



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 09:00 AM EDT

PDB ID : 5JYX
Title : Crystal structure of the covalent thioimide intermediate of the archaeosine synthase QueF-Like
Authors : Mei, X.; Swairjo, M.A.
Deposited on : 2016-05-15
Resolution : 2.74 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:

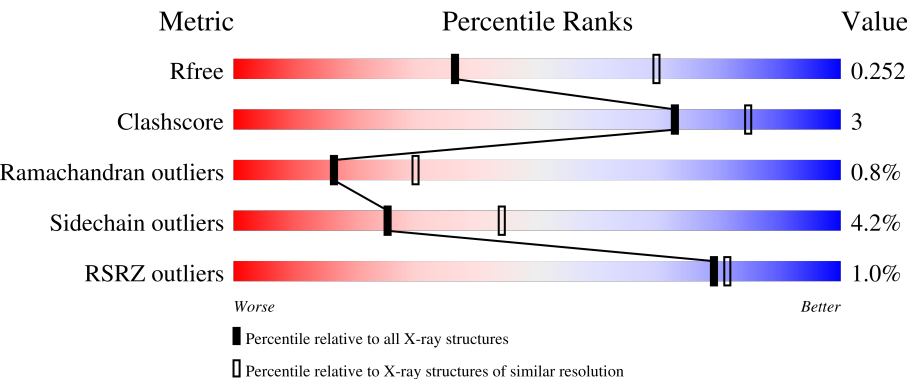
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.74 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}	164625	1649 (2.76-2.72)
Clashscore	180529	1744 (2.76-2.72)
Ramachandran outliers	177936	1710 (2.76-2.72)
Sidechain outliers	177891	1711 (2.76-2.72)
RSRZ outliers	164620	1649 (2.76-2.72)

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	109	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>77%18%••</div></div>
1	B	109	<div><div></div><div></div><div></div><div></div><div></div></div> <div>89%11%</div>
1	C	109	<div><div></div><div></div><div></div><div></div><div></div></div> <div>78%17%•5%</div>
1	D	109	<div><div></div><div></div><div></div><div></div><div></div></div> <div>78%17%••</div>
1	E	109	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>83%12%5%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	109	<div><div><div></div><div></div><div></div></div><div>2%</div><div>83%</div><div>12%</div><div>5%</div></div>
1	G	109	<div><div><div></div><div></div><div></div></div><div>3%</div><div>83%</div><div>13%</div><div>• • •</div></div>
1	H	109	<div><div><div></div><div></div><div></div></div><div>3%</div><div>85%</div><div>10%</div><div>5%</div></div>
1	I	109	<div><div><div></div><div></div><div></div></div><div>2%</div><div>89%</div><div>9%</div><div>•</div></div>
1	J	109	<div><div><div></div><div></div><div></div></div><div>%</div><div>84%</div><div>10%</div><div>• 5%</div></div>
1	K	109	<div><div><div></div><div></div><div></div></div><div>%</div><div>80%</div><div>15%</div><div>• •</div></div>
1	L	109	<div><div><div></div><div></div><div></div></div><div></div><div>85%</div><div>11%</div><div>•</div></div>
1	M	109	<div><div><div></div><div></div><div></div></div><div>%</div><div>84%</div><div>10%</div><div>6%</div></div>
1	N	109	<div><div><div></div><div></div><div></div></div><div></div><div>88%</div><div>6%</div><div>• 5%</div></div>
1	O	109	<div><div><div></div><div></div><div></div></div><div></div><div>86%</div><div>8%</div><div>6%</div></div>

2 Entry composition

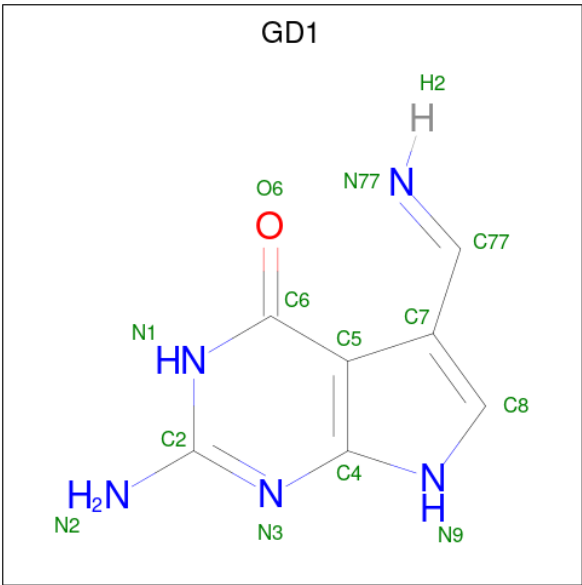
There are 4 unique types of molecules in this entry. The entry contains 12565 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Archaeosine synthase QueF-Like.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	Se	0	1	0
			819	527	133	156	1	2			
1	B	109	Total	C	N	O	S	Se	0	1	0
			853	552	137	161	1	2			
1	C	104	Total	C	N	O	S	Se	0	0	0
			806	518	132	153	1	2			
1	D	105	Total	C	N	O	S	Se	0	0	0
			813	523	133	154	1	2			
1	E	104	Total	C	N	O	S	Se	0	0	0
			806	518	132	153	1	2			
1	F	104	Total	C	N	O	S	Se	0	0	0
			805	518	132	153	1	1			
1	G	107	Total	C	N	O	S	Se	0	2	0
			839	541	135	160	1	2			
1	H	104	Total	C	N	O	S	Se	0	0	0
			805	518	132	153	1	1			
1	I	107	Total	C	N	O	S	Se	0	1	0
			835	538	138	156	1	2			
1	J	104	Total	C	N	O	S	Se	0	1	0
			812	522	132	155	1	2			
1	K	106	Total	C	N	O	S	Se	0	0	0
			820	528	134	155	1	2			
1	L	105	Total	C	N	O	S	Se	0	0	0
			813	523	133	154	1	2			
1	M	103	Total	C	N	O	S	Se	0	2	0
			809	519	132	156	1	1			
1	N	104	Total	C	N	O	S	Se	0	0	0
			806	518	132	153	1	2			
1	O	103	Total	C	N	O	S	Se	0	0	0
			799	513	131	152	1	2			

