



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:13 AM UTC

PDB ID : 1XSI / pdb_00001xsi
Title : Structure of a Family 31 alpha glycosidase
Authors : Lovering, A.L.; Lee, S.S.; Kim, Y.W.; Withers, S.G.; Strynadka, N.C.
Deposited on : 2004-10-19
Resolution : 2.20 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:

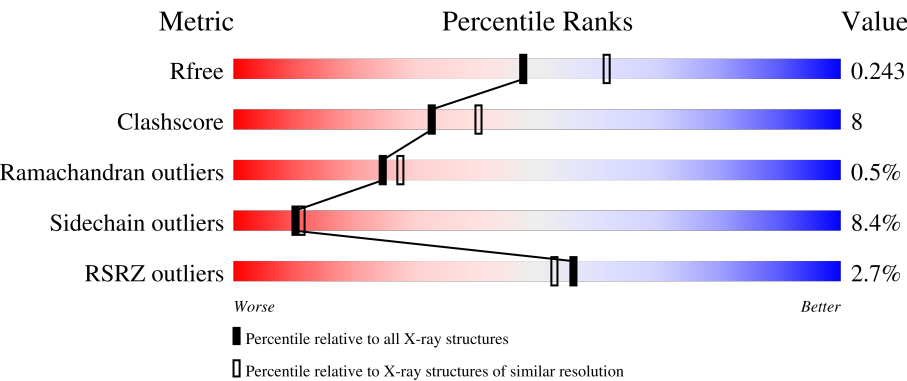
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	778	% 82%14% . .
1	B	778	3% 77%19% . .
1	C	778	% 79%16% . .
1	D	778	6% 77%18% . .
1	E	778	3% 76%20% . .

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Mol	Chain	Length	Quality of chain
1	F	778	% 78%18% . ..

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	SO4	F	3009	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 38490 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 Putative family 31 glucosidase yicI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	B	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	C	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	D	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	E	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	F	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			

There are 36 discrepancies between the modelled and reference sequences:

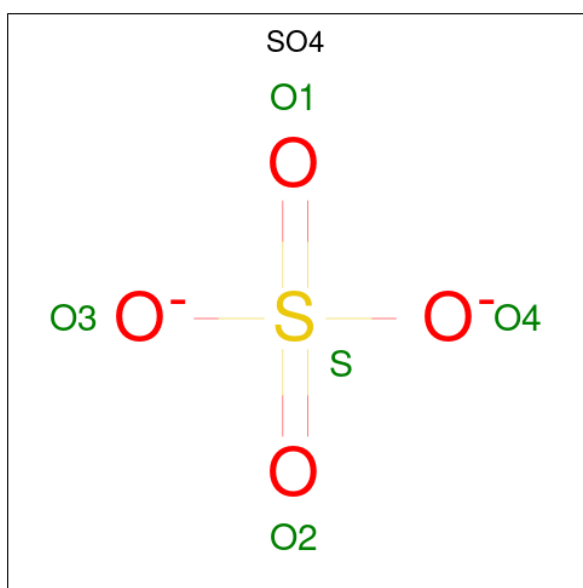
Chain	Residue	Modelled	Actual	Comment	Reference
A	773	HIS	-	expression tag	UNP P31434
A	774	HIS	-	expression tag	UNP P31434
A	775	HIS	-	expression tag	UNP P31434
A	776	HIS	-	expression tag	UNP P31434
A	777	HIS	-	expression tag	UNP P31434
A	778	HIS	-	expression tag	UNP P31434
B	773	HIS	-	expression tag	UNP P31434
B	774	HIS	-	expression tag	UNP P31434
B	775	HIS	-	expression tag	UNP P31434
B	776	HIS	-	expression tag	UNP P31434
B	777	HIS	-	expression tag	UNP P31434
B	778	HIS	-	expression tag	UNP P31434
C	773	HIS	-	expression tag	UNP P31434
C	774	HIS	-	expression tag	UNP P31434
C	775	HIS	-	expression tag	UNP P31434
C	776	HIS	-	expression tag	UNP P31434
C	777	HIS	-	expression tag	UNP P31434

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Chain	Residue	Modelled	Actual	Comment	Reference
C	778	HIS	-	expression tag	UNP P31434
D	773	HIS	-	expression tag	UNP P31434
D	774	HIS	-	expression tag	UNP P31434
D	775	HIS	-	expression tag	UNP P31434
D	776	HIS	-	expression tag	UNP P31434
D	777	HIS	-	expression tag	UNP P31434
D	778	HIS	-	expression tag	UNP P31434
E	773	HIS	-	expression tag	UNP P31434
E	774	HIS	-	expression tag	UNP P31434
E	775	HIS	-	expression tag	UNP P31434
E	776	HIS	-	expression tag	UNP P31434
E	777	HIS	-	expression tag	UNP P31434
E	778	HIS	-	expression tag	UNP P31434
F	773	HIS	-	expression tag	UNP P31434
F	774	HIS	-	expression tag	UNP P31434
F	775	HIS	-	expression tag	UNP P31434
F	776	HIS	-	expression tag	UNP P31434
F	777	HIS	-	expression tag	UNP P31434
F	778	HIS	-	expression tag	UNP P31434

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



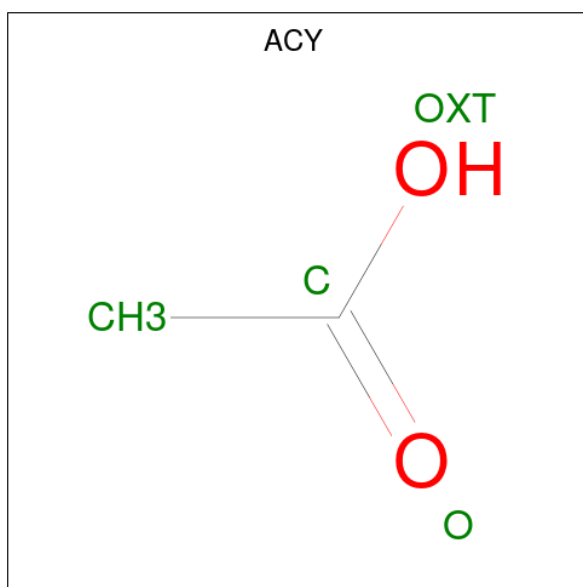
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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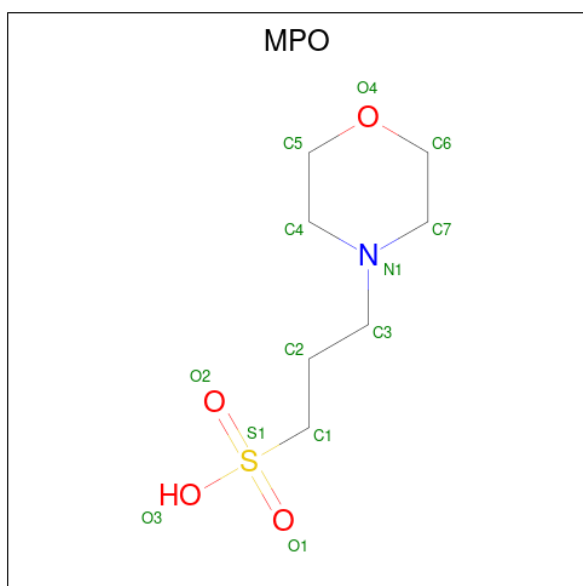
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total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

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	E	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

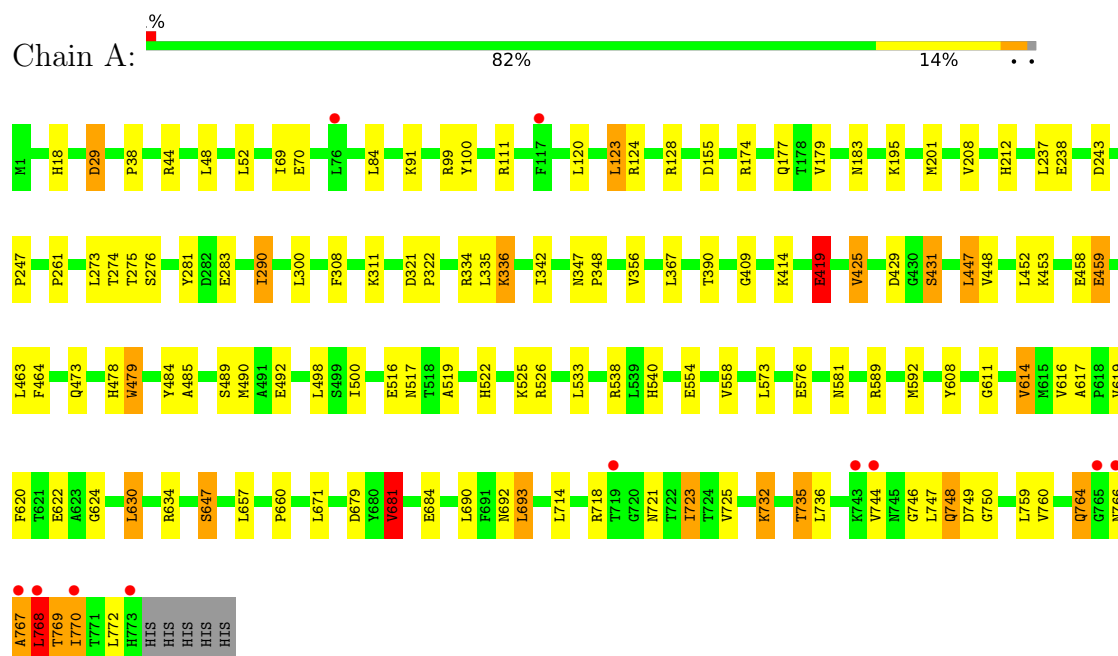
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	170	Total	O	0	0
			170	170		
5	B	140	Total	O	0	0
			140	140		
5	C	189	Total	O	0	0
			189	189		
5	D	162	Total	O	0	0
			162	162		
5	E	152	Total	O	0	0
			152	152		
5	F	167	Total	O	0	0
			167	167		

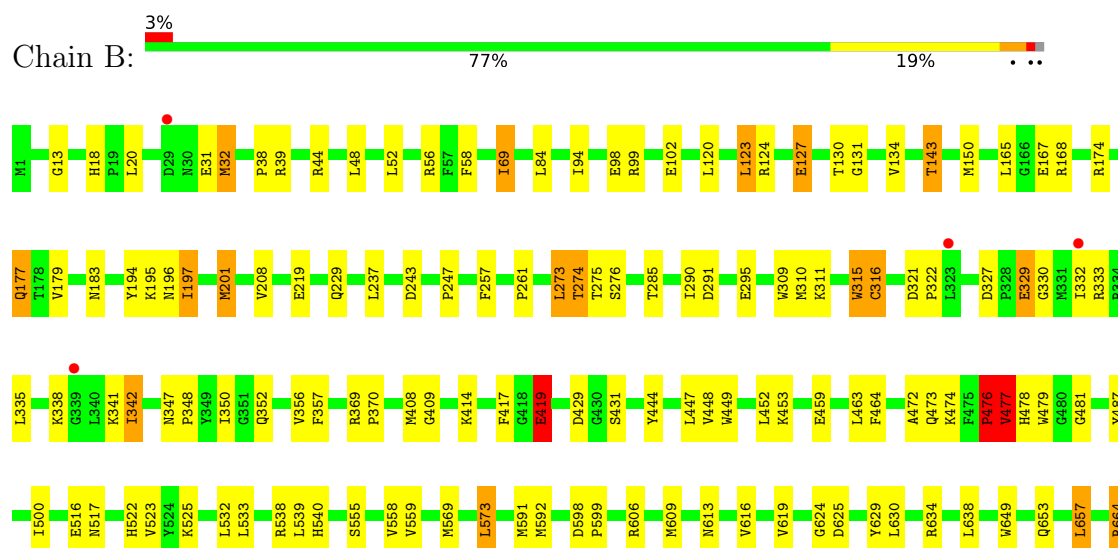
3 Residue-property plots

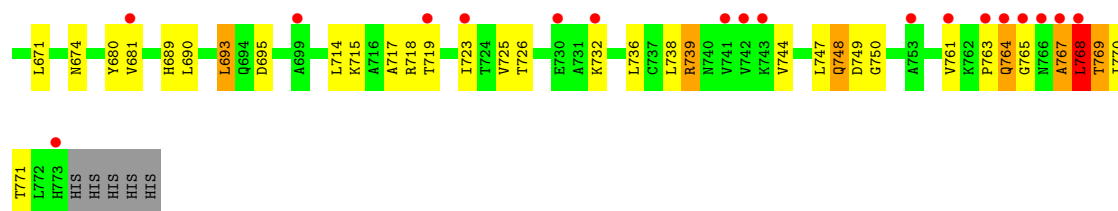
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Putative family 31 glucosidase yicI

