



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:40 PM UTC

PDB ID : 1XSK / pdb_00001xsk
Title : Structure of a Family 31 alpha glycosidase glycosyl-enzyme intermediate
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

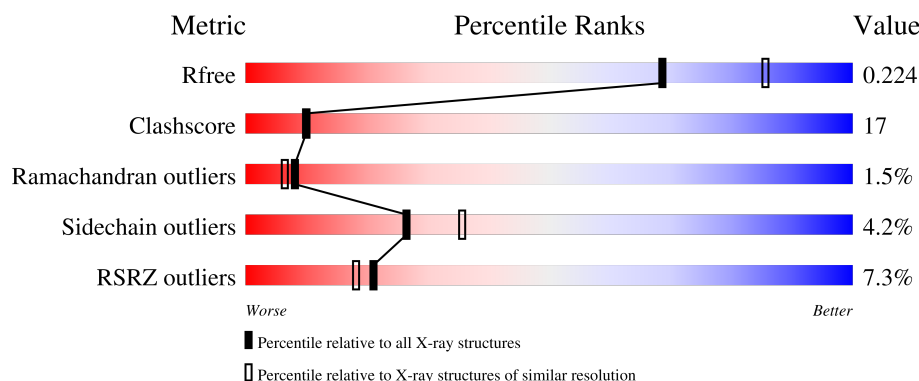
1 Overall quality at a glance

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	5% 67% 29% ...
1	B	778	9% 64% 33% ...
1	C	778	4% 65% 30% ...
1	D	778	11% 64% 31% ...
1	E	778	8% 64% 31% ...

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Mol	Chain	Length	Quality of chain
1	F	778	

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	3005	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 38360 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).



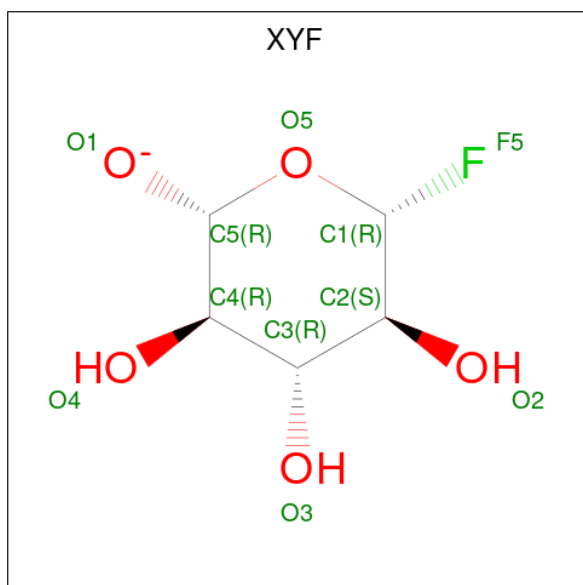
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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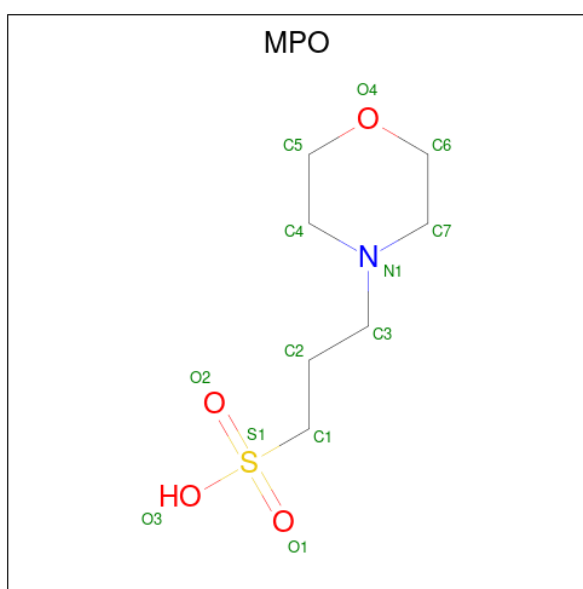
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total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

- Molecule 3 is 5(R)-fluoro-beta-D-xylopyranose (CCD ID: XYF) (formula: C₅H₈FO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			10	5	1	4		
3	B	1	Total	C	F	O	0	0
			10	5	1	4		
3	C	1	Total	C	F	O	0	0
			10	5	1	4		
3	E	1	Total	C	F	O	0	0
			10	5	1	4		

