	0.44
2:J:288:HIS:HE1	2:J:290:ALA:HB3	1.82	0.44
2:J:200:SER:O	2:J:201:LEU:HD23	2.18	0.43
1:A:94:PRO:HB3	3:L:55:ALA:HB1	2.00	0.43
1:B:70:PRO:HD2	1:B:78:TYR:CE1	2.53	0.43
3:M:69:SER:O	3:M:130:ALA:N	2.51	0.43
2:J:355:THR:HG21	2:J:357:TYR:CZ	2.53	0.43
3:L:101:GLU:HG2	3:L:102:PHE:CD2	2.53	0.43
1:A:24:ASP:OD1	1:A:48:ARG:NE	2.48	0.43
1:A:45:TRP:CD2	1:A:55:VAL:HG11	2.53	0.43
1:A:16:VAL:HG22	1:A:18:ASP:H	1.83	0.43
3:L:114:ASP:O	3:L:115:ASP:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:69:SER:HB2	6:M:2051:HOH:O	2.19	0.43
1:B:95:HIS:HB3	1:B:97:PHE:CZ	2.53	0.43
3:L:20:ILE:HA	3:L:25:TYR:CG	2.54	0.43
2:H:270[A]:GLU:CD	2:H:270[A]:GLU:H	2.21	0.43
2:J:197:ARG:HB2	6:M:2068:HOH:O	2.19	0.43
2:H:188:ALA:HB1	2:H:189:PRO:CD	2.49	0.43
2:H:188:ALA:HB1	2:H:189:PRO:HD2	2.01	0.43
2:J:290:ALA:HB3	2:J:291:LEU:CD1	2.48	0.43
1:B:105:GLU:OXT	6:B:2109:HOH:O	2.21	0.43
2:J:307:LYS:HZ1	3:M:94:GLU:CD	2.27	0.43
1:B:97:PHE:HB2	2:J:180[A]:ASP:CG	2.44	0.42
2:J:88:ASP:OD1	2:J:88:ASP:C	2.61	0.42
2:J:327:PHE:CG	2:J:364:GLY:HA3	2.53	0.42
2:J:161:ALA:HA	2:J:176:LEU:O	2.20	0.42
2:J:186:PRO:HA	2:J:192:PHE:HA	2.00	0.42
2:H:152:LEU:HD12	2:H:186:PRO:HG3	2.02	0.42
2:H:302:ASP:CG	2:H:303:GLU:N	2.78	0.42
2:J:201:LEU:HD21	2:J:220:PHE:CE1	2.54	0.42
2:J:295:TYR:CD1	2:J:295:TYR:N	2.87	0.42
3:M:80:TYR:HB2	3:M:120:HIS:HB2	2.01	0.42
2:H:249:ILE:HB	2:H:265:VAL:HG12	2.02	0.41
3:L:33:GLY:O	3:L:87:PRO:HA	2.20	0.41
3:L:66:ASP:OD2	3:L:70:TYR:OH	2.30	0.41
3:M:20:ILE:HG22	3:M:25:TYR:CZ	2.55	0.41
2:J:89:GLY:HA3	2:J:385:MET:HE3	2.02	0.41
3:M:68:GLN:HB2	3:M:70:TYR:CE1	2.55	0.41
1:A:30:TYR:OH	1:A:54:ASN:O	2.35	0.41
1:A:73:LYS:HB2	1:A:73:LYS:HE3	1.98	0.41
3:M:7:THR:CG2	6:M:2002:HOH:O	2.68	0.41
2:H:115:ASP:O	2:H:119:LEU:HA	2.20	0.41
3:L:70:TYR:HB3	3:L:126:ILE:HG23	2.02	0.41
3:L:107:ILE:HD12	3:L:119:TYR:HB2	2.02	0.41
1:B:45:TRP:O	1:B:77:ALA:HA	2.20	0.41
1:B:97:PHE:HB2	2:J:180[B]:ASP:CG	2.45	0.41
2:J:13:THR:HA	2:J:16:GLN:HG2	2.02	0.41
2:J:166:ASP:CG	2:J:169:GLY:H	2.27	0.41
2:J:200:SER:C	2:J:201:LEU:HD23	2.46	0.41
3:L:34:ASN:ND2	3:L:82:VAL:CG2	2.84	0.41
2:H:280:GLY:HA3	2:H:301:ARG:CZ	2.51	0.41
2:J:343:LYS:HA	2:J:344:PRO:HD3	1.90	0.41
1:A:18:ASP:C	1:A:20:ALA:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:66:ASP:OD1	3:L:66:ASP:C	2.64	0.41
1:B:57:PHE:CD1	1:B:57:PHE:N	2.89	0.40
2:J:16:GLN:CB	3:L:18:ASN:O	2.70	0.40
2:J:289:ARG:HB3	6:J:2187:HOH:O	2.20	0.40
