



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:22 AM UTC

PDB ID : 8OZU / pdb_00008ozu
Title : Fucosidase crystal structure
Authors : Gallego del Sol, F.; Marina, A.
Deposited on : 2023-05-09
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

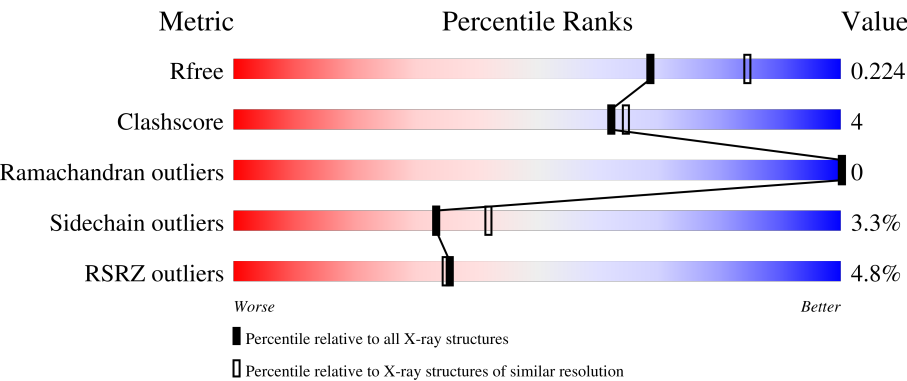
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	414	9% 89% 7% ..
1	B	414	9% 90% 7% ..
1	C	414	9% 89% 9% ..
1	D	414	9% 88% 9% ..
1	E	414	9% 87% 9% ..

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Mol	Chain	Length	Quality of chain
1	F	414	10% 85% 11% ..
1	G	414	% 85% 11% ..
1	H	414	4% 84% 12% ..

2 Entry composition

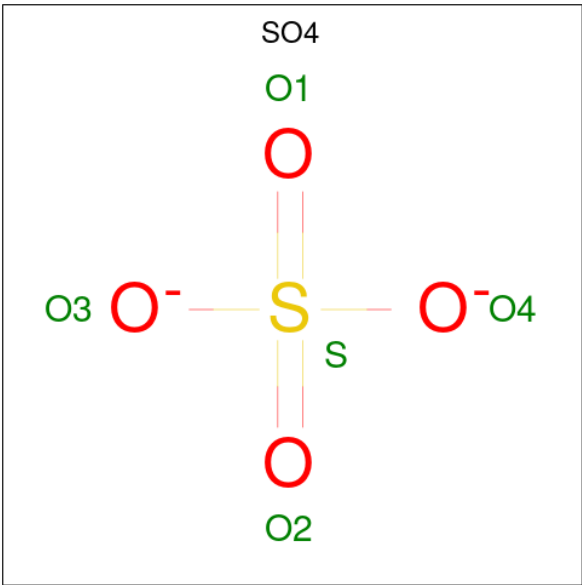
There are 3 unique types of molecules in this entry. The entry contains 52241 atoms, of which 25155 are hydrogens and 0 are deuteriums.

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 Alpha-L-fucosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	407	Total	C	H	N	O	S	103	0	0
			6406	2096	3148	554	599	9			
1	B	406	Total	C	H	N	O	S	102	0	0
			6381	2086	3138	553	595	9			
1	C	408	Total	C	H	N	O	S	103	1	0
			6434	2104	3163	558	600	9			
1	D	406	Total	C	H	N	O	S	101	0	0
			6388	2092	3138	553	596	9			
1	E	405	Total	C	H	N	O	S	102	0	0
			6385	2090	3138	552	596	9			
1	F	405	Total	C	H	N	O	S	102	0	0
			6385	2090	3138	552	596	9			
1	G	408	Total	C	H	N	O	S	102	0	0
			6418	2100	3153	556	600	9			
1	H	406	Total	C	H	N	O	S	103	0	0
			6390	2091	3139	553	598	9			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	C	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	D	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	E	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

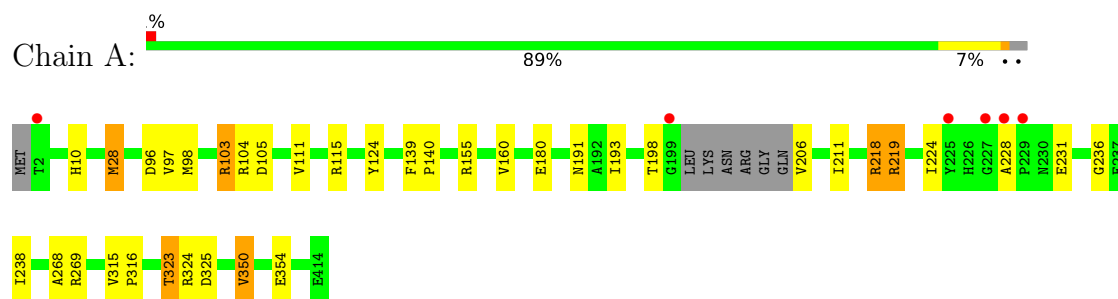
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	160	Total	O	0	0
			160	160		
3	B	207	Total	O	0	0
			207	207		
3	C	225	Total	O	0	0
			225	225		
3	D	59	Total	O	0	0
			59	59		
3	E	21	Total	O	0	0
			21	21		
3	F	30	Total	O	0	0
			30	30		
3	G	203	Total	O	0	0
			203	203		
3	H	34	Total	O	0	0
			34	34		

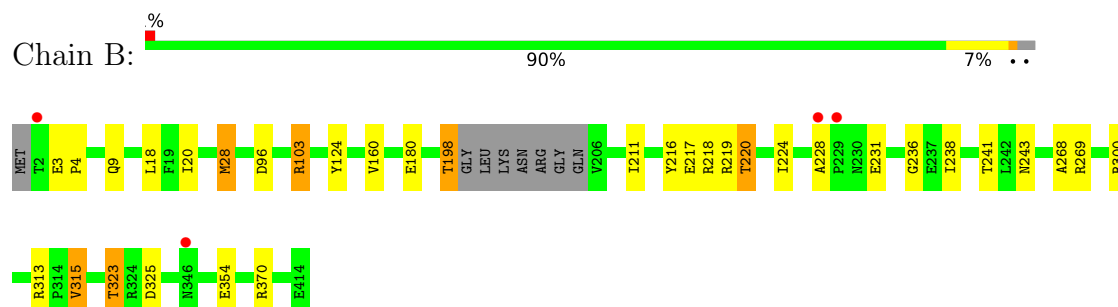
3 Residue-property plots [i](#)

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.

