Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 12:20 am GMT

PDB ID	:	4D1J
Title	:	The structure of the GH35 beta-galactosidase Bgl35A from Cellvibrio japonicas in complex with 1-Deoxygalactonojirimycin
Authors	:	Larsbrink, J.; Thompson, A.J.; Lundqvist, M.; Gardner, J.G.; Davies, G.J.; Brumer, H.
Deposited on	:	2014-05-02
Resolution	:	1.80 Å(reported)

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

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

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

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

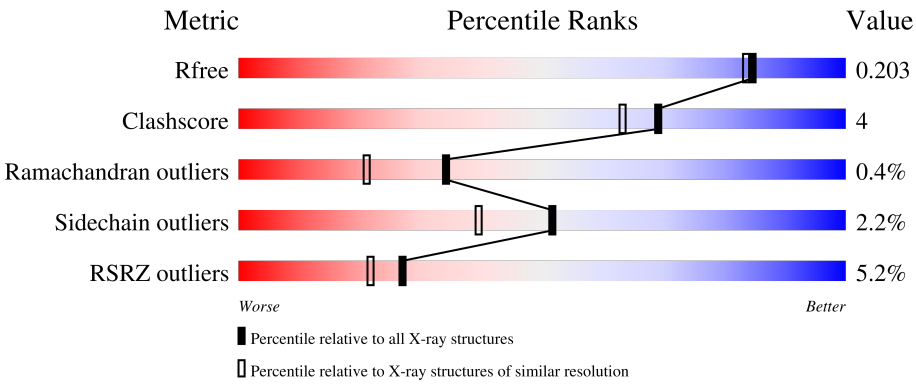
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 <=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	540	5% 92% 6% •
1	B	540	5% 91% 8% •
1	C	540	6% 92% 7% •
1	D	540	5% 92% 7% •
1	E	540	4% 91% 7% •

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Mol	Chain	Length	Quality of chain
1	F	540	5% 91% 7%
1	G	540	4% 92% 6%
1	H	540	8% 92% 6%

2 Entry composition (i)

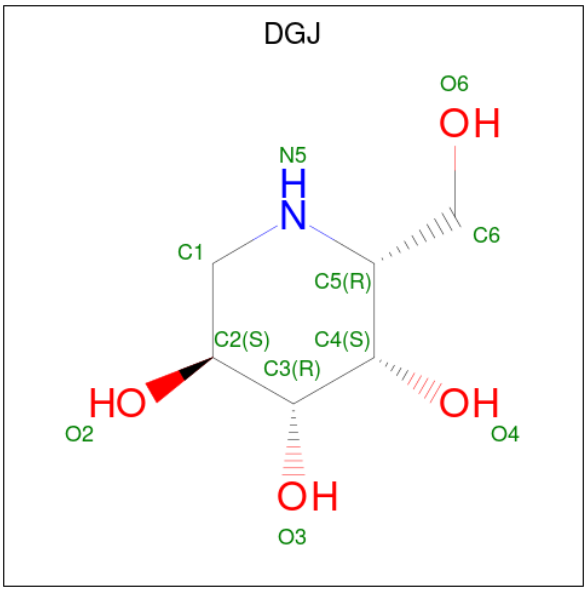
There are 5 unique types of molecules in this entry. The entry contains 37796 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-GALACTOSIDASE, PUTATIVE, BGL35A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	539	4185	2681	711	777	16	0	3	0
1	B	539	4167	2671	703	777	16	0	3	0
1	C	539	4190	2689	710	775	16	0	6	0
1	D	540	4222	2712	715	779	16	0	7	0
1	E	539	4234	2713	718	787	16	0	5	0
1	F	539	4244	2725	712	790	17	0	12	0
1	G	540	4224	2712	712	783	17	0	7	0
1	H	539	4181	2677	714	775	15	0	4	0

- Molecule 2 is (2R,3S,4R,5S)-2-(hydroxymethyl)piperidine-3,4,5-triol (three-letter code: DGJ) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	11	6	1	4	0	0
2	B	1	11	6	1	4	0	0
2	C	1	11	6	1	4	0	0
2	D	1	11	6	1	4	0	0
2	E	1	11	6	1	4	0	0
2	F	1	11	6	1	4	0	0
2	G	1	11	6	1	4	0	0
2	H	1	11	6	1	4	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	4	4	4	0	0
3	B	2	2	2	0	0
3	D	4	4	4	0	0
3	E	4	4	4	0	0

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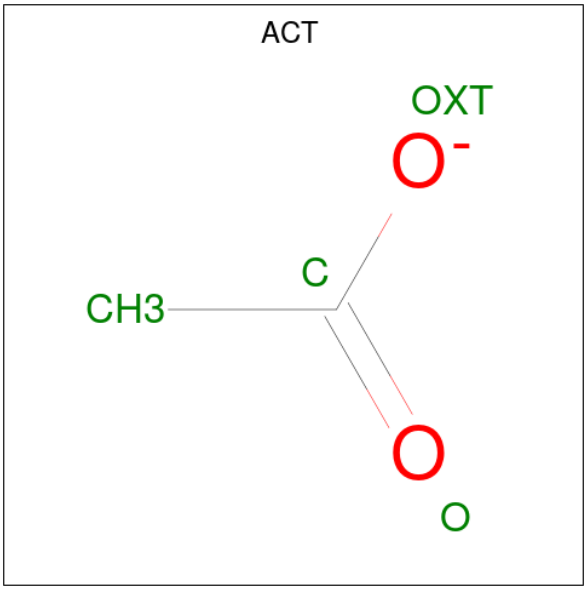
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	4	Total Na 4 4	0	0
3	G	4	Total Na 4 4	0	0
3	H	1	Total Na 1 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	493	Total O 493 493	0	0

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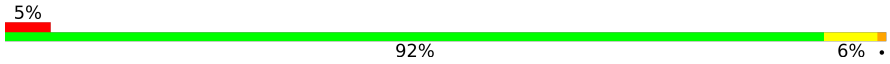
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	491	491	491	0	0
			Total	O		
5	C	409	409	409	0	0
			Total	O		
5	D	535	535	535	0	0
			Total	O		
5	E	567	571	571	0	4
			Total	O		
5	F	564	564	564	0	0
			Total	O		
5	G	556	559	559	0	3
			Total	O		
5	H	396	396	396	0	0

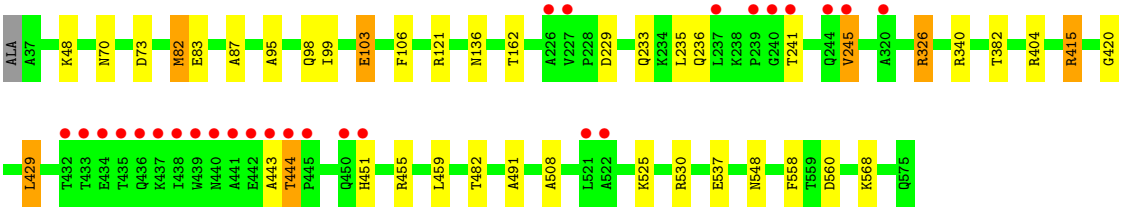
3 Residue-property plots (i)

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: BETA-GALACTOSIDASE, PUTATIVE, BGL35A

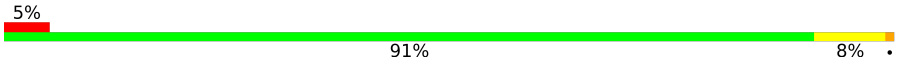
Chain A:

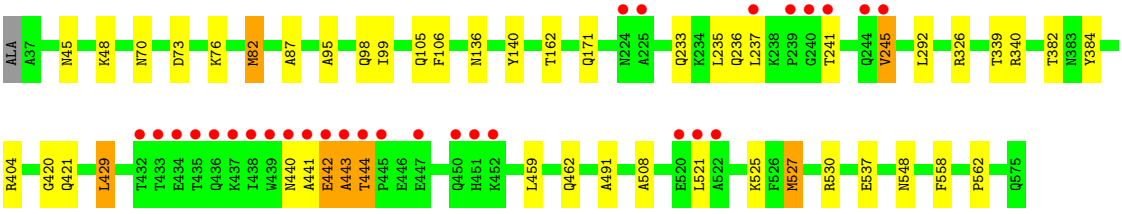




• Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A

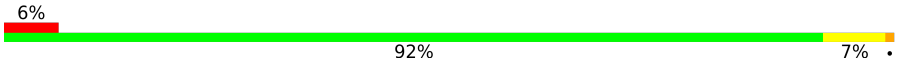
Chain B:

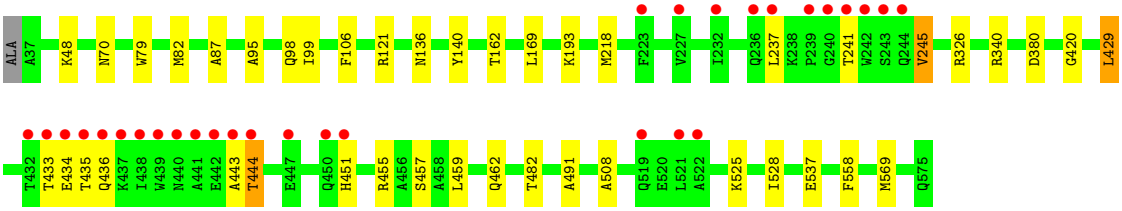




• Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A

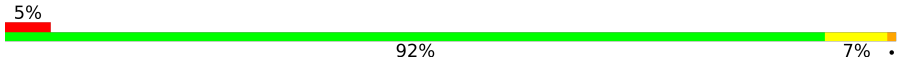
Chain C:

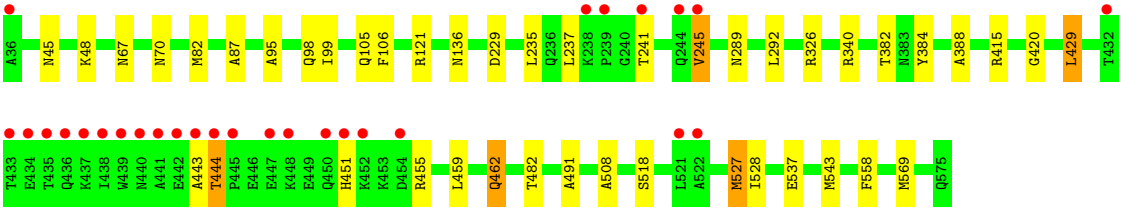




• Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A

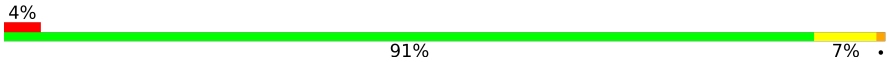
Chain D:

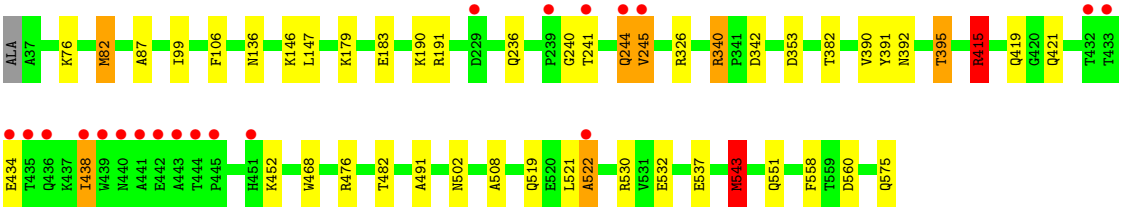




• Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A

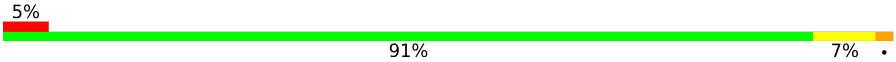
Chain E:

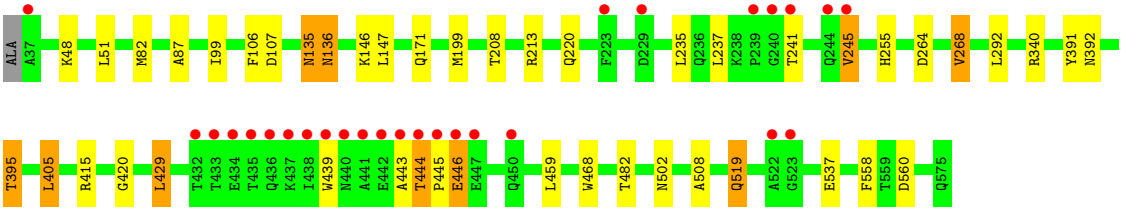




• Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A

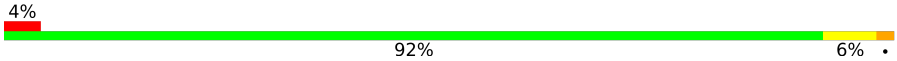
Chain F:

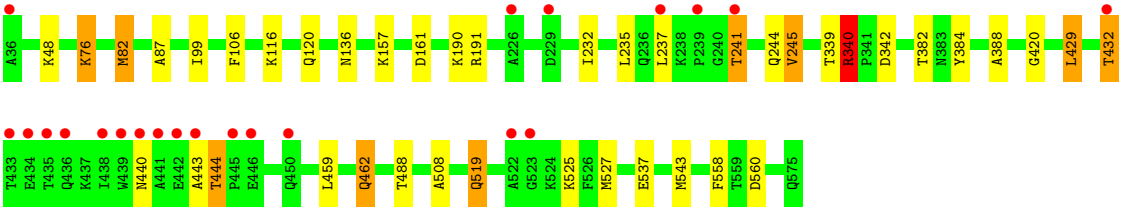




• Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A

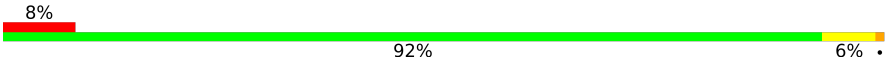
Chain G:

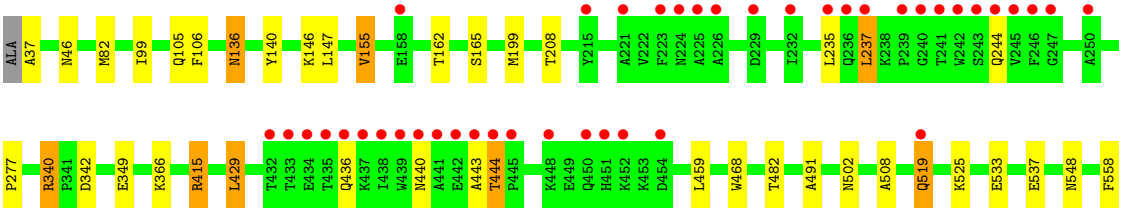




• Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A

Chain H:





H563
Q575

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	99.26Å 116.09Å 116.11Å 90.00° 90.05° 90.04°	Depositor
Resolution (Å)	116.11 – 1.80 46.03 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.1 (116.11-1.80) 97.1 (46.03-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.172 , 0.195 0.181 , 0.203	Depositor DCC
R_{free} test set	23426 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.077 for h,l,-k 0.077 for h,-l,k 0.057 for h,-k,-l 0.027 for -h,k,-l 0.028 for -h,-k,l 0.028 for -h,l,k 0.035 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	37796	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DGJ, NA, ACT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.58	0/4305	0.77	8/5873 (0.1%)
1	B	0.54	0/4287	0.77	7/5854 (0.1%)
1	C	0.56	0/4321	0.76	4/5899 (0.1%)
1	D	0.59	0/4356	0.76	8/5944 (0.1%)
1	E	0.61	1/4361 (0.0%)	0.97	14/5945 (0.2%)
1	F	0.61	0/4393	0.77	7/5997 (0.1%)
1	G	0.61	0/4358	0.94	7/5945 (0.1%)
1	H	0.54	0/4304	0.91	6/5875 (0.1%)
All	All	0.58	1/34685 (0.0%)	0.84	61/47332 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	183	GLU	CD-OE2	-5.55	1.19	1.25