2:H:168:GLU:HG3	6:H:2091:HOH:O	2.21	0.40
2:J:9:GLN:H	2:J:12:GLU:HG3	1.87	0.40
3:L:35:ILE:HG22	3:L:37:ASP:H	1.87	0.40
3:M:27:ARG:HD2	3:M:43:LEU:HD21	2.04	0.40
1:A:6:PRO:HB2	1:A:7:SER:H	1.71	0.40
2:J:335:SER:HB2	2:J:349:LEU:HB3	2.04	0.40

All (2) 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)
6:B:2028:HOH:O	6:H:2034:HOH:O[8_665]	1.99	0.21
6:B:2011:HOH:O	6:H:2272:HOH:O[8_665]	2.10	0.10

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	103/105 (98%)	90 (87%)	6 (6%)	7 (7%)	1	0
1	B	103/105 (98%)	100 (97%)	2 (2%)	1 (1%)	12	8
2	H	383/386 (99%)	369 (96%)	12 (3%)	2 (0%)	24	20
2	J	380/386 (98%)	350 (92%)	25 (7%)	5 (1%)	9	5
3	L	122/131 (93%)	115 (94%)	6 (5%)	1 (1%)	16	10
3	M	122/131 (93%)	113 (93%)	7 (6%)	2 (2%)	7	3
All	All	1213/1244 (98%)	1137 (94%)	58 (5%)	18 (2%)	9	4

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ALA
1	A	15	GLU
1	A	17	ALA
2	H	6	ALA
2	J	9	GLN
2	J	180[A]	ASP
2	J	180[B]	ASP
3	L	67	GLY
3	M	130	ALA
1	A	6	PRO
1	B	17	ALA
1	A	18	ASP
2	H	102	ILE
2	J	102	ILE
2	J	325	ALA
1	A	58	VAL
1	A	39	VAL
3	M	127	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/85 (99%)	75 (89%)	9 (11%)	6	3
1	B	84/85 (99%)	79 (94%)	5 (6%)	17	13
2	H	311/311 (100%)	298 (96%)	13 (4%)	26	25
2	J	308/311 (99%)	292 (95%)	16 (5%)	21	17
3	L	104/106 (98%)	102 (98%)	2 (2%)	50	56
3	M	104/106 (98%)	97 (93%)	7 (7%)	15	10
All	All	995/1004 (99%)	943 (95%)	52 (5%)	21	17

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	ILE
1	A	29	LYS
1	A	32	THR
1	A	41	ASP
1	A	64	GLU
1	A	67	LEU
1	A	73	LYS
1	A	80	LEU
1	B	7	SER
1	B	8	GLU
1	B	27	LYS
1	B	32	THR
1	B	73	LYS
2	H	5	GLU
2	H	9	GLN
2	H	13	THR
2	H	117	VAL
2	H	208	THR
2	H	214	ILE
2	H	218	GLU
2	H	240	LEU
2	H	262	LEU
2	H	265	VAL
2	H	270[A]	GLU
2	H	270[B]	GLU
2	H	354	LYS
2	J	7	GLU
2	J	13	THR
2	J	117	VAL
2	J	208	THR
2	J	209	GLU
2	J	213	GLU
2	J	218	GLU
2	J	240	LEU
2	J	242	TRP
2	J	249	ILE
2	J	252	ILE
2	J	291	LEU
2	J	300	GLN
2	J	322	GLU
2	J	328	GLU
2	J	342	GLU

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Mol	Chain	Res	Type
3	L	16	GLN
3	L	60	SER
3	M	12	LYS
3	M	16	GLN
3	M	18	ASN
3	M	60	SER
3	M	69	SER
3	M	127	VAL
3	M	129	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	50	ASN
2	H	61	GLN
2	H	155	GLN
2	H	183	HIS
2	J	50	ASN
2	J	54	HIS
2	J	61	GLN
2	J	288	HIS
2	J	375	HIS
2	J	378	GLN
3	L	16	GLN
3	L	34	ASN
3	M	16	GLN
3	M	18	ASN
3	M	34	ASN
3	M	68	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