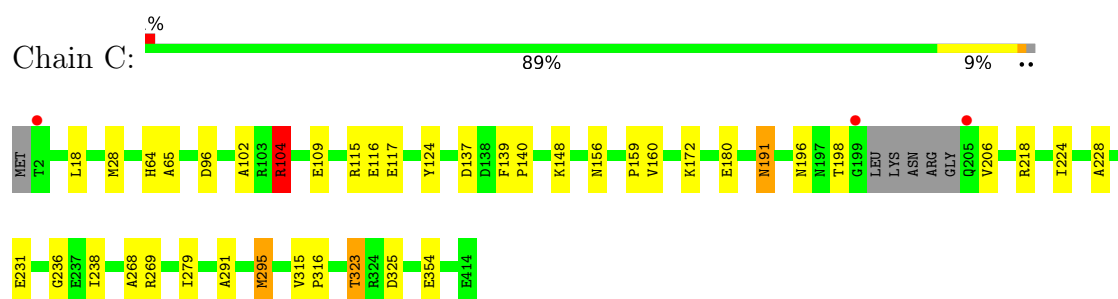
• Molecule 1: Alpha-L-fucosidase



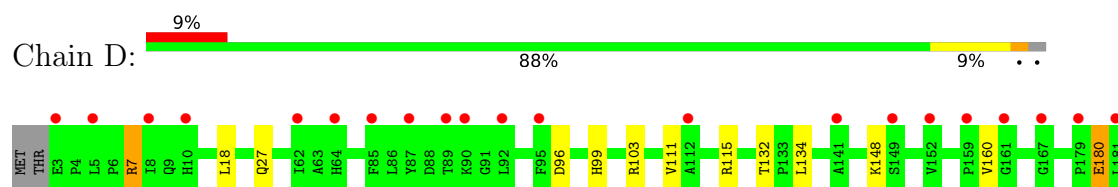
• Molecule 1: Alpha-L-fucosidase

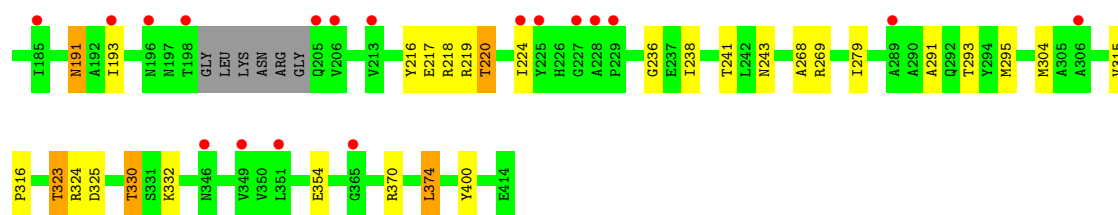


• Molecule 1: Alpha-L-fucosidase

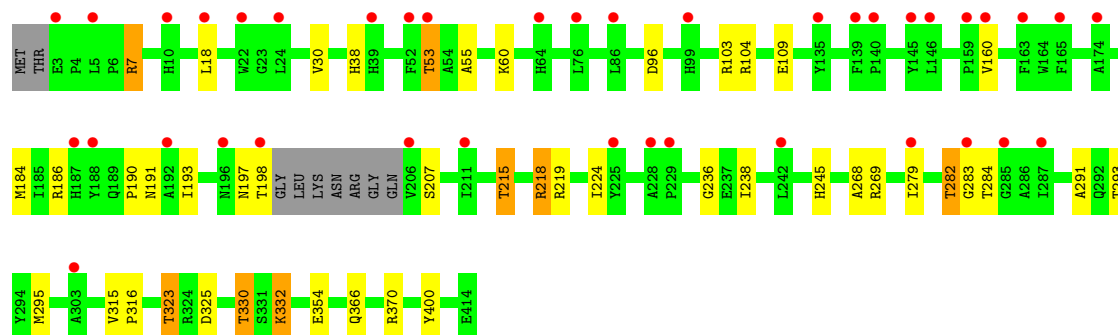
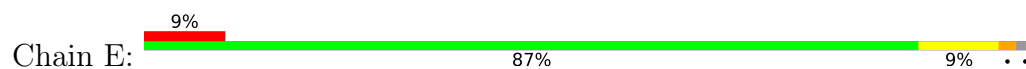


• Molecule 1: Alpha-L-fucosidase

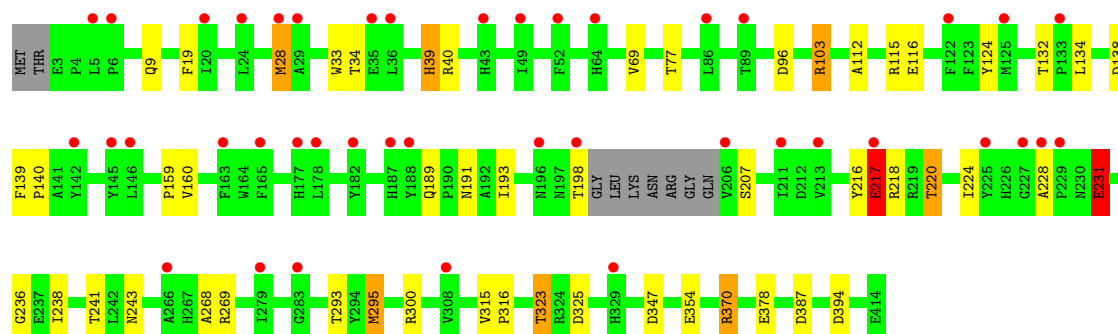
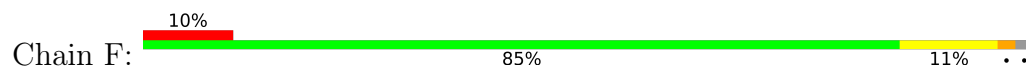




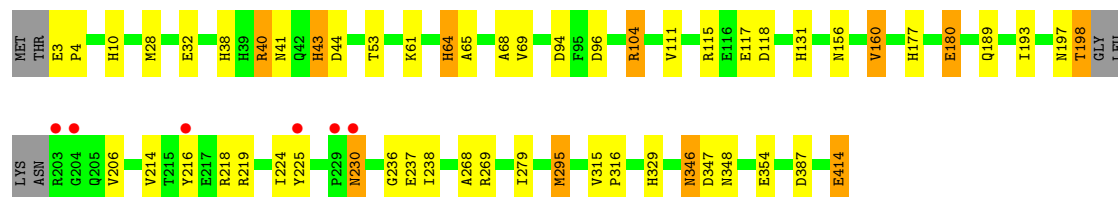
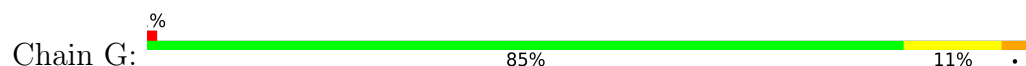
● Molecule 1: Alpha-L-fucosidase



