



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 04:10 AM UTC

PDB ID : 4D1I / pdb_00004d1i
Title : The structure of the GH35 beta-galactosidase Bgl35A from *Cellvibrio japonicus*
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

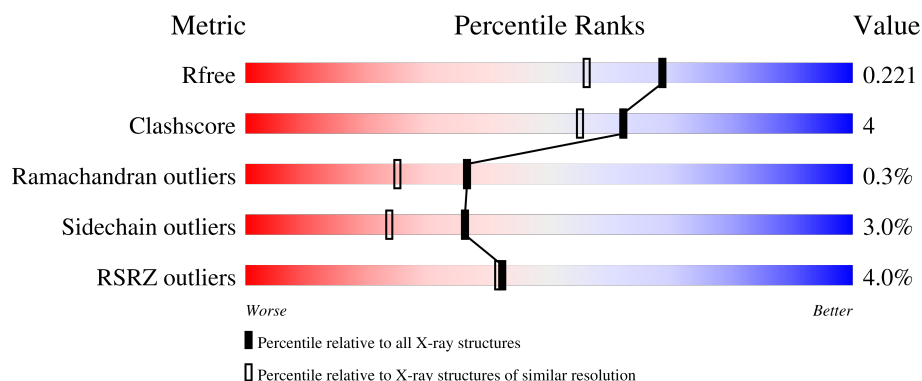
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	540	6% 92% 7%
1	B	540	5% 91% 7%
1	C	540	4% 92% 7%
1	D	540	2% 92% 7%
1	E	540	2% 90% 7%

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Mol	Chain	Length	Quality of chain
1	F	540	3% 89% 9% •
1	G	540	4% 90% 8% •
1	H	540	5% 90% 8% ••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 37302 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
1	A	539	Total	C	N	O	S	0	2	0
			4196	2687	713	780	16			
1	B	539	Total	C	N	O	S	0	3	0
			4206	2695	714	781	16			
1	C	539	Total	C	N	O	S	0	6	0
			4216	2702	718	780	16			
1	D	539	Total	C	N	O	S	0	6	0
			4238	2714	719	789	16			
1	E	539	Total	C	N	O	S	0	3	0
			4201	2688	714	784	15			
1	F	539	Total	C	N	O	S	0	4	0
			4231	2706	717	793	15			
1	G	540	Total	C	N	O	S	0	4	0
			4233	2713	721	783	16			
1	H	539	Total	C	N	O	S	0	4	0
			4159	2658	702	783	16			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	2	Total	Na	0	0
			2	2		
2	D	3	Total	Na	0	0
			3	3		
2	E	3	Total	Na	0	0
			3	3		
2	F	3	Total	Na	0	0
			3	3		

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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 8	C 4	O 4	0	1
3	H	1	Total 4	C 2	O 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	373	Total 375	O 375	0	2
4	B	445	Total 445	O 445	0	0
4	C	419	Total 420	O 420	0	1
4	D	542	Total 543	O 543	0	1

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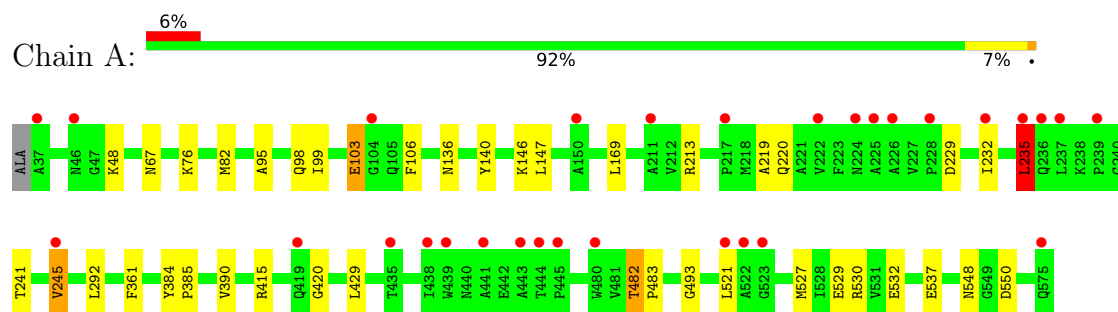
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	520	Total 520	O 520	0	0
4	F	475	Total 476	O 476	0	1
4	G	426	Total 427	O 427	0	1
4	H	381	Total 383	O 383	0	2

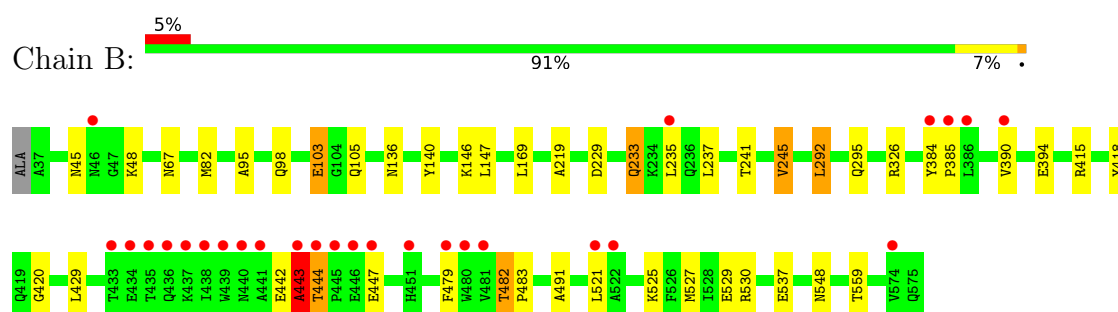
3 Residue-property plots [i](#)

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.

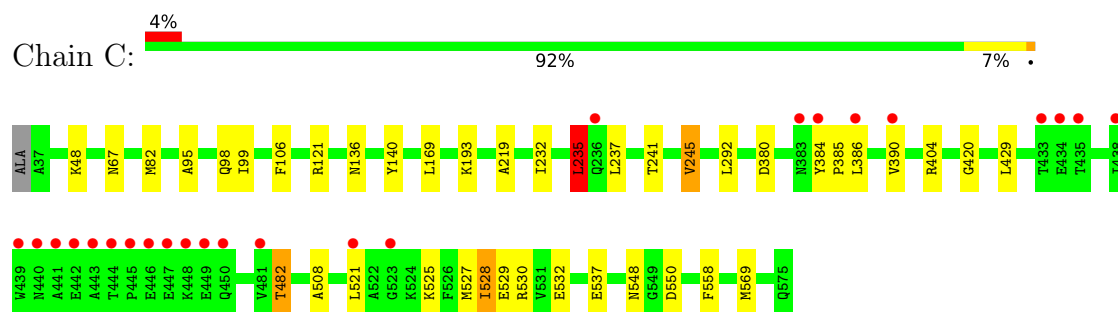
- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A