- Molecule 2 is 2-amino-5-[(Z)-iminomethyl]-3,7-dihydro-4H-pyrrolo[2,3-d]pyrimidin-4-one (three-letter code: GD1) (formula: C₇H₇N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	7	5	1		
2	B	1	Total	C	N	O	0	0
			13	7	5	1		
2	C	1	Total	C	N	O	0	0
			13	7	5	1		
2	D	1	Total	C	N	O	0	0
			13	7	5	1		
2	E	1	Total	C	N	O	0	0
			13	7	5	1		
2	F	1	Total	C	N	O	0	0
			13	7	5	1		
2	G	1	Total	C	N	O	0	0
			13	7	5	1		
2	H	1	Total	C	N	O	0	0
			13	7	5	1		
2	I	1	Total	C	N	O	0	0
			13	7	5	1		
2	J	1	Total	C	N	O	0	0
			13	7	5	1		
2	K	1	Total	C	N	O	0	0
			13	7	5	1		
2	L	1	Total	C	N	O	0	0
			13	7	5	1		
2	M	1	Total	C	N	O	0	0
			13	7	5	1		
2	N	1	Total	C	N	O	0	0
			13	7	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total	C	N	O	0	0
			13	7	5	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	L	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	12	Total	O	0	0
			12	12		
4	C	13	Total	O	0	0
			13	13		
4	D	13	Total	O	0	0
			13	13		
4	E	11	Total	O	0	0
			11	11		
4	F	9	Total	O	0	0
			9	9		
4	G	7	Total	O	0	0
			7	7		
4	H	3	Total	O	0	0
			3	3		
4	I	7	Total	O	0	0
			7	7		
4	J	5	Total	O	0	0
			5	5		
4	K	6	Total	O	0	0
			6	6		
4	L	4	Total	O	0	0
			4	4		
4	M	10	Total	O	0	0
			10	10		

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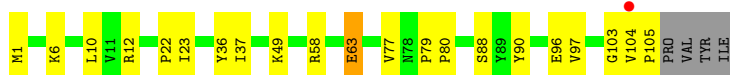
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	N	2	Total	O	0	0
			2	2		
4	O	9	Total	O	0	0
			9	9		

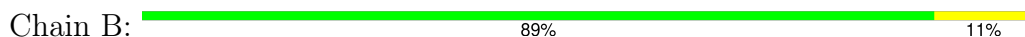
3 Residue-property plots [i](#)

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.

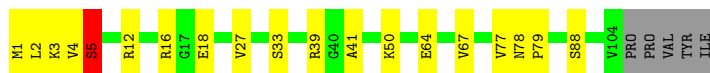
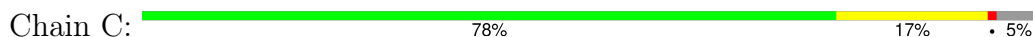
- Molecule 1: Archeosine synthase QueF-Like



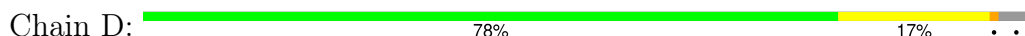
- Molecule 1: Archeosine synthase QueF-Like



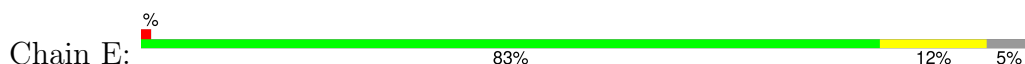
- Molecule 1: Archeosine synthase QueF-Like



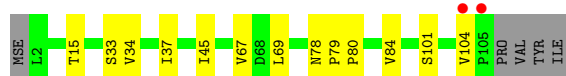
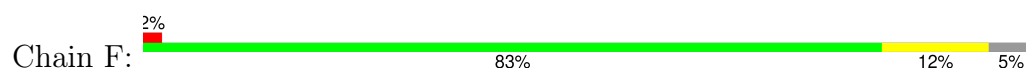
- Molecule 1: Archeosine synthase QueF-Like



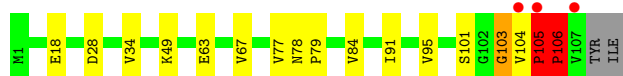
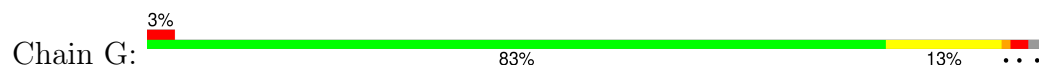
- Molecule 1: Archeosine synthase QueF-Like



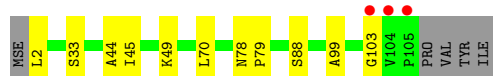
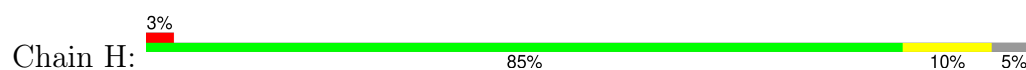
- Molecule 1: Archeosine synthase QueF-Like