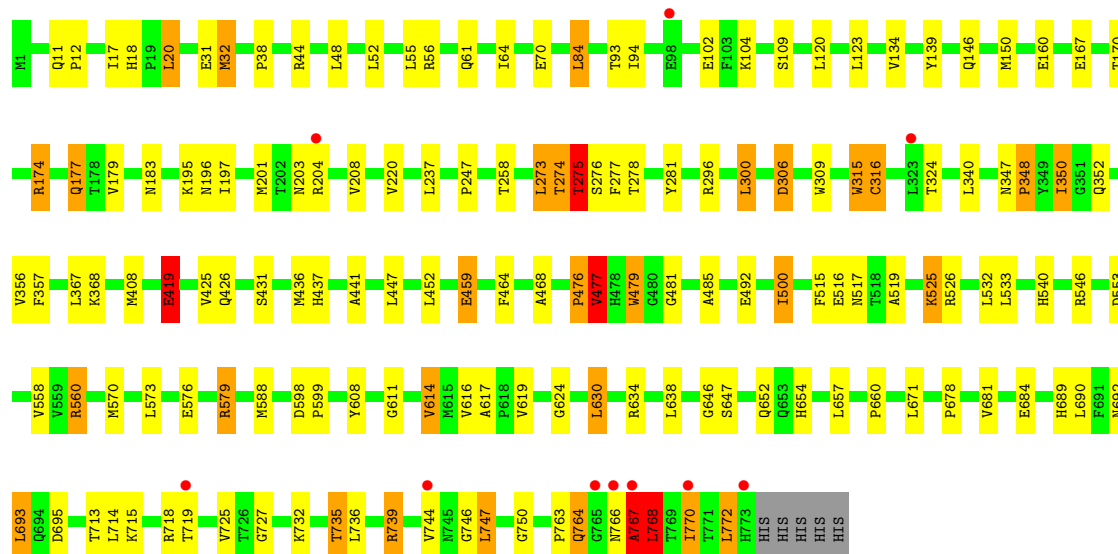
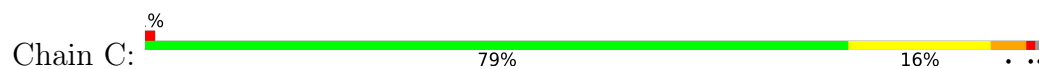


• Molecule 1: Putative family 31 glucosidase yicI

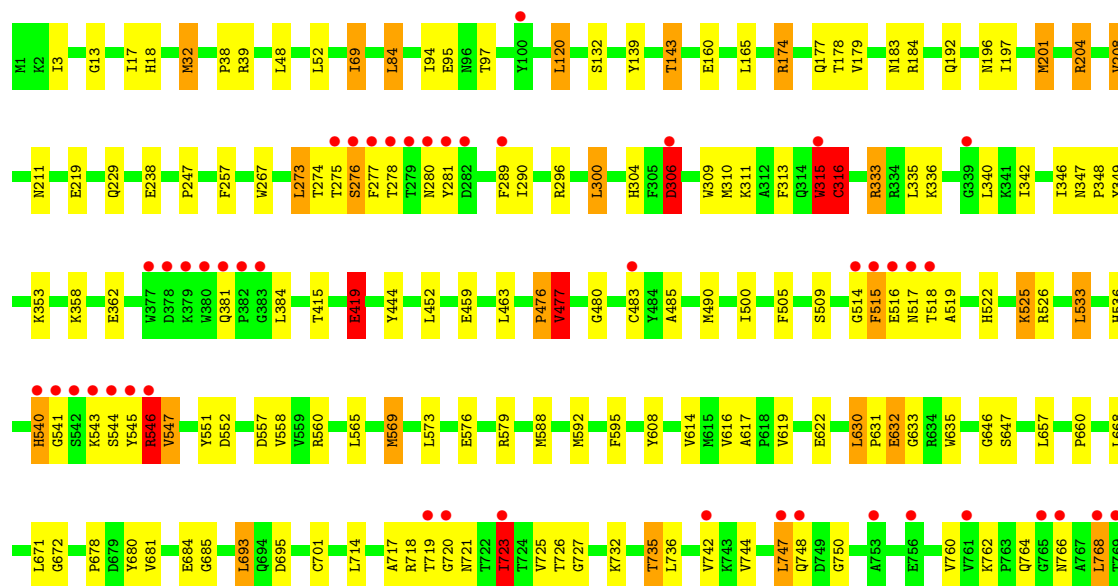
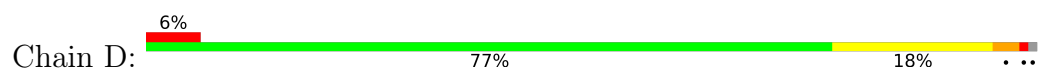




• Molecule 1: Putative family 31 glucosidase yicI

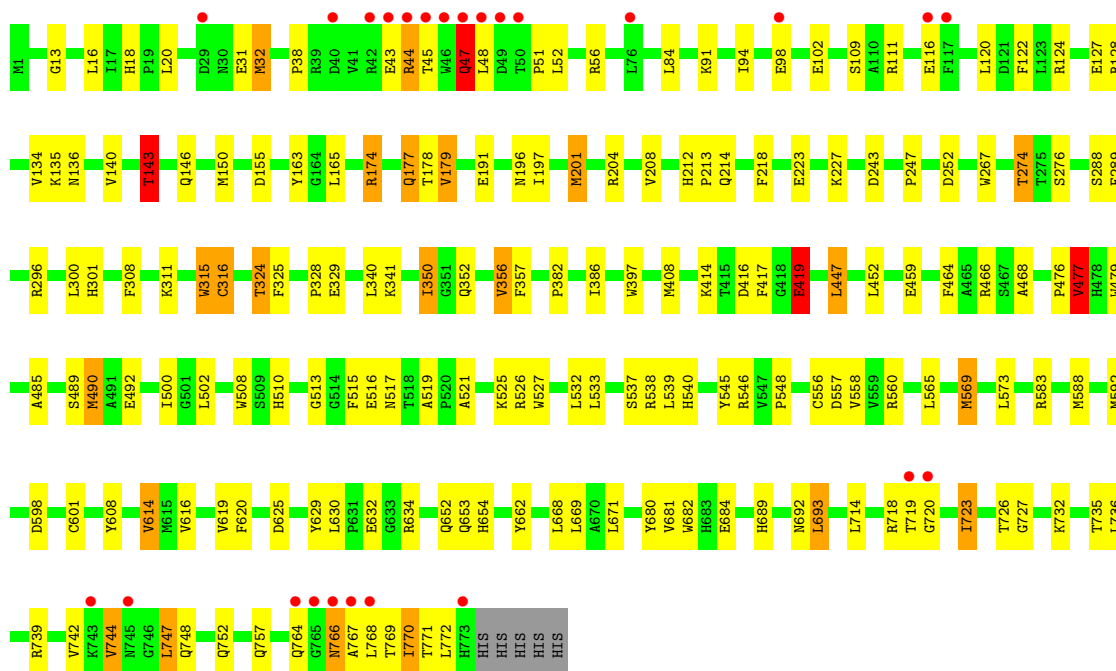
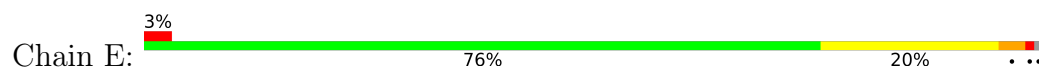


• Molecule 1: Putative family 31 glucosidase yicI

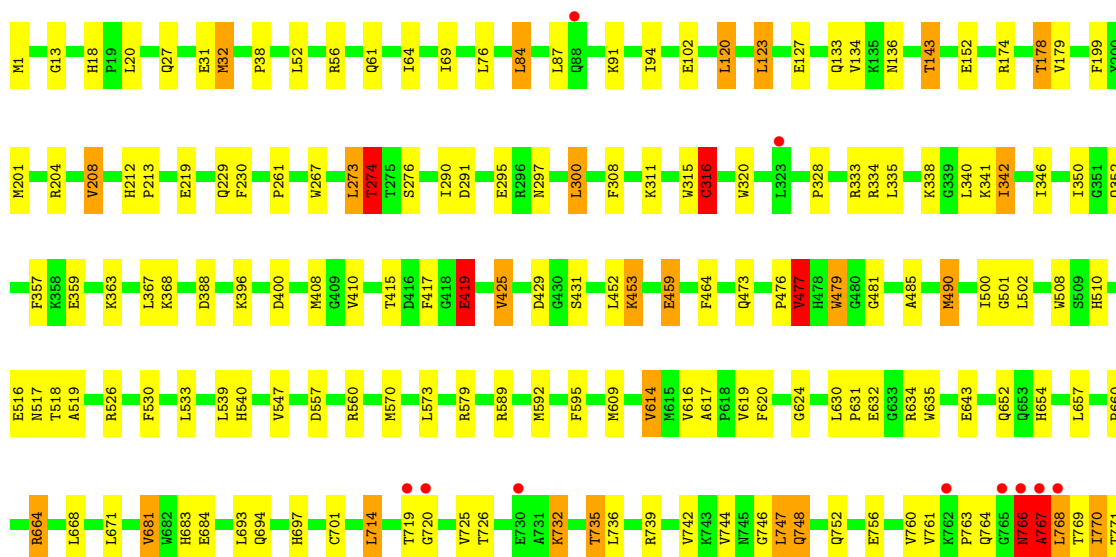
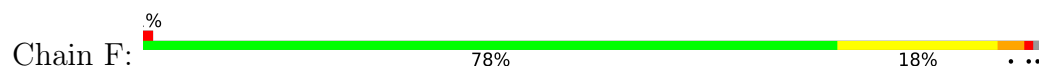




- Molecule 1: Putative family 31 glucosidase yicI



- Molecule 1: Putative family 31 glucosidase yicI



L772	HIS
H773	HIS
	HIS
	HIS
	HIS
	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	161.69Å 174.93Å 209.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-2.20) 98.7 (30.00-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.239 0.208 , 0.243	Depositor DCC
R_{free} test set	14939 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 23.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	38490	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MPO, ACY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	2/6409 (0.0%)	1.12	11/8711 (0.1%)
1	B	1.01	7/6409 (0.1%)	1.10	11/8711 (0.1%)
1	C	1.05	3/6409 (0.0%)	1.13	21/8711 (0.2%)
1	D	1.06	9/6409 (0.1%)	1.14	21/8711 (0.2%)
1	E	1.02	6/6409 (0.1%)	1.11	22/8711 (0.3%)
1	F	1.09	9/6409 (0.1%)	1.14	25/8711 (0.3%)
All	All	1.05	36/38454 (0.1%)	1.12	111/52266 (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	1	1
1	C	2	1
1	D	1	2
1	E	2	1
1	F	2	0
All	All	8	6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	32	MET	SD-CE	-13.99	1.44	1.79
1	F	32	MET	SD-CE	-10.56	1.53	1.79
1	D	32	MET	SD-CE	-10.52	1.53	1.79
1	D	490	MET	SD-CE	-9.41	1.56	1.79
1	D	306	ASP	CB-CG	8.19	1.72	1.52
1	F	609	MET	SD-CE	7.82	1.99	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	569	MET	SD-CE	-7.69	1.60	1.79
1	B	201	MET	SD-CE	-7.50	1.60	1.79
1	D	306	ASP	CA-CB	7.50	1.65	1.53
1	B	609	MET	SD-CE	7.11	1.97	1.79
1	D	201	MET	SD-CE	-6.96	1.62	1.79
1	E	150	MET	SD-CE	-6.76	1.62	1.79
1	F	570	MET	SD-CE	6.73	1.96	1.79
1	F	681	VAL	CA-CB	6.49	1.60	1.53
1	B	32	MET	SD-CE	-6.26	1.63	1.79
1	F	178	THR	CA-CB	6.26	1.62	1.53
1	E	490	MET	SD-CE	-6.17	1.64	1.79
1	A	681	VAL	CA-CB	6.02	1.61	1.53
1	D	306	ASP	N-CA	5.85	1.52	1.46
1	F	316	CYS	CA-C	-5.83	1.45	1.52
1	C	441	ALA	CA-CB	5.79	1.62	1.53
1	B	591	MET	SD-CE	5.79	1.94	1.79
1	D	723	ILE	CA-CB	5.75	1.61	1.54
1	A	723	ILE	CA-CB	5.61	1.60	1.54
1	F	316	CYS	N-CA	-5.57	1.39	1.46
1	E	468	ALA	C-O	5.52	1.29	1.23
1	F	490	MET	SD-CE	-5.43	1.66	1.79
1	C	316	CYS	N-CA	-5.39	1.38	1.46
1	F	84	LEU	CA-C	5.33	1.59	1.52
1	D	477	VAL	N-CA	-5.32	1.39	1.46
1	B	197	ILE	CA-CB	5.27	1.60	1.54
1	E	32	MET	SD-CE	-5.24	1.66	1.79
1	E	386	ILE	CA-CB	-5.12	1.48	1.54
1	D	569	MET	SD-CE	-5.11	1.66	1.79
1	B	316	CYS	CA-C	-5.06	1.46	1.52
1	B	523	VAL	CA-CB	5.01	1.60	1.54