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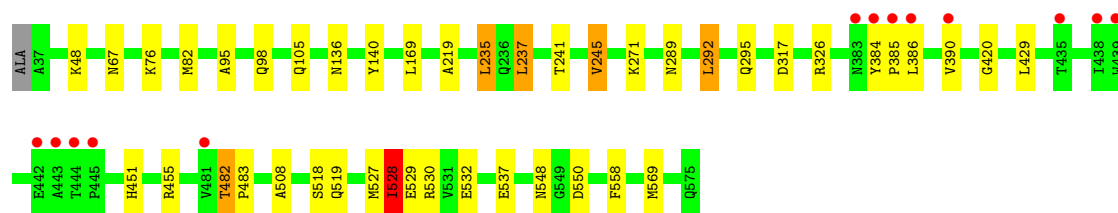


- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A

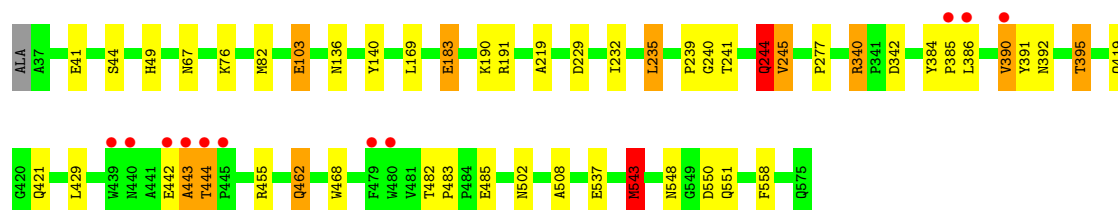
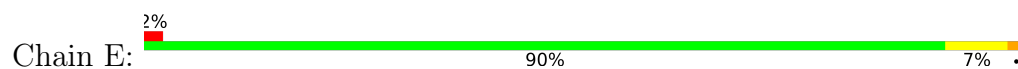


- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A

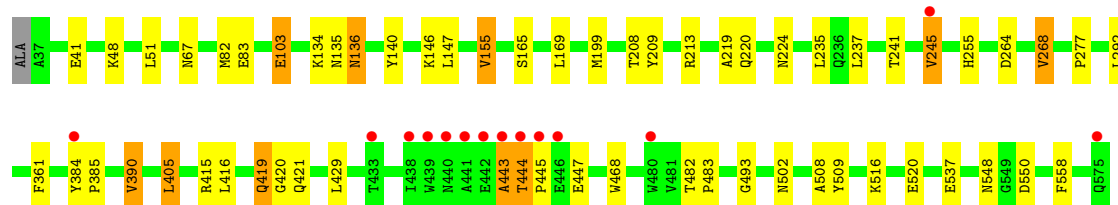
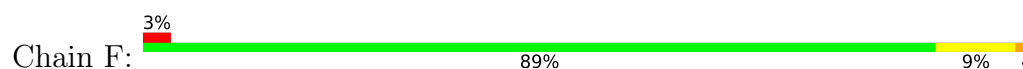




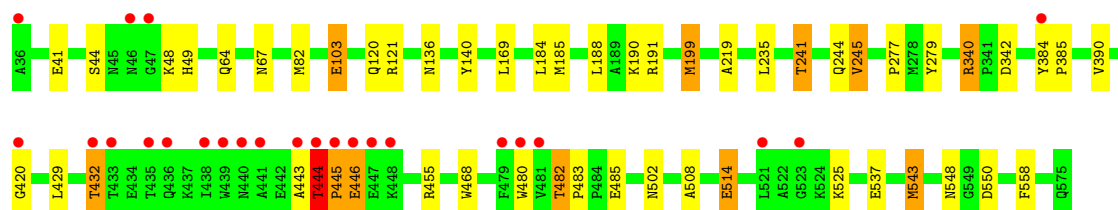
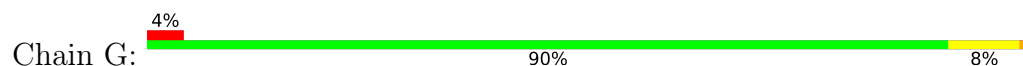
- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A



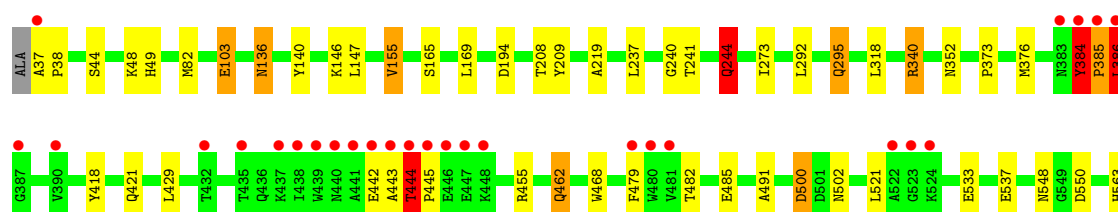
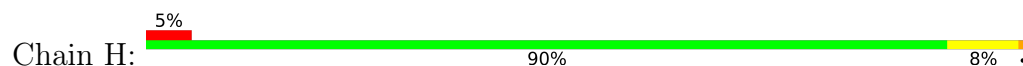
- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A



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- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	98.91Å 115.78Å 116.04Å 90.21° 90.25° 90.38°	Depositor
Resolution (Å)	116.03 – 1.80 116.03 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.4 (116.03-1.80) 96.4 (116.03-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.185 , 0.212 0.195 , 0.221	Depositor DCC
R_{free} test set	23101 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.075 for h,l,-k 0.075 for h,-l,k 0.053 for h,-k,-l 0.036 for -h,k,-l 0.036 for -h,-k,l 0.037 for -h,l,k 0.038 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	37302	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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: 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	0.73	1/4313 (0.0%)	0.83	5/5882 (0.1%)
1	B	0.72	1/4326 (0.0%)	0.80	2/5898 (0.0%)
1	C	0.73	0/4344	0.84	4/5922 (0.1%)
1	D	0.79	1/4364 (0.0%)	0.81	1/5949 (0.0%)
1	E	0.83	4/4320 (0.1%)	0.91	11/5894 (0.2%)
1	F	0.81	1/4351 (0.0%)	0.84	2/5932 (0.0%)
1	G	0.79	0/4356	0.84	4/5936 (0.1%)
1	H	0.77	0/4280	0.98	17/5846 (0.3%)
All	All	0.77	8/34654 (0.0%)	0.86	46/47259 (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
1	E	0	2
1	F	0	2
1	G	0	1
1	H	0	3
All	All	0	10

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	239	PRO	CA-C	8.15	1.62	1.52
1	E	443	ALA	CA-C	6.84	1.56	1.52
1	E	483	PRO	CA-C	6.48	1.55	1.51
1	B	443	ALA	CA-C	6.18	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	483	PRO	CA-C	6.12	1.55	1.51
1	E	239	PRO	C-O	-6.09	1.16	1.23
1	D	483	PRO	CA-C	6.06	1.55	1.51
1	F	483	PRO	CA-C	5.09	1.54	1.51