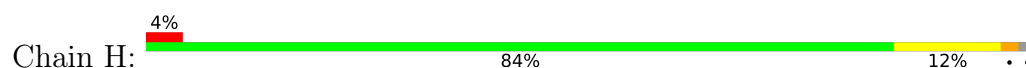
● Molecule 1: Alpha-L-fucosidase

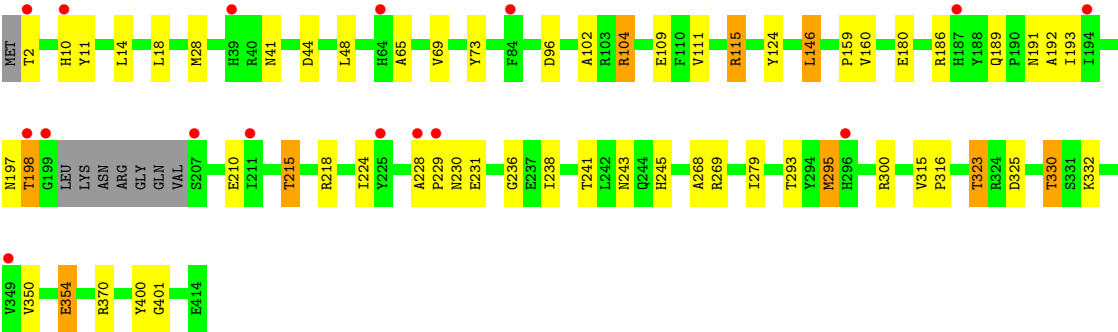


● Molecule 1: Alpha-L-fucosidase



● Molecule 1: Alpha-L-fucosidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	308.10Å 81.17Å 194.24Å 90.00° 123.88° 90.00°	Depositor
Resolution (Å)	148.63 – 2.25 148.63 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (148.63-2.25) 100.0 (148.63-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.193 , 0.224 0.193 , 0.224	Depositor DCC
R_{free} test set	9501 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52241	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: SO4

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	0.90	0/3355	1.11	6/4578 (0.1%)
1	B	0.95	0/3339	1.12	8/4557 (0.2%)
1	C	1.03	2/3371 (0.1%)	1.18	9/4599 (0.2%)
1	D	0.71	0/3347	1.06	4/4567 (0.1%)
1	E	0.66	0/3344	1.02	3/4563 (0.1%)
1	F	0.69	0/3344	1.06	8/4563 (0.2%)
1	G	1.04	7/3362 (0.2%)	1.22	16/4587 (0.3%)
1	H	0.71	0/3348	1.04	5/4568 (0.1%)
All	All	0.85	9/26810 (0.0%)	1.10	59/36582 (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	5
1	B	0	4
1	C	0	2
1	D	0	4
1	E	0	4
1	F	0	3
1	G	0	3
1	H	0	5
All	All	0	30

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	43	HIS	CE1-NE2	6.96	1.39	1.32
1	G	96	ASP	CG-OD2	6.29	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	32	GLU	CD-OE1	5.99	1.36	1.25
1	C	180	GLU	CD-OE2	5.91	1.36	1.25
1	C	116	GLU	CD-OE2	5.37	1.35	1.25
1	G	38	HIS	CD2-NE2	5.30	1.43	1.37
1	G	237	GLU	CD-OE1	5.26	1.35	1.25
1	G	131	HIS	CD2-NE2	-5.21	1.32	1.37
1	G	329	HIS	CE1-NE2	5.00	1.37	1.32

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	414	GLU	CB-CG-CD	9.86	129.37	112.60
1	G	198	THR	CA-C-O	-8.06	107.09	120.80
1	C	295	MET	CG-SD-CE	-7.59	84.19	100.90
1	C	218	ARG	CB-CA-C	-7.38	98.55	110.79
1	G	387	ASP	CA-CB-CG	7.29	119.89	112.60
1	D	180	GLU	CB-CG-CD	7.22	124.87	112.60
1	F	39	HIS	N-CA-CB	6.96	122.00	111.70
1	D	218	ARG	CB-CA-C	-6.96	99.24	110.79
1	B	218	ARG	CB-CA-C	-6.92	99.30	110.79
1	C	96	ASP	CA-CB-CG	6.89	119.49	112.60
1	B	198	THR	CA-C-O	-6.85	109.16	120.80
1	G	96	ASP	CA-CB-CG	6.65	119.25	112.60
1	H	215	THR	CA-CB-OG1	6.64	119.56	109.60
1	F	217	GLU	CB-CG-CD	6.42	123.52	112.60
1	F	387	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	218	ARG	CB-CA-C	-6.37	100.21	110.79
1	F	217	GLU	N-CA-CB	6.33	119.28	110.17
1	B	96	ASP	CA-CB-CG	6.32	118.92	112.60
1	D	96	ASP	CA-CB-CG	6.29	118.89	112.60
1	D	191	ASN	CA-CB-CG	-6.20	106.40	112.60
1	H	96	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	219	ARG	CG-CD-NE	-6.14	98.48	112.00
1	G	118	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	103	ARG	CB-CG-CD	5.95	124.99	111.30
1	E	96	ASP	CA-CB-CG	5.93	118.53	112.60
1	G	197	ASN	CA-C-N	5.90	132.33	121.70
1	G	197	ASN	C-N-CA	5.90	132.33	121.70
1	A	96	ASP	CA-CB-CG	5.89	118.49	112.60
1	B	315	VAL	N-CA-CB	5.88	117.94	111.64
1	G	104	ARG	NE-CZ-NH1	-5.87	115.63	121.50
1	G	225	TYR	CA-CB-CG	5.82	124.38	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	MET	CG-SD-CE	-5.78	88.17	100.90
1	A	350	VAL	N-CA-CB	5.71	117.90	111.21
1	C	156	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	B	103	ARG	CB-CG-CD	5.59	124.17	111.30
1	C	191	ASN	CA-CB-CG	-5.59	107.01	112.60
1	F	231	GLU	CB-CG-CD	5.57	122.06	112.60
1	F	218	ARG	CB-CA-C	-5.52	101.63	110.79
1	F	19	PHE	CA-CB-CG	5.51	119.31	113.80
1	C	137	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	198	THR	CA-CB-OG1	-5.47	101.39	109.60
1	F	96	ASP	CA-CB-CG	5.47	118.07	112.60
1	G	206	VAL	N-CA-C	5.43	114.56	106.85
1	C	104	ARG	NE-CZ-NH1	5.40	126.90	121.50
1	E	218	ARG	CB-CA-C	-5.38	101.86	110.79
1	B	313	ARG	NE-CZ-NH2	5.37	124.04	119.20
1	C	196	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	G	346	ASN	CA-CB-CG	5.30	117.90	112.60
1	H	218	ARG	CB-CA-C	-5.29	100.85	110.63
1	H	354	GLU	CB-CA-C	-5.27	101.05	110.70
1	B	180	GLU	CB-CG-CD	5.25	121.52	112.60
1	G	64	HIS	CB-CG-CD2	-5.16	124.50	131.20
1	H	198	THR	CB-CA-C	5.15	119.48	109.33
1	E	282	THR	CA-CB-CG2	5.13	119.23	110.50
1	C	159	PRO	CB-CA-C	-5.13	105.18	111.64
1	G	156	ASN	OD1-CG-ND2	-5.11	117.50	122.60
1	G	94	ASP	CA-CB-CG	5.08	117.68	112.60
1	G	104	ARG	CG-CD-NE	-5.08	100.83	112.00
1	G	218	ARG	CB-CA-C	-5.07	101.26	110.63