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	340	ARG	NE-CZ-NH1	30.58	135.59	120.30
1	E	340	ARG	NE-CZ-NH2	-30.37	105.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	340	ARG	NE-CZ-NH1	30.31	135.45	120.30
1	G	340	ARG	NE-CZ-NH2	-29.62	105.49	120.30
1	H	340	ARG	NE-CZ-NH1	28.64	134.62	120.30
1	H	340	ARG	NE-CZ-NH2	-27.80	106.40	120.30
1	G	76	LYS	CD-CE-NZ	14.33	144.66	111.70
1	A	340	ARG	NE-CZ-NH1	13.19	126.89	120.30
1	C	340	ARG	NE-CZ-NH1	12.41	126.51	120.30
1	B	340	ARG	NE-CZ-NH1	12.30	126.45	120.30
1	B	340	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	A	340	ARG	NE-CZ-NH2	-11.73	114.43	120.30
1	D	340	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	C	340	ARG	NE-CZ-NH2	-11.15	114.72	120.30
1	E	543[A]	MET	CG-SD-CE	11.06	117.90	100.20
1	E	543[B]	MET	CG-SD-CE	11.06	117.90	100.20
1	D	340	ARG	NE-CZ-NH2	-10.91	114.84	120.30
1	F	340	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	E	340	ARG	CD-NE-CZ	9.64	137.10	123.60
1	G	340	ARG	CD-NE-CZ	9.10	136.34	123.60
1	H	340	ARG	CD-NE-CZ	8.97	136.16	123.60
1	F	340	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	B	326	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	A	103	GLU	CA-C-N	7.37	130.94	116.20
1	C	326	ARG	NE-CZ-NH2	7.15	123.87	120.30
1	F	405	LEU	CB-CG-CD1	7.11	123.09	111.00
1	C	326	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	E	244	GLN	CB-CA-C	6.81	124.01	110.40
1	B	326	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	E	183	GLU	CG-CD-OE2	-6.54	105.23	118.30
1	D	527[A]	MET	CG-SD-CE	-6.43	89.91	100.20
1	D	527[B]	MET	CG-SD-CE	-6.43	89.91	100.20
1	E	183	GLU	CG-CD-OE1	6.42	131.13	118.30
1	E	476	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	527[A]	MET	CG-SD-CE	-6.20	90.28	100.20
1	B	527[B]	MET	CG-SD-CE	-6.20	90.28	100.20
1	E	415	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	103	GLU	O-C-N	-6.13	112.77	123.20
1	E	340	ARG	CB-CG-CD	-5.98	96.05	111.60
1	F	415	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	G	340	ARG	CB-CG-CD	-5.95	96.12	111.60
1	H	340	ARG	CB-CG-CD	-5.81	96.50	111.60
1	E	476	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	326	ARG	NE-CZ-NH1	-5.62	117.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	GLU	C-N-CA	5.59	134.04	122.30
1	F	405	LEU	CA-CB-CG	5.55	128.06	115.30
1	E	560	ASP	CB-CG-OD1	5.51	123.26	118.30
1	G	560	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	443	ALA	N-CA-C	-5.38	96.49	111.00
1	F	560	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	537	GLU	CG-CD-OE2	-5.33	107.63	118.30
1	F	268	VAL	CA-CB-CG1	5.32	118.87	110.90
1	H	415[A]	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	H	415[B]	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	E	530	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	D	543	MET	CG-SD-CE	-5.18	91.91	100.20
1	D	537	GLU	CA-CB-CG	5.12	124.67	113.40
1	G	237	LEU	CB-CG-CD1	5.12	119.69	111.00
1	A	560	ASP	CB-CG-OD1	5.09	122.89	118.30
1	D	415	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	415	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	GLU	Peptide
1	B	442	GLU	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	4185	0	3989	30	0
1	B	4167	0	3951	34	0
1	C	4190	0	3985	29	0
1	D	4222	0	4051	35	0
1	E	4234	0	4084	40	0
1	F	4244	0	4071	35	0
1	G	4224	0	4050	34	0
1	H	4181	0	3974	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	11	0	13	0	0
2	B	11	0	13	0	0
2	C	11	0	13	0	0
2	D	11	0	13	0	0
2	E	11	0	13	0	0
2	F	11	0	13	1	0
2	G	11	0	13	0	0
2	H	11	0	13	1	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	1	0	0	0	0
4	C	8	0	6	0	0
4	D	8	0	6	0	0
4	F	4	0	3	0	0
5	A	493	0	0	12	0
5	B	491	0	0	10	0
5	C	409	0	0	5	0
5	D	535	0	0	10	0
5	E	571	0	0	12	0
5	F	564	0	0	4	0
5	G	559	0	0	9	0
5	H	396	0	0	10	0
All	All	37796	0	32274	242	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (242) 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:146:LYS:HE3	1:G:527[A]:MET:HE3	1.37	1.06
1:D:527[A]:MET:HE3	1:F:146:LYS:HE3	1.38	1.03
1:F:468:TRP:HE1	1:F:502:ASN:HD22	1.09	1.00
1:B:527[A]:MET:HE3	1:H:146:LYS:HE3	1.44	0.96
1:H:468:TRP:HE1	1:H:502:ASN:HD22	1.12	0.93
1:E:468:TRP:HE1	1:E:502:ASN:HD22	1.07	0.92
1:H:105:GLN:HG3	5:H:2084:HOH:O	1.68	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326[B]:ARG:NH1	5:D:2322:HOH:O	2.09	0.86
1:B:45:ASN:CB	5:B:2014:HOH:O	2.24	0.85
1:E:146:LYS:HE3	1:G:527[A]:MET:CE	2.07	0.84
1:D:105:GLN:HG3	5:D:2105:HOH:O	1.78	0.83
1:D:527[A]:MET:CE	1:F:146:LYS:HE3	2.08	0.83
1:F:392:ASN:H	1:F:395:THR:HG23	1.45	0.80
1:G:382[B]:THR:CG2	1:G:388:ALA:O	2.30	0.80
1:A:95:ALA:H	1:A:98:GLN:HE21	1.31	0.79
1:C:193:LYS:H	1:D:289:ASN:HD21	1.29	0.79
1:C:380:ASP:OD2	1:H:563:HIS:HE1	1.64	0.79
1:E:392:ASN:H	1:E:395:THR:HG23	1.46	0.79
1:B:95:ALA:H	1:B:98:GLN:HE21	1.30	0.78
1:F:48:LYS:NZ	1:F:420:GLY:O	2.15	0.77
1:D:95:ALA:H	1:D:98:GLN:HE21	1.32	0.76
1:B:48:LYS:NZ	1:B:420:GLY:O	2.16	0.76
1:C:48:LYS:NZ	1:C:420:GLY:O	2.16	0.76
1:B:339:THR:O	5:B:2307:HOH:O	2.04	0.76
1:A:326:ARG:NH1	5:A:2292:HOH:O	2.17	0.75
1:C:218:MET:HE1	5:C:2141:HOH:O	1.85	0.75
1:G:440:ASN:CB	5:G:2416:HOH:O	2.34	0.75
1:F:392:ASN:H	1:F:395:THR:CG2	2.00	0.75
1:C:95:ALA:H	1:C:98:GLN:HE21	1.32	0.74
1:B:105:GLN:HG3	5:B:2095:HOH:O	1.89	0.73
1:B:527[A]:MET:CE	1:H:146:LYS:HE3	2.18	0.73
1:D:382[B]:THR:CG2	1:D:388:ALA:O	2.36	0.72
1:B:521:LEU:CB	5:B:2422:HOH:O	2.38	0.72
1:A:48:LYS:NZ	1:A:420:GLY:O	2.15	0.72
1:A:229:ASP:CB	5:A:2110:HOH:O	2.37	0.71
1:D:48:LYS:NZ	1:D:420:GLY:O	2.17	0.71
1:C:528[A]:ILE:CD1	1:C:569:MET:SD	2.79	0.70
1:D:528[A]:ILE:CD1	1:D:569:MET:SD	2.80	0.70
1:E:392:ASN:H	1:E:395:THR:CG2	2.04	0.70
1:E:236:GLN:CB	5:E:2121:HOH:O	2.39	0.70
1:A:236:GLN:CB	5:A:2235:HOH:O	2.39	0.70
1:G:432:THR:HG21	5:G:2426:HOH:O	1.93	0.69
1:D:518:SER:O	5:D:2466:HOH:O	2.10	0.69
1:B:421:GLN:CB	5:B:2203:HOH:O	2.40	0.69
1:E:532:GLU:CD	1:E:543[B]:MET:HE3	2.13	0.68
1:G:382[B]:THR:HG21	1:G:388:ALA:O	1.93	0.68
1:F:264:ASP:O	1:F:268:VAL:HG13	1.94	0.67
1:B:236:GLN:CB	5:B:2240:HOH:O	2.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:THR:O	1:C:435:THR:N	2.29	0.65
1:H:340:ARG:HD3	1:H:342:ASP:OD1	1.97	0.65
1:E:340:ARG:HD3	1:E:342:ASP:OD1	1.98	0.64
1:G:339:THR:O	5:G:2331:HOH:O	2.14	0.64
1:F:213:ARG:HH22	1:F:220:GLN:HE22	1.46	0.63
1:G:340:ARG:HD3	1:G:342:ASP:OD1	1.99	0.63
1:H:440:ASN:CB	5:H:2299:HOH:O	2.45	0.63
1:G:232:ILE:CB	5:G:2256:HOH:O	2.46	0.63
1:D:528[A]:ILE:HD12	1:D:569:MET:SD	2.39	0.62
1:D:382[B]:THR:HG22	1:D:384:TYR:H	1.65	0.61
1:C:528[A]:ILE:HD12	1:C:569:MET:SD	2.39	0.61
1:E:452:LYS:HE2	5:E:2448:HOH:O	1.98	0.61
1:C:457:SER:O	5:C:2324:HOH:O	2.17	0.60
1:F:99[A]:ILE:CD1	1:F:107:ASP:O	2.50	0.60
1:F:443:ALA:O	1:F:444:THR:CB	2.49	0.60
1:D:527[A]:MET:HE2	1:F:147:LEU:HD21	1.85	0.59
1:G:76:LYS:HE2	5:G:2052:HOH:O	2.02	0.59
1:A:382:THR:OG1	5:A:2319:HOH:O	2.17	0.59
1:F:445:PRO:O	1:F:446:GLU:CB	2.50	0.59
1:F:99[A]:ILE:HD13	1:F:107:ASP:O	2.03	0.58
1:B:171:GLN:HG2	5:B:2081:HOH:O	2.02	0.58
1:E:147:LEU:HD21	1:G:527[A]:MET:HE2	1.84	0.58
1:A:326:ARG:HG3	1:A:326:ARG:HH11	1.69	0.57
1:E:240:GLY:HA2	1:E:244:GLN:HE21	1.68	0.57
1:E:382[A]:THR:HG23	5:E:2380:HOH:O	2.03	0.57
1:C:443:ALA:O	1:C:444:THR:CB	2.53	0.57
1:D:67:ASN:HB2	1:E:551:GLN:HE22	1.70	0.57
1:E:390:VAL:O	1:E:395:THR:HG21	2.05	0.56
1:D:527[A]:MET:CE	1:F:147:LEU:HD21	2.36	0.56
1:D:382[B]:THR:HG21	1:D:388:ALA:O	2.05	0.56
1:F:439:TRP:CB	5:F:2416:HOH:O	2.54	0.56
1:H:155:VAL:HG13	1:H:165:SER:O	2.05	0.56
1:H:349:GLU:OE1	2:H:600:DGJ:H1	2.05	0.56
1:E:146:LYS:HG3	1:G:527[A]:MET:HE1	1.88	0.55