3	TRQ	M	57	3	16,17,18	1.92	5 (31%)	16,24,26	1.68	3 (18%)
3	TRQ	L	57	3	16,17,18	1.67	4 (25%)	16,24,26	1.65	4 (25%)

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
3	TRQ	M	57	3	-	0/5/19/21	0/2/2/2
3	TRQ	L	57	3	-	0/5/19/21	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	57	TRQ	CD2-CG	4.94	1.52	1.42
3	L	57	TRQ	CD2-CG	3.74	1.49	1.42
3	L	57	TRQ	CZ3-CH2	-3.39	1.36	1.45
3	M	57	TRQ	O7-CZ2	2.96	1.30	1.23
3	M	57	TRQ	CE3-CZ3	2.73	1.41	1.35
3	M	57	TRQ	CD2-CE2	2.36	1.48	1.42
3	M	57	TRQ	CZ3-CH2	-2.15	1.40	1.45
3	L	57	TRQ	CE3-CZ3	2.12	1.40	1.35
3	L	57	TRQ	CB-CA	2.07	1.58	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	57	TRQ	CZ2-CE2-NE1	3.78	136.46	127.25
3	L	57	TRQ	CG-CD1-NE1	3.53	113.77	109.22
3	L	57	TRQ	CD1-CG-CD2	-3.17	103.09	105.95
3	M	57	TRQ	CD1-NE1-CE2	2.99	113.18	109.49
3	L	57	TRQ	CZ2-CE2-NE1	2.66	133.72	127.25
3	L	57	TRQ	CB-CG-CD2	2.61	132.92	127.63
3	M	57	TRQ	CZ3-CH2-CZ2	2.23	121.90	118.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	57	TRQ	6	0
3	L	57	TRQ	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	H	1388	-	5,5,5	0.73	0	5,5,5	1.12	0
5	GOL	H	1389	-	5,5,5	0.64	0	5,5,5	1.46	1 (20%)
5	GOL	L	1132	-	5,5,5	0.53	0	5,5,5	1.13	0
5	GOL	H	1387	-	5,5,5	0.56	0	5,5,5	1.04	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	H	1388	-	-	1/4/4/4	-
5	GOL	H	1389	-	-	4/4/4/4	-
5	GOL	L	1132	-	-	2/4/4/4	-
5	GOL	H	1387	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	H	1389	GOL	O3-C3-C2	3.22	124.88	110.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	1387	GOL	C1-C2-C3-O3
5	H	1387	GOL	O2-C2-C3-O3
5	H	1389	GOL	O1-C1-C2-O2
5	H	1389	GOL	O1-C1-C2-C3
5	H	1389	GOL	C1-C2-C3-O3
5	H	1387	GOL	O1-C1-C2-C3
5	H	1388	GOL	C1-C2-C3-O3
5	L	1132	GOL	C1-C2-C3-O3
5	H	1389	GOL	O2-C2-C3-O3
5	L	1132	GOL	O2-C2-C3-O3
5	H	1387	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1389	GOL	12	0
5	L	1132	GOL	3	0
5	H	1387	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	105/105 (100%)	2.22	67 (63%) 0 0	62, 79, 91, 97	0
1	B	105/105 (100%)	0.96	6 (5%) 29 33	48, 56, 68, 81	0
2	H	382/386 (98%)	0.44	11 (2%) 53 57	29, 48, 64, 86	3 (0%)
2	J	381/386 (98%)	1.67	129 (33%) 1 1	41, 71, 89, 97	1 (0%)
3	L	124/131 (94%)	1.40	30 (24%) 2 2	48, 61, 74, 104	0
3	M	124/131 (94%)	0.67	8 (6%) 25 28	40, 54, 72, 102	0
All	All	1221/1244 (98%)	1.14	251 (20%) 2 3	29, 59, 87, 104	4 (0%)