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ARG	Sidechain
1	A	155	ARG	Sidechain
1	A	219	ARG	Sidechain
1	A	269	ARG	Sidechain
1	A	324	ARG	Sidechain
1	B	103	ARG	Sidechain
1	B	219	ARG	Sidechain
1	B	269	ARG	Sidechain
1	B	300	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	104	ARG	Sidechain
1	C	269	ARG	Sidechain
1	D	103	ARG	Sidechain
1	D	269	ARG	Sidechain
1	D	324	ARG	Sidechain
1	D	7	ARG	Sidechain
1	E	218	ARG	Sidechain
1	E	219	ARG	Sidechain
1	E	269	ARG	Sidechain
1	E	7	ARG	Sidechain
1	F	269	ARG	Sidechain
1	F	300	ARG	Sidechain
1	F	370	ARG	Sidechain
1	G	219	ARG	Sidechain
1	G	269	ARG	Sidechain
1	G	40	ARG	Sidechain
1	H	104	ARG	Sidechain
1	H	115	ARG	Sidechain
1	H	269	ARG	Sidechain
1	H	300	ARG	Sidechain
1	H	370	ARG	Sidechain

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	3258	3148	3125	21	0
1	B	3243	3138	3111	14	0
1	C	3271	3163	3140	20	0
1	D	3250	3138	3112	31	0
1	E	3247	3138	3115	40	0
1	F	3247	3138	3115	30	1
1	G	3265	3153	3128	27	0
1	H	3251	3139	3116	42	0
2	A	20	0	0	1	0
2	B	15	0	0	0	0
2	C	20	0	0	0	0
2	D	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	10	0	0	1	0
2	F	5	0	0	0	0
2	G	25	0	0	2	0
2	H	10	0	0	0	0
3	A	160	0	0	2	0
3	B	207	0	0	3	0
3	C	225	0	0	4	0
3	D	59	0	0	4	0
3	E	21	0	0	1	0
3	F	30	0	0	3	0
3	G	203	0	0	5	0
3	H	34	0	0	1	0
All	All	27086	25155	24962	211	1