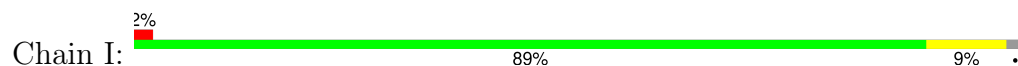
- Molecule 1: Archaeosine synthase QueF-Like



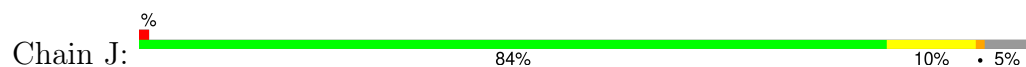
- Molecule 1: Archaeosine synthase QueF-Like



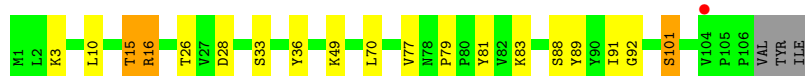
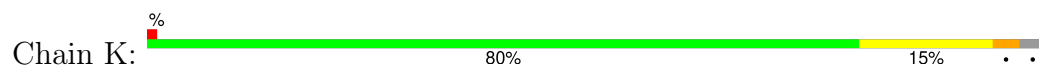
- Molecule 1: Archaeosine synthase QueF-Like



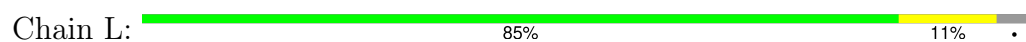
- Molecule 1: Archaeosine synthase QueF-Like



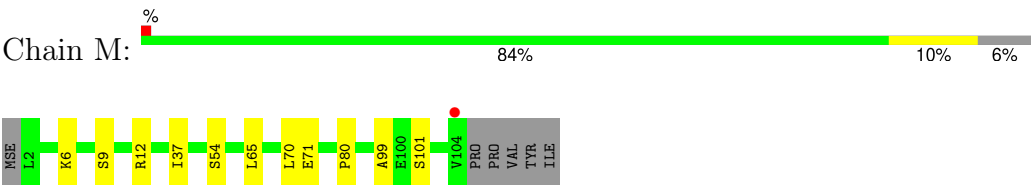
- Molecule 1: Archaeosine synthase QueF-Like



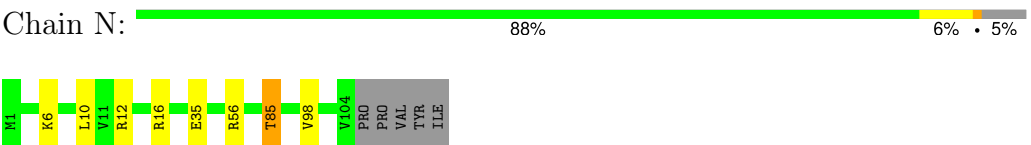
- Molecule 1: Archaeosine synthase QueF-Like



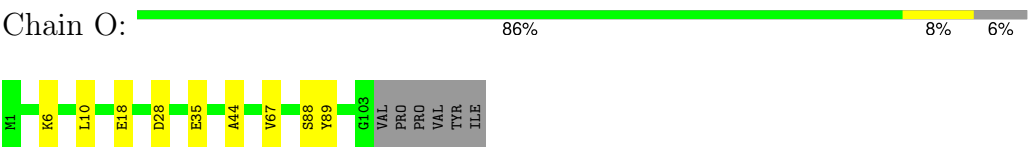
● Molecule 1: Archaeosine synthase QueF-Like



● Molecule 1: Archaeosine synthase QueF-Like



● Molecule 1: Archaeosine synthase QueF-Like



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.32Å 126.78Å 65.08Å 90.00° 102.58° 90.00°	Depositor
Resolution (Å)	108.56 – 2.74 108.56 – 2.74	Depositor EDS
% Data completeness (in resolution range)	96.3 (108.56-2.74) 96.4 (108.56-2.74)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.75 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.171 , 0.259 0.173 , 0.252	Depositor DCC
R_{free} test set	1975 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 23.7	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	0.96	EDS
Total number of atoms	12565	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: GD1, NA