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	444	THR	CA-C-N	20.45	145.41	119.84
1	H	444	THR	C-N-CA	20.45	145.41	119.84
1	E	235	LEU	N-CA-C	-12.76	92.09	110.59
1	C	235	LEU	N-CA-C	-12.49	92.48	110.59
1	A	235	LEU	N-CA-C	-11.71	93.61	110.59
1	E	239	PRO	O-C-N	-10.46	110.15	122.71
1	H	384	TYR	CA-C-N	10.26	132.66	119.84
1	H	384	TYR	C-N-CA	10.26	132.66	119.84
1	B	521	LEU	N-CA-C	-9.99	95.73	110.52
1	G	444	THR	CA-C-N	9.62	131.87	119.84
1	G	444	THR	C-N-CA	9.62	131.87	119.84
1	E	239	PRO	CA-C-N	9.37	138.57	121.70
1	E	239	PRO	C-N-CA	9.37	138.57	121.70
1	A	521	LEU	N-CA-C	-9.32	96.72	110.52
1	H	521	LEU	N-CA-C	-9.09	97.06	110.52
1	H	340	ARG	NE-CZ-NH2	-8.90	111.19	119.20
1	C	521	LEU	N-CA-C	-8.85	97.36	110.46
1	H	340	ARG	NE-CZ-NH1	8.44	129.94	121.50
1	H	273	ILE	CB-CG1-CD1	8.17	130.96	113.80
1	H	442	GLU	N-CA-C	8.15	121.27	111.82
1	C	235	LEU	CA-C-N	-8.12	111.91	122.79
1	C	235	LEU	C-N-CA	-8.12	111.91	122.79
1	H	273	ILE	CG1-CB-CG2	-7.62	87.83	110.70
1	E	443	ALA	N-CA-C	7.61	121.03	108.48
1	E	235	LEU	CA-C-N	-7.41	112.86	122.79
1	E	235	LEU	C-N-CA	-7.41	112.86	122.79
1	A	235	LEU	CA-C-N	-7.24	113.09	122.79
1	A	235	LEU	C-N-CA	-7.24	113.09	122.79
1	E	244	GLN	CB-CA-C	6.92	123.37	110.70
1	H	244	GLN	CB-CA-C	6.78	123.11	110.70
1	H	386	LEU	CA-CB-CG	6.52	139.10	116.30
1	F	390	VAL	CA-CB-CG2	6.24	121.01	110.40
1	G	483	PRO	N-CA-C	5.95	116.18	110.47
1	F	103	GLU	O-C-N	-5.73	115.90	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	239	PRO	CA-C-O	-5.67	114.15	122.31
1	E	543	MET	CG-SD-CE	5.67	113.36	100.90
1	H	340	ARG	CD-NE-CZ	5.66	132.33	124.40
1	B	103	GLU	O-C-N	-5.62	116.04	122.89
1	G	103	GLU	O-C-N	-5.48	116.20	122.89
1	E	103	GLU	O-C-N	-5.47	116.22	122.89
1	A	103	GLU	O-C-N	-5.29	116.44	122.89
1	H	295	GLN	CA-CB-CG	5.28	124.66	114.10
1	D	528	ILE	CA-CB-CG1	5.25	119.33	110.40
1	H	103	GLU	O-C-N	-5.17	116.58	122.89
1	H	384	TYR	O-C-N	5.08	127.16	121.32
1	H	462	GLN	CA-CB-CG	5.06	124.22	114.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	GLU	Peptide
1	B	103	GLU	Peptide
1	E	103	GLU	Peptide
1	E	442	GLU	Peptide
1	F	103	GLU	Peptide
1	F	444	THR	Peptide
1	G	103	GLU	Peptide
1	H	103	GLU	Peptide
1	H	384	TYR	Peptide,Mainchain

