



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:41 PM GMT

PDB ID : 4D1I
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

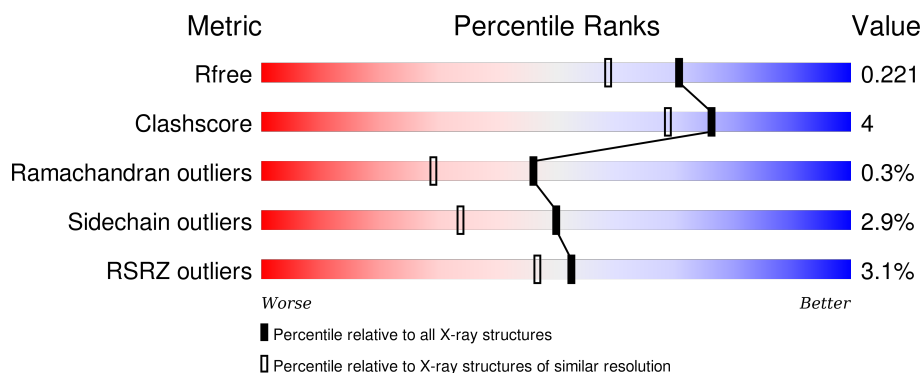
1 Overall quality at a glance ⓘ

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.



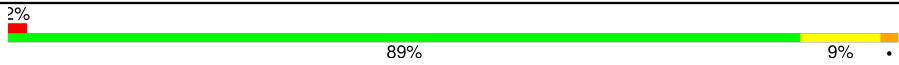
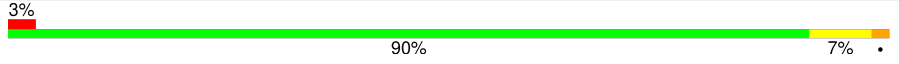
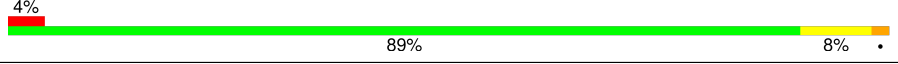
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>92%</div> <div>7%</div> </div>
1	B	540	<div> <div>5%</div> <div>91%</div> <div>7%</div> </div>
1	C	540	<div> <div>4%</div> <div>91%</div> <div>8%</div> </div>
1	D	540	<div> <div>2%</div> <div>92%</div> <div>7%</div> </div>
1	E	540	<div> <div>0%</div> <div>90%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	540	
1	G	540	
1	H	540	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	D	601	-	-	-	X

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 (three-letter code: NA) (formula: Na).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	F	3	Total	Na	0	0
			3	3		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is water.

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

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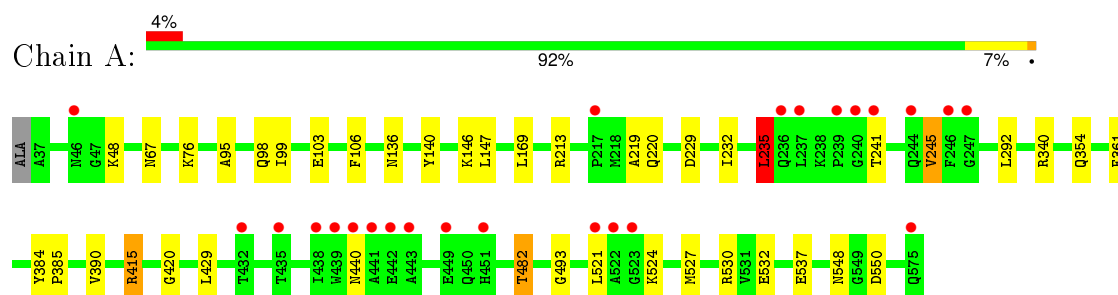
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	520	Total 520	O 520	0	0
4	F	475	Total 476	O 476	0	1
4	G	426	Total 427	O 427	0	1
4	H	381	Total 383	O 383	0	2

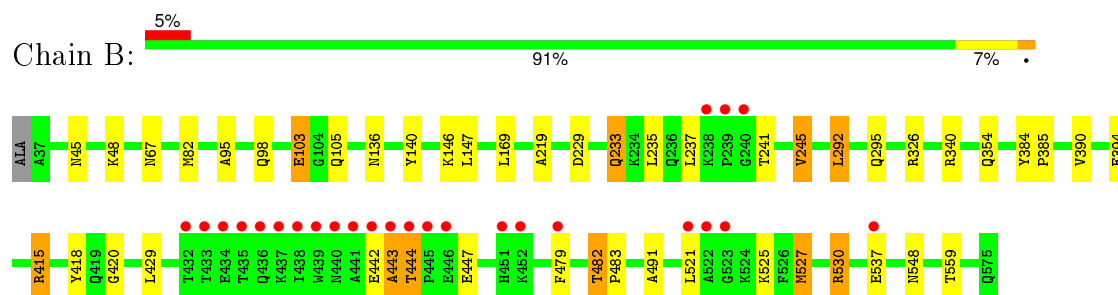
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