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	767	ALA	N-CA-C	-13.27	97.71	114.56
1	C	315	TRP	CA-C-N	11.11	138.74	122.74
1	C	315	TRP	C-N-CA	11.11	138.74	122.74
1	E	316	CYS	N-CA-C	10.79	126.31	111.74
1	E	315	TRP	CA-C-N	10.47	136.96	122.19
1	E	315	TRP	C-N-CA	10.47	136.96	122.19
1	C	476	PRO	CA-C-N	9.81	139.64	121.97
1	C	476	PRO	C-N-CA	9.81	139.64	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	476	PRO	CA-C-N	9.31	138.74	121.97
1	E	476	PRO	C-N-CA	9.31	138.74	121.97
1	F	476	PRO	CA-C-N	9.17	138.48	121.97
1	F	476	PRO	C-N-CA	9.17	138.48	121.97
1	C	316	CYS	N-CA-C	8.93	123.47	112.58
1	D	476	PRO	CA-C-N	8.35	137.00	121.97
1	D	476	PRO	C-N-CA	8.35	137.00	121.97
1	B	477	VAL	CB-CA-C	7.96	124.34	111.29
1	D	477	VAL	N-CA-C	7.69	125.33	109.34
1	F	477	VAL	CB-CA-C	7.65	123.83	111.29
1	C	477	VAL	N-CA-C	7.61	125.16	109.34
1	D	316	CYS	N-CA-C	7.56	126.91	110.80
1	E	476	PRO	N-CA-C	7.54	121.78	111.22
1	E	223	GLU	N-CA-C	-7.49	102.08	112.12
1	F	767	ALA	N-CA-C	-7.31	95.23	110.80
1	C	560	ARG	NE-CZ-NH1	-7.27	114.23	121.50
1	E	767	ALA	N-CA-C	-7.21	104.62	113.41
1	C	477	VAL	CB-CA-C	7.11	122.94	111.29
1	F	315	TRP	CA-C-N	7.06	135.02	121.54
1	F	315	TRP	C-N-CA	7.06	135.02	121.54
1	C	324	THR	N-CA-C	-7.05	105.20	113.88
1	B	315	TRP	N-CA-C	6.99	120.79	110.30
1	D	419	GLU	N-CA-C	6.72	121.79	112.45
1	A	419	GLU	CA-CB-CG	6.61	127.32	114.10
1	E	477	VAL	N-CA-C	6.57	123.00	109.34
1	D	315	TRP	CA-C-N	6.54	134.02	121.54
1	D	315	TRP	C-N-CA	6.54	134.02	121.54
1	D	208	VAL	N-CA-C	6.30	116.91	108.27
1	C	274	THR	OG1-CB-CG2	-6.30	96.70	109.30
1	C	767	ALA	N-CA-C	-6.27	97.44	110.80
1	F	315	TRP	O-C-N	6.17	130.52	122.93
1	C	275	THR	N-CA-CB	-6.12	99.91	110.32
1	D	419	GLU	CA-CB-CG	6.09	126.28	114.10
1	A	29	ASP	CB-CA-C	-6.07	108.97	117.23
1	E	315	TRP	O-C-N	6.06	130.32	122.87
1	C	315	TRP	O-C-N	6.05	130.31	122.87
1	B	194	TYR	N-CA-C	-6.03	105.41	112.89
1	C	419	GLU	CA-CB-CG	6.00	126.09	114.10
1	C	419	GLU	N-CA-C	5.99	120.77	112.45
1	E	476	PRO	CA-C-O	5.96	130.72	122.31
1	F	739	ARG	CG-CD-NE	-5.92	98.97	112.00
1	B	476	PRO	CA-C-N	5.90	132.59	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	476	PRO	C-N-CA	5.90	132.59	121.97
1	D	480	GLY	N-CA-C	5.87	121.50	113.99
1	F	315	TRP	N-CA-CB	5.76	118.44	109.85
1	B	315	TRP	CA-C-N	5.74	132.50	121.54
1	B	315	TRP	C-N-CA	5.74	132.50	121.54
1	F	410	VAL	N-CA-C	-5.71	102.21	109.58
1	A	721	ASN	N-CA-C	-5.69	104.92	112.94
1	E	350	ILE	CA-C-N	5.68	125.74	120.34
1	E	350	ILE	C-N-CA	5.68	125.74	120.34
1	F	476	PRO	O-C-N	5.67	129.51	122.71
1	F	419	GLU	N-CA-C	5.67	120.32	112.45
1	A	347	ASN	CB-CA-C	5.66	118.13	110.37
1	C	476	PRO	N-CA-C	5.66	119.42	111.33
1	C	177	GLN	CB-CA-C	5.66	119.72	109.37
1	F	614	VAL	CB-CA-C	5.63	118.96	110.63
1	D	306	ASP	OD1-CG-OD2	-5.62	109.41	122.90
1	B	69	ILE	CB-CA-C	5.60	119.17	110.83
1	F	316	CYS	N-CA-C	5.58	122.69	110.80
1	D	3	ILE	N-CA-C	-5.57	106.77	111.56
1	C	739	ARG	CG-CD-NE	-5.53	99.83	112.00
1	A	390	THR	N-CA-C	-5.53	106.58	113.38
1	F	476	PRO	N-CA-C	5.51	119.21	111.33
1	F	274	THR	N-CA-CB	-5.46	102.36	111.20
1	B	316	CYS	CA-CB-SG	-5.41	101.95	114.40
1	D	685	GLY	N-CA-C	-5.40	107.87	115.32
1	E	477	VAL	CB-CA-C	5.40	120.14	111.29
1	D	477	VAL	CB-CA-C	5.37	120.09	111.29
1	D	547	VAL	N-CA-C	5.36	113.17	107.76
1	A	614	VAL	N-CA-C	5.34	115.58	108.11
1	E	143	THR	N-CA-CB	-5.34	101.44	110.41
1	E	315	TRP	N-CA-CB	5.31	117.85	109.83
1	C	614	VAL	N-CA-C	5.30	115.53	108.11
1	F	530	PHE	CA-C-N	5.30	125.87	119.98
1	F	530	PHE	C-N-CA	5.30	125.87	119.98
1	F	664	ARG	CB-CA-C	-5.29	99.88	110.42
1	B	257	PHE	N-CA-C	5.29	117.46	111.11
1	A	589	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	C	735	THR	OG1-CB-CG2	-5.25	98.79	109.30
1	E	601	CYS	N-CA-C	5.23	119.64	113.16
1	E	614	VAL	N-CA-C	5.23	115.65	108.12
1	F	342	ILE	N-CA-C	5.22	115.36	107.75
1	F	76	LEU	N-CA-C	5.18	116.73	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	201	MET	CG-SD-CE	-5.17	89.52	100.90
1	D	306	ASP	N-CA-CB	5.17	117.39	109.94
1	A	177	GLN	N-CA-C	5.17	118.17	109.95
1	E	316	CYS	CB-CA-C	5.14	119.03	111.73
1	D	546	ARG	N-CA-C	-5.13	105.49	112.26
1	B	419	GLU	N-CA-C	5.12	119.57	112.45
1	E	419	GLU	N-CA-C	5.11	119.56	112.45
1	C	316	CYS	CB-CA-C	5.09	119.28	111.39
1	E	476	PRO	O-C-N	5.08	129.16	122.86
1	F	476	PRO	CA-C-O	5.08	129.62	122.31
1	A	281	TYR	N-CA-C	5.07	116.12	108.46
1	D	721	ASN	N-CA-C	-5.07	105.82	112.41
1	A	647	SER	CB-CA-C	5.05	119.21	111.39
1	F	547	VAL	N-CA-CB	5.04	115.18	109.99
1	F	178	THR	CB-CA-C	5.03	117.83	109.53
1	D	69	ILE	CA-C-N	-5.01	114.80	122.62
1	D	69	ILE	C-N-CA	-5.01	114.80	122.62
1	D	306	ASP	CB-CG-OD1	5.01	129.93	118.40
1	F	419	GLU	CA-CB-CG	5.00	124.11	114.10

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	477	VAL	CA
1	C	316	CYS	CA
1	C	477	VAL	CA
1	D	477	VAL	CA
1	E	316	CYS	CA
1	E	477	VAL	CA
1	F	316	CYS	CA
1	F	477	VAL	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	766	ASN	Peptide
1	B	476	PRO	Peptide
1	C	476	PRO	Peptide
1	D	315	TRP	Peptide
1	D	476	PRO	Peptide
1	E	766	ASN	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	6226	0	5934	80	0
1	B	6226	0	5934	94	0
1	C	6226	0	5934	113	0
1	D	6226	0	5934	99	0
1	E	6226	0	5934	103	0
1	F	6226	0	5934	95	0
2	A	15	0	0	0	0
2	B	25	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	1	0
2	F	25	0	0	4	0
3	A	4	0	3	0	0
3	E	4	0	3	0	0
3	F	4	0	3	0	0
4	B	13	0	15	0	0
4	C	13	0	15	0	0
4	D	13	0	15	0	0
4	E	13	0	15	0	0
5	A	170	0	0	2	0
5	B	140	0	0	4	0
5	C	189	0	0	1	0
5	D	162	0	0	2	0
5	E	152	0	0	7	0
5	F	167	0	0	2	0
All	All	38490	0	35673	581	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 8.