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	1.15	4/834 (0.5%)	1.01	3/1126 (0.3%)
1	B	1.06	3/870 (0.3%)	1.03	2/1177 (0.2%)
1	C	1.08	2/817 (0.2%)	1.00	1/1102 (0.1%)
1	D	1.02	1/825 (0.1%)	1.04	0/1114
1	E	1.03	1/817 (0.1%)	1.01	2/1102 (0.2%)
1	F	0.95	0/817	1.01	1/1104 (0.1%)
1	G	0.95	0/858	1.04	1/1160 (0.1%)
1	H	0.90	0/817	0.96	0/1104
1	I	0.82	0/851	0.89	0/1150
1	J	0.82	0/826	0.92	0/1114
1	K	0.85	0/833	0.98	1/1126 (0.1%)
1	L	0.80	0/825	0.86	1/1114 (0.1%)
1	M	0.95	0/823	0.97	0/1111
1	N	0.77	0/817	0.92	1/1102 (0.1%)
1	O	0.86	0/810	0.96	0/1092
All	All	0.94	11/12440 (0.1%)	0.98	13/16798 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	18	GLU	CD-OE1	8.67	1.35	1.25
1	A	63	GLU	CD-OE2	6.44	1.32	1.25
1	A	96	GLU	CD-OE1	6.43	1.32	1.25
1	B	59	GLU	CD-OE1	6.42	1.32	1.25
1	A	96	GLU	CD-OE2	6.26	1.32	1.25
1	C	64	GLU	CD-OE1	6.00	1.32	1.25
1	B	94	GLU	CD-OE1	5.35	1.31	1.25
1	B	59	GLU	CD-OE2	5.29	1.31	1.25
1	E	47	GLU	CD-OE1	5.20	1.31	1.25
1	A	90	TYR	CE1-CZ	5.19	1.45	1.38
1	D	46	GLU	CG-CD	5.13	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	12	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	E	77	VAL	N-CA-C	-5.87	95.15	111.00
1	L	12	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	E	28	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	K	28	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	96	GLU	OE1-CD-OE2	5.69	130.13	123.30
1	B	58	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	G	106	PRO	CA-N-CD	-5.19	104.23	111.50
1	N	56	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	F	69	LEU	CB-CG-CD1	5.03	119.54	111.00
1	A	58	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	33	SER	CB-CA-C	-5.02	100.56	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	819	0	860	6	0
1	B	853	0	896	3	0
1	C	806	0	847	8	0
1	D	813	0	854	11	0
1	E	806	0	847	5	0
1	F	805	0	842	7	0
1	G	839	0	882	13	0
1	H	805	0	842	5	0
1	I	835	0	883	4	0
1	J	812	0	853	5	0
1	K	820	0	861	10	0
1	L	813	0	854	6	0
1	M	809	0	843	3	0
1	N	806	0	847	3	0
1	O	799	0	838	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	13	0	5	0	0
2	B	13	0	5	0	0
2	C	13	0	5	0	0
2	D	13	0	5	2	0
2	E	13	0	5	0	0
2	F	13	0	5	1	0
2	G	13	0	5	0	0
2	H	13	0	5	0	0
2	I	13	0	5	1	0
2	J	13	0	5	2	0
2	K	13	0	5	0	0
2	L	13	0	5	0	0
2	M	13	0	5	0	0
2	N	13	0	5	0	0
2	O	13	0	5	2	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	L	1	0	0	0	0
4	A	16	0	0	0	0
4	B	12	0	0	0	0
4	C	13	0	0	1	0
4	D	13	0	0	0	0
4	E	11	0	0	0	0
4	F	9	0	0	0	0
4	G	7	0	0	0	0
4	H	3	0	0	0	0
4	I	7	0	0	0	0
4	J	5	0	0	0	0
4	K	6	0	0	0	0
4	L	4	0	0	0	0
4	M	10	0	0	0	0
4	N	2	0	0	0	0
4	O	9	0	0	0	0
All	All	12565	0	12924	78	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 3.