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	130	ALA	6.5
2	J	265	VAL	5.1
3	L	130	ALA	4.9
2	J	6	ALA	4.8
2	J	264	ALA	4.7
2	J	364	GLY	4.6
2	J	26	LEU	4.5
2	J	262	LEU	4.5
1	A	13	ALA	4.4
1	A	5	ILE	4.3
2	J	276	GLY	4.3
3	L	70	TYR	4.2
2	J	316	LEU	4.2
2	J	261	PHE	4.2
2	J	249	ILE	4.2
2	J	295	TYR	4.2
1	A	65	ALA	4.2
3	M	131	SER	4.1
1	A	7	SER	4.0

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Mol	Chain	Res	Type	RSRZ
2	H	386	GLY	4.0
2	J	296	LEU	3.9
2	J	290	ALA	3.9
1	B	19	GLY	3.9
1	A	39	VAL	3.9
2	J	28	ALA	3.9
2	J	348	ALA	3.8
2	J	315	VAL	3.8
1	A	17	ALA	3.8
2	J	259	ALA	3.7
2	J	274	ALA	3.6
3	L	72	ILE	3.6
2	J	246	THR	3.6
3	L	64	PRO	3.5
2	J	345	LEU	3.5
2	J	358	ILE	3.5
2	J	85	VAL	3.5
2	J	287	TYR	3.5
2	J	44	ALA	3.4
2	H	209	GLU	3.4
2	J	220	PHE	3.4
1	A	3	ALA	3.3
1	A	12	ALA	3.3
2	J	201	LEU	3.3
2	J	227	LEU	3.3
2	J	268	LEU	3.3
2	J	263	PRO	3.2
1	A	66	ALA	3.2
2	J	357	TYR	3.2
2	J	252	ILE	3.2
2	J	23	ALA	3.2
2	J	267	ALA	3.2
3	L	44	THR	3.2
2	J	242	TRP	3.1
2	J	285	VAL	3.1
2	J	247	GLY	3.1
2	J	318	ALA	3.1
2	J	277	TRP	3.1
2	J	324	LEU	3.1
2	J	320	THR	3.1
1	A	87	THR	3.1
2	J	289	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
2	J	10	ALA	3.1
2	J	24	ALA	3.1
1	A	10	PRO	3.0
1	A	11	PHE	3.0
1	A	26	ALA	3.0
3	L	126	ILE	3.0
3	M	128	GLY	3.0
2	H	9	GLN	3.0
2	J	219	VAL	3.0
2	J	298	VAL	3.0
2	J	187	THR	3.0
1	A	67	LEU	3.0
2	J	338	VAL	3.0
2	J	346	LEU	3.0
2	H	5	GLU	3.0
1	A	14	ALA	2.9
2	J	279	PRO	2.9
2	J	312	PHE	2.9
3	L	26	TRP	2.9
2	J	297	LEU	2.9
1	A	43	VAL	2.9
1	A	58	VAL	2.9
2	J	327	PHE	2.9
2	J	286	ALA	2.9
1	A	56	HIS	2.9
1	A	95	HIS	2.9
2	J	226	PHE	2.8
2	J	288	HIS	2.8
2	J	17	ALA	2.8
3	L	71	LEU	2.8
2	J	342	GLU	2.8
1	A	22	VAL	2.8
1	B	9	SER	2.8
2	J	359	HIS	2.8
2	J	271	ALA	2.8
1	A	96	PRO	2.8
2	J	294	ILE	2.8
2	J	291	LEU	2.8
1	A	33	PRO	2.8
2	J	71	VAL	2.7
2	J	216	HIS	2.7
1	A	2	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	J	325	ALA	2.7
1	A	99	ARG	2.7
2	J	367	LEU	2.7
2	J	317	ASP	2.7
2	J	269	THR	2.7
1	A	88	TYR	2.7
3	L	58	VAL	2.7
1	A	60	GLY	2.7
2	J	205	ALA	2.6
2	J	370	VAL	2.6
2	J	322	GLU	2.6
2	J	27	ALA	2.6
1	A	82	PHE	2.6
2	J	64	ILE	2.6
2	J	340	GLN	2.6
1	A	53	HIS	2.6
3	L	63	ASN	2.6
1	A	59	ALA	2.6
1	A	9	SER	2.6
2	J	193	PHE	2.6
1	B	16	VAL	2.6
1	A	92	CYS	2.6
2	J	236	LYS	2.6
2	H	6	ALA	2.6
2	H	320	THR	2.6
3	L	59	ALA	2.6
1	A	6	PRO	2.6
2	J	344	PRO	2.6
2	J	313	VAL	2.5
1	A	55	VAL	2.5
3	L	25	TYR	2.5
2	J	341	ASP	2.5
1	A	77	ALA	2.5
2	J	383	ALA	2.5
3	L	124	SER	2.5