All (581) 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:F:274:THR:HG22	1:F:276:SER:H	0.98	1.10
1:B:274:THR:HG22	1:B:276:SER:H	1.13	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:MET:HE2	1:D:94:ILE:HG23	1.23	1.08
1:E:274:THR:HG21	1:E:540:HIS:ND1	1.68	1.08
1:C:93:THR:HG22	1:C:104:LYS:HB3	1.36	1.07
1:B:274:THR:HG21	1:B:540:HIS:ND1	1.69	1.06
1:C:367:LEU:HD11	1:C:425:VAL:HG21	1.33	1.06
1:F:274:THR:HG21	1:F:540:HIS:ND1	1.72	1.03
1:E:274:THR:HG22	1:E:276:SER:H	1.24	1.00
1:E:565:LEU:HG	1:E:569:MET:HE2	1.39	1.00
1:D:32:MET:CE	1:D:94:ILE:HG23	1.95	0.96
1:B:32:MET:HE2	1:B:94:ILE:HG23	1.47	0.96
1:F:735:THR:HG22	5:F:3174:HOH:O	1.66	0.94
1:F:274:THR:HG22	1:F:276:SER:N	1.81	0.94
1:A:274:THR:HG22	1:A:276:SER:H	1.31	0.93
1:C:274:THR:HG21	1:C:540:HIS:ND1	1.84	0.93
1:D:381:GLN:HB2	1:D:384:LEU:HD12	1.50	0.93
1:C:274:THR:HG23	1:C:276:SER:H	1.36	0.91
1:A:274:THR:HG21	1:A:540:HIS:ND1	1.85	0.91
1:E:274:THR:CG2	1:E:276:SER:H	1.84	0.91
1:F:32:MET:HE3	1:F:94:ILE:HG23	1.52	0.91
1:E:32:MET:HE3	1:E:94:ILE:HG23	1.50	0.90
1:C:32:MET:HE2	1:C:94:ILE:HG23	1.54	0.89
1:C:367:LEU:CD1	1:C:425:VAL:HG21	2.01	0.89
1:E:201:MET:HE1	1:E:247:PRO:HB3	1.55	0.89
1:B:274:THR:CG2	1:B:276:SER:H	1.85	0.89
1:C:32:MET:CE	1:C:94:ILE:HG23	2.04	0.87
1:D:273:LEU:HB2	1:D:300:LEU:HD21	1.57	0.86
1:D:13:GLY:O	1:D:143:THR:HB	1.74	0.86
1:E:533:LEU:HD21	1:E:569:MET:HE1	1.54	0.86
1:A:770:ILE:HD11	1:A:772:LEU:HD23	1.59	0.85
1:D:540:HIS:CD2	1:D:541:GLY:N	2.45	0.84
1:D:693:LEU:HD13	1:D:718:ARG:HB2	1.60	0.84
1:B:32:MET:CE	1:B:94:ILE:HG23	2.07	0.84
1:B:274:THR:HG22	1:B:276:SER:N	1.94	0.82
1:F:290:ILE:CD1	1:F:335:LEU:HD22	2.09	0.82
1:E:533:LEU:CD2	1:E:569:MET:HE1	2.08	0.82
1:D:565:LEU:HG	1:D:569:MET:HE2	1.62	0.81
1:E:744:VAL:HG21	1:E:770:ILE:CG2	2.11	0.81
1:C:368:LYS:O	1:C:425:VAL:HG23	1.83	0.79
1:A:274:THR:HG22	1:A:276:SER:N	1.97	0.79
1:C:638:LEU:O	1:C:739:ARG:NH2	2.15	0.79
1:A:525:LYS:HG2	1:A:558:VAL:HG21	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:727:GLY:H	1:D:766:ASN:HD21	1.31	0.78
1:C:201:MET:HE1	1:C:247:PRO:HB3	1.65	0.78
1:C:274:THR:CG2	1:C:540:HIS:HA	2.13	0.78
1:B:32:MET:HE1	1:B:102:GLU:O	1.83	0.78
1:C:273:LEU:HB2	1:C:300:LEU:HD21	1.66	0.78
1:C:425:VAL:HG22	1:C:426:GLN:N	1.96	0.77
1:A:684:GLU:HG2	1:A:732:LYS:HB2	1.66	0.77
1:C:93:THR:CG2	1:C:104:LYS:HB3	2.12	0.77
1:F:274:THR:CG2	1:F:276:SER:H	1.91	0.77
1:F:13:GLY:O	1:F:143:THR:HB	1.84	0.76
1:B:695:ASP:HA	1:B:718:ARG:HG2	1.68	0.76
1:D:315:TRP:HE3	1:D:381:GLN:CD	1.94	0.76
1:E:13:GLY:O	1:E:143:THR:HB	1.86	0.76
1:B:332:ILE:HD12	1:B:333:ARG:N	2.01	0.75
1:C:425:VAL:CG2	1:C:426:GLN:N	2.49	0.75
1:C:274:THR:HG21	1:C:540:HIS:HA	1.69	0.75
1:C:367:LEU:HD11	1:C:425:VAL:CG2	2.16	0.75
1:D:32:MET:HE2	1:D:94:ILE:CG2	2.09	0.74
1:B:761:VAL:HG11	1:B:768:LEU:HD21	1.68	0.74
1:D:735:THR:HG23	1:D:760:VAL:HG13	1.70	0.73
2:E:3006:SO4:O2	5:E:3083:HOH:O	2.06	0.72
1:C:770:ILE:HD11	1:C:772:LEU:HD13	1.73	0.71
1:D:540:HIS:CD2	1:D:540:HIS:C	2.68	0.71
1:E:744:VAL:HG21	1:E:770:ILE:HG22	1.71	0.71
1:A:767:ALA:O	1:A:769:THR:N	2.24	0.71
1:B:638:LEU:O	1:B:739:ARG:NH2	2.23	0.70
1:A:212:HIS:HE1	1:A:238:GLU:H	1.39	0.70
1:A:290:ILE:HD13	1:A:335:LEU:HD22	1.73	0.70
1:A:735:THR:HG23	1:A:760:VAL:HG13	1.74	0.70
1:C:32:MET:HE1	1:C:102:GLU:C	2.17	0.69
1:D:275:THR:O	1:D:276:SER:HB2	1.91	0.69
1:A:128:ARG:NH1	1:A:155:ASP:OD2	2.26	0.69
1:A:212:HIS:CE1	1:A:238:GLU:H	2.10	0.69
1:D:315:TRP:CE3	1:D:381:GLN:CD	2.71	0.69
1:A:748:GLN:HG2	1:A:769:THR:HG23	1.74	0.69
1:D:485:ALA:HB1	1:D:519:ALA:HB2	1.73	0.69
1:C:275:THR:HG23	1:C:281:TYR:CE1	2.29	0.68
1:D:672:GLY:HA3	1:D:680:TYR:OH	1.93	0.68
1:F:201:MET:CE	1:F:502:LEU:HD23	2.24	0.68
1:C:525:LYS:HG2	1:C:558:VAL:HG21	1.75	0.68
1:D:315:TRP:CE3	1:D:381:GLN:NE2	2.62	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:LEU:HD13	1:E:179:VAL:HG11	1.75	0.68
1:E:38:PRO:HD3	1:E:51:PRO:O	1.93	0.68
1:B:525:LYS:HG2	1:B:558:VAL:HG21	1.75	0.67
1:E:179:VAL:HG13	1:E:218:PHE:HB2	1.77	0.66
1:F:681:VAL:HG12	2:F:3005:SO4:O3	1.95	0.66
1:E:324:THR:HG22	1:E:325:PHE:CD2	2.29	0.66
1:E:274:THR:HG22	1:E:276:SER:N	2.04	0.66
1:B:32:MET:HE1	1:B:102:GLU:C	2.21	0.66
1:E:668:LEU:HD21	1:E:714:LEU:HD23	1.78	0.66
1:D:333:ARG:HG3	1:D:333:ARG:HH11	1.59	0.66
1:A:447:LEU:C	1:A:447:LEU:HD23	2.20	0.66
1:D:39:ARG:HD2	5:D:3063:HOH:O	1.96	0.66
1:E:356:VAL:HG11	1:E:397:TRP:HZ2	1.60	0.66
1:B:124:ARG:HD3	1:B:243:ASP:OD1	1.96	0.66
1:A:490:MET:HE2	1:A:620:PHE:CE1	2.31	0.65
1:C:275:THR:HG22	1:C:276:SER:O	1.97	0.65
1:B:13:GLY:O	1:B:143:THR:HB	1.97	0.65
1:A:201:MET:HE1	1:A:247:PRO:HB3	1.78	0.64
1:E:300:LEU:HD12	1:E:340:LEU:HD21	1.79	0.64
1:D:533:LEU:CD1	1:D:569:MET:HE1	2.28	0.64
1:B:201:MET:HE1	1:B:247:PRO:HB3	1.81	0.63
1:D:274:THR:HG23	1:D:304:HIS:HD2	1.63	0.63
1:E:684:GLU:HG2	1:E:732:LYS:HB2	1.79	0.63
1:D:300:LEU:HD13	1:D:340:LEU:HD21	1.81	0.63
1:E:592:MET:HE2	5:E:3145:HOH:O	1.99	0.63
1:F:290:ILE:CD1	1:F:335:LEU:CD2	2.77	0.63
1:E:44:ARG:HA	1:E:47:GLN:HB2	1.80	0.63
1:E:356:VAL:HG11	1:E:397:TRP:CZ2	2.34	0.62
1:F:516:GLU:O	1:F:517:ASN:HB2	1.97	0.62
1:D:315:TRP:CZ3	1:D:381:GLN:NE2	2.66	0.62
1:A:693:LEU:HD13	1:A:718:ARG:HB2	1.81	0.62
1:A:767:ALA:C	1:A:769:THR:N	2.58	0.62
1:D:519:ALA:O	1:D:551:TYR:HE2	1.82	0.62
1:B:174:ARG:O	1:B:177:GLN:HG3	1.98	0.62
1:F:273:LEU:HB2	1:F:300:LEU:HD21	1.82	0.62
1:B:347:ASN:HB2	1:B:348:PRO:HD3	1.82	0.61
1:D:201:MET:HE1	1:D:247:PRO:HB3	1.80	0.61
1:E:490:MET:HE2	1:E:620:PHE:CD1	2.35	0.61
1:C:693:LEU:HD13	1:C:718:ARG:HB2	1.81	0.61
1:E:128:ARG:NH1	1:E:155:ASP:OD2	2.32	0.61
1:A:749:ASP:HB3	1:A:764:GLN:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:540:HIS:HA	1:D:546:ARG:HG3	1.83	0.60
1:A:770:ILE:HD11	1:A:772:LEU:CD2	2.29	0.60
1:F:747:LEU:HD12	1:F:752:GLN:HE21	1.67	0.60
1:B:39:ARG:HD2	5:B:3140:HOH:O	2.00	0.60
1:E:328:PRO:HD2	5:E:3147:HOH:O	2.02	0.60
1:A:212:HIS:CE1	1:A:237:LEU:HD12	2.37	0.60
1:E:662:TYR:OH	5:E:3121:HOH:O	2.16	0.59
1:D:522:HIS:CG	1:D:622:GLU:HG3	2.38	0.59
1:E:592:MET:CE	5:E:3145:HOH:O	2.50	0.59
1:C:277:PHE:CD2	1:C:278:THR:HG23	2.38	0.59
1:F:735:THR:HG23	1:F:760:VAL:HG13	1.84	0.59
1:E:525:LYS:HG2	1:E:558:VAL:HG21	1.85	0.58
1:C:690:LEU:HD11	1:C:693:LEU:HG	1.84	0.58
1:E:693:LEU:HD13	1:E:718:ARG:HB2	1.85	0.58
1:D:290:ILE:HD13	1:D:335:LEU:HD22	1.85	0.58
1:A:485:ALA:HB1	1:A:519:ALA:HB2	1.86	0.58
1:F:290:ILE:HD13	1:F:335:LEU:HD22	1.83	0.58
1:F:526:ARG:HD2	1:F:619:VAL:HB	1.85	0.58
1:C:274:THR:HG22	1:C:540:HIS:HA	1.83	0.58
1:D:274:THR:HG22	1:D:276:SER:H	1.68	0.58
1:C:32:MET:HE3	1:C:94:ILE:HG23	1.84	0.58
1:A:290:ILE:HD13	1:A:335:LEU:CD2	2.33	0.57
1:F:20:LEU:HD22	1:F:134:VAL:CG2	2.34	0.57
1:B:689:HIS:ND1	1:B:739:ARG:NH1	2.52	0.57
1:E:744:VAL:HG22	1:E:771:THR:O	2.03	0.57
1:D:306:ASP:OD1	1:D:540:HIS:HE1	1.88	0.57
1:E:38:PRO:CD	1:E:51:PRO:O	2.52	0.57
1:E:652:GLN:NE2	5:E:3121:HOH:O	2.38	0.57
1:E:516:GLU:O	1:E:517:ASN:HB2	2.03	0.57
1:A:767:ALA:C	1:A:769:THR:H	2.13	0.57
1:B:449:TRP:CH2	1:B:476:PRO:HD2	2.39	0.57
1:C:689:HIS:CE1	1:C:739:ARG:HH11	2.23	0.57
1:F:579:ARG:HG3	1:F:579:ARG:HH11	1.69	0.57
1:E:447:LEU:HD23	1:E:447:LEU:C	2.30	0.56
1:B:261:PRO:HA	1:B:473:GLN:O	2.05	0.56
1:A:212:HIS:HE1	1:A:237:LEU:HD12	1.69	0.56
1:B:201:MET:CE	1:B:247:PRO:HB3	2.34	0.56
1:C:32:MET:HE2	1:C:94:ILE:CG2	2.30	0.56
1:D:557:ASP:OD1	1:D:560:ARG:NH2	2.38	0.56
1:B:767:ALA:O	1:B:768:LEU:C	2.48	0.56
1:E:557:ASP:OD1	1:E:560:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:GLU:O	1:B:517:ASN:HB2	2.05	0.56
1:C:32:MET:HE1	1:C:102:GLU:O	2.06	0.56
1:E:417:PHE:HA	1:E:419:GLU:OE2	2.05	0.56
1:C:681:VAL:HG23	1:C:681:VAL:O	2.05	0.56
1:F:557:ASP:OD1	1:F:560:ARG:NH2	2.39	0.56
1:B:763:PRO:HB3	1:B:768:LEU:HD12	1.88	0.55
1:F:490:MET:HE2	1:F:620:PHE:CD1	2.42	0.55
1:F:133:GLN:HB2	1:F:136:ASN:HD22	1.71	0.55
1:D:735:THR:CG2	1:D:760:VAL:HG13	2.34	0.55
1:F:725:VAL:HB	1:F:768:LEU:HB3	1.87	0.55
1:A:429:ASP:OD1	1:A:431:SER:OG	2.24	0.55
1:D:296:ARG:O	1:D:560:ARG:NH1	2.38	0.55
1:B:569:MET:HB2	1:B:573:LEU:HD22	1.89	0.54
1:C:183:ASN:HB3	1:C:419:GLU:HB3	1.87	0.54
1:C:652:GLN:NE2	1:C:654:HIS:NE2	2.55	0.54
1:C:515:PHE:CD1	1:C:516:GLU:HG2	2.42	0.54
1:E:124:ARG:HD3	1:E:243:ASP:OD1	2.07	0.54
1:E:727:GLY:H	1:E:766:ASN:HD21	1.56	0.54
1:E:174:ARG:O	1:E:177:GLN:HG3	2.07	0.54
1:C:275:THR:HG23	1:C:281:TYR:CD1	2.43	0.54
1:A:183:ASN:HB3	1:A:419:GLU:HB3	1.88	0.54
1:E:485:ALA:HB1	1:E:519:ALA:HB2	1.89	0.54
1:F:681:VAL:CG2	1:F:683:HIS:CE1	2.91	0.54
1:B:332:ILE:HG12	1:B:408:MET:O	2.07	0.54
1:D:525:LYS:NZ	1:D:552:ASP:OD2	2.40	0.54
1:A:617:ALA:O	1:A:660:PRO:HD2	2.08	0.54
1:C:747:LEU:HD13	1:C:750:GLY:O	2.08	0.54
1:D:630:LEU:O	1:D:647:SER:N	2.39	0.54