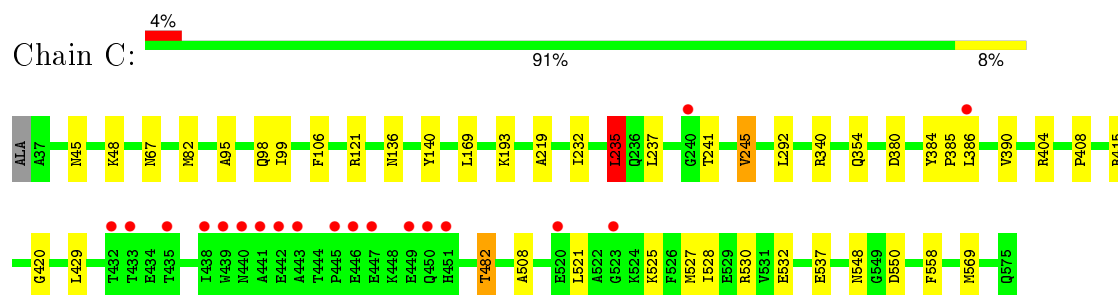
- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A



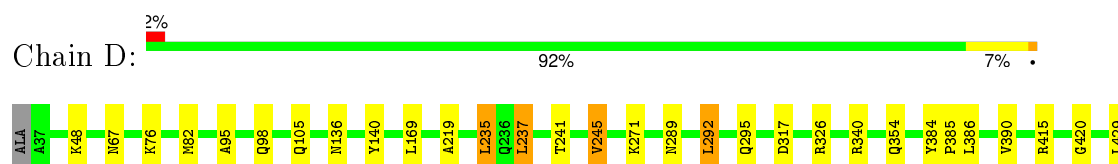
- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A



- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A

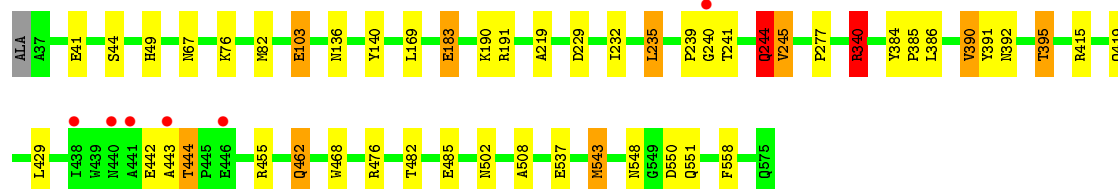
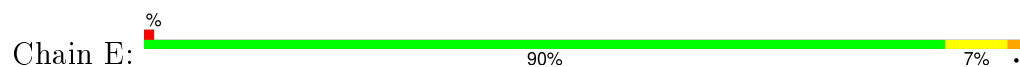


- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A

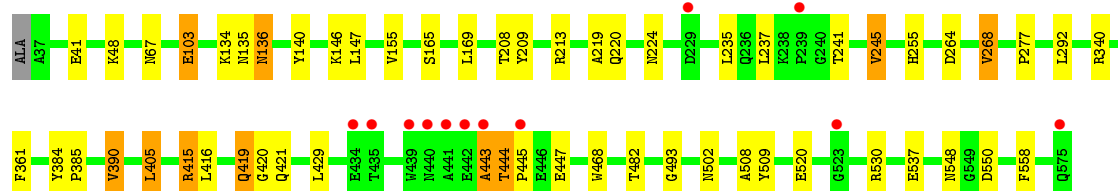
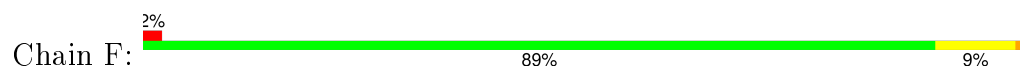




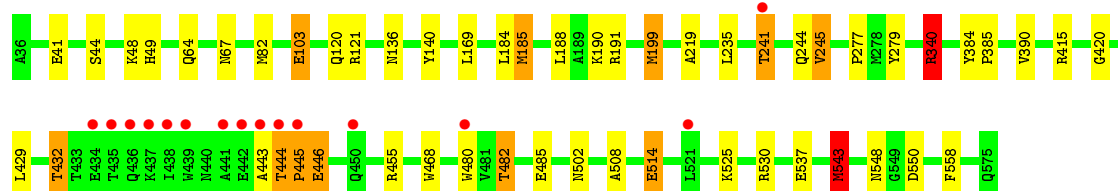
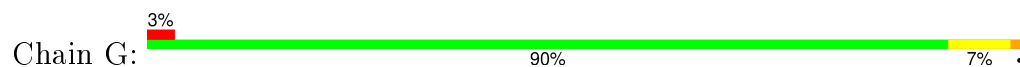
- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A