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	4196	0	4010	35	0
1	B	4206	0	4029	39	0
1	C	4216	0	4041	34	0
1	D	4238	0	4071	41	0
1	E	4201	0	4019	32	0
1	F	4231	0	4044	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4233	0	4084	46	0
1	H	4159	0	3913	47	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	1	0	0	0	0
3	D	12	0	9	0	0
3	H	4	0	3	0	0
4	A	375	0	0	9	0
4	B	445	0	0	9	0
4	C	420	0	0	8	0
4	D	543	0	0	14	0
4	E	520	0	0	8	0
4	F	476	0	0	9	0
4	G	427	0	0	12	0
4	H	383	0	0	4	0
All	All	37302	0	32223	269	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 (269) 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:H:352:ASN:HB3	1:H:376[A]:MET:HE1	1.32	1.11
1:H:352:ASN:CB	1:H:376[A]:MET:HE1	1.84	1.06
1:D:527[A]:MET:HE2	1:F:147:LEU:HD21	1.34	1.05
1:A:147:LEU:HD21	1:C:527[A]:MET:HE2	1.38	1.03
1:B:527[A]:MET:HE2	1:H:147:LEU:HD21	1.38	1.02
1:A:527[A]:MET:HE2	1:B:147:LEU:HD21	1.39	0.99
1:H:373:PRO:HB2	1:H:376[A]:MET:HE3	1.46	0.96
1:B:527[A]:MET:HE1	1:H:146:LYS:HE3	1.48	0.95
1:A:146:LYS:HE3	1:C:527[A]:MET:HE1	1.48	0.94
1:E:468:TRP:HE1	1:E:502:ASN:HD22	1.13	0.94
1:F:468:TRP:HE1	1:F:502:ASN:HD22	1.15	0.93
1:G:468:TRP:HE1	1:G:502:ASN:HD22	1.16	0.91
1:D:527[A]:MET:HE1	1:F:146:LYS:HE3	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:468:TRP:HE1	1:H:502:ASN:HD22	1.17	0.90
1:H:37:ALA:HB1	1:H:38:PRO:HD2	1.49	0.90
1:B:45:ASN:OD1	1:B:418:TYR:OH	1.89	0.89
1:G:480:TRP:CB	1:G:482:THR:HG22	2.02	0.89
1:A:67:ASN:HD22	1:C:550:ASP:H	1.18	0.88
1:A:527[A]:MET:HE1	1:B:146:LYS:HE3	1.54	0.88
1:D:550:ASP:H	1:F:67:ASN:HD22	1.19	0.87
1:C:482:THR:HG22	4:C:2373:HOH:O	1.75	0.84
1:A:530:ARG:NH1	1:A:532:GLU:OE2	2.10	0.84
1:D:530:ARG:NH1	1:D:532:GLU:OE2	2.11	0.84
1:G:525:LYS:HD2	4:G:2375:HOH:O	1.76	0.84
1:A:550:ASP:H	1:B:67:ASN:HD22	1.27	0.83
1:C:530[A]:ARG:NH1	1:C:532:GLU:OE2	2.12	0.82
1:C:193:LYS:H	1:D:289:ASN:HD21	1.24	0.82
1:E:67:ASN:HD22	1:G:550:ASP:H	1.26	0.81
1:H:373:PRO:CB	1:H:376[A]:MET:HE3	2.11	0.81
1:C:67:ASN:HD22	1:H:550:ASP:H	1.29	0.81
1:C:121[A]:ARG:NH1	4:C:2111:HOH:O	2.13	0.81
1:F:550:ASP:H	1:G:67:ASN:HD22	1.23	0.81
1:D:67:ASN:HD22	1:E:550:ASP:H	1.28	0.81
1:C:380:ASP:OD2	1:H:563:HIS:HE1	1.63	0.80
1:H:443:ALA:HB1	1:H:444:THR:CB	2.11	0.80
1:G:443:ALA:O	1:G:444:THR:O	2.00	0.79
1:B:95:ALA:H	1:B:98:GLN:HE21	1.29	0.78
1:A:146:LYS:HE3	1:C:527[A]:MET:CE	2.14	0.78
1:H:352:ASN:HB3	1:H:376[A]:MET:CE	2.12	0.78
1:A:95:ALA:H	1:A:98:GLN:HE21	1.32	0.77
1:A:147:LEU:CD2	1:C:527[A]:MET:HE2	2.14	0.77
1:C:95:ALA:H	1:C:98:GLN:HE21	1.28	0.77
1:D:527[A]:MET:HE2	1:F:147:LEU:CD2	2.14	0.77
1:C:48:LYS:NZ	1:C:420:GLY:O	2.18	0.77
1:F:48:LYS:NZ	1:F:420:GLY:O	2.19	0.76
1:B:527[A]:MET:HE2	1:H:147:LEU:CD2	2.16	0.76
1:D:95:ALA:H	1:D:98:GLN:HE21	1.31	0.75
1:B:48:LYS:NZ	1:B:420:GLY:O	2.20	0.75
1:H:352:ASN:HB2	1:H:376[A]:MET:HE1	1.66	0.75
1:D:482:THR:HG22	4:D:2459:HOH:O	1.85	0.75
1:D:48:LYS:NZ	1:D:420:GLY:O	2.19	0.75
1:A:527[A]:MET:HE2	1:B:147:LEU:CD2	2.14	0.74
1:B:527[A]:MET:CE	1:H:146:LYS:HE3	2.16	0.74
1:G:199:MET:CE	1:G:279:TYR:HD1	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:MET:HE1	1:G:279:TYR:HD1	1.52	0.74
1:G:48:LYS:NZ	1:G:420:GLY:O	2.20	0.73
1:G:199:MET:HE1	1:G:279:TYR:CD1	2.23	0.73
1:H:37:ALA:HB1	1:H:38:PRO:CD	2.17	0.73
1:A:48:LYS:NZ	1:A:420:GLY:O	2.19	0.73
1:A:527[A]:MET:CE	1:B:146:LYS:HE3	2.20	0.71
1:F:419:GLN:HG2	4:F:2341:HOH:O	1.90	0.70
1:D:527[A]:MET:CE	1:F:146:LYS:HE3	2.21	0.70
1:E:229:ASP:HB2	4:E:2246:HOH:O	1.92	0.70
1:H:48:LYS:HE3	1:H:418:TYR:O	1.90	0.70
1:E:386:LEU:HD13	4:E:2102:HOH:O	1.92	0.69
1:A:482:THR:HG22	4:A:2311:HOH:O	1.93	0.68
1:G:340[A]:ARG:NH2	4:G:2263:HOH:O	2.14	0.68
1:E:462[A]:GLN:OE1	4:E:2418:HOH:O	2.12	0.68
1:C:386[A]:LEU:HD13	4:C:2097:HOH:O	1.93	0.67
1:D:519[A]:GLN:CG	4:D:2446:HOH:O	2.43	0.67
1:H:384:TYR:CG	1:H:385:PRO:N	2.62	0.67
1:E:543:MET:HE3	1:E:543:MET:O	1.96	0.66
1:G:543:MET:SD	4:G:2385:HOH:O	2.53	0.66
1:G:241:THR:H	1:G:244:GLN:HE21	1.43	0.66
1:C:482:THR:CG2	4:C:2373:HOH:O	2.39	0.66
1:D:528:ILE:HD12	1:D:569:MET:SD	2.37	0.65
1:E:76:LYS:HE2	4:E:2040:HOH:O	1.97	0.65
1:D:271[B]:LYS:NZ	1:D:317:ASP:OD2	2.30	0.64
1:C:528[A]:ILE:HD12	1:C:569:MET:SD	2.37	0.64
1:G:445:PRO:O	1:G:446:GLU:CB	2.46	0.64
1:G:199:MET:CE	1:G:279:TYR:CD1	2.80	0.63
1:D:105:GLN:HG3	4:D:2115:HOH:O	1.98	0.63
1:E:392:ASN:H	1:E:395:THR:CG2	2.12	0.63