1:E:289:PHE:HZ	1:E:545:TYR:CD1	2.25	0.54
1:A:44:ARG:HD2	1:F:308:PHE:CE1	2.42	0.54
1:B:417:PHE:HA	1:B:419:GLU:OE2	2.08	0.54
1:D:274:THR:CG2	1:D:304:HIS:HD2	2.19	0.54
1:D:509:SER:HB3	1:D:536:HIS:HB2	1.89	0.54
1:E:252:ASP:HA	1:E:583:ARG:O	2.07	0.54
1:D:727:GLY:N	1:D:766:ASN:HD21	2.04	0.54
1:F:508:TRP:CZ3	1:F:510:HIS:CD2	2.96	0.53
1:A:735:THR:CG2	1:A:760:VAL:HG13	2.39	0.53
1:A:336:LYS:HE2	1:A:409:GLY:O	2.08	0.53
1:C:274:THR:HG23	1:C:276:SER:N	2.14	0.53
1:E:634:ARG:HG2	1:E:692:ASN:ND2	2.23	0.53
1:E:747:LEU:HD12	1:E:752:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLU:O	1:A:517:ASN:HB2	2.08	0.53
1:E:414:LYS:NZ	1:E:538:ARG:HH12	2.07	0.53
1:E:565:LEU:CG	1:E:569:MET:HE2	2.27	0.53
1:A:283:GLU:OE1	1:A:334:ARG:NH1	2.41	0.53
1:F:595:PHE:CE1	1:F:631:PRO:HG2	2.44	0.53
1:A:526:ARG:HD2	1:A:619:VAL:HB	1.90	0.53
1:C:367:LEU:CG	1:C:425:VAL:HG21	2.39	0.53
1:B:750:GLY:HA2	1:B:764:GLN:HG2	1.91	0.53
1:C:296:ARG:O	1:C:560:ARG:NH1	2.32	0.53
1:E:274:THR:CG2	1:E:276:SER:N	2.66	0.53
1:B:681:VAL:HG13	1:B:681:VAL:O	2.10	0.52
1:E:329:GLU:HB2	1:E:408:MET:HG2	1.91	0.52
1:C:560:ARG:HG3	1:C:560:ARG:HH11	1.73	0.52
1:C:695:ASP:OD1	1:C:719:THR:O	2.27	0.52
1:D:617:ALA:O	1:D:660:PRO:HD2	2.10	0.52
1:E:136:ASN:ND2	1:E:227:LYS:HE3	2.24	0.52
1:B:332:ILE:CD1	1:B:408:MET:O	2.57	0.52
1:B:748:GLN:HB2	1:B:769:THR:HB	1.92	0.52
1:C:689:HIS:ND1	1:C:739:ARG:NH1	2.47	0.52
1:C:44:ARG:HB3	1:E:308:PHE:CZ	2.45	0.52
1:C:347:ASN:HB2	1:C:348:PRO:CD	2.40	0.52
1:D:18:HIS:O	1:D:38:PRO:HA	2.09	0.52
1:E:521:ALA:O	1:E:525:LYS:HD3	2.10	0.52
1:D:632:GLU:HG3	1:D:633:GLY:N	2.26	0.52
1:E:102:GLU:HB2	1:E:111:ARG:HG3	1.91	0.52
1:E:414:LYS:HZ1	1:E:538:ARG:HH12	1.57	0.52
1:A:201:MET:CE	1:A:247:PRO:HB3	2.39	0.51
1:C:70:GLU:HG3	5:C:3103:HOH:O	2.11	0.51
1:D:500:ILE:HG12	1:D:505:PHE:HB2	1.92	0.51
1:D:576:GLU:O	1:D:579:ARG:HB2	2.10	0.51
1:D:717:ALA:O	1:D:723:ILE:HA	2.10	0.51
1:D:631:PRO:HD2	1:D:635:TRP:CZ2	2.45	0.51
1:E:744:VAL:CG2	1:E:770:ILE:HG22	2.39	0.51
1:F:634:ARG:HH21	1:F:643:GLU:HB3	1.74	0.51
1:A:274:THR:HG22	1:A:275:THR:N	2.26	0.51
1:B:463:LEU:O	1:B:477:VAL:HG22	2.10	0.51
1:D:533:LEU:HD12	1:D:569:MET:HE1	1.90	0.51
1:E:18:HIS:O	1:E:38:PRO:HA	2.10	0.51
1:E:16:LEU:HD22	1:E:140:VAL:HG22	1.92	0.51
1:C:634:ARG:HG2	1:C:692:ASN:OD1	2.10	0.51
1:D:300:LEU:CD1	1:D:340:LEU:HD21	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:544:SER:HG	1:D:546:ARG:HH12	1.57	0.51
1:E:32:MET:HE1	1:E:102:GLU:N	2.25	0.51
1:D:313:PHE:HA	1:D:381:GLN:HE22	1.76	0.51
1:A:735:THR:HG23	1:A:760:VAL:CG1	2.41	0.50
1:B:690:LEU:HD11	1:B:693:LEU:HG	1.93	0.50
1:F:359:GLU:OE2	1:F:363:LYS:NZ	2.40	0.50
1:A:576:GLU:HG3	1:A:611:GLY:HA3	1.92	0.50
1:C:18:HIS:O	1:C:38:PRO:HA	2.12	0.50
1:E:289:PHE:CZ	1:E:545:TYR:CD1	3.00	0.50
1:B:606:ARG:NH1	5:B:3101:HOH:O	2.41	0.50
1:F:267:TRP:CE3	1:F:341:LYS:HG3	2.47	0.50
1:B:689:HIS:CG	1:B:739:ARG:HH11	2.29	0.50
1:B:619:VAL:HG11	1:B:624:GLY:HA2	1.93	0.50
1:B:329:GLU:O	1:B:332:ILE:HG13	2.11	0.49
1:D:353:LYS:O	1:D:353:LYS:HG2	2.11	0.49
1:D:381:GLN:CB	1:D:384:LEU:HD12	2.34	0.49
1:E:747:LEU:HD11	1:E:752:GLN:HB3	1.94	0.49
1:C:275:THR:CG2	1:C:281:TYR:CZ	2.95	0.49
1:A:201:MET:HE1	1:A:247:PRO:CB	2.42	0.49
1:C:630:LEU:O	1:C:647:SER:N	2.45	0.49
1:C:425:VAL:CG2	1:C:426:GLN:H	2.24	0.49
1:F:201:MET:HE3	1:F:502:LEU:HD23	1.95	0.49
1:F:367:LEU:HG	1:F:425:VAL:CG2	2.43	0.49
1:F:766:ASN:HD22	1:F:767:ALA:N	2.10	0.49
1:A:630:LEU:O	1:A:647:SER:N	2.44	0.49
1:B:474:LYS:O	1:B:476:PRO:HD3	2.12	0.49
1:E:526:ARG:HD2	1:E:619:VAL:HB	1.94	0.49
1:F:267:TRP:CD2	1:F:341:LYS:HG3	2.47	0.49
1:B:273:LEU:HD22	1:B:274:THR:H	1.76	0.48
1:C:160:GLU:HA	1:C:203:ASN:OD1	2.13	0.48
1:B:738:LEU:HD11	1:B:770:ILE:HG21	1.95	0.48
1:D:120:LEU:HB3	1:D:132:SER:HB3	1.95	0.48
1:D:184:ARG:HD3	1:D:192:GLN:CD	2.37	0.48
1:C:515:PHE:HD1	1:C:516:GLU:HG2	1.78	0.48
1:C:20:LEU:HD22	1:C:134:VAL:CG2	2.43	0.48
1:F:501:GLY:HA3	5:F:3119:HOH:O	2.14	0.48
1:A:744:VAL:HG22	1:A:746:GLY:H	1.78	0.48
1:B:18:HIS:O	1:B:38:PRO:HA	2.14	0.48
1:B:167:GLU:HB3	1:B:195:LYS:HB2	1.96	0.48
1:E:533:LEU:HD23	1:E:569:MET:HE1	1.93	0.48
1:A:201:MET:HE1	1:A:247:PRO:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:GLU:OE1	1:C:56:ARG:HD3	2.14	0.48
1:B:347:ASN:HB2	1:B:348:PRO:CD	2.44	0.48
1:C:692:ASN:N	1:C:692:ASN:HD22	2.11	0.48
1:D:349:TYR:HB3	1:D:384:LEU:HD21	1.95	0.48
1:B:447:LEU:HD23	1:B:447:LEU:C	2.38	0.47
1:D:219:GLU:HB2	1:D:229:GLN:HB3	1.96	0.47
1:A:201:MET:HE1	1:A:247:PRO:CA	2.44	0.47
1:A:748:GLN:CG	1:A:769:THR:HG23	2.43	0.47
1:C:275:THR:CG2	1:C:276:SER:O	2.62	0.47
1:E:134:VAL:O	1:E:135:LYS:HB2	2.14	0.47
1:A:619:VAL:HG11	1:A:624:GLY:HA2	1.97	0.47
1:D:174:ARG:NH2	5:D:3028:HOH:O	2.31	0.47
1:D:183:ASN:HB3	1:D:419:GLU:HB3	1.96	0.47
1:A:679:ASP:OD1	1:A:679:ASP:N	2.47	0.47
1:D:346:ILE:HD11	1:D:415:THR:HG22	1.95	0.47
1:F:652:GLN:NE2	1:F:654:HIS:NE2	2.62	0.47
1:B:275:THR:O	1:B:276:SER:HB2	2.13	0.47
1:A:484:TYR:O	1:A:489:SER:HB3	2.14	0.47
1:A:522:HIS:CG	1:A:622:GLU:HG3	2.49	0.47
1:B:20:LEU:HD22	1:B:134:VAL:HG22	1.96	0.47
1:B:309:TRP:CE2	1:B:310:MET:HE2	2.49	0.47
1:B:332:ILE:HD13	1:B:409:GLY:HA3	1.96	0.47
1:B:348:PRO:HG3	1:B:444:TYR:CE1	2.50	0.47
1:B:352:GLN:HA	1:B:357:PHE:CD2	2.50	0.47
1:F:368:LYS:O	1:F:425:VAL:HG22	2.15	0.47
1:F:761:VAL:CG1	1:F:768:LEU:HD11	2.44	0.47
1:F:367:LEU:HG	1:F:425:VAL:HG21	1.95	0.47
1:C:167:GLU:OE2	1:C:195:LYS:NZ	2.44	0.47
1:C:560:ARG:HH11	1:C:560:ARG:CG	2.26	0.47
1:F:631:PRO:HD2	1:F:635:TRP:CZ2	2.50	0.47
1:C:274:THR:HG21	1:C:540:HIS:CG	2.50	0.46
1:C:104:LYS:HG3	1:C:109:SER:HB3	1.98	0.46
1:C:459:GLU:CD	1:C:459:GLU:H	2.22	0.46
1:C:744:VAL:HG22	1:C:746:GLY:H	1.79	0.46
1:E:31:GLU:OE1	1:E:56:ARG:HD3	2.15	0.46
1:B:98:GLU:H	1:B:98:GLU:CD	2.24	0.46
1:C:560:ARG:NH1	1:C:560:ARG:HG3	2.29	0.46
1:F:485:ALA:HB1	1:F:519:ALA:HB2	1.97	0.46
1:D:84:LEU:HG	1:D:257:PHE:CZ	2.51	0.46
1:D:540:HIS:CG	1:D:541:GLY:N	2.82	0.46
1:E:356:VAL:CG1	1:E:397:TRP:HZ2	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:GLU:HG2	1:D:97:THR:HG23	1.96	0.46
1:A:100:TYR:CG	1:A:111:ARG:HD2	2.50	0.46
1:C:516:GLU:O	1:C:517:ASN:HB2	2.15	0.46
1:E:300:LEU:C	1:E:300:LEU:HD13	2.40	0.46
1:A:70:GLU:HG3	5:A:3182:HOH:O	2.15	0.46
1:C:300:LEU:CD1	1:C:340:LEU:HD21	2.46	0.46
1:D:275:THR:O	1:D:276:SER:CB	2.60	0.46
1:D:384:LEU:C	1:D:384:LEU:HD23	2.40	0.46
1:F:300:LEU:CD1	1:F:340:LEU:HD21	2.45	0.46
1:A:725:VAL:HB	1:A:768:LEU:HB3	1.97	0.46
1:B:130:THR:OG1	1:B:131:GLY:N	2.48	0.46
1:C:617:ALA:O	1:C:660:PRO:HD2	2.16	0.46
1:E:165:LEU:HA	1:E:197:ILE:O	2.15	0.46
1:A:336:LYS:HG3	1:A:342:ILE:HD13	1.98	0.46
1:C:300:LEU:HD13	1:C:340:LEU:CD2	2.46	0.46
1:D:668:LEU:O	1:D:701:CYS:HB2	2.15	0.46
1:E:267:TRP:CD2	1:E:341:LYS:HG3	2.51	0.46
1:B:20:LEU:HD22	1:B:134:VAL:CG2	2.45	0.45
1:E:32:MET:HE1	1:E:102:GLU:H	1.80	0.45
1:E:513:GLY:H	1:E:527:TRP:CG	2.34	0.45
1:B:290:ILE:CD1	1:B:335:LEU:HD22	2.46	0.45
1:C:646:GLY:O	1:C:647:SER:HB3	2.16	0.45
1:D:747:LEU:HD13	1:D:750:GLY:O	2.15	0.45
1:E:540:HIS:C	1:E:546:ARG:HG3	2.41	0.45
1:A:690:LEU:HD11	1:A:693:LEU:HG	1.98	0.45
1:B:31:GLU:OE1	1:B:56:ARG:HD3	2.17	0.45
1:E:274:THR:HB	1:E:539:LEU:O	2.16	0.45
1:F:684:GLU:HG2	1:F:732:LYS:HB2	1.99	0.45
1:D:588:MET:HG3	1:D:608:TYR:CD1	2.51	0.45
1:D:684:GLU:HG2	1:D:732:LYS:HB2	1.98	0.45
1:A:308:PHE:CZ	1:B:44:ARG:HB3	2.52	0.45
1:A:453:LYS:HG3	1:A:458:GLU:HG3	1.97	0.45
1:C:540:HIS:C	1:C:546:ARG:HG3	2.41	0.45
1:D:267:TRP:HA	1:D:678:PRO:HG2	1.98	0.45
1:F:219:GLU:HB2	1:F:229:GLN:HB3	1.98	0.45
1:F:766:ASN:HD22	1:F:767:ALA:H	1.64	0.45
1:B:274:THR:HB	1:B:539:LEU:O	2.17	0.45
1:B:474:LYS:C	1:B:476:PRO:HD3	2.42	0.45
1:A:124:ARG:HD3	1:A:243:ASP:OD1	2.17	0.45
1:A:367:LEU:HD11	1:A:425:VAL:HG13	1.97	0.45
1:A:681:VAL:HG22	1:A:684:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:VAL:HG23	1:A:770:ILE:HD12	1.98	0.45
1:D:315:TRP:CE3	1:D:381:GLN:OE1	2.70	0.45
1:F:479:TRP:CD1	1:F:481:GLY:H	2.34	0.45
1:B:315:TRP:O	1:B:350:ILE:HA	2.16	0.45
1:B:327:ASP:OD2	1:B:330:GLY:HA3	2.16	0.45
1:D:483:CYS:SG	1:D:514:GLY:HA2	2.57	0.45
1:F:579:ARG:HD2	1:F:589:ARG:HH22	1.82	0.45
1:F:748:GLN:HG3	1:F:769:THR:HB	1.98	0.45
1:B:183:ASN:HA	1:B:196:ASN:ND2	2.32	0.45
1:D:274:THR:HG23	1:D:304:HIS:CD2	2.47	0.45
1:E:548:PRO:HB2	1:E:556:CYS:SG	2.57	0.45
1:F:417:PHE:HA	1:F:419:GLU:OE2	2.16	0.45
1:F:681:VAL:HG23	1:F:683:HIS:CE1	2.52	0.45
1:B:165:LEU:HA	1:B:197:ILE:O	2.16	0.44
1:B:369:ARG:HB3	1:B:370:PRO:HD2	1.99	0.44
1:F:694:GLN:O	1:F:697:HIS:HB2	2.17	0.44
1:C:17:ILE:HG13	1:C:139:TYR:HB3	1.99	0.44
1:C:598:ASP:HA	1:C:599:PRO:HD2	1.87	0.44
1:F:152:GLU:HB3	1:F:230:PHE:CE1	2.52	0.44
1:F:290:ILE:HD11	1:F:335:LEU:HD22	1.95	0.44
1:B:414:LYS:NZ	1:B:538:ARG:HH12	2.13	0.44