1:F:171:GLN:HG2	5:F:2092:HOH:O	2.07	0.55
1:H:199:MET:HG2	1:H:277:PRO:HB2	1.90	0.54
1:G:443:ALA:O	1:G:444:THR:CB	2.56	0.54
1:E:468:TRP:HE1	1:E:502:ASN:ND2	1.91	0.54
1:B:440:ASN:C	1:B:442:GLU:H	2.11	0.54
1:G:382[B]:THR:HG22	1:G:384:TYR:H	1.74	0.53
1:D:443:ALA:O	1:D:444:THR:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:391:TYR:HA	1:F:395:THR:HG21	1.90	0.53
1:F:136:ASN:HD22	1:F:208:THR:HA	1.73	0.53
1:E:391:TYR:HA	1:E:395:THR:HG21	1.90	0.53
1:E:326[B]:ARG:NH2	1:E:353:ASP:OD2	2.29	0.53
1:D:229:ASP:CB	5:D:2263:HOH:O	2.56	0.53
1:E:147:LEU:HD21	1:G:527[A]:MET:CE	2.39	0.53
1:E:575:GLN:HA	5:E:2564:HOH:O	2.08	0.53
1:H:443:ALA:O	1:H:444:THR:CB	2.57	0.53
1:E:452:LYS:CE	5:E:2448:HOH:O	2.56	0.52
1:B:382[B]:THR:HG23	1:B:384:TYR:H	1.75	0.52
1:H:436:GLN:CB	5:H:2298:HOH:O	2.57	0.52
1:D:382[B]:THR:HG23	5:D:2346:HOH:O	2.09	0.52
1:C:169:LEU:O	1:C:218:MET:HE1	2.10	0.51
1:A:443:ALA:O	1:A:444:THR:CB	2.57	0.51
1:F:208:THR:OG1	1:F:255:HIS:HE1	1.93	0.51
1:H:46:ASN:ND2	5:H:2016:HOH:O	2.37	0.51
1:A:326:ARG:HD3	5:A:2294:HOH:O	2.10	0.51
1:C:218:MET:CE	5:C:2141:HOH:O	2.52	0.51
1:B:76:LYS:HE2	5:B:2045:HOH:O	2.11	0.51
1:B:440:ASN:O	1:B:442:GLU:N	2.43	0.51
1:D:527[A]:MET:HE1	1:F:146:LYS:HG3	1.91	0.50
1:E:521:LEU:O	1:E:522:ALA:HB3	2.11	0.50
1:E:532:GLU:HG2	1:E:543[B]:MET:CE	2.41	0.50
1:B:443:ALA:O	1:B:444:THR:CB	2.59	0.50
1:G:488[A]:THR:HG23	5:G:2470:HOH:O	2.11	0.50
1:B:382[B]:THR:CG2	1:B:384:TYR:H	2.25	0.49
1:G:519:GLN:HG2	5:G:2444:HOH:O	2.11	0.49
1:G:508:ALA:HB3	1:G:558:PHE:CD1	2.47	0.49
1:H:415[A]:ARG:NH2	5:H:2280:HOH:O	2.46	0.49
1:A:568:LYS:HE2	5:A:2442:HOH:O	2.10	0.49
1:B:527[A]:MET:HE2	1:H:147:LEU:HD21	1.95	0.49
1:B:527[A]:MET:CE	1:H:147:LEU:HD21	2.43	0.49
1:C:380:ASP:OD2	1:H:563:HIS:CE1	2.54	0.49
1:H:136:ASN:HD22	1:H:208:THR:HA	1.77	0.49
1:E:382[A]:THR:HG22	5:E:2357:HOH:O	2.13	0.48
1:E:415:ARG:O	1:E:419:GLN:HG2	2.13	0.48
1:A:326:ARG:HH11	1:A:326:ARG:CG	2.24	0.48
1:A:70:ASN:HD22	1:A:98:GLN:NE2	2.11	0.48
1:B:527[A]:MET:HE1	1:H:146:LYS:HG3	1.96	0.48
1:G:241:THR:HG22	1:G:244:GLN:CG	2.44	0.48
1:A:415:ARG:NH1	5:A:2371:HOH:O	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:429:LEU:HD22	1:F:459:LEU:HG	1.96	0.48
1:A:229:ASP:CB	5:A:2228:HOH:O	2.61	0.47
1:C:162:THR:O	1:H:525:LYS:HE3	2.14	0.47
1:A:429:LEU:HD22	1:A:459:LEU:HG	1.97	0.47
1:G:157:LYS:HE3	1:G:161:ASP:HB2	1.95	0.47
1:G:241:THR:HG22	1:G:244:GLN:HG3	1.97	0.47
1:G:429:LEU:HD22	1:G:459:LEU:HG	1.97	0.47
1:A:525:LYS:HE3	1:B:162:THR:O	2.15	0.46
1:A:525:LYS:HE2	5:A:2438:HOH:O	2.15	0.46
1:D:482:THR:HG21	5:D:2236:HOH:O	2.14	0.46
1:G:48:LYS:NZ	1:G:420:GLY:O	2.48	0.46
1:H:429:LEU:HD22	1:H:459:LEU:HG	1.97	0.46
1:B:429:LEU:HD22	1:B:459:LEU:HG	1.97	0.46
1:B:525:LYS:HE3	1:H:162:THR:O	2.16	0.46
1:C:528[A]:ILE:HD13	1:C:569:MET:SD	2.56	0.46
1:C:140:TYR:CZ	1:H:548:ASN:HB3	2.51	0.46
1:C:429:LEU:HD22	1:C:459:LEU:HG	1.98	0.46
1:A:229:ASP:O	1:A:233:GLN:HG2	2.16	0.45
1:D:241:THR:O	1:D:245:VAL:HG13	2.17	0.45
1:E:241:THR:O	1:E:245:VAL:HG13	2.16	0.45
1:A:241:THR:O	1:A:245:VAL:HG13	2.16	0.45
1:D:528[A]:ILE:HD13	1:D:569:MET:SD	2.56	0.45
1:E:532:GLU:OE2	1:E:543[B]:MET:HE3	2.16	0.45
1:A:482:THR:HG23	5:A:2413:HOH:O	2.16	0.45
1:A:83:GLU:OE1	1:A:121[B]:ARG:NH2	2.50	0.45
1:F:508:ALA:HB3	1:F:558:PHE:CD1	2.52	0.45
1:A:508:ALA:HB3	1:A:558:PHE:CD1	2.52	0.44
1:B:70:ASN:HD22	1:B:98:GLN:NE2	2.15	0.44
1:E:482:THR:HG23	5:E:2482:HOH:O	2.16	0.44
1:G:241:THR:O	1:G:245:VAL:HG13	2.18	0.44
1:A:82:MET:HG2	1:A:87:ALA:HB3	2.00	0.44
1:B:241:THR:O	1:B:245:VAL:HG13	2.17	0.44
1:F:135:ASN:N	1:F:135:ASN:HD22	2.16	0.44
1:C:70:ASN:HD22	1:C:98:GLN:NE2	2.16	0.44
1:F:395:THR:HB	5:F:2365:HOH:O	2.17	0.44
1:A:99:ILE:O	1:A:106:PHE:HA	2.18	0.44
1:C:241:THR:O	1:C:245:VAL:HG13	2.17	0.44
1:D:382[B]:THR:HG23	1:D:388:ALA:O	2.17	0.44
1:D:508:ALA:HB3	1:D:558:PHE:CD1	2.52	0.44
1:E:421:GLN:NE2	5:E:2425:HOH:O	2.51	0.44
1:B:70:ASN:HD22	1:B:98:GLN:HE22	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ILE:O	1:D:106:PHE:HA	2.17	0.44
1:D:382[B]:THR:CG2	5:D:2346:HOH:O	2.64	0.44
1:G:116:LYS:O	1:G:120:GLN:HG2	2.17	0.44
1:D:121[B]:ARG:NH2	5:D:2065:HOH:O	2.48	0.43
1:G:99:ILE:O	1:G:106:PHE:HA	2.18	0.43
1:G:190:LYS:HG3	1:G:191[B]:ARG:HG2	2.01	0.43
1:B:76:LYS:CE	5:B:2045:HOH:O	2.66	0.43
1:E:190:LYS:HG3	1:E:191:ARG:HG2	2.01	0.43
1:E:99:ILE:O	1:E:106:PHE:HA	2.17	0.43
1:E:508:ALA:HB3	1:E:558:PHE:CD1	2.54	0.43
1:F:241:THR:O	1:F:245:VAL:HG13	2.17	0.43
1:H:508:ALA:HB3	1:H:558:PHE:CD1	2.54	0.43
1:B:404[B]:ARG:NH1	1:B:562:PRO:HD3	2.32	0.43
1:E:421:GLN:HG3	5:E:2424:HOH:O	2.19	0.43
1:H:366:LYS:NZ	5:H:2254:HOH:O	2.41	0.43
1:B:508:ALA:HB3	1:B:558:PHE:CD1	2.54	0.43
1:D:429:LEU:HD22	1:D:459:LEU:HG	2.00	0.43
1:A:162:THR:O	1:C:525:LYS:HE3	2.18	0.43
1:C:99:ILE:O	1:C:106:PHE:HA	2.19	0.43
1:H:99:ILE:O	1:H:106:PHE:HA	2.19	0.43
1:H:244:GLN:CB	5:H:2176:HOH:O	2.67	0.42
1:D:482:THR:HG23	5:D:2447:HOH:O	2.19	0.42
1:B:99:ILE:O	1:B:106:PHE:HA	2.19	0.42
1:F:519[B]:GLN:H	1:F:519[B]:GLN:NE2	2.17	0.42
1:G:76:LYS:HE3	5:G:2054:HOH:O	2.18	0.42
1:D:527[A]:MET:HE3	1:F:146:LYS:CE	2.28	0.42
1:E:236:GLN:CB	5:E:2260:HOH:O	2.67	0.42
1:E:240:GLY:CA	1:E:244:GLN:HE21	2.29	0.42
1:E:146:LYS:CE	1:G:527[A]:MET:HE3	2.27	0.42
1:G:82:MET:HG2	1:G:87:ALA:HB3	2.01	0.42
1:A:326:ARG:NH1	1:A:326:ARG:CG	2.82	0.42
1:F:135:ASN:HD21	2:F:600:DGJ:H2	1.84	0.42
1:H:519:GLN:HG2	5:H:2313:HOH:O	2.19	0.42
1:B:82:MET:HG2	1:B:87:ALA:HB3	2.02	0.42
1:C:433:THR:O	1:C:436:GLN:N	2.40	0.42
1:E:76:LYS:HE2	5:E:2051:HOH:O	2.20	0.42
1:G:190:LYS:HG3	1:G:191[A]:ARG:HG2	2.02	0.42
1:C:508:ALA:HB3	1:C:558:PHE:CD1	2.55	0.41
1:D:82:MET:HG2	1:D:87:ALA:HB3	2.01	0.41
1:D:451:HIS:CE1	1:D:455:ARG:HD2	2.55	0.41
1:D:462:GLN:HB3	5:D:2425:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:462:GLN:HB3	5:G:2435:HOH:O	2.20	0.41
1:A:451:HIS:CE1	1:A:455:ARG:HD2	2.55	0.41
1:H:482:THR:HG23	5:H:2322:HOH:O	2.19	0.41
1:G:241:THR:H	1:G:244:GLN:NE2	2.19	0.41
1:C:482[A]:THR:HG23	5:C:2345:HOH:O	2.21	0.41
1:C:482[B]:THR:HG23	5:C:2345:HOH:O	2.21	0.41
1:C:82:MET:HG2	1:C:87:ALA:HB3	2.02	0.41
1:D:70:ASN:HD22	1:D:98:GLN:NE2	2.18	0.41
1:B:73:ASP:HB2	5:B:2044:HOH:O	2.20	0.41
1:C:451:HIS:CE1	1:C:455:ARG:HD2	2.56	0.41
1:B:548:ASN:HB3	1:H:140:TYR:CZ	2.56	0.41
1:E:482:THR:HG21	5:E:2228:HOH:O	2.20	0.41
1:H:533:GLU:OE2	1:H:563:HIS:HD2	2.04	0.41
1:F:482[A]:THR:HG21	5:F:2457:HOH:O	2.20	0.41
1:C:121[B]:ARG:HG2	1:C:121[B]:ARG:HH11	1.86	0.41
1:H:235:LEU:HB2	1:H:237:LEU:HD22	2.02	0.41
1:F:264:ASP:O	1:F:268:VAL:CG1	2.67	0.40
1:G:190:LYS:CG	1:G:191[B]:ARG:HG2	2.51	0.40
1:A:548:ASN:HB3	1:B:140:TYR:CZ	2.56	0.40
1:C:79:TRP:HB3	1:C:121[B]:ARG:CZ	2.51	0.40
1:F:82:MET:HG2	1:F:87:ALA:HB3	2.03	0.40
1:F:51:LEU:HD13	1:F:199[A]:MET:HE1	2.02	0.40
1:E:434:GLU:O	1:E:438:ILE:HG23	2.20	0.40
1:H:37:ALA:N	5:H:2004:HOH:O	2.53	0.40
1:A:73:ASP:HB2	5:A:2045:HOH:O	2.21	0.40
1:A:404:ARG:HD2	5:A:2361:HOH:O	2.22	0.40
1:E:82:MET:HG2	1:E:87:ALA:HB3	2.03	0.40
1:F:199[A]:MET:HE3	1:F:199[A]:MET:HB2	1.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	540/540 (100%)	519 (96%)	19 (4%)	2 (0%)	34	21
1	B	540/540 (100%)	519 (96%)	18 (3%)	3 (1%)	25	12
1	C	543/540 (101%)	524 (96%)	16 (3%)	3 (1%)	25	12
1	D	545/540 (101%)	525 (96%)	18 (3%)	2 (0%)	34	21
1	E	542/540 (100%)	524 (97%)	16 (3%)	2 (0%)	34	21
1	F	549/540 (102%)	528 (96%)	19 (4%)	2 (0%)	34	21
1	G	545/540 (101%)	525 (96%)	19 (4%)	1 (0%)	47	33
1	H	541/540 (100%)	522 (96%)	17 (3%)	2 (0%)	34	21
All	All	4345/4320 (101%)	4186 (96%)	142 (3%)	17 (0%)	34	21