1:E:392:ASN:H	1:E:395:THR:HG23	1.62	0.63
1:D:76:LYS:HE2	4:D:2051:HOH:O	1.98	0.62
1:D:386:LEU:HD13	4:D:2122:HOH:O	1.99	0.62
1:G:241:THR:HG23	4:G:2187:HOH:O	1.99	0.61
1:H:37:ALA:HA	4:H:2001:HOH:O	2.01	0.61
1:G:432:THR:HG21	4:G:2329:HOH:O	2.00	0.61
1:H:421:GLN:CB	4:H:2320:HOH:O	2.49	0.61
1:A:146:LYS:CE	1:C:527[A]:MET:HE1	2.25	0.60
1:G:120:GLN:HE21	1:G:121:ARG:HH12	1.49	0.60
1:A:213:ARG:HH22	1:A:220:GLN:HE22	1.49	0.60
1:A:415:ARG:NH2	4:A:2272:HOH:O	2.35	0.60
1:D:67:ASN:HB2	1:E:551:GLN:HE22	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527[A]:MET:HE1	1:B:146:LYS:CE	2.31	0.59
1:G:543:MET:CG	4:G:2385:HOH:O	2.51	0.59
1:D:519[A]:GLN:HG3	4:D:2446:HOH:O	2.01	0.59
1:C:569:MET:O	4:C:2389:HOH:O	2.17	0.59
1:D:519[A]:GLN:NE2	4:D:2447:HOH:O	2.37	0.58
1:D:527[A]:MET:HE3	1:D:529:GLU:HA	1.86	0.58
1:D:482:THR:HG21	4:D:2240:HOH:O	2.04	0.57
1:G:184:LEU:HG	1:G:185[A]:MET:CE	2.35	0.56
1:B:443:ALA:O	1:B:447:GLU:CB	2.54	0.56
1:C:380:ASP:OD2	1:H:563:HIS:CE1	2.53	0.56
1:C:527[A]:MET:HE3	1:C:529:GLU:HA	1.87	0.56
1:F:264:ASP:O	1:F:268:VAL:HG12	2.05	0.56
1:E:455:ARG:NH2	1:E:485:GLU:O	2.39	0.56
1:G:455:ARG:NH2	1:G:485:GLU:O	2.39	0.55
1:D:528:ILE:CD1	1:D:569:MET:SD	2.94	0.55
1:B:525[A]:LYS:HD3	4:B:2387:HOH:O	2.05	0.55
1:E:240:GLY:HA2	4:E:2115:HOH:O	2.05	0.55
1:F:443:ALA:HB1	1:F:444:THR:CB	2.36	0.55
1:C:528[A]:ILE:CD1	1:C:569:MET:SD	2.94	0.55
1:B:527[A]:MET:HE1	1:H:146:LYS:CE	2.28	0.54
1:A:527[A]:MET:HE3	1:A:529:GLU:HA	1.89	0.54
1:H:455:ARG:NH2	1:H:485:GLU:O	2.40	0.54
1:B:527[A]:MET:HE3	1:B:529:GLU:HA	1.88	0.54
1:F:213:ARG:HH22	1:F:220:GLN:HE22	1.55	0.54
1:A:146:LYS:HG3	1:C:527[A]:MET:HE1	1.90	0.54
1:B:394:GLU:HG3	4:B:2161:HOH:O	2.08	0.54
1:A:384:TYR:CD1	1:A:385:PRO:HA	2.43	0.53
1:G:64:GLN:HB2	4:G:2027:HOH:O	2.07	0.53
1:A:482:THR:CG2	4:A:2311:HOH:O	2.54	0.53
1:G:185[A]:MET:CE	1:G:188:LEU:HD12	2.39	0.53
1:B:105:GLN:HG3	4:B:2087:HOH:O	2.08	0.53
1:B:292:LEU:HB2	1:B:295:GLN:HE21	1.72	0.53
1:B:384:TYR:CD1	1:B:385:PRO:HA	2.44	0.53
1:G:185[A]:MET:HE2	1:G:185[A]:MET:HA	1.91	0.53
1:E:190:LYS:HG3	1:E:191:ARG:HG2	1.91	0.53
1:F:390:VAL:HG12	4:F:2309:HOH:O	2.09	0.53
1:F:447:GLU:CB	4:F:2360:HOH:O	2.57	0.52
1:E:391:TYR:HA	1:E:395:THR:HG21	1.92	0.52
1:G:443:ALA:O	1:G:444:THR:C	2.52	0.52
1:D:384:TYR:CD1	1:D:385:PRO:HA	2.45	0.52
1:A:527[A]:MET:HE1	1:B:146:LYS:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:THR:HG21	4:A:2145:HOH:O	2.08	0.51
1:B:525[A]:LYS:NZ	4:B:2386:HOH:O	2.21	0.51
1:C:386[A]:LEU:CD1	4:C:2097:HOH:O	2.54	0.51
1:G:190:LYS:HG3	1:G:191:ARG:HG2	1.92	0.51
1:H:240:GLY:HA2	1:H:244:GLN:HE21	1.74	0.51
1:G:64:GLN:OE1	4:G:2027:HOH:O	2.19	0.51
1:D:326:ARG:NH1	4:D:2330:HOH:O	2.44	0.51
1:F:516:LYS:NZ	4:F:2405:HOH:O	2.42	0.51
1:B:415:ARG:NH2	4:B:2333:HOH:O	2.44	0.50
1:B:443:ALA:O	1:B:444:THR:CB	2.59	0.50
1:H:155:VAL:HG13	1:H:165:SER:O	2.11	0.50
1:B:479:PHE:CZ	1:H:386:LEU:HD11	2.46	0.50
1:D:455:ARG:NH1	4:D:2434:HOH:O	2.44	0.50
1:E:384:TYR:CD1	1:E:385:PRO:HA	2.47	0.50
1:G:384:TYR:CD1	1:G:385:PRO:HA	2.46	0.50
1:D:527[A]:MET:HE1	1:F:146:LYS:CE	2.33	0.50
4:A:2119:HOH:O	1:C:525:LYS:HE3	2.11	0.50
1:E:340[A]:ARG:NH2	4:E:2333:HOH:O	2.25	0.49
1:G:443:ALA:C	1:G:444:THR:O	2.55	0.49
1:D:482:THR:CG2	4:D:2459:HOH:O	2.51	0.49
1:F:384:TYR:CD1	1:F:385:PRO:HA	2.47	0.49
1:H:352:ASN:CB	1:H:376[A]:MET:CE	2.75	0.49
1:F:264:ASP:O	1:F:268:VAL:CG1	2.61	0.49
1:G:514[B]:GLU:OE1	4:G:2366:HOH:O	2.20	0.49
1:B:479:PHE:CZ	1:H:386:LEU:CD1	2.95	0.49
1:C:384:TYR:CD1	1:C:385:PRO:HA	2.47	0.49
1:B:479:PHE:CE1	1:H:386:LEU:CD1	2.96	0.48
1:D:292:LEU:HB2	1:D:295:GLN:HE21	1.78	0.48
1:E:543:MET:HE3	1:E:543:MET:C	2.38	0.48
1:A:415:ARG:CZ	4:A:2272:HOH:O	2.60	0.48
1:B:229:ASP:O	1:B:233:GLN:HG3	2.13	0.48
1:E:386:LEU:CD1	4:E:2102:HOH:O	2.54	0.48
1:D:386:LEU:CD1	4:D:2122:HOH:O	2.57	0.48
1:F:419:GLN:CG	4:F:2341:HOH:O	2.58	0.48
1:B:326:ARG:NH1	4:B:2270:HOH:O	2.47	0.48
1:F:155:VAL:HG13	1:F:165:SER:O	2.14	0.47
1:F:213:ARG:HH22	1:F:220:GLN:NE2	2.12	0.47
1:H:533:GLU:OE2	1:H:563:HIS:HD2	1.97	0.47
1:H:240:GLY:CA	1:H:244:GLN:HE21	2.28	0.47
1:B:527[A]:MET:HE1	1:H:146:LYS:HG3	1.95	0.47
1:F:208:THR:OG1	1:F:255:HIS:HE1	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:136:ASN:HD22	1:H:208:THR:HA	1.80	0.47
1:F:136:ASN:HD22	1:F:208:THR:HA	1.80	0.46
1:C:232:ILE:O	1:C:235:LEU:O	2.32	0.46