1:C:195:LYS:HB3	1:C:468:ALA:HB3	2.00	0.44
1:E:515:PHE:CD1	1:E:516:GLU:HG2	2.52	0.44
1:F:396:LYS:NZ	1:F:400:ASP:OD2	2.34	0.44
1:F:763:PRO:HB3	1:F:768:LEU:HD22	1.98	0.44
1:B:219:GLU:HB2	1:B:229:GLN:HB3	2.00	0.44
1:C:174:ARG:HB3	1:C:220:VAL:HG11	1.99	0.44
1:D:727:GLY:H	1:D:766:ASN:ND2	2.08	0.44
1:E:340:LEU:HD23	1:E:340:LEU:HA	1.84	0.44
1:B:725:VAL:HB	1:B:768:LEU:HB3	1.99	0.44
1:F:201:MET:CE	1:F:502:LEU:CD2	2.95	0.44
1:F:744:VAL:CG2	1:F:770:ILE:HD12	2.48	0.44
1:B:479:TRP:CD1	1:B:481:GLY:H	2.36	0.44
1:C:684:GLU:HG2	1:C:732:LYS:HB2	2.00	0.44
1:D:196:ASN:O	1:D:197:ILE:HD13	2.17	0.44
1:D:695:ASP:HA	1:D:718:ARG:HD3	2.00	0.44
1:E:324:THR:CG2	1:E:325:PHE:CD2	2.99	0.44
1:E:416:ASP:OD1	1:E:466:ARG:HD3	2.18	0.44
1:F:333:ARG:NH1	2:F:3009:SO4:O4	2.29	0.44
1:F:333:ARG:NH1	2:F:3009:SO4:S	2.90	0.44
1:F:767:ALA:O	1:F:768:LEU:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:GLN:HB2	1:C:64:ILE:HD12	2.00	0.44
1:E:109:SER:O	1:E:122:PHE:HA	2.18	0.44
1:E:723:ILE:HG12	1:E:770:ILE:HB	1.99	0.44
1:C:11:GLN:HA	1:C:12:PRO:HD3	1.83	0.44
1:D:17:ILE:HG13	1:D:139:TYR:HB3	2.00	0.44
1:F:297:ASN:O	1:F:560:ARG:HD3	2.17	0.44
1:A:770:ILE:O	1:A:770:ILE:HG13	2.16	0.43
1:B:629:TYR:HA	1:B:649:TRP:HA	2.00	0.43
1:D:277:PHE:CD2	1:D:278:THR:HG23	2.52	0.43
1:F:744:VAL:HG22	1:F:746:GLY:H	1.82	0.43
1:C:306:ASP:O	1:C:309:TRP:HD1	2.01	0.43
1:C:588:MET:HG3	1:C:608:TYR:CD1	2.53	0.43
1:A:321:ASP:HA	1:A:322:PRO:HD3	1.86	0.43
1:A:554:GLU:O	1:A:558:VAL:HG23	2.19	0.43
1:D:515:PHE:HB3	1:D:516:GLU:H	1.69	0.43
1:D:541:GLY:HA3	1:D:546:ARG:CZ	2.49	0.43
1:F:300:LEU:HD13	1:F:340:LEU:HD21	2.00	0.43
1:B:347:ASN:CB	1:B:348:PRO:CD	2.97	0.43
1:C:436:MET:O	1:C:437:HIS:C	2.61	0.43
1:D:165:LEU:HA	1:D:197:ILE:O	2.18	0.43
1:E:191:GLU:OE1	1:E:191:GLU:N	2.48	0.43
1:F:735:THR:HG23	1:F:760:VAL:CG1	2.48	0.43
1:A:634:ARG:HD2	1:A:692:ASN:OD1	2.18	0.43
1:C:619:VAL:HG11	1:C:624:GLY:HA2	2.01	0.43
1:D:280:ASN:O	1:D:281:TYR:HB3	2.18	0.43
1:E:352:GLN:HA	1:E:357:PHE:CD2	2.53	0.43
1:E:598:ASP:OD2	1:E:629:TYR:OH	2.35	0.43
1:F:123:LEU:N	1:F:123:LEU:HD22	2.33	0.43
1:D:381:GLN:HA	1:D:381:GLN:HE21	1.83	0.43
1:E:136:ASN:HD21	1:E:227:LYS:HE3	1.83	0.43
1:E:689:HIS:ND1	1:E:739:ARG:HD3	2.33	0.43
1:F:664:ARG:HH11	1:F:664:ARG:HD2	1.67	0.43
1:A:747:LEU:HD13	1:A:750:GLY:O	2.18	0.43
1:B:715:LYS:O	1:B:725:VAL:HA	2.19	0.43
1:C:174:ARG:O	1:C:177:GLN:HG2	2.19	0.43
1:C:763:PRO:HB3	1:C:768:LEU:HD22	2.00	0.43
1:C:764:GLN:O	1:C:764:GLN:HG2	2.19	0.43
1:F:61:GLN:HB2	1:F:64:ILE:HD12	1.99	0.43
1:F:346:ILE:HD11	1:F:415:THR:HG22	2.01	0.43
1:A:498:LEU:HD21	1:A:608:TYR:HB3	2.01	0.42
1:C:692:ASN:HD22	1:C:692:ASN:H	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:ILE:CD1	1:D:335:LEU:HD22	2.49	0.42
1:D:595:PHE:CE1	1:D:631:PRO:HG2	2.53	0.42
1:B:613:ASN:HA	1:B:664:ARG:HD2	2.00	0.42
1:C:55:LEU:N	1:C:55:LEU:HD12	2.33	0.42
1:F:18:HIS:O	1:F:38:PRO:HA	2.18	0.42
1:F:352:GLN:HA	1:F:357:PHE:CD2	2.54	0.42
1:F:735:THR:CG2	1:F:760:VAL:HG13	2.49	0.42
1:F:668:LEU:HD21	1:F:714:LEU:HD13	2.00	0.42
1:A:261:PRO:HA	1:A:473:GLN:O	2.19	0.42
1:A:448:VAL:HG12	1:A:463:LEU:HD21	2.02	0.42
1:B:472:ALA:HB1	5:B:3089:HOH:O	2.20	0.42
1:F:429:ASP:OD1	1:F:431:SER:OG	2.37	0.42
1:A:447:LEU:C	1:A:447:LEU:CD2	2.92	0.42
1:B:717:ALA:O	1:B:723:ILE:HA	2.19	0.42
1:C:576:GLU:HG3	1:C:611:GLY:HA3	2.01	0.42
1:F:261:PRO:HA	1:F:473:GLN:O	2.20	0.42
1:F:300:LEU:HD13	1:F:340:LEU:CD2	2.49	0.42
1:A:261:PRO:O	1:A:581:ASN:HA	2.20	0.42
1:A:414:LYS:NZ	1:A:538:ARG:HH12	2.17	0.42
1:C:20:LEU:HD22	1:C:134:VAL:HG22	2.00	0.42
1:C:275:THR:HG21	1:C:281:TYR:CE2	2.54	0.42
1:E:267:TRP:CE3	1:E:341:LYS:HG3	2.54	0.42
1:B:291:ASP:O	1:B:295:GLU:HG3	2.20	0.42
1:B:321:ASP:HA	1:B:322:PRO:HD3	1.86	0.42
1:B:429:ASP:OD1	1:B:431:SER:OG	2.36	0.42
1:B:657:LEU:HB2	5:B:3155:HOH:O	2.20	0.42
1:C:167:GLU:HB2	1:C:500:ILE:HG13	2.01	0.42
1:C:560:ARG:NH1	1:C:560:ARG:CG	2.81	0.42
1:C:689:HIS:CE1	1:C:739:ARG:NH1	2.87	0.42
1:D:211:ASN:ND2	1:D:238:GLU:OE1	2.48	0.42
1:A:767:ALA:O	1:A:768:LEU:C	2.63	0.42
1:B:555:SER:O	1:B:559:VAL:HG23	2.20	0.42
1:C:425:VAL:HG23	1:C:426:GLN:H	1.85	0.42
1:C:431:SER:HB3	1:C:436:MET:HG2	2.02	0.42
1:C:715:LYS:O	1:C:725:VAL:HA	2.19	0.42
1:B:598:ASP:HA	1:B:599:PRO:HD2	1.93	0.42
1:C:347:ASN:CB	1:C:348:PRO:CD	2.96	0.42
1:C:744:VAL:HG22	1:C:746:GLY:N	2.35	0.42
1:D:160:GLU:HG3	1:D:204:ARG:HG2	2.02	0.42
1:F:1:MET:N	1:F:219:GLU:OE2	2.48	0.42
1:A:336:LYS:HZ3	1:A:336:LYS:HG2	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:GLU:H	1:A:459:GLU:HG3	1.69	0.42
1:B:168:ARG:HG3	1:B:174:ARG:NH2	2.35	0.42
1:B:408:MET:O	1:B:408:MET:HG2	2.19	0.42
1:E:163:TYR:HB3	1:E:502:LEU:HD13	2.01	0.42
1:B:123:LEU:HA	1:B:127:GLU:O	2.20	0.41
1:D:347:ASN:HA	1:D:444:TYR:OH	2.19	0.41
1:D:540:HIS:N	1:D:546:ARG:HD2	2.35	0.41
1:C:767:ALA:O	1:C:768:LEU:O	2.37	0.41
1:D:358:LYS:O	1:D:362:GLU:HG3	2.20	0.41
1:D:631:PRO:O	1:D:646:GLY:HA3	2.20	0.41
1:D:725:VAL:HB	1:D:768:LEU:HD12	2.02	0.41
1:E:565:LEU:O	1:E:569:MET:HG3	2.20	0.41
1:B:195:LYS:HE2	1:B:478:HIS:HB3	2.03	0.41
1:C:315:TRP:O	1:C:350:ILE:HA	2.19	0.41
1:D:32:MET:HB2	1:D:32:MET:HE3	1.75	0.41
1:E:296:ARG:O	1:E:560:ARG:NH1	2.52	0.41
1:E:315:TRP:O	1:E:350:ILE:HA	2.20	0.41
1:F:273:LEU:HD23	1:F:539:LEU:HB2	2.02	0.41
1:A:414:LYS:HE3	1:A:479:TRP:CH2	2.56	0.41
1:C:579:ARG:NH1	1:C:579:ARG:HG3	2.36	0.41
1:D:309:TRP:CE2	1:D:310:MET:HE2	2.55	0.41
1:D:463:LEU:O	1:D:477:VAL:HG22	2.20	0.41
1:E:300:LEU:HD13	1:E:301:HIS:N	2.35	0.41
1:B:31:GLU:HG2	1:B:58:PHE:HB3	2.02	0.41
1:C:150:MET:HB3	1:C:237:LEU:HB2	2.01	0.41
1:C:479:TRP:CD1	1:C:481:GLY:H	2.38	0.41
1:F:32:MET:HE1	1:F:102:GLU:N	2.35	0.41
1:F:212:HIS:HA	1:F:213:PRO:HD3	1.87	0.41
1:A:123:LEU:HD12	1:A:128:ARG:HA	2.02	0.41
1:C:17:ILE:CG1	1:C:139:TYR:HB3	2.51	0.41
1:C:570:MET:HG3	1:C:678:PRO:HA	2.02	0.41
1:E:382:PRO:HG2	5:E:3049:HOH:O	2.20	0.41
1:E:489:SER:O	1:E:492:GLU:HG2	2.20	0.41
1:F:619:VAL:HG11	1:F:624:GLY:HA2	2.01	0.41
1:B:150:MET:HB3	1:B:237:LEU:HB2	2.01	0.41
1:B:167:GLU:OE2	1:B:195:LYS:NZ	2.46	0.41
1:F:579:ARG:HG3	1:F:579:ARG:NH1	2.32	0.41
1:B:674:ASN:HB3	1:B:680:TYR:CE1	2.56	0.41
1:E:165:LEU:HD12	1:E:174:ARG:HG2	2.03	0.41
1:F:120:LEU:C	1:F:120:LEU:CD2	2.93	0.41
1:A:18:HIS:O	1:A:38:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:LYS:O	1:B:342:ILE:HD12	2.20	0.41
1:B:448:VAL:HG12	1:B:463:LEU:HD21	2.02	0.41
1:C:32:MET:HB2	1:C:94:ILE:HD13	2.02	0.41
1:C:170:THR:HG1	1:C:177:GLN:HE22	1.61	0.41
1:C:526:ARG:HD2	1:C:619:VAL:HB	2.02	0.41
1:E:196:ASN:C	1:E:197:ILE:HG12	2.46	0.41
1:F:31:GLU:OE1	1:F:56:ARG:HD3	2.21	0.41
1:F:388:ASP:OD1	1:F:388:ASP:C	2.63	0.41
1:F:459:GLU:H	1:F:459:GLU:HG3	1.29	0.41
1:F:617:ALA:O	1:F:660:PRO:HD2	2.21	0.41
1:B:749:ASP:HB3	1:B:765:GLY:O	2.21	0.41
1:C:352:GLN:HA	1:C:357:PHE:CD2	2.56	0.41
1:C:692:ASN:N	1:C:692:ASN:ND2	2.69	0.41
1:E:680:TYR:CE2	1:E:682:TRP:HD1	2.39	0.41
1:C:485:ALA:HB1	1:C:519:ALA:HB2	2.03	0.40
1:D:278:THR:HG21	1:E:45:THR:HA	2.03	0.40
1:E:652:GLN:NE2	1:E:654:HIS:NE2	2.69	0.40
1:F:291:ASP:OD1	1:F:338:LYS:NZ	2.54	0.40
1:A:367:LEU:HD11	1:A:425:VAL:CG1	2.51	0.40
1:A:622:GLU:HA	5:A:3158:HOH:O	2.22	0.40
1:A:768:LEU:HD23	1:A:768:LEU:HA	1.66	0.40
1:D:509:SER:HB3	1:D:536:HIS:CB	2.52	0.40
1:E:508:TRP:CZ3	1:E:510:HIS:CD2	3.09	0.40
1:F:681:VAL:HG13	1:F:684:GLU:HB2	2.02	0.40
1:A:195:LYS:HE2	1:A:478:HIS:HB3	2.03	0.40
1:C:196:ASN:C	1:C:197:ILE:HG12	2.46	0.40
1:E:212:HIS:HA	1:E:213:PRO:HD3	1.87	0.40
1:F:320:TRP:CD2	1:F:328:PRO:HB3	2.56	0.40
1:F:333:ARG:NH1	2:F:3009:SO4:O3	2.54	0.40
1:F:668:LEU:O	1:F:701:CYS:HB2	2.22	0.40
1:B:32:MET:HE3	1:B:94:ILE:HG23	1.97	0.40
1:C:275:THR:HG23	1:C:281:TYR:CZ	2.56	0.40
1:C:713:THR:O	1:C:727:GLY:HA2	2.21	0.40
1:D:526:ARG:HD2	1:D:619:VAL:HB	2.03	0.40
1:F:199:PHE:HA	1:F:208:VAL:O	2.20	0.40
1:F:767:ALA:O	1:F:769:THR:N	2.55	0.40
1:B:487:TYR:OH	1:B:522:HIS:ND1	2.45	0.40
1:C:84:LEU:HD12	1:C:258:THR:HG22	2.04	0.40
1:D:525:LYS:HG2	1:D:558:VAL:HG21	2.03	0.40
1:D:540:HIS:C	1:D:540:HIS:HD2	2.28	0.40
1:E:38:PRO:HG2	1:E:51:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:THR:CG2	1:E:540:HIS:ND1	2.60	0.40
1:E:588:MET:HG3	1:E:608:TYR:CD1	2.57	0.40
1:E:747:LEU:HD12	1:E:752:GLN:HE21	1.85	0.40
1:F:453:LYS:HE3	1:F:453:LYS:HB3	1.77	0.40
1:F:634:ARG:HH21	1:F:643:GLU:CB	2.35	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	771/778 (99%)	744 (96%)	25 (3%)	2 (0%)	36	42
1	B	771/778 (99%)	731 (95%)	37 (5%)	3 (0%)	30	34
1	C	771/778 (99%)	740 (96%)	27 (4%)	4 (0%)	24	27
1	D	771/778 (99%)	733 (95%)	32 (4%)	6 (1%)	16	16
1	E	771/778 (99%)	738 (96%)	29 (4%)	4 (0%)	24	27
1	F	771/778 (99%)	739 (96%)	26 (3%)	6 (1%)	16	16
All	All	4626/4668 (99%)	4425 (96%)	176 (4%)	25 (0%)	24	27