- 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	168	Total	O	0	0
			168	168		

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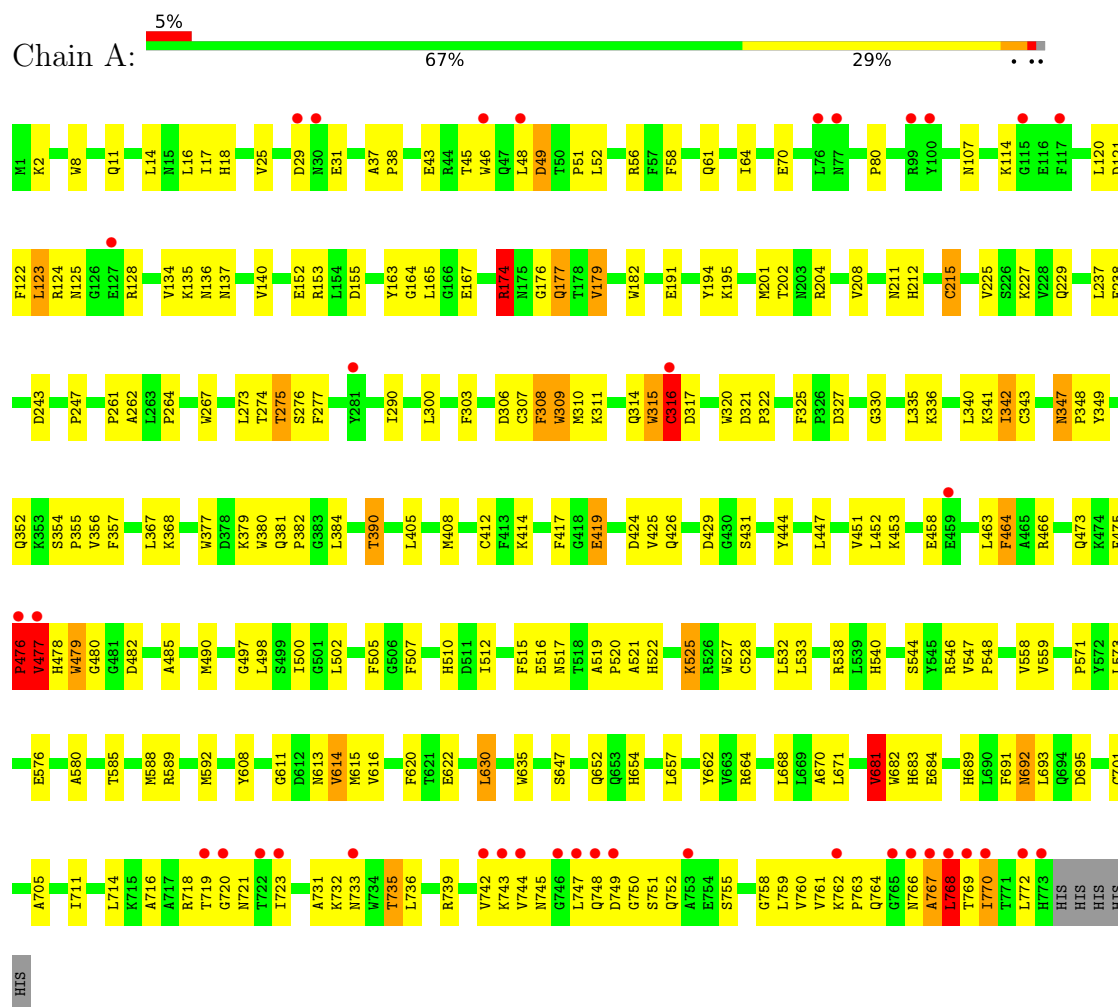
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	114	Total 114	O 114	0	0
5	C	167	Total 167	O 167	0	0
5	D	145	Total 145	O 145	0	0
5	E	122	Total 122	O 122	0	0
5	F	131	Total 131	O 131	0	0