1:C:528[A]:ILE:HD13	1:C:569:MET:HE1	1.97	0.46
1:A:548:ASN:HB3	1:B:140:TYR:CZ	2.50	0.46
1:E:183:GLU:HG3	4:E:2191:HOH:O	2.13	0.46
1:B:548:ASN:HB3	1:H:140:TYR:CZ	2.51	0.46
1:H:169:LEU:HD13	1:H:219:ALA:HA	1.98	0.46
1:D:527[A]:MET:HE1	1:F:146:LYS:HG3	1.97	0.46
1:E:241:THR:H	1:E:244:GLN:NE2	2.14	0.46
1:G:199:MET:HE2	1:G:279:TYR:HD1	1.78	0.46
1:C:140:TYR:CZ	1:H:548:ASN:HB3	2.51	0.45
1:D:528:ILE:HD13	1:D:569:MET:HE1	1.98	0.45
1:H:384:TYR:CD2	1:H:385:PRO:N	2.84	0.45
1:B:525[A]:LYS:CD	4:B:2387:HOH:O	2.60	0.45
4:C:2314:HOH:O	1:H:479:PHE:CB	2.65	0.45
1:G:184:LEU:HG	1:G:185[A]:MET:HE3	1.98	0.45
1:E:241:THR:O	1:E:245:VAL:HG13	2.17	0.45
1:H:241:THR:H	1:H:244:GLN:NE2	2.15	0.45
1:B:530[B]:ARG:NH2	4:B:2397:HOH:O	2.46	0.44
1:H:48:LYS:CE	1:H:418:TYR:O	2.62	0.44
1:F:416:LEU:HG	4:F:2331:HOH:O	2.16	0.44
1:G:169:LEU:HD13	1:G:219:ALA:HA	1.99	0.44
1:G:514[A]:GLU:HG3	4:G:2340:HOH:O	2.18	0.44
1:A:232:ILE:O	1:A:235:LEU:O	2.35	0.44
1:B:169:LEU:HD13	1:B:219:ALA:HA	1.98	0.44
1:G:185[A]:MET:HE1	1:G:188:LEU:HD12	1.98	0.44
1:G:241:THR:O	1:G:245:VAL:HG13	2.18	0.44
1:A:140:TYR:CZ	1:C:548:ASN:HB3	2.53	0.44
1:F:224:ASN:ND2	4:F:2202:HOH:O	2.49	0.44
1:A:241:THR:O	1:A:245:VAL:HG13	2.18	0.44
1:E:232:ILE:O	1:E:235:LEU:O	2.35	0.43
1:C:241:THR:O	1:C:245:VAL:HG13	2.19	0.43
1:C:404:ARG:NH1	4:C:2329:HOH:O	2.29	0.43
1:A:530:ARG:NH2	4:A:2338:HOH:O	2.51	0.43
1:B:241:THR:O	1:B:245:VAL:HG13	2.18	0.43
1:D:271[B]:LYS:HE2	4:D:2297:HOH:O	2.19	0.43
1:F:415:ARG:NH2	4:F:2331:HOH:O	2.51	0.43
1:E:169:LEU:HD13	1:E:219:ALA:HA	2.00	0.43
1:D:548:ASN:HB3	1:F:140:TYR:CZ	2.54	0.43
1:G:508:ALA:HB3	1:G:558:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:THR:O	1:F:245:VAL:HG13	2.18	0.43
1:F:405:LEU:HD11	1:F:509:TYR:HB2	2.01	0.43
1:E:41:GLU:HA	1:E:277:PRO:HG3	2.01	0.42
1:F:169:LEU:HD13	1:F:219:ALA:HA	2.01	0.42
1:A:361:PHE:CD2	1:A:493:GLY:HA3	2.55	0.42
1:F:136:ASN:ND2	1:F:209:TYR:H	2.18	0.42
1:C:169:LEU:HD13	1:C:219:ALA:HA	2.01	0.42
1:D:241:THR:O	1:D:245:VAL:HG13	2.19	0.42
1:F:41:GLU:HA	1:F:277:PRO:HG3	2.01	0.42
1:G:199:MET:HE2	1:G:199:MET:HB3	1.55	0.42
1:H:37:ALA:CB	1:H:38:PRO:CD	2.94	0.42
1:A:169:LEU:HD13	1:A:219:ALA:HA	2.01	0.42
1:D:518:SER:C	1:D:519[A]:GLN:HG3	2.45	0.42
1:F:67:ASN:ND2	1:F:134:LYS:HZ1	2.17	0.42
1:B:559:THR:HG22	4:B:2209:HOH:O	2.20	0.42
1:H:318:LEU:HD12	1:H:318:LEU:C	2.45	0.42
1:E:443:ALA:O	1:E:444:THR:CB	2.68	0.42
1:H:292:LEU:HB3	4:H:2212:HOH:O	2.20	0.42
1:E:140:TYR:CZ	1:G:548:ASN:HB3	2.54	0.41
1:G:64:GLN:NE2	4:G:2028:HOH:O	2.31	0.41
1:H:136:ASN:ND2	1:H:209:TYR:H	2.16	0.41
1:A:229:ASP:CB	4:A:2159:HOH:O	2.67	0.41
1:G:342:ASP:OD1	1:G:342:ASP:C	2.63	0.41
1:F:508:ALA:HB3	1:F:558:PHE:CD1	2.55	0.41
1:G:199:MET:HE2	1:G:279:TYR:CD1	2.53	0.41
1:F:421:GLN:N	4:F:2337:HOH:O	2.41	0.41
1:A:76:LYS:HD3	4:A:2023:HOH:O	2.20	0.41
1:D:169:LEU:HD13	1:D:219:ALA:HA	2.03	0.41
1:E:342:ASP:OD1	1:E:342:ASP:C	2.62	0.41
1:C:508:ALA:HB3	1:C:558:PHE:CD1	2.56	0.41
1:E:508:ALA:HB3	1:E:558:PHE:CD1	2.56	0.41
1:A:99:ILE:O	1:A:106:PHE:HA	2.21	0.41
1:E:44:SER:OG	1:E:49:HIS:HD2	2.03	0.41
1:C:99:ILE:O	1:C:106:PHE:HA	2.21	0.41
1:E:390:VAL:O	1:E:395:THR:HG21	2.20	0.41
1:F:51:LEU:HD22	1:F:199:MET:HE1	2.03	0.41
1:F:445:PRO:O	1:F:447:GLU:N	2.49	0.41
1:G:41:GLU:HA	1:G:277:PRO:HG3	2.02	0.41
1:G:543:MET:HE2	4:G:2385:HOH:O	2.21	0.41
1:B:482:THR:HA	1:B:483:PRO:HD3	1.96	0.40
1:F:444:THR:CB	1:F:445:PRO:O	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:LEU:O	1:D:237:LEU:HD13	2.21	0.40
1:G:44:SER:OG	1:G:49:HIS:HD2	2.03	0.40
1:H:386:LEU:HA	4:H:2270:HOH:O	2.20	0.40
1:D:140:TYR:CZ	1:E:548:ASN:HB3	2.56	0.40
1:F:361:PHE:CD2	1:F:493:GLY:HA3	2.56	0.40
1:F:548:ASN:HB3	1:G:140:TYR:CZ	2.57	0.40
1:D:451:HIS:CD2	4:D:2431:HOH:O	2.74	0.40
1:D:508:ALA:HB3	1:D:558:PHE:CD1	2.56	0.40
1:H:44:SER:OG	1:H:49:HIS:HD2	2.04	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	539/540 (100%)	521 (97%)	18 (3%)	0	100	100
1	B	540/540 (100%)	521 (96%)	15 (3%)	4 (1%)	18	8
1	C	543/540 (101%)	526 (97%)	17 (3%)	0	100	100
1	D	543/540 (101%)	527 (97%)	16 (3%)	0	100	100
1	E	540/540 (100%)	519 (96%)	20 (4%)	1 (0%)	43	31
1	F	541/540 (100%)	521 (96%)	19 (4%)	1 (0%)	43	31
1	G	542/540 (100%)	523 (96%)	16 (3%)	3 (1%)	21	11
1	H	541/540 (100%)	519 (96%)	18 (3%)	4 (1%)	18	8
All	All	4329/4320 (100%)	4177 (96%)	139 (3%)	13 (0%)	36	25