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	434	GLU
1	F	446	GLU
1	B	441	ALA
1	B	444	THR
1	E	522	ALA
1	F	444	THR
1	A	444	THR
1	C	444	THR
1	D	444	THR
1	G	444	THR
1	H	444	THR
1	A	491	ALA
1	C	491	ALA
1	E	491	ALA
1	B	491	ALA
1	D	491	ALA
1	H	491	ALA

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	423/452 (94%)	416 (98%)	7 (2%)	60	51
1	B	419/452 (93%)	408 (97%)	11 (3%)	46	32
1	C	421/452 (93%)	415 (99%)	6 (1%)	67	59
1	D	429/452 (95%)	421 (98%)	8 (2%)	57	46
1	E	436/452 (96%)	425 (98%)	11 (2%)	47	34
1	F	436/452 (96%)	424 (97%)	12 (3%)	43	30
1	G	430/452 (95%)	415 (96%)	15 (4%)	36	21
1	H	420/452 (93%)	413 (98%)	7 (2%)	60	51
All	All	3414/3616 (94%)	3337 (98%)	77 (2%)	52	37

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	MET
1	A	136	ASN
1	A	235	LEU
1	A	245	VAL
1	A	429	LEU
1	A	530	ARG
1	A	537	GLU
1	B	82	MET
1	B	136	ASN
1	B	233	GLN
1	B	235	LEU
1	B	237	LEU
1	B	245	VAL
1	B	292	LEU
1	B	429	LEU
1	B	462	GLN
1	B	530	ARG
1	B	537	GLU
1	C	136	ASN
1	C	237	LEU
1	C	245	VAL
1	C	429	LEU
1	C	462	GLN
1	C	537	GLU
1	D	45	ASN
1	D	136	ASN
1	D	235	LEU

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Mol	Chain	Res	Type
1	D	237	LEU
1	D	245	VAL
1	D	292	LEU
1	D	429	LEU
1	D	462	GLN
1	E	82	MET
1	E	136	ASN
1	E	179	LYS
1	E	245	VAL
1	E	395	THR
1	E	415	ARG
1	E	438	ILE
1	E	519	GLN
1	E	537	GLU
1	E	543[A]	MET
1	E	543[B]	MET
1	F	135	ASN
1	F	136	ASN
1	F	235	LEU
1	F	237	LEU
1	F	245	VAL
1	F	292	LEU
1	F	395	THR
1	F	405	LEU
1	F	429	LEU
1	F	519[A]	GLN
1	F	519[B]	GLN
1	F	537	GLU
1	G	82	MET
1	G	136	ASN
1	G	235	LEU
1	G	241	THR
1	G	245	VAL
1	G	340	ARG
1	G	429	LEU
1	G	432	THR
1	G	462	GLN
1	G	519	GLN
1	G	525[A]	LYS
1	G	525[B]	LYS
1	G	537	GLU
1	G	543[A]	MET