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 (211) 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:B:217:GLU:O	1:B:220:THR:HG22	1.49	1.10
1:D:217:GLU:O	1:D:220:THR:HG22	1.49	1.09
1:E:53:THR:CG2	1:E:55:ALA:HB2	1.84	1.07
1:F:217:GLU:O	1:F:220:THR:HG23	1.68	0.92
1:H:197:ASN:OD1	1:H:215:THR:HG21	1.70	0.92
1:E:53:THR:HG21	1:E:55:ALA:HB2	1.56	0.86
1:C:206:VAL:HA	3:C:636:HOH:O	1.78	0.82
1:E:30:VAL:CG1	1:E:38:HIS:HE1	1.93	0.82
1:E:30:VAL:HG12	1:E:38:HIS:HE1	1.45	0.82
1:E:53:THR:HG22	1:E:55:ALA:H	1.47	0.79
1:E:53:THR:HG22	1:E:55:ALA:N	1.97	0.79
1:A:97:VAL:HG13	1:A:98:MET:HE2	1.63	0.79
1:C:148:LYS:HE2	3:C:687:HOH:O	1.83	0.78
1:A:28:MET:CE	1:G:53:THR:HG22	2.14	0.78
1:F:34:THR:OG1	1:F:40:ARG:NH1	2.17	0.78
1:A:323:THR:HG21	3:A:632:HOH:O	1.83	0.77
1:G:68:ALA:HB3	3:G:697:HOH:O	1.83	0.77
1:E:30:VAL:CG1	1:E:38:HIS:CE1	2.68	0.77
1:D:27:GLN:HG3	3:D:636:HOH:O	1.84	0.76
1:F:378:GLU:OE1	3:F:601:HOH:O	2.04	0.75
1:A:28:MET:HE1	1:G:53:THR:HG22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:503:SO4:O1	3:G:601:HOH:O	2.04	0.74
1:D:304:MET:SD	1:D:374:LEU:CD1	2.75	0.74
1:E:323:THR:HG21	3:E:608:HOH:O	1.88	0.73
1:H:11:TYR:HA	1:H:14:LEU:HD13	1.70	0.72
1:A:98:MET:HE1	1:A:104:ARG:C	2.14	0.72
1:D:217:GLU:O	1:D:220:THR:CG2	2.35	0.72
1:H:41:ASN:HD22	1:H:44:ASP:H	1.33	0.72
1:C:104:ARG:HD2	1:C:109:GLU:OE2	1.91	0.71
1:H:323:THR:HG21	3:H:604:HOH:O	1.88	0.71
1:E:53:THR:CG2	1:E:55:ALA:CB	2.68	0.69
1:H:186:ARG:HD2	1:H:210:GLU:OE1	1.93	0.68
1:H:186:ARG:NH2	1:H:192:ALA:O	2.27	0.68
1:B:217:GLU:O	1:B:220:THR:CG2	2.37	0.67
1:E:30:VAL:HG12	1:E:30:VAL:O	1.94	0.67
1:E:18:LEU:HD21	1:E:295:MET:CE	2.25	0.67
1:F:216:TYR:HB3	1:F:220:THR:HG21	1.77	0.66
1:E:53:THR:HG22	1:E:55:ALA:HB2	1.76	0.66
1:H:11:TYR:HA	1:H:14:LEU:CD1	2.26	0.66
1:D:216:TYR:HB3	1:D:220:THR:HG21	1.78	0.65
1:A:98:MET:HE1	1:A:105:ASP:N	2.11	0.65
1:F:69:VAL:HB	1:F:295:MET:HG3	1.78	0.65
1:H:10:HIS:O	1:H:14:LEU:HD12	1.96	0.64
1:E:30:VAL:HG12	1:E:38:HIS:CE1	2.29	0.64
1:C:64:HIS:HE1	3:G:779:HOH:O	1.81	0.64
1:A:28:MET:CE	1:G:53:THR:CG2	2.76	0.64
1:E:245:HIS:NE2	1:H:400:TYR:O	2.32	0.63
1:D:323:THR:HG21	3:D:612:HOH:O	1.99	0.62
1:D:99:HIS:CE1	3:D:646:HOH:O	2.52	0.62
1:D:99:HIS:HE1	3:D:646:HOH:O	1.82	0.61
1:H:350:VAL:HG13	1:H:354:GLU:OE2	2.01	0.61
1:D:330:THR:HG22	1:D:332:LYS:H	1.65	0.61
1:D:304:MET:SD	1:D:374:LEU:HD11	2.42	0.60
1:E:330:THR:HG22	1:E:332:LYS:H	1.65	0.60
1:H:330:THR:HG22	1:H:332:LYS:H	1.66	0.60
1:H:69:VAL:HB	1:H:295:MET:HG3	1.83	0.60
1:H:2:THR:HB	1:H:229:PRO:O	2.02	0.59
1:B:323:THR:HG21	3:B:667:HOH:O	2.02	0.59
1:E:197:ASN:OD1	1:E:215:THR:HG21	2.02	0.59
1:G:69:VAL:HB	1:G:295:MET:HG3	1.83	0.59
1:E:53:THR:HG22	1:E:55:ALA:CB	2.31	0.59
1:A:228:ALA:HB3	1:A:231:GLU:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:VAL:CG1	1:E:30:VAL:O	2.51	0.58
1:E:186:ARG:NH1	1:E:190:PRO:O	2.36	0.58
1:E:7:ARG:NH1	1:E:186:ARG:NH1	2.51	0.58
1:E:293:THR:HG21	1:H:293:THR:OG1	2.03	0.58
1:F:132:THR:HG22	1:F:134:LEU:H	1.68	0.58
1:E:30:VAL:HG13	1:H:401:GLY:HA3	1.85	0.58
1:G:160:VAL:H	1:G:189:GLN:NE2	2.02	0.57
1:C:65:ALA:HB1	1:C:295:MET:HE3	1.85	0.57
1:E:18:LEU:HD21	1:E:295:MET:HE1	1.85	0.57
1:D:132:THR:HG22	1:D:134:LEU:H	1.70	0.57
1:E:400:TYR:O	1:H:245:HIS:NE2	2.37	0.57
1:C:148:LYS:CE	3:C:687:HOH:O	2.48	0.57
1:E:291:ALA:O	1:E:295:MET:HG3	2.04	0.57
1:D:293:THR:HG21	1:F:293:THR:OG1	2.03	0.57
1:G:224:ILE:HD13	1:G:236:GLY:HA3	1.86	0.57
1:F:217:GLU:O	1:F:220:THR:CG2	2.46	0.57
1:E:104:ARG:HD2	1:E:109:GLU:OE2	2.05	0.56
1:A:28:MET:HA	1:A:28:MET:HE2	1.87	0.56
1:A:315:VAL:HG22	1:A:316:PRO:HD2	1.88	0.56
1:D:293:THR:HG21	1:F:293:THR:CG2	2.35	0.56
1:B:18:LEU:HD23	1:B:20:ILE:HD11	1.86	0.56
1:G:214:VAL:HG23	1:G:216:TYR:CE1	2.41	0.56
1:H:65:ALA:HB1	1:H:295:MET:HE3	1.86	0.56
1:D:293:THR:CG2	1:F:293:THR:HG21	2.35	0.56
1:H:104:ARG:HD2	1:H:109:GLU:OE2	2.05	0.56
1:B:370:ARG:NH1	3:B:607:HOH:O	2.39	0.55
1:H:228:ALA:HB3	1:H:231:GLU:HG3	1.87	0.55
1:H:18:LEU:HD22	1:H:279:ILE:HD11	1.88	0.55
1:G:224:ILE:CD1	1:G:236:GLY:HA3	2.37	0.55
1:G:238:ILE:HD11	1:G:268:ALA:HB2	1.90	0.54
1:C:291:ALA:O	1:C:295:MET:HG2	2.07	0.54
1:H:115:ARG:HH12	1:H:159:PRO:HD2	1.74	0.53
1:C:323:THR:HG21	3:C:701:HOH:O	2.08	0.53
1:A:111:VAL:O	1:A:115:ARG:HG3	2.09	0.52
1:B:224:ILE:HD13	1:B:236:GLY:HA3	1.90	0.52
1:D:293:THR:OG1	1:F:293:THR:HG21	2.10	0.52
1:B:323:THR:HG23	1:B:325:ASP:H	1.75	0.52
1:D:18:LEU:HD22	1:D:279:ILE:HD11	1.90	0.52
1:E:30:VAL:HG11	1:E:38:HIS:CE1	2.43	0.52
1:F:323:THR:HG21	3:F:615:HOH:O	2.08	0.52
1:G:41:ASN:HD21	1:G:43:HIS:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:LEU:CD2	1:H:73:TYR:CD1	2.93	0.52
1:H:159:PRO:HA	1:H:189:GLN:NE2	2.25	0.52
1:F:112:ALA:O	1:F:116:GLU:HG3	2.10	0.51
1:D:18:LEU:HD11	1:D:295:MET:HE1	1.93	0.51
1:H:14:LEU:HD23	1:H:73:TYR:CD1	2.46	0.51
1:G:10:HIS:HB2	3:G:770:HOH:O	2.11	0.50
1:A:323:THR:HG23	1:A:325:ASP:H	1.75	0.50
1:H:111:VAL:O	1:H:115:ARG:HG3	2.11	0.50
1:F:103:ARG:HH21	1:F:103:ARG:HB3	1.76	0.50
1:G:65:ALA:HB1	1:G:295:MET:HE3	1.94	0.50
1:D:291:ALA:O	1:D:295:MET:HG2	2.11	0.50
1:E:18:LEU:HD21	1:E:295:MET:HE3	1.94	0.50
1:F:159:PRO:HA	1:F:189:GLN:NE2	2.27	0.50
1:G:28:MET:HE1	1:G:40:ARG:HE	1.75	0.49
1:E:224:ILE:HD13	1:E:236:GLY:HA3	1.94	0.49
1:F:323:THR:HG23	1:F:325:ASP:H	1.76	0.49
1:A:224:ILE:HD13	1:A:236:GLY:HA3	1.95	0.49
1:C:224:ILE:HD13	1:C:236:GLY:HA3	1.94	0.49
1:C:238:ILE:HD11	1:C:268:ALA:HB2	1.95	0.49
1:D:323:THR:HG23	1:D:325:ASP:H	1.76	0.49
1:F:228:ALA:HB3	1:F:231:GLU:HG3	1.95	0.49
1:H:224:ILE:HD13	1:H:236:GLY:HA3	1.95	0.49
1:G:41:ASN:ND2	1:G:43:HIS:HB3	2.28	0.48
1:F:315:VAL:HG22	1:F:316:PRO:HD2	1.94	0.48
1:H:28:MET:HE2	1:H:48:LEU:HD11	1.96	0.48
1:E:315:VAL:HG22	1:E:316:PRO:HD2	1.95	0.48
1:B:211:ILE:HD13	3:B:722:HOH:O	2.13	0.48
1:B:216:TYR:HB3	1:B:220:THR:HG21	1.96	0.48
1:D:224:ILE:HD13	1:D:236:GLY:HA3	1.96	0.48
1:E:323:THR:HG23	1:E:325:ASP:H	1.77	0.48
1:G:111:VAL:O	1:G:115:ARG:HG3	2.12	0.48
1:H:323:THR:HG23	1:H:325:ASP:H	1.79	0.47
1:H:400:TYR:O	1:H:400:TYR:CD1	2.67	0.47
1:A:206:VAL:HG13	1:A:211:ILE:HG12	1.97	0.47
1:A:238:ILE:HD11	1:A:268:ALA:HB2	1.96	0.47
1:C:323:THR:HG23	1:C:325:ASP:H	1.79	0.47
1:D:7:ARG:HB3	1:D:191:ASN:OD1	2.15	0.47
1:E:400:TYR:O	1:E:400:TYR:CD1	2.68	0.47
1:H:14:LEU:CD2	1:H:73:TYR:HB3	2.45	0.47
1:B:228:ALA:HB3	1:B:231:GLU:HG3	1.97	0.47
1:G:279:ILE:HD13	1:G:295:MET:HE1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:ILE:HD11	1:D:268:ALA:HB2	1.97	0.46
1:H:146:LEU:C	1:H:146:LEU:HD13	2.40	0.46
1:E:366:GLN:NE2	2:E:502:SO4:O1	2.47	0.46
1:C:65:ALA:HB1	1:C:295:MET:CE	2.45	0.46
1:D:132:THR:HG22	1:D:134:LEU:HG	1.96	0.46
1:F:224:ILE:HD13	1:F:236:GLY:HA3	1.97	0.46
1:G:3:GLU:HG3	1:G:4:PRO:HD2	1.97	0.46
1:A:28:MET:HE3	1:G:53:THR:CG2	2.46	0.46
1:A:206:VAL:HG13	1:A:211:ILE:CG1	2.45	0.46
1:E:238:ILE:HD11	1:E:268:ALA:HB2	1.98	0.46
1:A:218:ARG:HD3	2:A:502:SO4:O2	2.17	0.45
1:D:293:THR:CG2	1:F:293:THR:CG2	2.95	0.45
1:B:238:ILE:HD11	1:B:268:ALA:HB2	1.97	0.45
1:H:104:ARG:HH11	1:H:109:GLU:CD	2.25	0.45
1:F:28:MET:HA	1:F:28:MET:HE2	1.99	0.45
1:G:160:VAL:H	1:G:189:GLN:HE22	1.65	0.45
1:H:238:ILE:HD11	1:H:268:ALA:HB2	1.98	0.45
1:H:315:VAL:HG22	1:H:316:PRO:HD2	1.99	0.44
1:E:282:THR:HG22	1:E:284:THR:H	1.82	0.44
1:H:115:ARG:NH1	1:H:159:PRO:HD2	2.32	0.44
1:G:41:ASN:HD22	1:G:44:ASP:H	1.64	0.44
1:F:241:THR:HG23	1:F:243:ASN:O	2.18	0.44
1:G:61:LYS:HG2	2:G:504:SO4:O1	2.18	0.44
1:B:124:TYR:C	1:B:124:TYR:CD1	2.96	0.44
1:F:115:ARG:NH1	1:F:159:PRO:HD2	2.33	0.44
1:F:132:THR:HG22	1:F:134:LEU:HG	2.00	0.43
1:D:18:LEU:HD22	1:D:279:ILE:CD1	2.47	0.43
1:G:230:ASN:HD22	1:G:230:ASN:HA	1.52	0.43
1:E:7:ARG:CZ	1:E:186:ARG:NH1	2.82	0.43
1:H:14:LEU:HD22	1:H:73:TYR:CD1	2.53	0.43
1:C:18:LEU:HD11	1:C:295:MET:HE1	1.99	0.43
1:D:304:MET:SD	1:D:374:LEU:HD13	2.57	0.43
1:A:139:PHE:N	1:A:140:PRO:CD	2.82	0.43
1:C:124:TYR:CD1	1:C:124:TYR:C	2.97	0.42
1:D:400:TYR:CZ	1:F:33:TRP:HB2	2.54	0.42
1:H:18:LEU:HD22	1:H:279:ILE:CD1	2.47	0.42
1:A:10:HIS:HB2	3:A:720:HOH:O	2.18	0.42
1:E:400:TYR:O	1:E:400:TYR:CG	2.72	0.42
1:F:394:ASP:OD1	3:F:602:HOH:O	2.21	0.42
1:G:315:VAL:HG22	1:G:316:PRO:HD2	2.01	0.42
1:C:139:PHE:N	1:C:140:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ARG:NH2	2:D:501:SO4:O2	2.53	0.42
1:H:102:ALA:O	1:H:104:ARG:HG3	2.20	0.42
1:A:124:TYR:CD1	1:A:124:TYR:C	2.98	0.42
1:H:400:TYR:O	1:H:400:TYR:CG	2.71	0.42
1:C:102:ALA:O	1:C:104:ARG:HG3	2.20	0.42
1:C:315:VAL:HG22	1:C:316:PRO:HD2	2.02	0.42
1:D:241:THR:HG23	1:D:243:ASN:O	2.20	0.42
1:E:53:THR:HG22	1:E:55:ALA:CA	2.49	0.42
1:G:64:HIS:HE1	3:G:719:HOH:O	2.01	0.42
1:C:279:ILE:HD13	1:C:279:ILE:HG21	1.76	0.41
1:E:282:THR:CG2	1:E:283:GLY:N	2.83	0.41
1:E:282:THR:HG22	1:E:283:GLY:N	2.35	0.41
1:H:241:THR:HG23	1:H:243:ASN:O	2.21	0.41
1:B:3:GLU:HG3	1:B:4:PRO:HD2	2.03	0.41
1:D:315:VAL:HG22	1:D:316:PRO:HD2	2.02	0.41
1:F:124:TYR:C	1:F:124:TYR:CD1	2.99	0.41
1:H:124:TYR:C	1:H:124:TYR:CD1	2.99	0.41
1:C:117:GLU:OE1	1:G:117:GLU:OE1	2.38	0.41
1:H:41:ASN:ND2	1:H:44:ASP:H	2.09	0.41
1:F:238:ILE:HD11	1:F:268:ALA:HB2	2.02	0.41
1:F:77:THR:HA	1:F:124:TYR:HB3	2.03	0.40
1:D:111:VAL:O	1:D:115:ARG:HG3	2.20	0.40
1:G:177:HIS:O	1:G:180:GLU:HG2	2.22	0.40
1:B:241:THR:HG23	1:B:243:ASN:O	2.21	0.40
1:C:228:ALA:HB3	1:C:231:GLU:HG3	2.03	0.40
1:F:139:PHE:N	1:F:140:PRO:CD	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:ASP:OD2	1:F:138:ASP:OD2[2_656]	1.77	0.43