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	444	THR

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Mol	Chain	Res	Type
1	G	445	PRO
1	H	385	PRO
1	H	444	THR
1	H	445	PRO
1	B	442	GLU
1	B	443	ALA
1	B	444	THR
1	E	444	THR
1	F	443	ALA
1	G	446	GLU
1	H	491	ALA
1	B	491	ALA

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	426/452 (94%)	417 (98%)	9 (2%)	47	36
1	B	428/452 (95%)	417 (97%)	11 (3%)	40	28
1	C	428/452 (95%)	416 (97%)	12 (3%)	38	26
1	D	435/452 (96%)	424 (98%)	11 (2%)	42	30
1	E	428/452 (95%)	411 (96%)	17 (4%)	28	15
1	F	433/452 (96%)	416 (96%)	17 (4%)	28	16
1	G	433/452 (96%)	417 (96%)	16 (4%)	30	18
1	H	417/452 (92%)	401 (96%)	16 (4%)	29	17
All	All	3428/3616 (95%)	3319 (97%)	109 (3%)	36	22

All (109) 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

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Mol	Chain	Res	Type
1	A	245	VAL
1	A	292	LEU
1	A	390	VAL
1	A	429	LEU
1	A	482	THR
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	390	VAL
1	B	429	LEU
1	B	482	THR
1	B	537	GLU
1	C	82	MET
1	C	136	ASN
1	C	235	LEU
1	C	237	LEU
1	C	245	VAL
1	C	292	LEU
1	C	390	VAL
1	C	429	LEU
1	C	482	THR
1	C	528[A]	ILE
1	C	528[B]	ILE
1	C	537	GLU
1	D	82	MET
1	D	136	ASN
1	D	235	LEU
1	D	237	LEU
1	D	245	VAL
1	D	292	LEU
1	D	390	VAL
1	D	429	LEU
1	D	482	THR
1	D	528	ILE
1	D	537	GLU
1	E	82	MET
1	E	136	ASN

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Mol	Chain	Res	Type
1	E	183	GLU
1	E	244	GLN
1	E	245	VAL
1	E	340[A]	ARG
1	E	340[B]	ARG
1	E	390	VAL
1	E	395	THR
1	E	419	GLN
1	E	421	GLN
1	E	429	LEU
1	E	462[A]	GLN
1	E	462[B]	GLN
1	E	482	THR
1	E	537	GLU
1	E	543	MET
1	F	82	MET
1	F	83[A]	GLU
1	F	83[B]	GLU
1	F	135	ASN
1	F	136	ASN
1	F	155	VAL
1	F	235	LEU
1	F	237	LEU
1	F	245	VAL
1	F	268	VAL
1	F	292	LEU
1	F	405	LEU
1	F	419	GLN
1	F	429	LEU
1	F	482	THR
1	F	520	GLU
1	F	537	GLU
1	G	82	MET
1	G	136	ASN
1	G	199	MET
1	G	235	LEU
1	G	241	THR
1	G	245	VAL
1	G	340[A]	ARG
1	G	340[B]	ARG
1	G	390	VAL
1	G	429	LEU

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Mol	Chain	Res	Type
1	G	432	THR
1	G	482	THR
1	G	514[A]	GLU
1	G	514[B]	GLU
1	G	537	GLU
1	G	543	MET
1	H	82	MET
1	H	136	ASN
1	H	155	VAL
1	H	194[A]	ASP
1	H	194[B]	ASP
1	H	237	LEU
1	H	244	GLN
1	H	295	GLN
1	H	340	ARG
1	H	386	LEU
1	H	429	LEU
1	H	462	GLN
1	H	482	THR
1	H	500[A]	ASP
1	H	500[B]	ASP
1	H	537	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	98	GLN
1	A	172	ASN
1	A	201	GLN
1	A	220	GLN
1	A	275	ASN
1	A	315	ASN
1	A	440	ASN
1	A	451	HIS
1	B	67	ASN
1	B	98	GLN
1	B	172	ASN
1	B	275	ASN
1	B	295	GLN
1	B	315	ASN
1	B	451	HIS

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Mol	Chain	Res	Type
1	C	64	GLN
1	C	67	ASN
1	C	98	GLN
1	C	172	ASN
1	C	201	GLN
1	C	275	ASN
1	C	315	ASN
1	C	354	GLN
1	C	451	HIS
1	D	67	ASN
1	D	98	GLN
1	D	275	ASN
1	D	289	ASN
1	D	295	GLN
1	D	354	GLN
1	D	451	HIS
1	E	49	HIS
1	E	67	ASN
1	E	105	GLN
1	E	171	GLN
1	E	172	ASN
1	E	275	ASN
1	E	451	HIS
1	E	502	ASN
1	E	551	GLN
1	F	46	ASN
1	F	49	HIS
1	F	67	ASN
1	F	105	GLN
1	F	135	ASN
1	F	136	ASN
1	F	201	GLN
1	F	220	GLN
1	F	224	ASN
1	F	233	GLN
1	F	255	HIS
1	F	275	ASN
1	F	502	ASN
1	G	49	HIS
1	G	67	ASN
1	G	105	GLN
1	G	120	GLN