1	A	68	LYS	2.5
2	J	386	GLY	2.5
2	J	239	ARG	2.5
3	M	62	TYR	2.5
3	L	65	THR	2.5
2	J	34	PRO	2.5
2	J	300	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	4	THR	2.4
2	J	217	THR	2.4
2	J	260	LYS	2.4
2	J	221	HIS	2.4
1	A	105	GLU	2.4
3	L	13	TRP	2.4
2	J	18	ALA	2.4
2	J	66	GLY	2.4
3	L	93	GLY	2.4
1	B	97	PHE	2.4
1	A	37	VAL	2.4
1	A	104	VAL	2.4
3	L	129	LYS	2.4
1	A	61	VAL	2.4
1	A	103	VAL	2.4
2	J	228	ILE	2.4
2	J	339	SER	2.4
2	J	243	PRO	2.4
1	A	30	TYR	2.3
1	A	85	ALA	2.3
2	H	270[A]	GLU	2.3
1	A	86	GLY	2.3
2	J	281	GLY	2.3
2	J	319	LYS	2.3
1	A	93	THR	2.3
3	M	13	TRP	2.3
3	L	52	LEU	2.3
1	A	57	PHE	2.3
3	L	42	SER	2.3
2	J	379	VAL	2.3
1	A	44	THR	2.3
2	J	22	ALA	2.3
3	L	73	ALA	2.3
3	L	103	ALA	2.3
2	J	273	ARG	2.3
2	J	369	SER	2.3
2	J	314	VAL	2.3
2	J	208	THR	2.3
3	L	125	PRO	2.3
2	J	218	GLU	2.2
1	A	79	SER	2.2
2	J	117	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	244	THR	2.2
3	L	127	VAL	2.2
2	H	10	ALA	2.2
2	J	199	GLY	2.2
2	J	237	ALA	2.2
1	A	62	LEU	2.2
2	J	349	LEU	2.2
2	J	347	TYR	2.2
1	A	45	TRP	2.2
1	A	83	THR	2.2
3	L	20	ILE	2.2
2	J	135	VAL	2.2
1	B	18	ASP	2.2
1	A	40	GLY	2.2
2	J	37	LEU	2.2
3	L	68	GLN	2.2
2	J	363	SER	2.2
2	H	20	ARG	2.2
2	J	20	ARG	2.2
1	A	25	ILE	2.2
1	A	42	THR	2.2
2	J	333	ILE	2.2
3	L	15	PRO	2.2
2	H	259	ALA	2.2
2	J	361	ALA	2.2
1	A	80	LEU	2.2
3	M	60	SER	2.2
1	A	78	TYR	2.2
1	A	38	LYS	2.2
2	J	304	TRP	2.2
2	J	212	PRO	2.1
1	A	8	GLU	2.1
2	J	206	PHE	2.1
1	A	50	ALA	2.1
2	J	248	LYS	2.1
1	A	98	MET	2.1
1	A	1	ASP	2.1
2	J	29	GLY	2.1
2	J	257	GLY	2.1
2	H	202	ALA	2.1
2	J	68	ALA	2.1
2	J	232	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	L	55	ALA	2.1
2	J	254	LEU	2.1
3	L	18	ASN	2.1
2	J	146	PRO	2.1
3	L	123	ILE	2.1
1	A	15	GLU	2.1
1	A	63	GLY	2.1
1	B	25	ILE	2.1
3	M	127	VAL	2.1
1	A	20	ALA	2.1
2	J	270	GLU	2.0
2	J	15	GLY	2.0
3	L	128	GLY	2.0
1	A	16	VAL	2.0
1	A	102	VAL	2.0
2	J	335	SER	2.0
2	J	19	ALA	2.0
1	A	54	ASN	2.0
2	J	251	GLN	2.0
2	J	32	ASP	2.0
2	J	191	THR	2.0
3	M	98	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TRQ	L	57	16/17	0.94	0.10	54,57,60,61	0
3	TRQ	M	57	16/17	0.96	0.08	54,57,59,59	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	L	1132	6/6	0.78	0.18	75,76,77,77	0
5	GOL	H	1387	6/6	0.83	0.15	66,71,74,75	0
5	GOL	H	1389	6/6	0.90	0.20	39,46,54,58	0
4	CU	A	1106	1/1	0.93	0.09	66,66,66,66	0
5	GOL	H	1388	6/6	0.94	0.13	27,42,45,51	0
4	CU	B	1106	1/1	0.98	0.06	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.