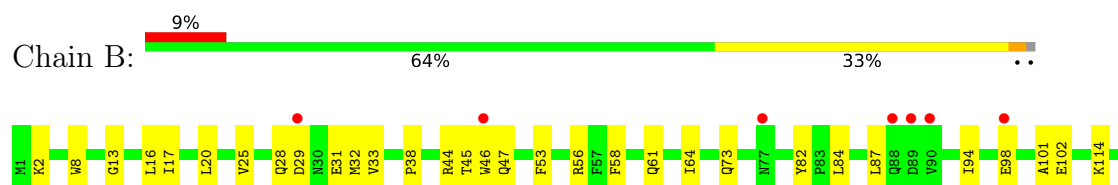
3 Residue-property plots

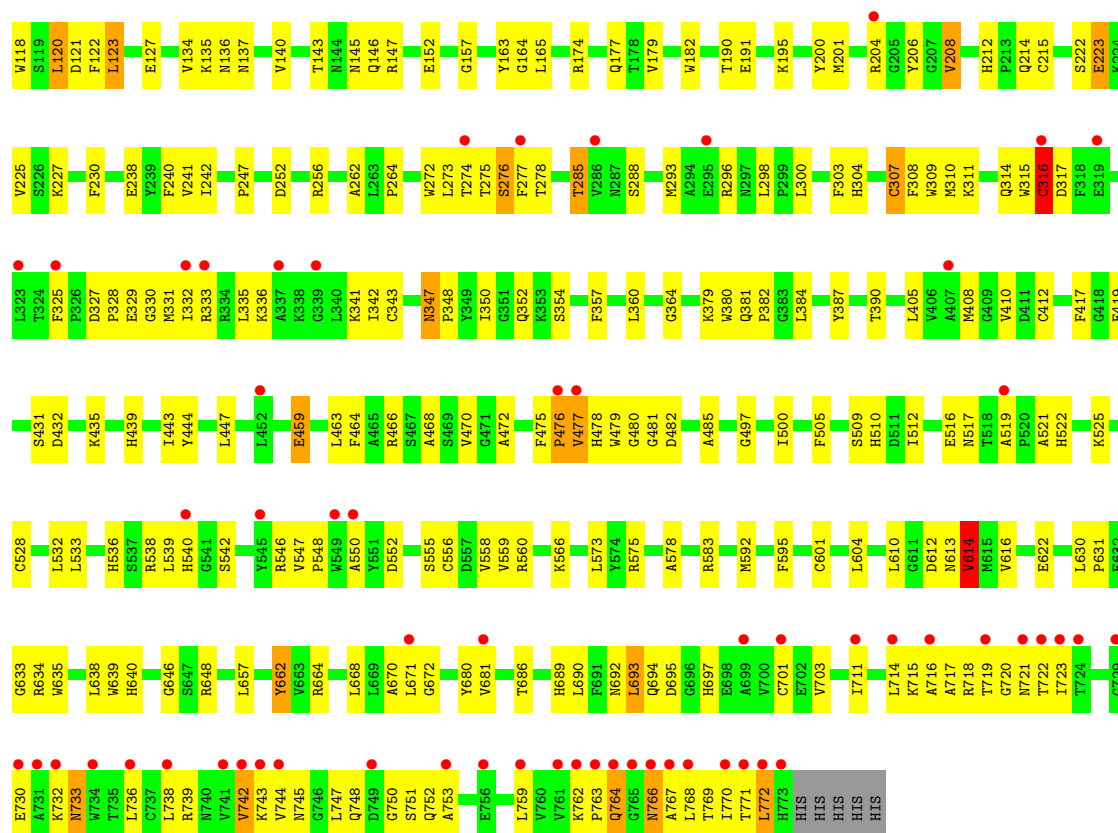
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