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	768	LEU
1	B	767	ALA
1	C	766	ASN
1	C	768	LEU
1	E	768	LEU
1	F	767	ALA
1	B	768	LEU

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Mol	Chain	Res	Type
1	C	477	VAL
1	C	767	ALA
1	D	276	SER
1	D	316	CYS
1	D	477	VAL
1	F	768	LEU
1	F	316	CYS
1	D	720	GLY
1	B	477	VAL
1	E	477	VAL
1	F	477	VAL
1	F	720	GLY
1	A	348	PRO
1	D	515	PHE
1	E	47	GLN
1	F	766	ASN
1	D	348	PRO
1	E	720	GLY

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	659/665 (99%)	610 (93%)	49 (7%)	13	14
1	B	659/665 (99%)	605 (92%)	54 (8%)	10	12
1	C	659/665 (99%)	610 (93%)	49 (7%)	13	14
1	D	659/665 (99%)	599 (91%)	60 (9%)	9	9
1	E	659/665 (99%)	597 (91%)	62 (9%)	8	9
1	F	659/665 (99%)	600 (91%)	59 (9%)	9	9
All	All	3954/3990 (99%)	3621 (92%)	333 (8%)	10	11

All (333) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	48	LEU
1	A	52	LEU
1	A	69	ILE
1	A	84	LEU
1	A	91	LYS
1	A	99	ARG
1	A	120	LEU
1	A	123	LEU
1	A	174	ARG
1	A	179	VAL
1	A	208	VAL
1	A	273	LEU
1	A	290	ILE
1	A	300	LEU
1	A	311	LYS
1	A	336	LYS
1	A	356	VAL
1	A	419	GLU
1	A	425	VAL
1	A	431	SER
1	A	447	LEU
1	A	452	LEU
1	A	459	GLU
1	A	464	PHE
1	A	479	TRP
1	A	492	GLU
1	A	500	ILE
1	A	533	LEU
1	A	573	LEU
1	A	592	MET
1	A	614	VAL
1	A	616	VAL
1	A	630	LEU
1	A	657	LEU
1	A	671	LEU
1	A	681	VAL
1	A	693	LEU
1	A	714	LEU
1	A	723	ILE
1	A	732	LYS
1	A	735	THR
1	A	736	LEU

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Mol	Chain	Res	Type
1	A	748	GLN
1	A	759	LEU
1	A	764	GLN
1	A	768	LEU
1	A	769	THR
1	A	770	ILE
1	B	48	LEU
1	B	52	LEU
1	B	69	ILE
1	B	84	LEU
1	B	99	ARG
1	B	120	LEU
1	B	123	LEU
1	B	127	GLU
1	B	143	THR
1	B	177	GLN
1	B	179	VAL
1	B	208	VAL
1	B	273	LEU
1	B	274	THR
1	B	285	THR
1	B	311	LYS
1	B	316	CYS
1	B	329	GLU
1	B	338	LYS
1	B	342	ILE
1	B	356	VAL
1	B	419	GLU
1	B	452	LEU
1	B	453	LYS
1	B	459	GLU
1	B	464	PHE
1	B	477	VAL
1	B	500	ILE
1	B	532	LEU
1	B	533	LEU
1	B	573	LEU
1	B	592	MET
1	B	616	VAL
1	B	625	ASP
1	B	630	LEU
1	B	634	ARG

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Mol	Chain	Res	Type
1	B	653	GLN
1	B	657	LEU
1	B	664	ARG
1	B	671	LEU
1	B	693	LEU
1	B	714	LEU
1	B	719	THR
1	B	726	THR
1	B	732	LYS
1	B	736	LEU
1	B	739	ARG
1	B	744	VAL
1	B	747	LEU
1	B	748	GLN
1	B	764	GLN
1	B	768	LEU
1	B	769	THR
1	B	771	THR
1	C	20	LEU
1	C	48	LEU
1	C	52	LEU
1	C	84	LEU
1	C	120	LEU
1	C	123	LEU
1	C	146	GLN
1	C	174	ARG
1	C	179	VAL
1	C	204	ARG
1	C	208	VAL
1	C	273	LEU
1	C	275	THR
1	C	300	LEU
1	C	306	ASP
1	C	316	CYS
1	C	348	PRO
1	C	350	ILE
1	C	356	VAL
1	C	408	MET
1	C	419	GLU
1	C	447	LEU
1	C	452	LEU
1	C	459	GLU

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Mol	Chain	Res	Type
1	C	464	PHE
1	C	477	VAL
1	C	479	TRP
1	C	492	GLU
1	C	500	ILE
1	C	525	LYS
1	C	532	LEU
1	C	533	LEU
1	C	553	ASP
1	C	573	LEU
1	C	579	ARG
1	C	614	VAL
1	C	616	VAL
1	C	630	LEU
1	C	657	LEU
1	C	671	LEU
1	C	693	LEU
1	C	714	LEU
1	C	735	THR
1	C	736	LEU
1	C	747	LEU
1	C	764	GLN
1	C	768	LEU
1	C	770	ILE
1	C	772	LEU
1	D	48	LEU
1	D	52	LEU
1	D	69	ILE
1	D	84	LEU
1	D	120	LEU
1	D	143	THR
1	D	174	ARG
1	D	177	GLN
1	D	178	THR
1	D	179	VAL
1	D	204	ARG
1	D	208	VAL
1	D	273	LEU
1	D	289	PHE
1	D	300	LEU
1	D	306	ASP
1	D	311	LYS

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Mol	Chain	Res	Type
1	D	316	CYS
1	D	333	ARG
1	D	336	LYS
1	D	342	ILE
1	D	419	GLU
1	D	452	LEU
1	D	459	GLU
1	D	477	VAL
1	D	517	ASN
1	D	518	THR
1	D	525	LYS
1	D	533	LEU
1	D	540	HIS
1	D	543	LYS
1	D	545	TYR
1	D	546	ARG
1	D	547	VAL
1	D	573	LEU
1	D	592	MET
1	D	614	VAL
1	D	616	VAL
1	D	630	LEU
1	D	632	GLU
1	D	657	LEU
1	D	671	LEU
1	D	681	VAL
1	D	693	LEU
1	D	714	LEU
1	D	719	THR
1	D	723	ILE
1	D	726	THR
1	D	735	THR
1	D	736	LEU
1	D	742	VAL
1	D	744	VAL
1	D	747	LEU
1	D	748	GLN
1	D	762	LYS
1	D	764	GLN
1	D	768	LEU
1	D	770	ILE
1	D	771	THR

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Mol	Chain	Res	Type
1	D	772	LEU
1	E	20	LEU
1	E	43	GLU
1	E	44	ARG
1	E	47	GLN
1	E	48	LEU
1	E	52	LEU
1	E	84	LEU
1	E	91	LYS
1	E	98	GLU
1	E	116	GLU
1	E	120	LEU
1	E	127	GLU
1	E	143	THR
1	E	146	GLN
1	E	174	ARG
1	E	177	GLN
1	E	178	THR
1	E	179	VAL
1	E	204	ARG
1	E	208	VAL
1	E	214	GLN
1	E	274	THR
1	E	288	SER
1	E	311	LYS
1	E	316	CYS
1	E	324	THR
1	E	356	VAL
1	E	419	GLU
1	E	447	LEU
1	E	452	LEU
1	E	459	GLU
1	E	464	PHE
1	E	477	VAL
1	E	479	TRP
1	E	500	ILE
1	E	532	LEU
1	E	537	SER
1	E	573	LEU
1	E	614	VAL
1	E	616	VAL
1	E	625	ASP

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Mol	Chain	Res	Type
1	E	630	LEU
1	E	632	GLU
1	E	653	GLN
1	E	669	LEU
1	E	671	LEU
1	E	681	VAL
1	E	693	LEU
1	E	719	THR
1	E	723	ILE
1	E	726	THR
1	E	735	THR
1	E	736	LEU
1	E	742	VAL
1	E	744	VAL
1	E	747	LEU
1	E	748	GLN
1	E	757	GLN
1	E	764	GLN
1	E	769	THR
1	E	770	ILE
1	E	772	LEU
1	F	27	GLN
1	F	52	LEU
1	F	69	ILE
1	F	84	LEU
1	F	87	LEU
1	F	91	LYS
1	F	120	LEU
1	F	123	LEU
1	F	127	GLU
1	F	143	THR
1	F	174	ARG
1	F	178	THR
1	F	179	VAL
1	F	204	ARG
1	F	208	VAL
1	F	273	LEU
1	F	274	THR
1	F	295	GLU
1	F	300	LEU
1	F	311	LYS
1	F	316	CYS