All (78) 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:G:49:LYS:HE3	1:K:91:ILE:O	1.87	0.74
1:F:67:VAL:HG11	1:O:6:LYS:HB2	1.75	0.67
1:C:1:MSE:HE3	1:C:77:VAL:HA	1.77	0.66
1:G:103:GLY:O	1:G:105:PRO:HD3	1.96	0.65
1:F:37:ILE:O	1:F:80:PRO:HD2	1.99	0.63
1:K:49:LYS:HE3	1:L:91:ILE:O	1.99	0.63
1:N:85:THR:HG23	1:N:98:VAL:HG22	1.81	0.63
1:E:93:VAL:HG22	1:F:15:THR:HB	1.82	0.61
1:D:63:GLU:HA	1:D:97:VAL:HG11	1.84	0.59
1:E:95:VAL:HG21	1:F:45:ILE:HD11	1.85	0.59
1:C:1:MSE:HG3	1:C:77:VAL:HG12	1.89	0.54
1:C:1:MSE:HE2	1:C:41:ALA:CB	2.37	0.54
1:L:37:ILE:O	1:L:79:PRO:HB3	2.09	0.52
1:H:78:ASN:N	1:H:79:PRO:HD3	2.25	0.52
1:A:77:VAL:HG23	1:A:79:PRO:HG3	1.91	0.52
1:K:89:TYR:CZ	1:K:92:GLY:HA2	2.46	0.51
1:N:12:ARG:NE	1:N:35:GLU:OE1	2.44	0.51
1:K:70:LEU:HD11	1:K:101:SER:HB2	1.92	0.50
1:D:91:ILE:O	1:H:49:LYS:HE2	2.11	0.50
1:K:77:VAL:HG23	1:K:79:PRO:HG3	1.94	0.50
1:C:78:ASN:N	1:C:79:PRO:HD3	2.27	0.49
1:D:95:VAL:HG21	1:H:45:ILE:HD11	1.94	0.49
1:G:18:GLU:HA	1:G:28:ASP:O	2.12	0.49
1:F:34:VAL:HG22	1:F:84:VAL:HG22	1.93	0.49
1:I:6:LYS:HB2	1:O:67:VAL:HG11	1.95	0.49
1:A:10:LEU:HD12	1:A:36:TYR:O	2.13	0.49
1:G:34:VAL:HG22	1:G:84:VAL:HG22	1.94	0.48
1:F:78:ASN:N	1:F:79:PRO:HD3	2.28	0.48
1:L:34:VAL:HG22	1:L:84:VAL:HG22	1.95	0.48
1:N:10:LEU:HD11	1:N:35:GLU:HG2	1.95	0.48
1:E:81:TYR:HD1	1:E:103:GLY:H	1.61	0.48
1:D:34:VAL:HG22	1:D:84:VAL:HG22	1.96	0.47
1:G:49:LYS:CE	1:K:91:ILE:O	2.58	0.47
1:G:77:VAL:HG23	1:G:79:PRO:HG3	1.96	0.47
1:J:90:TYR:CD2	1:J:91:ILE:HG12	2.50	0.46
1:L:87:LYS:HG2	1:L:96:GLU:HG2	1.97	0.46
1:O:28:ASP:OD2	2:O:201:GD1:N77	2.49	0.46
1:F:67:VAL:HG11	1:O:6:LYS:CB	2.46	0.46
1:I:37:ILE:O	1:I:79:PRO:HB3	2.16	0.46
1:M:65:LEU:C	1:M:65:LEU:HD23	2.35	0.46
1:B:95:VAL:HG21	1:E:45:ILE:HD11	1.98	0.45
1:J:34:VAL:HG22	1:J:84:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLY:O	1:A:105:PRO:HD3	2.17	0.45
1:B:63:GLU:HA	1:B:97:VAL:HG11	1.99	0.45
1:D:13:LEU:HD23	1:G:95:VAL:HG13	1.99	0.45
1:D:28:ASP:OD2	2:D:201:GD1:N77	2.51	0.44
1:H:70:LEU:HD22	1:H:99:ALA:HB1	1.99	0.44
1:I:45:ILE:HD12	2:O:201:GD1:C4	2.48	0.44
1:A:37:ILE:O	1:A:80:PRO:HD2	2.18	0.43
1:C:67:VAL:HG11	1:J:6:LYS:HB3	2.01	0.43