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	403/414 (97%)	390 (97%)	13 (3%)	0	100	100
1	B	402/414 (97%)	390 (97%)	12 (3%)	0	100	100
1	C	405/414 (98%)	392 (97%)	13 (3%)	0	100	100
1	D	402/414 (97%)	390 (97%)	12 (3%)	0	100	100
1	E	401/414 (97%)	386 (96%)	15 (4%)	0	100	100
1	F	401/414 (97%)	387 (96%)	14 (4%)	0	100	100
1	G	404/414 (98%)	387 (96%)	17 (4%)	0	100	100
1	H	402/414 (97%)	389 (97%)	13 (3%)	0	100	100
All	All	3220/3312 (97%)	3111 (97%)	109 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	340/346 (98%)	332 (98%)	8 (2%)	43	54
1	B	338/346 (98%)	330 (98%)	8 (2%)	43	54
1	C	341/346 (99%)	332 (97%)	9 (3%)	40	50
1	D	338/346 (98%)	328 (97%)	10 (3%)	36	45
1	E	339/346 (98%)	323 (95%)	16 (5%)	23	26
1	F	339/346 (98%)	322 (95%)	17 (5%)	22	24
1	G	340/346 (98%)	328 (96%)	12 (4%)	32	39
1	H	339/346 (98%)	329 (97%)	10 (3%)	37	47
All	All	2714/2768 (98%)	2624 (97%)	90 (3%)	33	42