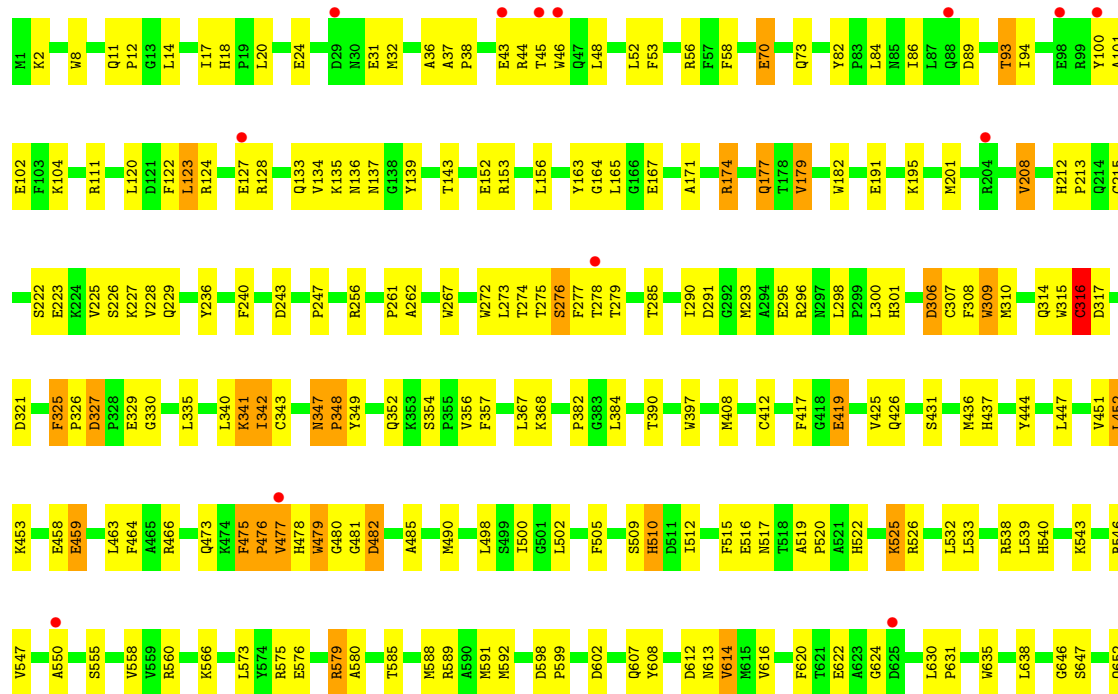


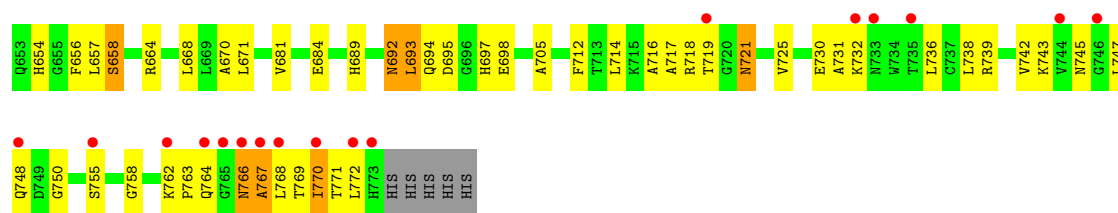
- Molecule 1: Putative family 31 glucosidase yicI