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Mol	Chain	Res	Type
1	G	543[B]	MET
1	H	82	MET
1	H	136	ASN
1	H	155	VAL
1	H	237	LEU
1	H	429	LEU
1	H	519	GLN
1	H	537	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	172	ASN
1	A	421	GLN
1	A	451	HIS
1	A	462	GLN
1	B	98	GLN
1	B	172	ASN
1	B	451	HIS
1	C	98	GLN
1	C	172	ASN
1	C	451	HIS
1	D	45	ASN
1	D	98	GLN
1	D	172	ASN
1	D	289	ASN
1	D	354	GLN
1	D	451	HIS
1	E	49	HIS
1	E	172	ASN
1	E	244	GLN
1	E	421	GLN
1	E	487	ASN
1	E	502	ASN
1	E	519	GLN
1	E	551	GLN
1	F	49	HIS
1	F	135	ASN
1	F	136	ASN
1	F	220	GLN
1	F	224	ASN

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Mol	Chain	Res	Type
1	F	255	HIS
1	F	462	GLN
1	F	502	ASN
1	G	49	HIS
1	G	224	ASN
1	G	244	GLN
1	G	401	GLN
1	G	519	GLN
1	H	49	HIS
1	H	136	ASN
1	H	172	ASN
1	H	502	ASN
1	H	563	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 23 are monoatomic - leaving 13 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	DGJ	G	600	-	11,11,11	0.95	0	13,15,15	1.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DGJ	F	600	-	11,11,11	0.97	1 (9%)	13,15,15	1.12	0
2	DGJ	A	600	-	11,11,11	0.88	1 (9%)	13,15,15	1.07	0
2	DGJ	E	600	-	11,11,11	1.16	1 (9%)	13,15,15	0.72	0
2	DGJ	D	600	-	11,11,11	1.09	1 (9%)	13,15,15	1.33	2 (15%)
2	DGJ	H	600	-	11,11,11	0.54	0	13,15,15	0.87	0
4	ACT	C	601	-	3,3,3	0.71	0	3,3,3	0.63	0
4	ACT	D	605	-	3,3,3	0.87	0	3,3,3	0.18	0
4	ACT	D	606	-	3,3,3	1.03	0	3,3,3	0.48	0
4	ACT	F	605	-	3,3,3	0.76	0	3,3,3	1.07	0
4	ACT	C	602	-	3,3,3	0.92	0	3,3,3	0.61	0
2	DGJ	B	600	-	11,11,11	0.70	0	13,15,15	0.86	1 (7%)
2	DGJ	C	600	-	11,11,11	0.82	0	13,15,15	0.97	1 (7%)

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	DGJ	G	600	-	-	0/2/19/19	0/1/1/1
2	DGJ	F	600	-	-	0/2/19/19	0/1/1/1
2	DGJ	A	600	-	-	0/2/19/19	0/1/1/1
2	DGJ	E	600	-	-	0/2/19/19	0/1/1/1
2	DGJ	D	600	-	-	0/2/19/19	0/1/1/1
2	DGJ	H	600	-	-	0/2/19/19	0/1/1/1
2	DGJ	B	600	-	-	0/2/19/19	0/1/1/1
2	DGJ	C	600	-	-	0/2/19/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	600	DGJ	C1-C2	3.19	1.55	1.52
2	D	600	DGJ	C1-N5	2.84	1.51	1.47
2	A	600	DGJ	O2-C2	2.07	1.47	1.43
2	F	600	DGJ	C1-C2	-2.02	1.50	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	600	DGJ	C1-C2-C3	2.57	113.34	110.33
2	D	600	DGJ	O2-C2-C1	2.26	114.04	109.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	600	DGJ	C2-C3-C4	-2.06	107.33	110.89
2	B	600	DGJ	O4-C4-C3	-2.01	105.70	110.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	600	DGJ	1	0
2	H	600	DGJ	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	539/540 (99%)	0.02	27 (5%)	28	23	17, 26, 49, 93	0
1	B	539/540 (99%)	0.08	29 (5%)	25	20	19, 28, 51, 101	0
1	C	539/540 (99%)	0.14	30 (5%)	24	19	18, 29, 56, 108	0
1	D	540/540 (100%)	0.02	28 (5%)	27	22	15, 25, 52, 107	0
1	E	539/540 (99%)	-0.04	20 (3%)	41	36	16, 24, 47, 87	0
1	F	539/540 (99%)	0.03	27 (5%)	28	23	15, 23, 47, 97	0
1	G	540/540 (100%)	-0.00	22 (4%)	37	31	16, 24, 48, 82	0
1	H	539/540 (99%)	0.17	42 (7%)	13	10	20, 29, 62, 102	0
All	All	4314/4320 (99%)	0.05	225 (5%)	27	22	15, 26, 53, 108	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	441	ALA	10.1
1	B	438	ILE	9.7
1	B	439	TRP	9.7
1	F	441	ALA	9.0
1	D	439	TRP	8.9
1	A	441	ALA	8.4
1	D	441	ALA	8.0
1	D	440	ASN	8.0
1	C	438	ILE	7.9
1	H	442	GLU	7.7
1	H	441	ALA	7.6
1	H	439	TRP	7.6
1	F	439	TRP	7.5
1	A	438	ILE	7.4
1	H	438	ILE	7.3
1	F	440	ASN	7.2