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	MET
1	A	160	VAL
1	A	180	GLU
1	A	191	ASN
1	A	193	ILE
1	A	323	THR
1	A	350	VAL
1	A	354	GLU
1	B	9	GLN
1	B	28	MET
1	B	160	VAL
1	B	198	THR
1	B	220	THR
1	B	315	VAL
1	B	323	THR
1	B	354	GLU
1	C	28	MET
1	C	115[A]	ARG
1	C	115[B]	ARG
1	C	160	VAL
1	C	172	LYS
1	C	191	ASN
1	C	198	THR
1	C	323	THR
1	C	354	GLU
1	D	148	LYS
1	D	160	VAL
1	D	180	GLU
1	D	193	ILE
1	D	220	THR
1	D	323	THR
1	D	330	THR
1	D	354	GLU
1	D	370	ARG
1	D	374	LEU
1	E	53	THR
1	E	60	LYS
1	E	103	ARG
1	E	160	VAL
1	E	184	MET
1	E	191	ASN
1	E	193	ILE
1	E	198	THR

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Mol	Chain	Res	Type
1	E	207	SER
1	E	215	THR
1	E	279	ILE
1	E	323	THR
1	E	330	THR
1	E	332	LYS
1	E	354	GLU
1	E	370	ARG
1	F	9	GLN
1	F	28	MET
1	F	39	HIS
1	F	103	ARG
1	F	160	VAL
1	F	191	ASN
1	F	193	ILE
1	F	198	THR
1	F	207	SER
1	F	217	GLU
1	F	220	THR
1	F	231	GLU
1	F	295	MET
1	F	323	THR
1	F	347	ASP
1	F	354	GLU
1	F	370	ARG
1	G	104	ARG
1	G	160	VAL
1	G	180	GLU
1	G	193	ILE
1	G	198	THR
1	G	230	ASN
1	G	295	MET
1	G	346	ASN
1	G	347	ASP
1	G	348	ASN
1	G	354	GLU
1	G	414	GLU
1	H	146	LEU
1	H	160	VAL
1	H	180	GLU
1	H	191	ASN
1	H	193	ILE

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Mol	Chain	Res	Type
1	H	198	THR
1	H	230	ASN
1	H	295	MET
1	H	323	THR
1	H	330	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	147	GLN
1	A	187	HIS
1	A	372	HIS
1	A	410	GLN
1	B	10	HIS
1	B	42	GLN
1	B	43	HIS
1	B	170	ASN
1	B	187	HIS
1	B	191	ASN
1	B	410	GLN
1	C	64	HIS
1	C	372	HIS
1	C	410	GLN
1	D	9	GLN
1	D	147	GLN
1	D	187	HIS
1	D	372	HIS
1	E	9	GLN
1	E	321	HIS
1	E	372	HIS
1	E	410	GLN
1	F	27	GLN
1	F	147	GLN
1	F	189	GLN
1	F	244	GLN
1	F	372	HIS
1	F	410	GLN
1	G	9	GLN
1	G	41	ASN
1	G	42	GLN
1	G	64	HIS

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Mol	Chain	Res	Type
1	G	177	HIS
1	G	187	HIS
1	G	189	GLN
1	G	191	ASN
1	G	230	ASN
1	G	410	GLN
1	H	41	ASN
1	H	42	GLN
1	H	187	HIS
1	H	189	GLN
1	H	230	ASN
1	H	292	GLN
1	H	321	HIS
1	H	372	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](#)