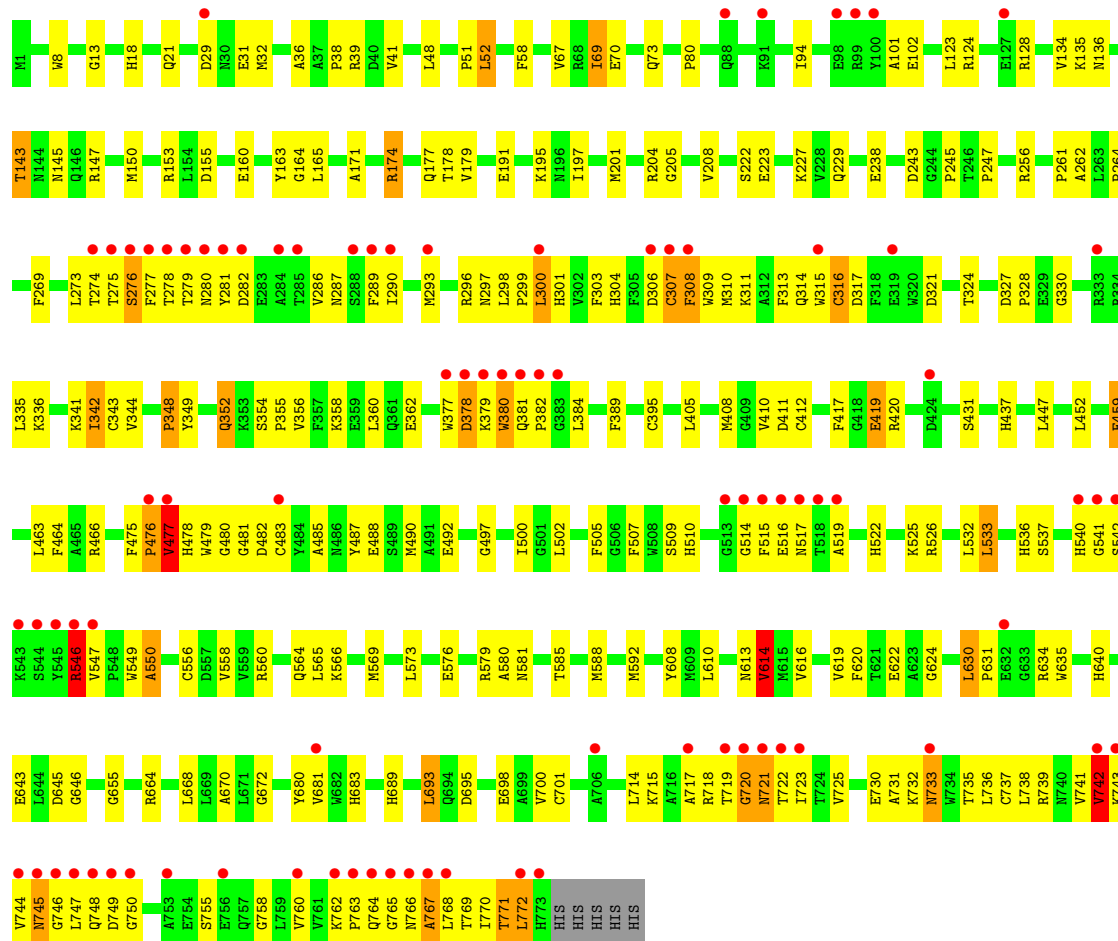


● Molecule 1: Putative family 31 glucosidase yicI

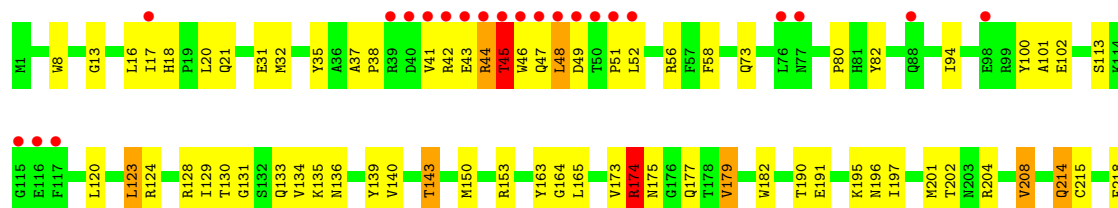


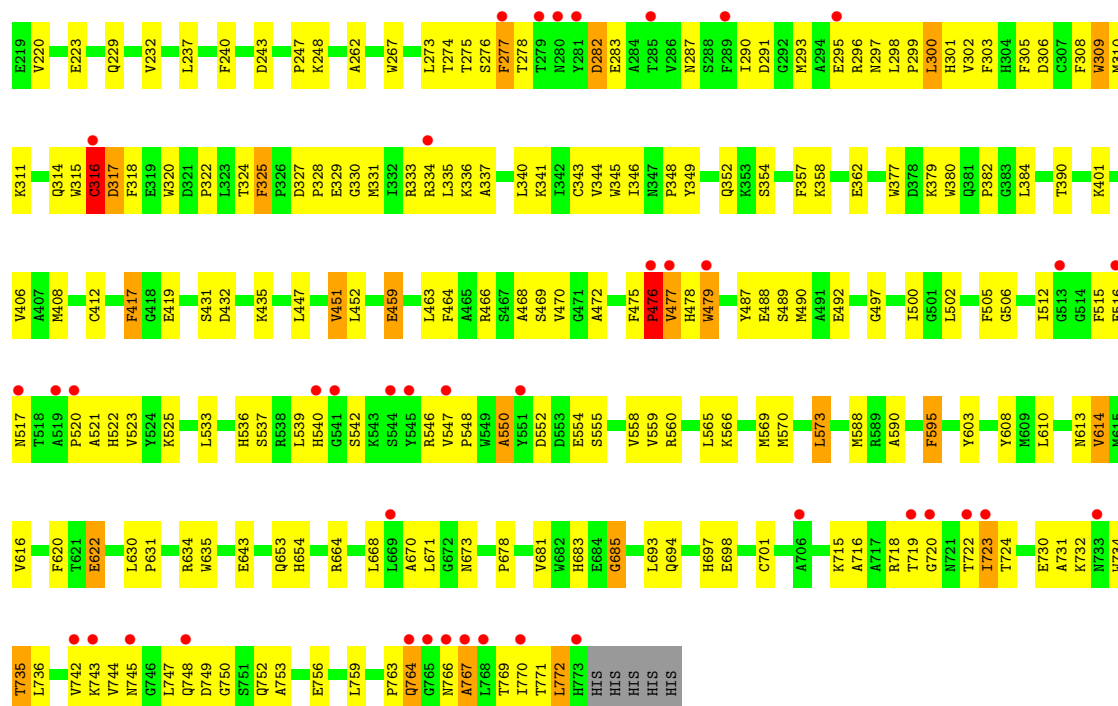


- Molecule 1: Putative family 31 glucosidase yicI

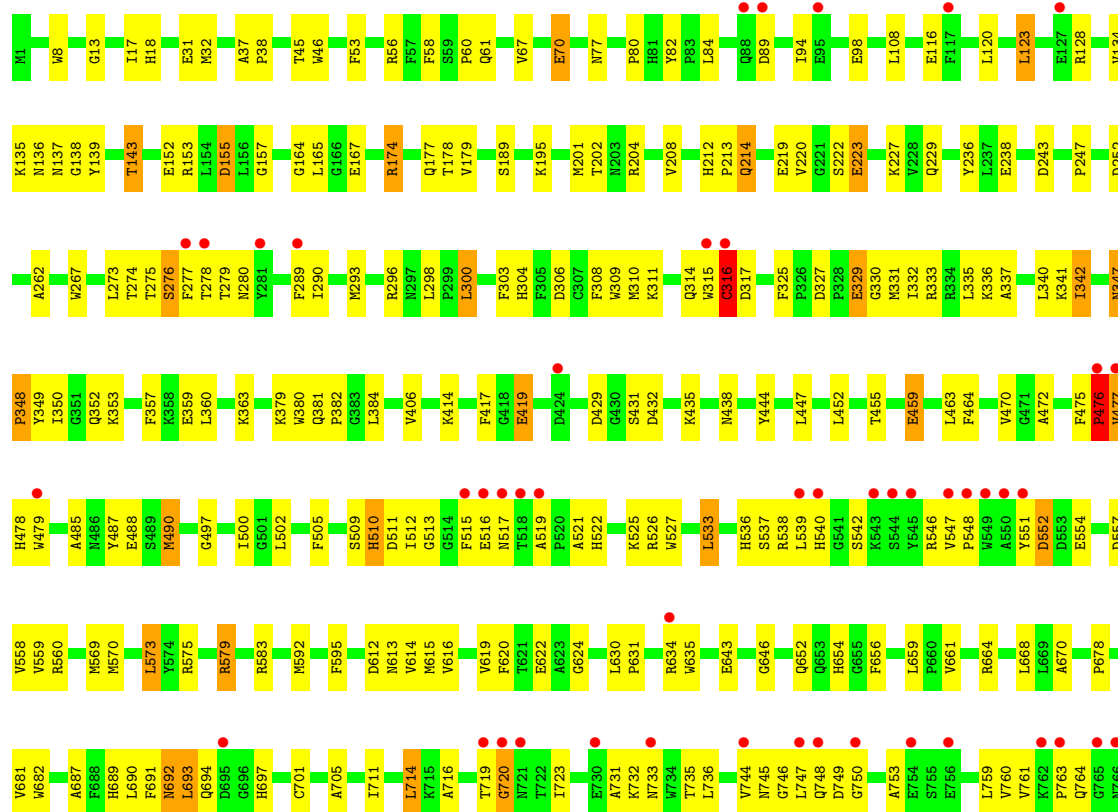


- Molecule 1: Putative family 31 glucosidase yicI





- Molecule 1: Putative family 31 glucosidase yicI



A767	L768	T769	T770	T771	L772	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	162.14Å 175.47Å 210.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.20 29.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.88-2.20) 97.8 (29.88-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.272 0.228 , 0.224	Depositor DCC
R_{free} test set	15006 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	38360	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: MPO, SO4, XYF

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	0.47	0/6409	1.00	31/8711 (0.4%)
1	B	0.39	0/6409	0.94	22/8711 (0.3%)
1	C	0.47	0/6409	0.99	37/8711 (0.4%)
1	D	0.46	0/6409	0.96	23/8711 (0.3%)
1	E	0.45	0/6409	0.97	27/8711 (0.3%)
1	F	0.45	0/6409	0.96	26/8711 (0.3%)
All	All	0.45	0/38454	0.97	166/52266 (0.3%)

There are no bond length outliers.