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Mol	Chain	Res	Type
1	F	334	ARG
1	F	342	ILE
1	F	350	ILE
1	F	408	MET
1	F	419	GLU
1	F	425	VAL
1	F	452	LEU
1	F	453	LYS
1	F	459	GLU
1	F	464	PHE
1	F	477	VAL
1	F	479	TRP
1	F	500	ILE
1	F	518	THR
1	F	533	LEU
1	F	573	LEU
1	F	592	MET
1	F	614	VAL
1	F	616	VAL
1	F	630	LEU
1	F	632	GLU
1	F	657	LEU
1	F	671	LEU
1	F	693	LEU
1	F	714	LEU
1	F	719	THR
1	F	726	THR
1	F	732	LYS
1	F	735	THR
1	F	736	LEU
1	F	742	VAL
1	F	747	LEU
1	F	748	GLN
1	F	756	GLU
1	F	764	GLN
1	F	766	ASN
1	F	770	ILE
1	F	771	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	27	GLN
1	A	47	GLN
1	A	125	ASN
1	A	212	HIS
1	A	287	ASN
1	A	426	GLN
1	A	445	ASN
1	A	517	ASN
1	A	692	ASN
1	A	733	ASN
1	B	27	GLN
1	B	47	GLN
1	B	73	GLN
1	B	107	ASN
1	B	133	GLN
1	B	177	GLN
1	B	426	GLN
1	B	517	ASN
1	B	564	GLN
1	B	652	GLN
1	B	683	HIS
1	B	752	GLN
1	B	764	GLN
1	C	15	ASN
1	C	27	GLN
1	C	47	GLN
1	C	107	ASN
1	C	125	ASN
1	C	141	GLN
1	C	146	GLN
1	C	177	GLN
1	C	445	ASN
1	C	517	ASN
1	C	564	GLN
1	C	652	GLN
1	C	692	ASN
1	C	697	HIS
1	C	764	GLN
1	D	27	GLN
1	D	73	GLN
1	D	81	HIS
1	D	88	GLN

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Mol	Chain	Res	Type
1	D	107	ASN
1	D	125	ASN
1	D	133	GLN
1	D	146	GLN
1	D	287	ASN
1	D	381	GLN
1	D	564	GLN
1	D	613	ASN
1	D	652	GLN
1	D	683	HIS
1	D	745	ASN
1	D	766	ASN
1	E	15	ASN
1	E	27	GLN
1	E	47	GLN
1	E	73	GLN
1	E	133	GLN
1	E	141	GLN
1	E	144	ASN
1	E	211	ASN
1	E	517	ASN
1	E	652	GLN
1	E	697	HIS
1	E	748	GLN
1	E	752	GLN
1	E	764	GLN
1	E	766	ASN
1	F	47	GLN
1	F	73	GLN
1	F	125	ASN
1	F	133	GLN
1	F	146	GLN
1	F	177	GLN
1	F	517	ASN
1	F	564	GLN
1	F	613	ASN
1	F	652	GLN
1	F	653	GLN
1	F	692	ASN
1	F	752	GLN
1	F	766	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

25 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$
3	ACY	A	2003	-	3,3,3	0.96	0	3,3,3	1.09	0
2	SO4	F	3005	-	4,4,4	0.57	0	6,6,6	0.89	0
2	SO4	B	3016	-	4,4,4	0.35	0	6,6,6	0.32	0
2	SO4	F	3003	-	4,4,4	0.29	0	6,6,6	0.55	0
3	ACY	E	2001	-	3,3,3	1.22	0	3,3,3	0.66	0
2	SO4	C	3012	-	4,4,4	0.38	0	6,6,6	0.63	0
4	MPO	B	1001	-	13,13,13	1.82	2 (15%)	17,17,17	1.48	2 (11%)
2	SO4	B	3010	-	4,4,4	0.30	0	6,6,6	0.43	0
2	SO4	F	3002	-	4,4,4	0.24	0	6,6,6	0.41	0
2	SO4	F	3001	-	4,4,4	0.36	0	6,6,6	0.21	0
2	SO4	B	3008	-	4,4,4	0.29	0	6,6,6	0.39	0
3	ACY	F	2002	-	3,3,3	0.90	0	3,3,3	1.23	0
2	SO4	D	3011	-	4,4,4	0.30	0	6,6,6	0.41	0
2	SO4	A	3018	-	4,4,4	0.30	0	6,6,6	0.11	0
2	SO4	E	3006	-	4,4,4	0.22	0	6,6,6	0.45	0
2	SO4	D	3004	-	4,4,4	0.39	0	6,6,6	0.42	0
2	SO4	F	3009	-	4,4,4	0.41	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	3007	-	4,4,4	0.18	0	6,6,6	0.15	0
4	MPO	E	1004	-	13,13,13	1.77	2 (15%)	17,17,17	1.10	1 (5%)
2	SO4	B	3015	-	4,4,4	0.36	0	6,6,6	0.22	0
2	SO4	A	3017	-	4,4,4	0.27	0	6,6,6	0.44	0
4	MPO	C	1002	-	13,13,13	1.41	1 (7%)	17,17,17	1.28	2 (11%)
2	SO4	A	3014	-	4,4,4	0.27	0	6,6,6	0.33	0
2	SO4	B	3013	-	4,4,4	0.30	0	6,6,6	0.36	0
4	MPO	D	1003	-	13,13,13	1.28	1 (7%)	17,17,17	1.42	3 (17%)

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
4	MPO	D	1003	-	-	4/7/15/15	0/1/1/1
4	MPO	B	1001	-	-	0/7/15/15	0/1/1/1
4	MPO	E	1004	-	-	1/7/15/15	0/1/1/1
4	MPO	C	1002	-	-	0/7/15/15	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	MPO	C1-S1	5.42	1.85	1.77
4	E	1004	MPO	C1-S1	4.50	1.83	1.77
4	C	1002	MPO	C1-S1	4.16	1.83	1.77
4	D	1003	MPO	C1-S1	3.59	1.82	1.77
4	B	1001	MPO	O2-S1	2.25	1.51	1.45
4	E	1004	MPO	O4-C5	2.08	1.50	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1001	MPO	O1-S1-C1	3.15	111.49	106.73
4	D	1003	MPO	O4-C6-C7	-3.10	105.10	111.77
4	E	1004	MPO	O2-S1-C1	2.38	110.33	106.73
4	D	1003	MPO	C7-N1-C4	2.37	113.95	108.84
4	C	1002	MPO	C5-C4-N1	-2.26	106.69	110.12
4	D	1003	MPO	O2-S1-C1	2.26	110.14	106.73
4	B	1001	MPO	O4-C5-C4	-2.18	107.07	111.77
4	C	1002	MPO	C3-N1-C7	-2.10	105.65	111.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1003	MPO	C2-C3-N1-C7
4	D	1003	MPO	C2-C3-N1-C4
4	D	1003	MPO	C2-C1-S1-O2
4	D	1003	MPO	C2-C1-S1-O3
4	E	1004	MPO	C1-C2-C3-N1

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3005	SO4	1	0
2	E	3006	SO4	1	0
2	F	3009	SO4	3	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	773/778 (99%)	-0.25	11 (1%) 73 71	18, 29, 47, 71	0
1	B	773/778 (99%)	0.12	22 (2%) 55 52	23, 36, 60, 81	0
1	C	773/778 (99%)	-0.21	10 (1%) 75 73	20, 30, 47, 75	0
1	D	773/778 (99%)	0.07	48 (6%) 26 23	19, 32, 64, 78	0
1	E	773/778 (99%)	-0.07	25 (3%) 50 47	20, 33, 57, 89	0
1	F	773/778 (99%)	-0.16	11 (1%) 73 71	21, 31, 50, 69	0
All	All	4638/4668 (99%)	-0.08	127 (2%) 56 53	18, 32, 55, 89	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	278	THR	7.0
1	D	545	TYR	5.9
1	B	766	ASN	5.7
1	D	275	THR	5.7
1	F	773	HIS	5.7
1	D	281	TYR	5.4
1	D	279	THR	5.0
1	B	767	ALA	4.9
1	B	765	GLY	4.9
1	B	773	HIS	4.9
1	D	380	TRP	4.8
1	C	773	HIS	4.7
1	F	768	LEU	4.7
1	C	767	ALA	4.6
1	D	277	PHE	4.5
1	E	773	HIS	4.5
1	D	773	HIS	4.5
1	D	540	HIS	4.4
1	D	541	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	719	THR	4.3
1	D	546	ARG	4.2
1	E	766	ASN	4.2
1	D	383	GLY	4.1
1	A	768	LEU	4.0
1	D	280	ASN	4.0
1	A	766	ASN	3.9
1	A	773	HIS	3.9
1	D	766	ASN	3.8
1	C	766	ASN	3.7
1	D	381	GLN	3.7
1	D	515	PHE	3.6
1	D	289	PHE	3.6
1	A	719	THR	3.6
1	B	768	LEU	3.5
1	D	276	SER	3.5
1	D	544	SER	3.5
1	D	282	ASP	3.4
1	B	742	VAL	3.4
1	E	45	THR	3.3
1	F	767	ALA	3.2
1	D	765	GLY	3.2
1	B	323	LEU	3.2
1	E	46	TRP	3.2
1	D	768	LEU	3.2
1	D	382	PRO	3.1
1	D	542	SER	3.1
1	D	306	ASP	3.1
1	D	723	ILE	3.0
1	F	766	ASN	3.0
1	A	767	ALA	3.0
1	D	747	LEU	3.0
1	E	40	ASP	3.0
1	D	377	TRP	3.0
1	C	765	GLY	2.9
1	B	332	ILE	2.9
1	A	744	VAL	2.9
1	D	719	THR	2.9
1	E	43	GLU	2.9
1	E	720	GLY	2.8
1	F	720	GLY	2.8
1	D	753	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	117	PHE	2.7
1	B	681	VAL	2.7
1	B	764	GLN	2.7
1	E	765	GLY	2.7
1	D	514	GLY	2.7
1	C	98	GLU	2.6
1	E	48	LEU	2.6
1	F	762	LYS	2.6
1	B	29	ASP	2.6
1	B	732	LYS	2.6
1	D	543	LYS	2.5
1	E	768	LEU	2.5
1	E	745	ASN	2.5
1	C	744	VAL	2.5
1	E	49	ASP	2.5
1	E	44	ARG	2.4
1	A	117	PHE	2.4
1	B	723	ILE	2.4
1	F	323	LEU	2.4
1	F	765	GLY	2.4
1	D	761	VAL	2.4
1	A	770	ILE	2.4
1	E	42	ARG	2.4
1	E	98	GLU	2.3
1	E	719	THR	2.3
1	D	742	VAL	2.3
1	D	483	CYS	2.3
1	B	743	LYS	2.3
1	D	720	GLY	2.3
1	B	730	GLU	2.3
1	D	516	GLU	2.3
1	C	323	LEU	2.3
1	D	379	LYS	2.3
1	D	517	ASN	2.3
1	D	518	THR	2.3
1	B	763	PRO	2.2
1	A	765	GLY	2.2
1	B	719	THR	2.2
1	E	116	GLU	2.2
1	E	743	LYS	2.2
1	E	50	THR	2.2
1	B	761	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	47	GLN	2.2
1	A	76	LEU	2.1
1	C	770	ILE	2.1
1	D	378	ASP	2.1
1	B	753	ALA	2.1
1	C	719	THR	2.1
1	E	29	ASP	2.1
1	F	88	GLN	2.1
1	D	756	GLU	2.1
1	F	730	GLU	2.1
1	D	100	TYR	2.1
1	E	764	GLN	2.1
1	B	339	GLY	2.1
1	C	204	ARG	2.1
1	A	743	LYS	2.1
1	E	76	LEU	2.1
1	B	741	VAL	2.1
1	D	315	TRP	2.1
1	B	699	ALA	2.0
1	D	339	GLY	2.0
1	D	769	THR	2.0
1	E	767	ALA	2.0
1	D	748	GLN	2.0
1	D	772	LEU	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	B	3015	5/5	0.65	0.13	79,81,82,82	0
2	SO4	A	3014	5/5	0.70	0.13	78,79,80,82	0
2	SO4	B	3016	5/5	0.71	0.15	72,72,73,75	0
2	SO4	D	3011	5/5	0.74	0.12	86,87,88,88	0
2	SO4	A	3018	5/5	0.75	0.12	84,85,85,86	0
3	ACY	A	2003	4/4	0.75	0.18	40,40,42,42	0
2	SO4	F	3009	5/5	0.76	0.16	64,66,68,69	0
3	ACY	F	2002	4/4	0.76	0.19	46,46,47,48	0
2	SO4	B	3013	5/5	0.77	0.11	77,78,79,80	0
3	ACY	E	2001	4/4	0.79	0.15	38,39,41,41	0
2	SO4	B	3010	5/5	0.82	0.12	76,77,77,78	0
2	SO4	C	3012	5/5	0.84	0.15	66,66,69,70	0
2	SO4	F	3005	5/5	0.85	0.16	50,53,56,56	0
2	SO4	F	3001	5/5	0.86	0.16	65,66,67,68	0
2	SO4	A	3017	5/5	0.86	0.13	73,75,77,78	0
2	SO4	F	3003	5/5	0.89	0.17	57,57,59,60	0
2	SO4	B	3008	5/5	0.89	0.16	59,61,62,63	0
4	MPO	B	1001	13/13	0.89	0.15	46,54,64,66	0
2	SO4	D	3004	5/5	0.90	0.12	65,65,66,67	0
4	MPO	E	1004	13/13	0.90	0.14	51,53,58,58	0
2	SO4	F	3002	5/5	0.91	0.12	60,63,65,66	0
4	MPO	C	1002	13/13	0.92	0.11	43,48,53,55	0
4	MPO	D	1003	13/13	0.93	0.11	43,52,58,58	0
2	SO4	C	3007	5/5	0.94	0.15	61,62,63,63	0
2	SO4	E	3006	5/5	0.94	0.15	56,58,59,62	0

6.5 Other polymers ⓘ

There are no such residues in this entry.