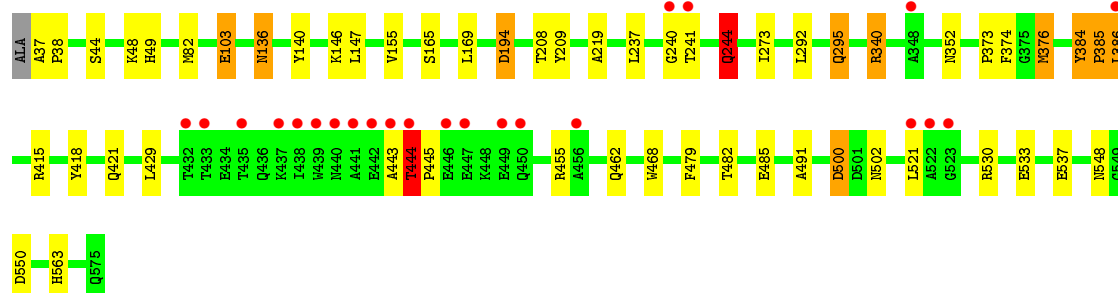
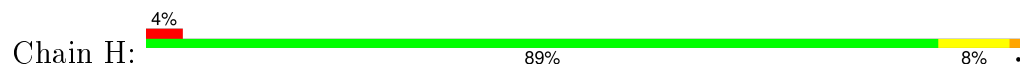
- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A



- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A



- 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 46.02 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.4 (116.03-1.80) 96.2 (46.02-1.80)	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 (5.29%)	DCC
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.2	EDS
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
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 459885 reflections	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.55	0/4313	0.73	6/5882 (0.1%)
1	B	0.55	0/4326	0.73	10/5898 (0.2%)
1	C	0.55	0/4344	0.74	5/5922 (0.1%)
1	D	0.59	0/4364	0.73	3/5949 (0.1%)
1	E	0.63	0/4320	0.92	16/5894 (0.3%)
1	F	0.62	0/4351	0.76	8/5932 (0.1%)
1	G	0.60	0/4356	0.86	13/5936 (0.2%)
1	H	0.62	2/4280 (0.0%)	0.89	18/5846 (0.3%)
All	All	0.59	2/34654 (0.0%)	0.80	79/47259 (0.2%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	194[A]	ASP	CB-CG	8.35	1.69	1.51
1	H	194[B]	ASP	CB-CG	8.35	1.69	1.51

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	340	ARG	NE-CZ-NH1	19.27	129.94	120.30
1	H	340	ARG	NE-CZ-NH2	-18.22	111.19	120.30
1	E	340[A]	ARG	NE-CZ-NH1	17.74	129.17	120.30
1	E	340[B]	ARG	NE-CZ-NH1	17.74	129.17	120.30
1	G	340[A]	ARG	NE-CZ-NH1	16.64	128.62	120.30
1	G	340[B]	ARG	NE-CZ-NH1	16.64	128.62	120.30
1	E	340[A]	ARG	NE-CZ-NH2	-15.71	112.45	120.30
1	E	340[B]	ARG	NE-CZ-NH2	-15.71	112.45	120.30
1	G	340[A]	ARG	NE-CZ-NH2	-15.69	112.45	120.30
1	G	340[B]	ARG	NE-CZ-NH2	-15.69	112.45	120.30
1	H	273	ILE	CG1-CB-CG2	-10.71	87.83	111.40
1	H	386	LEU	CA-CB-CG	10.35	139.10	115.30
1	E	239	PRO	CA-C-N	9.73	135.65	116.20
1	C	340	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	E	543	MET	CG-SD-CE	8.23	113.36	100.20
1	C	340	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	A	340	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	A	340	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	E	239	PRO	C-N-CA	7.75	138.57	122.30
1	E	239	PRO	O-C-N	-7.67	110.15	123.20
1	H	415	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	H	376[A]	MET	CG-SD-CE	-7.30	88.52	100.20
1	H	376[B]	MET	CG-SD-CE	-7.30	88.52	100.20
1	E	415	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	B	340	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	D	340	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	D	340	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	E	235	LEU	N-CA-C	-7.00	92.09	111.00
1	B	340	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	G	415	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	C	235	LEU	N-CA-C	-6.86	92.48	111.00
1	F	415	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	F	390	VAL	CA-CB-CG2	6.74	121.01	110.90
1	A	415	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	E	244	GLN	CB-CA-C	6.49	123.37	110.40
1	F	405	LEU	CB-CG-CD1	6.47	122.00	111.00
1	A	235	LEU	N-CA-C	-6.44	93.61	111.00
1	D	415	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	H	244	GLN	CB-CA-C	6.35	123.11	110.40
1	G	185[A]	MET	CG-SD-CE	6.33	110.32	100.20
1	G	185[B]	MET	CG-SD-CE	6.33	110.32	100.20
1	H	340	ARG	CD-NE-CZ	6.24	132.33	123.60
1	H	386	LEU	CB-CG-CD1	-6.21	100.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	273	ILE	CB-CG1-CD1	6.09	130.96	113.90
1	B	415	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	H	415	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	G	543	MET	CG-SD-CE	-5.93	90.72	100.20
1	E	340[A]	ARG	CD-NE-CZ	5.88	131.82	123.60
1	E	340[B]	ARG	CD-NE-CZ	5.88	131.82	123.60
1	H	386	LEU	CB-CG-CD2	5.82	120.89	111.00
1	G	530	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	E	415	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	G	340[A]	ARG	CD-NE-CZ	5.67	131.54	123.60
1	G	340[B]	ARG	CD-NE-CZ	5.67	131.54	123.60
1	B	521	LEU	N-CA-C	-5.65	95.73	111.00
1	C	415	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	H	444	THR	C-N-CA	5.57	145.41	122.00
1	E	476	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	F	530	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	527[A]	MET	CG-SD-CE	-5.46	91.46	100.20
1	B	527[B]	MET	CG-SD-CE	-5.46	91.46	100.20
1	B	530[A]	ARG	CG-CD-NE	5.46	123.26	111.80
1	B	530[B]	ARG	CG-CD-NE	5.46	123.26	111.80
1	F	340	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	415	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	F	405	LEU	CA-CB-CG	5.38	127.68	115.30
1	F	103	GLU	CA-C-N	5.38	126.95	116.20
1	F	415	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	521	LEU	N-CA-C	-5.29	96.72	111.00
1	B	103	GLU	CA-C-N	5.28	126.77	116.20
1	G	415	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	E	103	GLU	CA-C-N	5.19	126.58	116.20
1	B	415	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	H	521	LEU	N-CA-C	-5.16	97.06	111.00
1	H	103	GLU	CA-C-N	5.14	126.48	116.20
1	H	295	GLN	CA-CB-CG	5.12	124.66	113.40
1	G	103	GLU	CA-C-N	5.08	126.37	116.20
1	C	521	LEU	N-CA-C	-5.05	97.36	111.00
1	H	530	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	GLU	Peptide