1:M:70:LEU:HD22	1:M:99:ALA:HB1	2.00	0.43
1:L:90:TYR:CD2	1:L:91:ILE:HG12	2.53	0.43
1:K:10:LEU:HD12	1:K:36:TYR:O	2.19	0.43
1:D:49:LYS:HE2	1:G:91:ILE:O	2.19	0.43
1:D:13:LEU:CD2	1:G:95:VAL:HG13	2.50	0.42
1:B:45:ILE:HD12	2:I:201:GD1:C4	2.50	0.42
1:A:63:GLU:HA	1:A:97:VAL:HG11	2.01	0.42
1:K:15:THR:HG23	1:K:16:ARG:N	2.35	0.42
1:C:4:VAL:HG12	1:C:5:SER:N	2.35	0.41
1:E:81:TYR:HD1	1:E:103:GLY:N	2.19	0.41
1:J:28:ASP:OD2	2:J:201:GD1:N77	2.52	0.41
1:A:49:LYS:HE3	1:C:27:VAL:HG11	2.01	0.41
1:I:70:LEU:HD22	1:I:99:ALA:HB1	2.01	0.41
1:O:10:LEU:HD11	1:O:35:GLU:CG	2.50	0.41
1:M:37:ILE:O	1:M:80:PRO:HD2	2.21	0.41
1:G:78:ASN:N	1:G:79:PRO:HD3	2.35	0.41
1:H:2:LEU:HD12	1:H:44:ALA:HA	2.02	0.41
1:K:49:LYS:NZ	1:O:18:GLU:OE1	2.54	0.41
1:L:77:VAL:HG23	1:L:79:PRO:HG3	2.01	0.41
1:G:63:GLU:N	1:G:63:GLU:OE1	2.54	0.41
1:K:81:TYR:OH	1:K:83:LYS:HB2	2.22	0.40
1:C:16:ARG:HD2	4:C:313:HOH:O	2.21	0.40
1:J:90:TYR:CE2	2:J:201:GD1:H7	2.56	0.40
1:D:37:ILE:O	1:D:80:PRO:HD2	2.20	0.40
1:D:61:LEU:HD22	2:D:201:GD1:C6	2.52	0.40
1:G:104:VAL:O	1:G:106:PRO:CD	2.69	0.40
1:D:6:LYS:HB3	1:G:67:VAL:HG11	2.04	0.40
2:F:201:GD1:H5	1:O:44:ALA:HA	1.85	0.40

There are no symmetry-related clashes.

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	104/109 (95%)	99 (95%)	3 (3%)	2 (2%)	6	11
1	B	108/109 (99%)	101 (94%)	7 (6%)	0	100	100
1	C	102/109 (94%)	100 (98%)	1 (1%)	1 (1%)	13	23
1	D	103/109 (94%)	95 (92%)	7 (7%)	1 (1%)	13	23
1	E	102/109 (94%)	93 (91%)	9 (9%)	0	100	100
1	F	102/109 (94%)	97 (95%)	4 (4%)	1 (1%)	13	23
1	G	107/109 (98%)	99 (92%)	5 (5%)	3 (3%)	4	6
1	H	102/109 (94%)	96 (94%)	5 (5%)	1 (1%)	13	23
1	I	106/109 (97%)	99 (93%)	6 (6%)	1 (1%)	14	27
1	J	103/109 (94%)	91 (88%)	9 (9%)	3 (3%)	3	5
1	K	104/109 (95%)	96 (92%)	8 (8%)	0	100	100
1	L	103/109 (94%)	95 (92%)	8 (8%)	0	100	100
1	M	103/109 (94%)	96 (93%)	7 (7%)	0	100	100
1	N	102/109 (94%)	92 (90%)	10 (10%)	0	100	100
1	O	101/109 (93%)	95 (94%)	6 (6%)	0	100	100
All	All	1552/1635 (95%)	1444 (93%)	95 (6%)	13 (1%)	16	30

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	106	PRO
1	A	23	ILE
1	A	104	VAL
1	G	103	GLY
1	G	105	PRO
1	H	103	GLY
1	D	25	LYS
1	J	54	SER