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Mol	Chain	Res	Type
1	G	171	GLN
1	G	224	ASN
1	G	244	GLN
1	G	275	ASN
1	G	401	GLN
1	G	451	HIS
1	G	502	ASN
1	H	45	ASN
1	H	46	ASN
1	H	49	HIS
1	H	64	GLN
1	H	136	ASN
1	H	172	ASN
1	H	233	GLN
1	H	244	GLN
1	H	275	ASN
1	H	451	HIS
1	H	462	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 17 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	$\# Z > 2$
3	ACT	D	603	-	3,3,3	0.80	0	3,3,3	0.98	0
3	ACT	D	604[A]	-	3,3,3	0.91	0	3,3,3	0.72	0
3	ACT	D	604[B]	-	3,3,3	0.87	0	3,3,3	0.50	0
3	ACT	H	601	-	3,3,3	0.87	0	3,3,3	0.54	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	539/540 (99%)	0.29	30 (5%)	30	29	20, 31, 60, 73	2 (0%)
1	B	539/540 (99%)	0.15	27 (5%)	34	33	18, 28, 57, 100	3 (0%)
1	C	539/540 (99%)	0.08	24 (4%)	38	37	18, 28, 60, 96	6 (1%)
1	D	539/540 (99%)	-0.16	13 (2%)	59	60	14, 24, 48, 74	6 (1%)
1	E	539/540 (99%)	-0.15	11 (2%)	65	65	14, 25, 46, 76	3 (0%)
1	F	539/540 (99%)	-0.00	14 (2%)	57	57	13, 26, 52, 94	4 (0%)
1	G	540/540 (100%)	0.04	24 (4%)	39	38	15, 26, 54, 102	4 (0%)
1	H	539/540 (99%)	0.21	29 (5%)	31	30	16, 29, 58, 104	4 (0%)
All	All	4313/4320 (99%)	0.06	172 (3%)	42	41	13, 27, 55, 104	32 (0%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	439	TRP	6.2
1	B	443	ALA	5.1
1	G	480	TRP	5.0
1	C	386[A]	LEU	4.9
1	C	438	ILE	4.8
1	A	224	ASN	4.6
1	G	445	PRO	4.5
1	H	444	THR	4.3
1	B	480	TRP	4.2
1	B	479	PHE	4.2
1	H	445	PRO	4.1
1	A	46	ASN	4.1
1	H	439	TRP	4.1
1	C	384	TYR	4.0
1	H	384	TYR	4.0
1	B	433	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	435	THR	4.0
1	H	438	ILE	4.0
1	B	386	LEU	3.8
1	B	441	ALA	3.8
1	H	386	LEU	3.7
1	C	433	THR	3.7
1	B	444	THR	3.6
1	F	445	PRO	3.6
1	E	386	LEU	3.6
1	A	522	ALA	3.6
1	G	438	ILE	3.6
1	D	435	THR	3.6
1	H	441	ALA	3.6
1	B	438	ILE	3.5
1	A	237	LEU	3.5
1	D	439	TRP	3.5
1	H	385	PRO	3.5
1	F	575	GLN	3.4
1	G	444	THR	3.4
1	H	440	ASN	3.3
1	G	440	ASN	3.3
1	B	434	GLU	3.3
1	D	385	PRO	3.2
1	G	443	ALA	3.2
1	E	444	THR	3.2
1	B	445	PRO	3.2
1	H	481	VAL	3.2
1	D	386	LEU	3.2
1	A	225	ALA	3.1
1	D	384	TYR	3.1
1	A	444	THR	3.1
1	G	435	THR	3.1
1	C	441	ALA	3.1
1	C	439	TRP	3.1
1	B	385	PRO	3.1
1	C	434	GLU	3.1
1	A	211	ALA	3.1
1	C	444	THR	3.0
1	E	445	PRO	3.0
1	G	446	GLU	3.0
1	D	445	PRO	3.0
1	C	383	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	443	ALA	3.0
1	A	521	LEU	2.9
1	C	447	GLU	2.9
1	F	439	TRP	2.9
1	H	479	PHE	2.9
1	B	440	ASN	2.8
1	F	440	ASN	2.8
1	H	435	THR	2.8
1	E	479	PHE	2.8
1	B	446	GLU	2.8
1	G	47	GLY	2.8
1	G	439	TRP	2.8
1	H	390	VAL	2.8
1	H	574	VAL	2.8
1	C	521	LEU	2.8
1	H	443	ALA	2.7
1	H	448	LYS	2.7
1	C	445	PRO	2.7
1	A	236	GLN	2.7
1	B	46	ASN	2.7
1	F	442	GLU	2.7
1	B	481	VAL	2.7
1	E	439	TRP	2.7
1	E	385	PRO	2.7
1	A	150	ALA	2.6
1	G	384	TYR	2.6
1	B	521	LEU	2.6
1	A	438	ILE	2.6
1	B	522	ALA	2.6
1	G	441	ALA	2.6
1	F	433	THR	2.6
1	A	232	ILE	2.6
1	G	420	GLY	2.6
1	H	523	GLY	2.6
1	G	433	THR	2.6
1	A	480	TRP	2.6
1	H	524	LYS	2.6
1	G	36	ALA	2.6
1	A	217	PRO	2.5
1	B	384	TYR	2.5
1	A	235	LEU	2.5
1	C	443	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	443	ALA	2.5
1	G	46	ASN	2.5
1	C	450	GLN	2.5
1	D	442	GLU	2.5
1	H	446	GLU	2.5
1	G	479	PHE	2.5
1	A	104	GLY	2.5
1	D	390	VAL	2.5
1	A	575	GLN	2.5
1	C	446	GLU	2.5
1	H	442	GLU	2.5
1	H	480	TRP	2.5
1	A	37	ALA	2.5
1	F	444	THR	2.5
1	B	390	VAL	2.5
1	C	448	LYS	2.4
1	F	441	ALA	2.4
1	E	480	TRP	2.4
1	A	239	PRO	2.4
1	D	444	THR	2.4
1	H	37	ALA	2.4
1	A	523	GLY	2.4
1	A	439	TRP	2.4
1	A	435	THR	2.3
1	C	435	THR	2.3
1	G	447	GLU	2.3
1	H	575	GLN	2.3
1	F	438	ILE	2.3
1	C	440	ASN	2.3
1	D	383	ASN	2.3
1	A	222	VAL	2.3
1	E	440	ASN	2.3
1	F	245	VAL	2.3
1	H	447	GLU	2.3
1	A	445	PRO	2.3
1	H	522	ALA	2.3
1	C	449	GLU	2.3
1	D	481	VAL	2.3
1	A	226	ALA	2.2
1	B	436	GLN	2.2
1	G	481	VAL	2.2
1	C	236	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	436	GLN	2.2
1	A	443	ALA	2.2
1	C	390	VAL	2.2
1	A	441	ALA	2.2
1	G	448	LYS	2.2
1	H	432	THR	2.2
1	C	523	GLY	2.2
1	B	437	LYS	2.2
1	B	447	GLU	2.1
1	C	481	VAL	2.1
1	B	235	LEU	2.1
1	B	451	HIS	2.1
1	E	442	GLU	2.1
1	B	574	VAL	2.1
1	G	523	GLY	2.1
1	F	446	GLU	2.1
1	D	443	ALA	2.1
1	D	438	ILE	2.1
1	C	442	GLU	2.1
1	F	480	TRP	2.1
1	A	419	GLN	2.1
1	F	384	TYR	2.0
1	G	432	THR	2.0
1	H	387	GLY	2.0
1	A	228	PRO	2.0
1	E	390	VAL	2.0
1	G	521	LEU	2.0
1	H	437	LYS	2.0
1	H	383	ASN	2.0
1	A	245	VAL	2.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	ACT	D	604[A]	4/4	0.47	0.25	40,42,43,45	4
3	ACT	D	604[B]	4/4	0.47	0.25	46,47,48,49	4
3	ACT	H	601	4/4	0.84	0.12	49,51,52,52	0
3	ACT	D	603	4/4	0.86	0.17	36,37,38,39	0
2	NA	C	601	1/1	0.88	0.09	50,50,50,50	0
2	NA	C	600	1/1	0.90	0.08	46,46,46,46	0
2	NA	F	600	1/1	0.93	0.08	43,43,43,43	0
2	NA	G	600	1/1	0.93	0.07	41,41,41,41	0
2	NA	G	601	1/1	0.95	0.07	34,34,34,34	0
2	NA	H	600	1/1	0.96	0.05	36,36,36,36	0
2	NA	A	600	1/1	0.97	0.04	37,37,37,37	0
2	NA	F	601	1/1	0.97	0.05	40,40,40,40	0
2	NA	D	601	1/1	0.97	0.07	36,36,36,36	0
2	NA	E	601	1/1	0.98	0.04	26,26,26,26	0
2	NA	D	600	1/1	0.98	0.08	25,25,25,25	0
2	NA	G	602	1/1	0.98	0.05	23,23,23,23	0
2	NA	B	600	1/1	0.98	0.04	35,35,35,35	0
2	NA	E	602	1/1	0.99	0.02	29,29,29,29	0
2	NA	E	600	1/1	0.99	0.09	26,26,26,26	0
2	NA	D	602	1/1	0.99	0.05	27,27,27,27	0
2	NA	F	602	1/1	0.99	0.03	24,24,24,24	0

6.5 Other polymers

There are no such residues in this entry.