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Mol	Chain	Res	Type	Group
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	Mainchain,Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4196	0	4010	33	0
1	B	4206	0	4029	36	0
1	C	4216	0	4041	31	0
1	D	4238	0	4071	37	0
1	E	4201	0	4019	29	0
1	F	4231	0	4044	38	0
1	G	4233	0	4084	41	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	10	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	8	0
4	G	427	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	383	0	0	4	0
All	All	37302	0	32223	250	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 (250) 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:A:146:LYS:HE3	1:C:527[A]:MET:HE3	1.35	1.07
1:B:527[A]:MET:HE3	1:H:146:LYS:HE3	1.39	1.05
1:A:527[A]:MET:HE3	1:B:146:LYS:HE3	1.42	0.99
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:D:527[A]:MET:HE3	1:F:146:LYS:HE3	1.49	0.92
1:G:468:TRP:HE1	1:G:502:ASN:HD22	1.16	0.91
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:G:480:TRP:CB	1:G:482:THR:HG22	2.02	0.89
1:B:45:ASN:OD1	1:B:418:TYR:OH	1.89	0.89
1:A:67:ASN:HD22	1:C:550:ASP:H	1.18	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:G:199:MET:HE2	1:G:279:TYR:HD1	1.46	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:H:443:ALA:HB1	1:H:444:THR:CB	2.11	0.80
1:C:380:ASP:OD2	1:H:563:HIS:HE1	1.63	0.80
1:G:199:MET:HE2	1:G:279:TYR:CD1	2.16	0.80
1:H:352:ASN:HB3	1:H:376[A]:MET:HE1	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:95:ALA:H	1:C:98:GLN:HE21	1.28	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: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:D:482:THR:HG22	4:D:2459:HOH:O	1.85	0.75
1:A:146:LYS:HE3	1:C:527[A]:MET:CE	2.14	0.75
1:D:48:LYS:NZ	1:D:420:GLY:O	2.19	0.75
1:G:199:MET:CE	1:G:279:TYR:HD1	2.00	0.74
1:G:48:LYS:NZ	1:G:420:GLY:O	2.20	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:B:527[A]:MET:CE	1:H:146:LYS:HE3	2.16	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: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:H:352:ASN:CB	1:H:376[A]:MET:CE	2.75	0.65
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: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:D:527[A]:MET:HE2	1:F:147:LEU:HD21	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:LEU:HD13	4:D:2122:HOH:O	1.99	0.62
1:D:527[A]:MET:CE	1:F:147:LEU:HD21	2.30	0.61
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: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
1:A:527[A]:MET:HE2	1:B:147:LEU:HD21	1.83	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:G:199:MET:CE	1:G:279:TYR:CD1	2.80	0.59
1:A:147:LEU:HD21	1:C:527[A]:MET:HE2	1.86	0.58
1:D:519[A]:GLN:NE2	4:D:2447:HOH:O	2.37	0.58
1:D:482:THR:HG21	4:D:2240:HOH:O	2.04	0.57
1:A:147:LEU:HD21	1:C:527[A]:MET:CE	2.35	0.57
1:A:527[A]:MET:CE	1:B:147:LEU:HD21	2.35	0.57
1:G:184:LEU:HG	1:G:185[A]:MET:CE	2.35	0.56
1:C:380:ASP:OD2	1:H:563:HIS:CE1	2.53	0.56
1:B:443:ALA:O	1:B:447:GLU:CB	2.54	0.56
1:F:264:ASP:O	1:F:268:VAL:HG12	2.05	0.56
1:H:373:PRO:HB2	1:H:376[A]:MET:HE2	1.87	0.56
1:B:527[A]:MET:CE	1:H:147:LEU:HD21	2.35	0.56
1:E:455:ARG:NH2	1:E:485:GLU:O	2.39	0.56
1:G:184:LEU:HG	1:G:185[A]:MET:HE3	1.88	0.55
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:H:352:ASN:CB	1:H:376[A]:MET:HE3	2.35	0.55
1:B:527[A]:MET:HE2	1:H:147:LEU:HD21	1.88	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:525[A]:LYS:NZ	4:B:2386:HOH:O	2.21	0.54
1:H:455:ARG:NH2	1:H:485:GLU:O	2.40	0.54
1:F:213:ARG:HH22	1:F:220:GLN:HE22	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:GLN:HB2	4:G:2027:HOH:O	2.07	0.53
1:H:352:ASN:HB3	1:H:376[A]:MET:HE3	1.89	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:384:TYR:CD1	1:B:385:PRO:HA	2.44	0.53
1:B:292:LEU:HB2	1:B:295:GLN:HE21	1.72	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:D:384:TYR:CD1	1:D:385:PRO:HA	2.45	0.52