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Mol	Chain	Res	Type
1	F	104	VAL
1	I	105	PRO
1	J	101	SER
1	J	75	ALA
1	C	5	SER

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	94/95 (99%)	90 (96%)	4 (4%)	25	43
1	B	98/95 (103%)	94 (96%)	4 (4%)	26	45
1	C	92/95 (97%)	85 (92%)	7 (8%)	11	20
1	D	93/95 (98%)	87 (94%)	6 (6%)	14	25
1	E	92/95 (97%)	87 (95%)	5 (5%)	18	33
1	F	92/95 (97%)	90 (98%)	2 (2%)	47	68
1	G	97/95 (102%)	95 (98%)	2 (2%)	48	69
1	H	92/95 (97%)	90 (98%)	2 (2%)	47	68
1	I	96/95 (101%)	93 (97%)	3 (3%)	35	56
1	J	93/95 (98%)	89 (96%)	4 (4%)	25	43
1	K	94/95 (99%)	87 (93%)	7 (7%)	11	20
1	L	93/95 (98%)	91 (98%)	2 (2%)	47	68
1	M	93/95 (98%)	87 (94%)	6 (6%)	14	25
1	N	92/95 (97%)	89 (97%)	3 (3%)	33	54
1	O	91/95 (96%)	89 (98%)	2 (2%)	47	68
All	All	1402/1425 (98%)	1343 (96%)	59 (4%)	25	44

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE

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Mol	Chain	Res	Type
1	A	6	LYS
1	A	22	PRO
1	A	88	SER
1	B	1	MSE
1	B	6	LYS
1	B	7	SER
1	B	101	SER
1	C	2	LEU
1	C	3	LYS
1	C	5	SER
1	C	33	SER
1	C	39	ARG
1	C	50	LYS
1	C	88	SER
1	D	2	LEU
1	D	6	LYS
1	D	33	SER
1	D	47	GLU
1	D	65	LEU
1	D	100	GLU
1	E	3	LYS
1	E	39	ARG
1	E	88	SER
1	E	101	SER
1	E	104	VAL
1	F	33	SER
1	F	101	SER
1	G	101	SER
1	G	105	PRO
1	H	33	SER
1	H	88	SER
1	I	1	MSE
1	I	9	SER
1	I	33	SER
1	J	1	MSE
1	J	6	LYS
1	J	26	THR
1	J	88	SER
1	K	3	LYS
1	K	15	THR
1	K	16	ARG
1	K	26	THR

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Mol	Chain	Res	Type
1	K	33	SER
1	K	88	SER
1	K	101	SER
1	L	9	SER
1	L	16	ARG
1	M	6	LYS
1	M	9	SER
1	M	12	ARG
1	M	54	SER
1	M	71	GLU
1	M	101	SER
1	N	6	LYS
1	N	16	ARG
1	N	85	THR
1	O	88	SER
1	O	89	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	78	ASN
1	C	78	ASN
1	H	62	HIS
1	I	78	ASN
1	L	78	ASN
1	O	62	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 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
2	GD1	G	201	1	11,14,14	1.93	3 (27%)	10,20,20	2.54	6 (60%)
2	GD1	H	201	1	11,14,14	2.25	2 (18%)	10,20,20	1.50	3 (30%)
2	GD1	I	201	1	11,14,14	2.31	2 (18%)	10,20,20	1.62	2 (20%)
2	GD1	F	201	1	11,14,14	1.77	2 (18%)	10,20,20	1.84	5 (50%)
2	GD1	J	201	1	11,14,14	1.98	2 (18%)	10,20,20	1.82	3 (30%)
2	GD1	C	201	1	11,14,14	2.15	3 (27%)	10,20,20	1.72	2 (20%)
2	GD1	A	201	1	11,14,14	2.20	2 (18%)	10,20,20	1.78	4 (40%)
2	GD1	K	201	1	11,14,14	2.54	3 (27%)	10,20,20	1.94	4 (40%)
2	GD1	N	201	1	11,14,14	2.23	4 (36%)	10,20,20	1.89	4 (40%)
2	GD1	E	201	1	11,14,14	1.92	2 (18%)	10,20,20	2.61	6 (60%)
2	GD1	M	201	1	11,14,14	2.06	2 (18%)	10,20,20	1.89	4 (40%)
2	GD1	O	201	1	11,14,14	2.34	2 (18%)	10,20,20	1.98	5 (50%)
2	GD1	D	201	1	11,14,14	2.12	2 (18%)	10,20,20	1.51	3 (30%)
2	GD1	L	201	1	11,14,14	1.64	1 (9%)	10,20,20	1.44	1 (10%)
2	GD1	B	201	1	11,14,14	2.30	2 (18%)	10,20,20	2.83	7 (70%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GD1	G	201	1	-	0/0/2/2	0/2/2/2
2	GD1	H	201	1	-	0/0/2/2	0/2/2/2
2	GD1	I	201	1	-	0/0/2/2	0/2/2/2
2	GD1	F	201	1	-	0/0/2/2	0/2/2/2
2	GD1	J	201	1	-	0/0/2/2	0/2/2/2
2	GD1	C	201	1	-	0/0/2/2	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GD1	A	201	1	-	0/0/2/2	0/2/2/2
2	GD1	K	201	1	-	0/0/2/2	0/2/2/2
2	GD1	N	201	1	-	0/0/2/2	0/2/2/2
2	GD1	E	201	1	-	0/0/2/2	0/2/2/2
2	GD1	M	201	1	-	0/0/2/2	0/2/2/2
2	GD1	O	201	1	-	0/0/2/2	0/2/2/2
2	GD1	D	201	1	-	0/0/2/2	0/2/2/2
2	GD1	L	201	1	-	0/0/2/2	0/2/2/2
2	GD1	B	201	1	-	0/0/2/2	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	201	GD1	O6-C6	7.32	1.40	1.23
2	I	201	GD1	O6-C6	6.34	1.38	1.23
2	O	201	GD1	O6-C6	6.28	1.38	1.23
2	D	201	GD1	O6-C6	6.23	1.37	1.23
2	H	201	GD1	O6-C6	6.15	1.37	1.23
2	A	201	GD1	O6-C6	6.10	1.37	1.23
2	B	201	GD1	O6-C6	6.05	1.37	1.23
2	M	201	GD1	O6-C6	5.94	1.37	1.23
2	N	201	GD1	O6-C6	5.94	1.37	1.23
2	C	201	GD1	O6-C6	5.75	1.36	1.23
2	E	201	GD1	O6-C6	5.43	1.36	1.23
2	J	201	GD1	O6-C6	5.31	1.35	1.23
2	G	201	GD1	O6-C6	5.15	1.35	1.23
2	F	201	GD1	O6-C6	5.02	1.35	1.23
2	L	201	GD1	O6-C6	4.54	1.33	1.23
2	H	201	GD1	C7-C77	3.43	1.53	1.47
2	O	201	GD1	C5-C4	-3.42	1.37	1.42
2	M	201	GD1	C7-C77	2.87	1.52	1.47
2	K	201	GD1	C7-C77	2.71	1.51	1.47
2	B	201	GD1	C6-N1	2.65	1.41	1.37
2	N	201	GD1	C7-C77	2.64	1.51	1.47
2	J	201	GD1	C7-C77	2.57	1.51	1.47
2	I	201	GD1	C5-C4	-2.40	1.38	1.42
2	E	201	GD1	C5-C4	-2.34	1.38	1.42
2	G	201	GD1	C5-C6	2.30	1.51	1.47
2	N	201	GD1	C5-C6	2.29	1.51	1.47
2	G	201	GD1	C2-N3	2.27	1.38	1.33
2	N	201	GD1	C5-C4	-2.23	1.38	1.42
2	F	201	GD1	C7-C77	2.19	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	GD1	C7-C77	2.17	1.50	1.47
2	K	201	GD1	C5-C6	2.12	1.51	1.47
2	A	201	GD1	C7-C77	2.09	1.50	1.47
2	D	201	GD1	C5-C6	2.07	1.51	1.47
2	C	201	GD1	C5-C4	-2.03	1.39	1.42