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Mol	Chain	Res	Type	RSRZ
1	F	438	ILE	7.1
1	G	439	TRP	6.9
1	C	441	ALA	6.9
1	C	439	TRP	6.9
1	D	438	ILE	6.9
1	E	438	ILE	6.8
1	A	439	TRP	6.7
1	A	443	ALA	6.7
1	H	443	ALA	6.5
1	C	435	THR	6.2
1	F	442	GLU	5.8
1	B	432	THR	5.8
1	A	440	ASN	5.8
1	B	444	THR	5.8
1	F	443	ALA	5.8
1	B	435	THR	5.7
1	A	522	ALA	5.7
1	H	223	PHE	5.6
1	E	441	ALA	5.6
1	E	435	THR	5.5
1	B	440	ASN	5.4
1	D	433	THR	5.2
1	G	438	ILE	5.2
1	B	442	GLU	5.2
1	E	439	TRP	5.2
1	C	442	GLU	5.2
1	H	435	THR	5.1
1	G	443	ALA	5.1
1	H	445	PRO	5.0
1	G	441	ALA	5.0
1	A	435	THR	4.9
1	C	443	ALA	4.9
1	C	434	GLU	4.9
1	D	522	ALA	4.9
1	H	440	ASN	4.8
1	D	435	THR	4.8
1	F	445	PRO	4.7
1	C	440	ASN	4.7
1	F	435	THR	4.7
1	B	434	GLU	4.7
1	D	443	ALA	4.7
1	H	241	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	436	GLN	4.6
1	H	243	SER	4.6
1	C	223	PHE	4.6
1	G	442	GLU	4.5
1	H	436	GLN	4.5
1	G	440	ASN	4.5
1	B	443	ALA	4.5
1	B	433	THR	4.5
1	G	435	THR	4.5
1	D	436	GLN	4.4
1	E	444	THR	4.4
1	E	443	ALA	4.3
1	A	442	GLU	4.3
1	H	239	PRO	4.3
1	C	522	ALA	4.3
1	F	522	ALA	4.2
1	A	432	THR	4.2
1	E	440	ASN	4.2
1	B	445	PRO	4.2
1	D	442	GLU	4.2
1	H	432	THR	4.2
1	D	445	PRO	4.2
1	H	244	GLN	4.1
1	E	442	GLU	4.1
1	D	432	THR	3.9
1	H	433	THR	3.9
1	H	451	HIS	3.9
1	A	444	THR	3.9
1	H	242	TRP	3.8
1	C	433	THR	3.8
1	H	444	THR	3.8
1	B	521	LEU	3.7
1	C	432	THR	3.7
1	A	521	LEU	3.7
1	B	436	GLN	3.7
1	C	241	THR	3.6
1	F	436	GLN	3.6
1	F	432	THR	3.6
1	B	522	ALA	3.5
1	H	232	ILE	3.5
1	B	437	LYS	3.5
1	A	226	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	523	GLY	3.5
1	D	434	GLU	3.5
1	C	519	GLN	3.4
1	G	522	ALA	3.4
1	F	433	THR	3.4
1	B	240	GLY	3.4
1	E	434	GLU	3.4
1	H	224	ASN	3.4
1	F	437	LYS	3.4
1	H	240	GLY	3.3
1	A	437	LYS	3.3
1	H	245	VAL	3.3
1	D	444	THR	3.3
1	C	244	GLN	3.3
1	A	245	VAL	3.3
1	B	237	LEU	3.3
1	F	434	GLU	3.3
1	D	437	LYS	3.2
1	C	444	THR	3.2
1	G	432	THR	3.2
1	H	437	LYS	3.2
1	C	447	GLU	3.1
1	D	239	PRO	3.1
1	G	433	THR	3.1
1	C	450	GLN	3.1
1	E	445	PRO	3.0
1	C	451	HIS	3.0
1	C	227	VAL	3.0
1	H	434	GLU	3.0
1	C	437	LYS	3.0
1	C	521	LEU	2.9
1	F	229	ASP	2.9
1	G	436	GLN	2.9
1	D	36	ALA	2.9
1	C	243	SER	2.9
1	A	227	VAL	2.9
1	C	239	PRO	2.9
1	D	448	LYS	2.8
1	B	451	HIS	2.8
1	E	433	THR	2.8
1	G	241	THR	2.8
1	H	246	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	229	ASP	2.8
1	D	521	LEU	2.8
1	F	240	GLY	2.8
1	F	244	GLN	2.8
1	A	436	GLN	2.7
1	G	434	GLU	2.7
1	A	241	THR	2.7
1	E	522	ALA	2.7
1	D	245	VAL	2.7
1	H	235	LEU	2.7
1	A	451	HIS	2.7
1	H	226	ALA	2.7
1	B	520	GLU	2.7
1	F	444	THR	2.7
1	G	226	ALA	2.7
1	G	450	GLN	2.7
1	B	239	PRO	2.7
1	E	244	GLN	2.6
1	G	36	ALA	2.6
1	C	232	ILE	2.6
1	G	239	PRO	2.6
1	B	244	GLN	2.6
1	D	244	GLN	2.6
1	D	241	THR	2.6
1	B	450	GLN	2.6
1	E	436	GLN	2.6
1	C	242	TRP	2.6
1	E	241	THR	2.6
1	G	237	LEU	2.5
1	A	445	PRO	2.5
1	E	432	THR	2.5
1	H	247	GLY	2.5
1	H	237	LEU	2.5
1	E	239	PRO	2.4
1	A	244	GLN	2.4
1	H	450	GLN	2.4
1	D	447	GLU	2.4
1	F	245	VAL	2.4
1	H	215	TYR	2.4
1	E	245	VAL	2.4
1	C	236	GLN	2.4
1	H	519	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	239	PRO	2.4
1	B	452	LYS	2.3
1	D	238	LYS	2.3
1	F	37	ALA	2.3
1	H	225	ALA	2.3
1	B	447	GLU	2.3
1	D	450	GLN	2.3
1	F	450	GLN	2.3
1	D	451	HIS	2.3
1	B	245	VAL	2.3
1	G	523	GLY	2.3
1	A	433	THR	2.3
1	A	237	LEU	2.3
1	B	225	ALA	2.2
1	D	452	LYS	2.2
1	G	445	PRO	2.2
1	E	451	HIS	2.2
1	H	452	LYS	2.2
1	F	447	GLU	2.2
1	A	240	GLY	2.2
1	H	448	LYS	2.2
1	A	450	GLN	2.2
1	G	446	GLU	2.1
1	H	236	GLN	2.1
1	B	224	ASN	2.1
1	C	237	LEU	2.1
1	H	250	ALA	2.1
1	D	454	ASP	2.1
1	B	241	THR	2.1
1	E	229	ASP	2.1
1	G	229	ASP	2.1
1	A	320	ALA	2.1
1	F	239	PRO	2.1
1	F	223	PHE	2.0
1	H	221	ALA	2.0
1	C	240	GLY	2.0
1	A	434	GLU	2.0
1	F	446	GLU	2.0
1	F	241	THR	2.0
1	H	158	GLU	2.0
1	H	454	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	C	601	4/4	0.84	0.22	36,44,45,45	0
4	ACT	D	605	4/4	0.87	0.22	37,37,41,44	0
3	NA	B	601	1/1	0.91	0.19	47,47,47,47	0
4	ACT	D	606	4/4	0.92	0.13	33,34,34,34	0
3	NA	F	603	1/1	0.93	0.08	30,30,30,30	0
4	ACT	C	602	4/4	0.93	0.19	36,36,36,38	0
4	ACT	F	605	4/4	0.93	0.15	37,40,44,45	0
3	NA	H	601	1/1	0.95	0.19	41,41,41,41	0
3	NA	B	602	1/1	0.95	0.23	42,42,42,42	0
3	NA	A	604	1/1	0.96	0.20	44,44,44,44	0
3	NA	D	602	1/1	0.96	0.24	41,41,41,41	0
3	NA	A	603	1/1	0.96	0.18	36,36,36,36	0
3	NA	G	602	1/1	0.97	0.11	31,31,31,31	0
2	DGJ	B	600	11/11	0.97	0.14	20,21,24,25	0
2	DGJ	D	600	11/11	0.97	0.17	17,18,20,20	0
3	NA	E	603	1/1	0.97	0.08	28,28,28,28	0
3	NA	E	604	1/1	0.97	0.04	31,31,31,31	0
3	NA	F	602	1/1	0.97	0.07	35,35,35,35	0
2	DGJ	E	600	11/11	0.97	0.17	17,18,20,21	0
2	DGJ	H	600	11/11	0.98	0.15	21,22,23,23	0
3	NA	G	603	1/1	0.98	0.22	38,38,38,38	0
3	NA	D	604	1/1	0.98	0.11	30,30,30,30	0
2	DGJ	A	600	11/11	0.98	0.17	17,19,21,21	0
2	DGJ	C	600	11/11	0.98	0.15	21,22,22,23	0
3	NA	F	601	1/1	0.98	0.08	26,26,26,26	0
2	DGJ	F	600	11/11	0.98	0.15	15,18,19,19	0
2	DGJ	G	600	11/11	0.98	0.16	18,18,19,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	D	603	1/1	0.99	0.07	40,40,40,40	0
3	NA	G	604	1/1	0.99	0.14	39,39,39,39	0
3	NA	D	601	1/1	0.99	0.13	33,33,33,33	0
3	NA	E	601	1/1	0.99	0.05	24,24,24,24	0
3	NA	E	602	1/1	0.99	0.16	27,27,27,27	0
3	NA	F	604	1/1	0.99	0.05	24,24,24,24	0
3	NA	G	601	1/1	0.99	0.07	35,35,35,35	0
3	NA	A	602	1/1	0.99	0.23	35,35,35,35	0
3	NA	A	601	1/1	1.00	0.06	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.