1:A:482:THR:HG21	4:A:2145:HOH:O	2.08	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: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:G:384:TYR:CD1	1:G:385:PRO:HA	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
4:A:2119:HOH:O	1:C:525:LYS:HE3	2.11	0.50
1:H:373:PRO:HB2	1:H:376[A]:MET:CE	2.42	0.49
1:G:185[A]:MET:HE2	1:G:188:LEU:HD12	1.92	0.49
1:E:340[A]:ARG:NH2	4:E:2333:HOH:O	2.25	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: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:A:415:ARG:CZ	4:A:2272:HOH:O	2.60	0.48
1:E:386:LEU:CD1	4:E:2102:HOH:O	2.54	0.48
1:B:229:ASP:O	1:B:233:GLN:HG3	2.13	0.48
1:A:146:LYS:HG3	1:C:527[A]:MET:HE1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:533:GLU:OE2	1:H:563:HIS:HD2	1.97	0.47
1:F:213:ARG:HH22	1:F:220:GLN:NE2	2.12	0.47
1:G:443:ALA:O	1:G:444:THR:C	2.52	0.47
1:H:240:GLY:CA	1:H:244:GLN:HE21	2.28	0.47
1:H:136:ASN:HD22	1:H:208:THR:HA	1.80	0.47
1:F:208:THR:OG1	1:F:255:HIS:HE1	1.98	0.47
1:F:136:ASN:HD22	1:F:208:THR:HA	1.80	0.46
1:A:527[A]:MET:HE1	1:B:146:LYS:HG3	1.96	0.46
1:C:232:ILE:O	1:C:235:LEU:O	2.32	0.46
1:E:183:GLU:HG3	4:E:2191:HOH:O	2.13	0.46
1:A:548:ASN:HB3	1:B:140:TYR:CZ	2.50	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:E:241:THR:H	1:E:244:GLN:NE2	2.14	0.46
1:C:140:TYR:CZ	1:H:548:ASN:HB3	2.51	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:443:ALA:C	1:G:444:THR:O	2.55	0.45
1:H:241:THR:H	1:H:244:GLN:NE2	2.15	0.45
1:E:241:THR:O	1:E:245:VAL:HG13	2.17	0.45
1:H:48:LYS:CE	1:H:418:TYR:O	2.62	0.44
1:B:530[B]:ARG:NH2	4:B:2397:HOH:O	2.46	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:524:LYS:NZ	4:A:2330:HOH:O	2.49	0.44
1:B:169:LEU:HD13	1:B:219:ALA:HA	1.98	0.44
1:A:232:ILE:O	1:A:235:LEU:O	2.35	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:G:185[A]:MET:HA	1:G:185[A]:MET:HE2	1.98	0.43
1:D:527[A]:MET:HE1	1:F:146:LYS:HG3	2.01	0.43
1:C:241:THR:O	1:C:245:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:241:THR:O	1:B:245:VAL:HG13	2.18	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
1:F:405:LEU:HD11	1:F:509:TYR:HB2	2.01	0.43
1:F:241:THR:O	1:F:245:VAL:HG13	2.18	0.43
1:B:527[A]:MET:HE1	1:H:146:LYS:HG3	2.01	0.42
1:F:169:LEU:HD13	1:F:219:ALA:HA	2.01	0.42
1:E:41:GLU:HA	1:E:277:PRO:HG3	2.01	0.42
1:F:136:ASN:ND2	1:F:209:TYR:H	2.18	0.42
1:A:361:PHE:CD2	1:A:493:GLY:HA3	2.55	0.42
1:H:37:ALA:CB	1:H:38:PRO:CD	2.94	0.42
1:D:241:THR:O	1:D:245:VAL:HG13	2.19	0.42
1:C:169:LEU:HD13	1:C:219:ALA:HA	2.01	0.42
1:F:41:GLU:HA	1:F:277:PRO:HG3	2.01	0.42
1:F:67:ASN:ND2	1:F:134:LYS:HZ2	2.17	0.42
1:A:169:LEU:HD13	1:A:219:ALA:HA	2.01	0.42
1:B:559:THR:HG22	4:B:2209:HOH:O	2.20	0.42
1:H:292:LEU:HB3	4:H:2212:HOH:O	2.20	0.42
1:E:443:ALA:O	1:E:444:THR:CB	2.68	0.42
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:E:140:TYR:CZ	1:G:548:ASN:HB3	2.54	0.41
1:A:229:ASP:CB	4:A:2159:HOH:O	2.67	0.41
1:F:508:ALA:HB3	1:F:558:PHE:CD1	2.55	0.41
1:F:421:GLN:N	4:F:2337:HOH:O	2.41	0.41
1:D:169:LEU:HD13	1:D:219:ALA:HA	2.03	0.41
1:A:76:LYS:HD3	4:A:2023:HOH:O	2.20	0.41
1:H:352:ASN:CB	1:H:376[A]:MET:HE1	2.38	0.41
1:E:508:ALA:HB3	1:E:558:PHE:CD1	2.56	0.41
1:C:508:ALA:HB3	1:C:558:PHE:CD1	2.56	0.41
1:A:99:ILE:O	1:A:106:PHE:HA	2.21	0.41
1:H:374:PHE:O	1:H:376[A]:MET:HE1	2.21	0.41
1:E:44:SER:OG	1:E:49:HIS:HD2	2.03	0.41
1:E:390:VAL:O	1:E:395:THR:HG21	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ILE:O	1:C:106:PHE:HA	2.21	0.41
1:F:444:THR:CB	1:F:445:PRO:O	2.69	0.40
1:B:482:THR:HA	1:B:483:PRO:HD3	1.96	0.40
1:H:386:LEU:HA	4:H:2270:HOH:O	2.20	0.40
1:G:44:SER:OG	1:G:49:HIS:HD2	2.03	0.40
1:D:235:LEU:O	1:D:237:LEU:HD13	2.21	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:140:TYR:CZ	1:E:548:ASN:HB3	2.56	0.40
1:H:44:SER:OG	1:H:49:HIS:HD2	2.04	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