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	GD1	C5-C6-N1	4.97	120.61	115.05
2	E	201	GD1	C5-C6-N1	3.91	119.42	115.05
2	E	201	GD1	N2-C2-N1	3.78	124.73	116.76
2	B	201	GD1	C5-C6-N1	3.74	119.23	115.05
2	B	201	GD1	O6-C6-C5	-3.68	116.14	124.11
2	K	201	GD1	N2-C2-N1	3.65	124.47	116.76
2	B	201	GD1	O6-C6-N1	3.38	124.62	120.62
2	B	201	GD1	N2-C2-N1	3.37	123.88	116.76
2	G	201	GD1	C2-N1-C6	-3.20	119.25	125.11
2	B	201	GD1	C7-C77-N77	-3.16	116.54	121.83
2	N	201	GD1	C5-C6-N1	3.16	118.59	115.05
2	E	201	GD1	N2-C2-N3	-3.13	113.56	119.67
2	O	201	GD1	N2-C2-N1	3.13	123.37	116.76
2	J	201	GD1	O6-C6-N1	-3.13	116.91	120.62
2	L	201	GD1	C5-C6-N1	3.08	118.50	115.05
2	E	201	GD1	C8-C7-C77	-2.99	116.26	127.93
2	B	201	GD1	C8-C7-C77	-2.96	116.35	127.93
2	E	201	GD1	C7-C77-N77	-2.92	116.94	121.83
2	C	201	GD1	O6-C6-N1	-2.92	117.15	120.62
2	J	201	GD1	C8-C7-C77	-2.86	116.76	127.93
2	O	201	GD1	C5-C6-N1	2.85	118.24	115.05
2	M	201	GD1	N2-C2-N1	2.80	122.67	116.76
2	A	201	GD1	C8-C7-C77	-2.78	117.06	127.93
2	I	201	GD1	N2-C2-N1	2.75	122.57	116.76
2	M	201	GD1	C5-C6-N1	2.72	118.09	115.05
2	F	201	GD1	N2-C2-N1	2.71	122.49	116.76
2	F	201	GD1	C5-C6-N1	2.70	118.07	115.05
2	K	201	GD1	N2-C2-N3	-2.68	114.44	119.67
2	A	201	GD1	C7-C77-N77	-2.68	117.35	121.83
2	J	201	GD1	C5-C6-N1	2.68	118.05	115.05
2	A	201	GD1	C5-C6-N1	2.67	118.04	115.05
2	G	201	GD1	O6-C6-C5	-2.67	118.33	124.11
2	D	201	GD1	N2-C2-N1	2.64	122.34	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	GD1	C8-C7-C77	-2.61	117.72	127.93
2	M	201	GD1	C8-C7-C77	-2.61	117.74	127.93
2	G	201	GD1	C8-C7-C77	-2.59	117.81	127.93
2	C	201	GD1	C5-C6-N1	2.56	117.92	115.05
2	N	201	GD1	C8-C7-C77	-2.55	117.95	127.93
2	M	201	GD1	C7-C77-N77	-2.47	117.70	121.83
2	E	201	GD1	C2-N1-C6	-2.44	120.64	125.11
2	O	201	GD1	C8-C7-C77	-2.41	118.50	127.93
2	I	201	GD1	C8-C7-C77	-2.35	118.73	127.93
2	N	201	GD1	N2-C2-N1	2.34	121.70	116.76
2	F	201	GD1	N2-C2-N3	-2.28	115.23	119.67
2	N	201	GD1	C2-N1-C6	-2.27	120.95	125.11
2	K	201	GD1	C8-C7-C77	-2.27	119.06	127.93
2	D	201	GD1	C8-C7-C77	-2.24	119.17	127.93
2	H	201	GD1	C8-C7-C77	-2.21	119.29	127.93
2	G	201	GD1	N2-C2-N1	2.19	121.38	116.76
2	G	201	GD1	C7-C8-N9	-2.13	105.02	108.59
2	H	201	GD1	N2-C2-N3	-2.12	115.53	119.67
2	A	201	GD1	C2-N1-C6	-2.12	121.24	125.11
2	O	201	GD1	C2-N1-C6	-2.11	121.25	125.11
2	H	201	GD1	C2-N1-C6	-2.11	121.26	125.11
2	K	201	GD1	O6-C6-N1	2.06	123.07	120.62
2	B	201	GD1	C2-N1-C6	-2.05	121.35	125.11
2	F	201	GD1	C2-N1-C6	-2.05	121.36	125.11
2	O	201	GD1	N2-C2-N3	-2.03	115.71	119.67
2	D	201	GD1	N2-C2-N3	-2.00	115.77	119.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	201	GD1	1	0
2	F	201	GD1	1	0
2	J	201	GD1	2	0
2	O	201	GD1	2	0
2	D	201	GD1	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	103/109 (94%)	-0.87	1 (0%) 79 81	24, 38, 59, 103	1 (0%)
1	B	107/109 (98%)	-0.86	0 100 100	26, 40, 72, 108	1 (0%)
1	C	102/109 (93%)	-0.85	0 100 100	28, 41, 74, 92	0
1	D	103/109 (94%)	-0.80	0 100 100	32, 43, 73, 101	0
1	E	102/109 (93%)	-0.82	1 (0%) 79 81	30, 43, 67, 106	0
1	F	103/109 (94%)	-0.73	2 (1%) 66 66	34, 45, 84, 115	0
1	G	105/109 (96%)	-0.64	3 (2%) 54 54	29, 47, 88, 134	2 (1%)
1	H	103/109 (94%)	-0.57	3 (2%) 54 54	37, 54, 93, 150	0
1	I	105/109 (96%)	-0.63	2 (1%) 66 66	28, 53, 99, 138	1 (0%)
1	J	102/109 (93%)	-0.59	1 (0%) 79 81	30, 59, 80, 102	1 (0%)
1	K	104/109 (95%)	-0.48	1 (0%) 79 81	43, 56, 98, 145	0
1	L	103/109 (94%)	-0.54	0 100 100	46, 64, 102, 142	0
1	M	102/109 (93%)	-0.69	1 (0%) 79 81	19, 48, 81, 111	2 (1%)
1	N	102/109 (93%)	-0.42	0 100 100	48, 68, 93, 106	0
1	O	101/109 (92%)	-0.56	0 100 100	39, 57, 75, 90	0
All	All	1547/1635 (94%)	-0.67	15 (0%) 79 81	19, 50, 90, 150	8 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	104	VAL	3.5
1	E	104	VAL	3.5
1	I	107	VAL	3.4
1	A	104	VAL	3.3
1	M	104	VAL	3.2
1	K	104	VAL	3.2
1	G	105	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	107	VAL	2.8
1	H	105	PRO	2.6
1	F	104	VAL	2.5
1	I	104	VAL	2.4
1	F	105	PRO	2.4
1	J	104	VAL	2.3
1	H	103	GLY	2.1
1	H	104	VAL	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	GD1	L	201	13/13	0.88	0.09	64,65,68,68	0
2	GD1	J	201	13/13	0.89	0.09	84,88,95,95	0
2	GD1	H	201	13/13	0.91	0.07	61,64,70,72	0
2	GD1	O	201	13/13	0.91	0.07	64,65,69,69	0
2	GD1	D	201	13/13	0.92	0.07	48,51,54,57	0
2	GD1	K	201	13/13	0.92	0.07	44,47,52,52	0
2	GD1	G	201	13/13	0.93	0.07	46,48,50,52	0
2	GD1	I	201	13/13	0.93	0.07	50,52,59,59	0
2	GD1	E	201	13/13	0.94	0.07	48,50,54,56	0
2	GD1	M	201	13/13	0.94	0.07	40,43,45,46	0
2	GD1	N	201	13/13	0.94	0.06	68,70,74,75	0
2	GD1	B	201	13/13	0.94	0.08	39,40,42,43	0
2	GD1	A	201	13/13	0.95	0.07	39,40,42,43	0
2	GD1	C	201	13/13	0.95	0.06	50,51,54,54	0
2	GD1	F	201	13/13	0.95	0.06	47,50,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	L	202	1/1	0.97	0.06	47,47,47,47	0
3	NA	C	202	1/1	0.98	0.04	37,37,37,37	0
3	NA	E	202	1/1	0.99	0.04	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.