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	502	-	4,4,4	0.08	0	6,6,6	0.55	0
2	SO4	G	502	-	4,4,4	0.43	0	6,6,6	0.69	0
2	SO4	H	502	-	4,4,4	0.33	0	6,6,6	0.24	0
2	SO4	G	504	-	4,4,4	0.47	0	6,6,6	0.17	0
2	SO4	A	502	-	4,4,4	0.18	0	6,6,6	0.50	0
2	SO4	C	503	-	4,4,4	0.26	0	6,6,6	0.39	0
2	SO4	C	501	-	4,4,4	0.50	0	6,6,6	0.67	0
2	SO4	H	501	-	4,4,4	0.42	0	6,6,6	0.42	0
2	SO4	B	502	-	4,4,4	0.22	0	6,6,6	0.32	0
2	SO4	D	501	-	4,4,4	0.56	0	6,6,6	0.51	0
2	SO4	E	502	-	4,4,4	0.27	0	6,6,6	0.26	0
2	SO4	G	505	-	4,4,4	0.31	0	6,6,6	0.21	0
2	SO4	C	504	-	4,4,4	0.19	0	6,6,6	0.46	0
2	SO4	B	501	-	4,4,4	0.27	0	6,6,6	0.19	0
2	SO4	B	503	-	4,4,4	0.32	0	6,6,6	0.25	0
2	SO4	D	502	-	4,4,4	0.20	0	6,6,6	0.33	0
2	SO4	F	501	-	4,4,4	0.51	0	6,6,6	0.39	0
2	SO4	G	503	-	4,4,4	0.23	0	6,6,6	0.39	0
2	SO4	G	501	-	4,4,4	0.28	0	6,6,6	0.46	0
2	SO4	E	501	-	4,4,4	0.22	0	6,6,6	0.45	0
2	SO4	A	503	-	4,4,4	0.33	0	6,6,6	0.44	0
2	SO4	A	501	-	4,4,4	0.39	0	6,6,6	0.51	0
2	SO4	A	504	-	4,4,4	0.63	0	6,6,6	0.68	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.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	504	SO4	1	0
2	A	502	SO4	1	0
2	D	501	SO4	1	0
2	E	502	SO4	1	0
2	G	503	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	407/414 (98%)	-0.24	6 (1%) 72 73	25, 38, 77, 127	0
1	B	406/414 (98%)	-0.54	4 (0%) 79 81	25, 33, 63, 128	0
1	C	408/414 (98%)	-0.56	3 (0%) 84 85	21, 30, 56, 120	1 (0%)
1	D	406/414 (98%)	0.95	39 (9%) 13 12	44, 68, 98, 129	0
1	E	405/414 (97%)	0.94	39 (9%) 13 12	41, 83, 117, 168	0
1	F	405/414 (97%)	1.00	42 (10%) 11 11	38, 78, 115, 149	0
1	G	408/414 (98%)	-0.43	6 (1%) 72 73	24, 32, 71, 122	0
1	H	406/414 (98%)	0.48	16 (3%) 43 43	35, 69, 99, 130	0
All	All	3251/3312 (98%)	0.20	155 (4%) 35 35	21, 53, 105, 168	1 (0%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	198	THR	7.3
1	A	199	GLY	7.1
1	F	206	VAL	6.4
1	G	203	ARG	5.5
1	C	199	GLY	5.5
1	E	206	VAL	5.5
1	H	199	GLY	5.3
1	E	198	THR	4.5
1	G	225	TYR	4.4
1	D	205	GLN	4.3
1	E	229	PRO	4.2
1	A	225	TYR	4.1
1	F	198	THR	4.0
1	E	160	VAL	3.9
1	D	225	TYR	3.8
1	E	225	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	76	LEU	3.6
1	B	229	PRO	3.6
1	F	225	TYR	3.5
1	H	225	TYR	3.5
1	D	62	ILE	3.5
1	A	229	PRO	3.4
1	F	227	GLY	3.3
1	F	125	MET	3.1
1	A	2	THR	3.1
1	H	229	PRO	3.1
1	D	306	ALA	3.1
1	D	227	GLY	3.0
1	D	10	HIS	3.0
1	C	2	THR	3.0
1	D	152	VAL	2.9
1	D	229	PRO	2.9
1	F	64	HIS	2.9
1	D	349	VAL	2.9
1	B	2	THR	2.9
1	F	229	PRO	2.9
1	F	5	LEU	2.9
1	F	86	LEU	2.9
1	G	204	GLY	2.8
1	E	135	TYR	2.8
1	F	145	TYR	2.8
1	G	229	PRO	2.8
1	D	228	ALA	2.8
1	D	92	LEU	2.8
1	E	163	PHE	2.7
1	D	346	ASN	2.7
1	F	196	ASN	2.7
1	H	2	THR	2.7
1	E	22	TRP	2.7
1	D	64	HIS	2.7
1	D	206	VAL	2.7
1	H	198	THR	2.7
1	H	187	HIS	2.7
1	H	228	ALA	2.7
1	E	188	TYR	2.7
1	F	228	ALA	2.6
1	F	122	PHE	2.6
1	F	279	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	211	ILE	2.6
1	E	64	HIS	2.6
1	E	86	LEU	2.6
1	F	43	HIS	2.6
1	F	146	LEU	2.6
1	C	205	GLN	2.6
1	D	196	ASN	2.6
1	D	159	PRO	2.6
1	F	20	ILE	2.6
1	E	145	TYR	2.6
1	E	287	ILE	2.6
1	H	207	SER	2.5
1	F	165	PHE	2.5
1	F	35	GLU	2.5
1	B	228	ALA	2.5
1	D	365	GLY	2.5
1	D	89	THR	2.5
1	D	351	LEU	2.5
1	D	181	LEU	2.4
1	G	216	TYR	2.4
1	E	285	GLY	2.4
1	D	193	ILE	2.4
1	H	10	HIS	2.4
1	E	159	PRO	2.4
1	E	283	GLY	2.4
1	F	283	GLY	2.4
1	E	279	ILE	2.4
1	E	39	HIS	2.4
1	F	188	TYR	2.4
1	D	112	ALA	2.4
1	D	224	ILE	2.4
1	G	230	ASN	2.3
1	E	174	ALA	2.3
1	D	185	ILE	2.3
1	E	24	LEU	2.3
1	F	177	HIS	2.3
1	F	187	HIS	2.3
1	F	308	VAL	2.3
1	E	192	ALA	2.3
1	F	266	ALA	2.3
1	D	85	PHE	2.3
1	D	3	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	3	GLU	2.3
1	E	187	HIS	2.3
1	H	39	HIS	2.3
1	F	49	ILE	2.3
1	F	36	LEU	2.2
1	D	87	TYR	2.2
1	E	303	ALA	2.2
1	F	89	THR	2.2
1	H	64	HIS	2.2
1	D	213	VAL	2.2
1	E	52	PHE	2.2
1	E	53	THR	2.2
1	F	29	ALA	2.2
1	F	211	ILE	2.2
1	F	24	LEU	2.2
1	F	213	VAL	2.2
1	F	52	PHE	2.2
1	D	167	GLY	2.2
1	E	10	HIS	2.2
1	E	228	ALA	2.2
1	F	142	TYR	2.2
1	B	346	ASN	2.2
1	H	349	VAL	2.2
1	F	163	PHE	2.2
1	F	6	PRO	2.2
1	F	133	PRO	2.2
1	D	90	LYS	2.2
1	A	227	GLY	2.2
1	H	296	HIS	2.2
1	E	18	LEU	2.1
1	F	178	LEU	2.1
1	D	95	PHE	2.1
1	F	217	GLU	2.1
1	H	84	PHE	2.1
1	D	5	LEU	2.1
1	F	28	MET	2.1
1	E	5	LEU	2.1
1	E	139	PHE	2.1
1	E	165	PHE	2.1
1	D	289	ALA	2.1
1	E	99	HIS	2.1
1	E	242	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	196	ASN	2.1
1	E	211	ILE	2.1
1	E	146	LEU	2.0
1	D	8	ILE	2.0
1	H	194	ILE	2.0
1	F	182	TYR	2.0
1	D	161	GLY	2.0
1	D	149	SER	2.0
1	A	228	ALA	2.0
1	D	141	ALA	2.0
1	F	329	HIS	2.0
1	D	179	PRO	2.0
1	E	140	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	G	504	5/5	0.81	0.14	52,98,105,110	0
2	SO4	E	502	5/5	0.82	0.09	89,89,114,123	0
2	SO4	B	503	5/5	0.82	0.11	84,89,95,95	0
2	SO4	H	502	5/5	0.82	0.11	72,79,102,110	0
2	SO4	A	503	5/5	0.84	0.12	62,63,93,100	0
2	SO4	G	503	5/5	0.84	0.16	57,91,120,128	0
2	SO4	G	501	5/5	0.85	0.09	57,58,73,78	0
2	SO4	G	505	5/5	0.85	0.14	58,89,110,144	0
2	SO4	F	501	5/5	0.85	0.11	61,75,81,92	0
2	SO4	D	502	5/5	0.86	0.10	63,67,81,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	504	5/5	0.86	0.14	60,60,110,150	0
2	SO4	G	502	5/5	0.87	0.14	69,72,79,79	0
2	SO4	A	504	5/5	0.88	0.09	42,55,74,105	0
2	SO4	H	501	5/5	0.90	0.10	57,70,78,109	0
2	SO4	C	503	5/5	0.91	0.13	54,63,88,94	0
2	SO4	A	502	5/5	0.91	0.08	58,65,76,86	0
2	SO4	E	501	5/5	0.92	0.08	60,62,84,115	0
2	SO4	C	502	5/5	0.92	0.07	54,56,68,71	0
2	SO4	D	501	5/5	0.93	0.07	55,61,63,100	0
2	SO4	B	502	5/5	0.94	0.10	50,56,66,67	0
2	SO4	A	501	5/5	0.96	0.08	54,57,63,69	0
2	SO4	B	501	5/5	0.96	0.06	55,56,71,81	0
2	SO4	C	501	5/5	0.96	0.08	45,53,57,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.