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	539/540 (100%)	521 (97%)	18 (3%)	0	100	100
1	B	540/540 (100%)	521 (96%)	15 (3%)	4 (1%)	26	11
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%)	52	35
1	F	541/540 (100%)	521 (96%)	19 (4%)	1 (0%)	52	35
1	G	542/540 (100%)	523 (96%)	16 (3%)	3 (1%)	30	14
1	H	541/540 (100%)	519 (96%)	18 (3%)	4 (1%)	26	11
All	All	4329/4320 (100%)	4177 (96%)	139 (3%)	13 (0%)	46	29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	444	THR
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%)	416 (98%)	10 (2%)	58	42
1	B	428/452 (95%)	416 (97%)	12 (3%)	51	35
1	C	428/452 (95%)	415 (97%)	13 (3%)	48	31
1	D	435/452 (96%)	422 (97%)	13 (3%)	48	31
1	E	428/452 (95%)	412 (96%)	16 (4%)	41	23
1	F	433/452 (96%)	421 (97%)	12 (3%)	51	35
1	G	433/452 (96%)	417 (96%)	16 (4%)	41	23
1	H	417/452 (92%)	403 (97%)	14 (3%)	44	26
All	All	3428/3616 (95%)	3322 (97%)	106 (3%)	50	30

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	235	LEU
1	A	245	VAL

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Mol	Chain	Res	Type
1	A	292	LEU
1	A	354	GLN
1	A	390	VAL
1	A	429	LEU
1	A	440	ASN
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	354	GLN
1	B	390	VAL
1	B	429	LEU
1	B	482	THR
1	B	537	GLU
1	C	45	ASN
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	354	GLN
1	C	390	VAL
1	C	408	PRO
1	C	429	LEU
1	C	482	THR
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	354	GLN
1	D	390	VAL
1	D	429	LEU
1	D	482	THR

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Mol	Chain	Res	Type
1	D	519[A]	GLN
1	D	519[B]	GLN
1	D	537	GLU
1	E	82	MET
1	E	136	ASN
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	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	135	ASN
1	F	136	ASN
1	F	235	LEU
1	F	237	LEU
1	F	245	VAL
1	F	268	VAL
1	F	292	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
1	G	432	THR

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Mol	Chain	Res	Type
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	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	429	LEU
1	H	462	GLN
1	H	482	THR
1	H	500[A]	ASP
1	H	500[B]	ASP
1	H	537	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	98	GLN
1	A	220	GLN
1	A	354	GLN
1	A	440	ASN
1	A	451	HIS
1	A	462	GLN
1	B	67	ASN
1	B	98	GLN
1	B	120	GLN
1	B	172	ASN
1	B	295	GLN
1	B	354	GLN
1	B	451	HIS
1	B	462	GLN
1	C	45	ASN
1	C	67	ASN
1	C	98	GLN
1	C	172	ASN

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Mol	Chain	Res	Type
1	C	354	GLN
1	C	451	HIS
1	C	462	GLN
1	D	67	ASN
1	D	98	GLN
1	D	289	ASN
1	D	295	GLN
1	D	354	GLN
1	D	451	HIS
1	D	462	GLN
1	E	49	HIS
1	E	67	ASN
1	E	171	GLN
1	E	244	GLN
1	E	487	ASN
1	E	502	ASN
1	E	551	GLN
1	F	49	HIS
1	F	67	ASN
1	F	135	ASN
1	F	136	ASN
1	F	220	GLN
1	F	224	ASN
1	F	255	HIS
1	F	502	ASN
1	G	49	HIS
1	G	64	GLN
1	G	67	ASN
1	G	224	ASN
1	G	244	GLN
1	G	401	GLN
1	G	502	ASN
1	H	45	ASN
1	H	46	ASN
1	H	49	HIS
1	H	136	ASN
1	H	244	GLN
1	H	502	ASN
1	H	563	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	1,3,3	1.92	0	0,3,3	0.00	-
3	ACT	D	604[A]	-	1,3,3	2.06	1 (100%)	0,3,3	0.00	-
3	ACT	D	604[B]	-	1,3,3	1.44	0	0,3,3	0.00	-
3	ACT	H	601	-	1,3,3	0.93	0	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	D	603	-	-	0/0/0/0	0/0/0/0
3	ACT	D	604[A]	-	-	0/0/0/0	0/0/0/0
3	ACT	D	604[B]	-	-	0/0/0/0	0/0/0/0
3	ACT	H	601	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	604[A]	ACT	CH3-C	2.06	1.51	1.48

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%)	-0.01	24 (4%)	37	31	21, 31, 60, 73	0
1	B	539/540 (99%)	-0.07	25 (4%)	36	30	21, 29, 57, 100	0
1	C	539/540 (99%)	-0.14	19 (3%)	48	42	19, 28, 60, 96	0
1	D	539/540 (99%)	-0.26	9 (1%)	73	69	16, 24, 48, 74	0
1	E	539/540 (99%)	-0.24	6 (1%)	82	80	17, 25, 46, 76	0
1	F	539/540 (99%)	-0.18	12 (2%)	65	60	17, 26, 52, 94	0
1	G	540/540 (100%)	-0.12	15 (2%)	56	51	18, 27, 54, 102	0
1	H	539/540 (99%)	-0.08	23 (4%)	39	32	21, 29, 58, 104	0
All	All	4313/4320 (99%)	-0.14	133 (3%)	52	47	16, 27, 55, 104	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	438	ILE	7.4
1	H	441	ALA	6.6
1	G	438	ILE	6.4
1	C	439	TRP	6.3
1	B	443	ALA	6.3
1	C	441	ALA	6.1
1	F	441	ALA	6.0
1	A	441	ALA	5.9
1	G	444	THR	5.4
1	B	440	ASN	5.3
1	H	438	ILE	5.2
1	G	445	PRO	5.1
1	G	435	THR	5.1
1	A	438	ILE	5.0
1	A	521	LEU	4.6
1	B	441	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	434	GLU	4.4
1	H	439	TRP	4.4
1	G	439	TRP	4.3
1	H	442	GLU	4.3
1	F	440	ASN	4.2
1	A	237	LEU	4.2
1	F	442	GLU	4.1
1	H	443	ALA	4.0
1	A	435	THR	4.0
1	B	436	GLN	3.9
1	B	521	LEU	3.9
1	H	521	LEU	3.9
1	C	386[A]	LEU	3.8
1	B	433	THR	3.8
1	B	439	TRP	3.8
1	E	443	ALA	3.7
1	C	438	ILE	3.6
1	B	444	THR	3.6
1	B	432	THR	3.6
1	H	440	ASN	3.6
1	A	443	ALA	3.5
1	F	443	ALA	3.4
1	A	439	TRP	3.4
1	F	439	TRP	3.3
1	A	522	ALA	3.3
1	H	447	GLU	3.3
1	G	441	ALA	3.2
1	A	523	GLY	3.2
1	C	449	GLU	3.2
1	F	445	PRO	3.1
1	A	241	THR	3.1
1	A	46	ASN	3.1
1	A	239	PRO	3.1
1	B	445	PRO	3.0
1	H	432	THR	3.0
1	D	443	ALA	3.0
1	H	522	ALA	3.0
1	G	442	GLU	2.9
1	C	443	ALA	2.9
1	F	575	GLN	2.9
1	H	523	GLY	2.9
1	C	440	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	441	ALA	2.9
1	D	434	GLU	2.9
1	B	451	HIS	2.9
1	H	241	THR	2.9
1	F	523	GLY	2.9
1	C	445	PRO	2.8
1	H	456	ALA	2.8
1	A	240	GLY	2.8
1	G	443	ALA	2.8
1	B	435	THR	2.8
1	B	442	GLU	2.8
1	B	446	GLU	2.8
1	D	442	GLU	2.7
1	C	447	GLU	2.7
1	C	451	HIS	2.7
1	E	441	ALA	2.7
1	H	433	THR	2.7
1	A	244	GLN	2.7
1	G	521	LEU	2.7
1	C	520	GLU	2.6
1	H	444	THR	2.6
1	B	437	LYS	2.6
1	E	440	ASN	2.6
1	C	432	THR	2.6
1	A	449	GLU	2.6
1	D	439	TRP	2.5
1	D	444	THR	2.6
1	C	450	GLN	2.5
1	A	575	GLN	2.5
1	G	434	GLU	2.5
1	H	240	GLY	2.5
1	E	438	ILE	2.5
1	G	436	GLN	2.5
1	H	435	THR	2.5
1	F	434	GLU	2.4
1	B	523	GLY	2.4
1	B	240	GLY	2.4
1	B	479	PHE	2.4
1	B	537	GLU	2.4
1	A	440	ASN	2.3
1	D	436	GLN	2.3
1	C	442	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	440	ASN	2.3
1	D	522	ALA	2.3
1	C	433	THR	2.3
1	A	247	GLY	2.3
1	H	386	LEU	2.2
1	G	480	TRP	2.2
1	H	450	GLN	2.2
1	A	236	GLN	2.2
1	C	446	GLU	2.2
1	F	435	THR	2.2
1	A	217	PRO	2.2
1	A	442	GLU	2.2
1	B	452	LYS	2.2
1	G	437	LYS	2.2
1	A	246	PHE	2.2
1	G	450	GLN	2.2
1	H	348	ALA	2.1
1	B	522	ALA	2.1
1	H	446	GLU	2.1
1	F	229	ASP	2.1
1	B	238	LYS	2.1
1	C	240	GLY	2.1
1	C	523	GLY	2.1
1	E	240	GLY	2.1
1	A	432	THR	2.1
1	F	239	PRO	2.1
1	H	437	LYS	2.0
1	G	241	THR	2.0
1	A	451	HIS	2.0
1	C	435	THR	2.0
1	B	239	PRO	2.0
1	E	446	GLU	2.0
1	H	449	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NA	D	601	1/1	0.97	0.16	3.33	36,36,36,36	0
2	NA	E	601	1/1	0.98	0.08	0.02	26,26,26,26	0
2	NA	A	600	1/1	0.95	0.13	-0.27	37,37,37,37	0
2	NA	G	602	1/1	0.99	0.10	-0.44	23,23,23,23	0
2	NA	B	600	1/1	0.95	0.12	-0.69	35,35,35,35	0
2	NA	F	602	1/1	0.99	0.06	-1.01	24,24,24,24	0
2	NA	D	602	1/1	0.99	0.06	-1.15	27,27,27,27	0
3	ACT	D	604[B]	4/4	0.80	0.28	-	46,47,48,49	4
2	NA	D	600	1/1	0.99	0.09	-	25,25,25,25	0
3	ACT	D	604[A]	4/4	0.80	0.28	-	40,42,43,45	4
2	NA	F	601	1/1	0.96	0.11	-	40,40,40,40	0
2	NA	H	600	1/1	0.96	0.07	-	36,36,36,36	0
2	NA	G	601	1/1	0.93	0.14	-	34,34,34,34	0
2	NA	C	600	1/1	0.90	0.16	-	46,46,46,46	0
3	ACT	D	603	4/4	0.89	0.20	-	36,37,38,39	0
2	NA	E	602	1/1	0.99	0.04	-	29,29,29,29	0
2	NA	C	601	1/1	0.91	0.10	-	50,50,50,50	0
2	NA	G	600	1/1	0.95	0.06	-	41,41,41,41	0
2	NA	E	600	1/1	0.99	0.07	-	26,26,26,26	0
2	NA	F	600	1/1	0.89	0.09	-	43,43,43,43	0
3	ACT	H	601	4/4	0.92	0.20	-	49,51,52,52	0

6.5 Other polymers

There are no such residues in this entry.