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	613	ASN	N-CA-C	10.81	126.67	113.38
1	D	613	ASN	N-CA-C	10.40	126.28	113.17
1	C	613	ASN	N-CA-C	10.27	126.01	113.38
1	B	475	PHE	CA-C-N	10.02	132.37	119.84
1	B	475	PHE	C-N-CA	10.02	132.37	119.84
1	E	613	ASN	N-CA-C	9.99	126.70	113.72
1	D	317	ASP	N-CA-C	-9.43	100.66	113.30
1	B	317	ASP	N-CA-C	-9.38	100.73	113.30
1	B	613	ASN	N-CA-C	9.26	124.84	113.17
1	F	613	ASN	N-CA-C	9.11	125.51	113.30
1	F	475	PHE	CA-C-N	9.11	131.22	119.84
1	F	475	PHE	C-N-CA	9.11	131.22	119.84
1	F	317	ASP	N-CA-C	-9.04	101.97	113.72
1	A	317	ASP	N-CA-C	-8.93	101.92	113.17
1	C	317	ASP	N-CA-C	-8.90	101.38	113.30
1	A	721	ASN	N-CA-C	-8.55	101.85	113.30
1	E	317	ASP	N-CA-C	-8.53	101.87	113.30
1	D	309	TRP	N-CA-C	-8.43	102.99	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	PHE	CA-C-N	8.40	130.34	119.84
1	A	475	PHE	C-N-CA	8.40	130.34	119.84
1	B	309	TRP	N-CA-C	-8.36	103.07	113.18
1	C	475	PHE	CA-C-N	8.35	130.28	119.84
1	C	475	PHE	C-N-CA	8.35	130.28	119.84
1	D	475	PHE	CA-C-N	8.09	129.95	119.84
1	D	475	PHE	C-N-CA	8.09	129.95	119.84
1	E	475	PHE	CA-C-N	8.00	129.84	119.84
1	E	475	PHE	C-N-CA	8.00	129.84	119.84
1	D	8	TRP	N-CA-C	7.86	122.69	113.18
1	D	480	GLY	N-CA-C	7.47	122.70	114.40
1	F	309	TRP	N-CA-C	-7.34	104.30	113.18
1	D	721	ASN	N-CA-C	-7.33	101.48	112.54
1	A	225	VAL	N-CA-C	7.32	118.09	110.62
1	A	315	TRP	N-CA-C	7.22	121.13	110.30
1	C	309	TRP	N-CA-C	-7.21	104.45	113.18
1	C	325	PHE	CA-C-N	7.19	127.19	119.28
1	C	325	PHE	C-N-CA	7.19	127.19	119.28
1	A	390	THR	N-CA-C	-6.80	104.98	113.28
1	E	595	PHE	CA-C-N	6.70	126.65	119.28
1	E	595	PHE	C-N-CA	6.70	126.65	119.28
1	E	309	TRP	N-CA-C	-6.60	105.20	113.18
1	A	8	TRP	N-CA-C	6.57	121.38	113.23
1	B	8	TRP	N-CA-C	6.57	121.37	113.23
1	A	309	TRP	N-CA-C	-6.54	105.26	113.18
1	C	451	VAL	N-CA-C	-6.54	104.38	110.53
1	D	281	TYR	N-CA-C	6.49	118.93	109.07
1	F	315	TRP	N-CA-C	6.49	120.24	110.64
1	C	614	VAL	N-CA-C	6.32	116.96	108.11
1	E	390	THR	N-CA-C	-6.29	105.61	113.28
1	C	612	ASP	N-CA-C	6.26	118.11	111.28
1	C	327	ASP	CA-C-N	6.25	125.75	119.24
1	C	327	ASP	C-N-CA	6.25	125.75	119.24
1	C	70	GLU	N-CA-C	6.24	119.36	109.50
1	F	342	ILE	N-CA-C	6.22	116.81	108.11
1	C	390	THR	N-CA-C	-6.21	105.70	113.28
1	D	308	PHE	N-CA-C	6.16	123.93	110.80
1	A	342	ILE	N-CA-C	6.15	116.72	108.11
1	A	476	PRO	N-CA-C	6.14	125.12	112.47
1	F	476	PRO	N-CA-C	6.13	125.10	112.47
1	C	482	ASP	N-CA-C	6.13	119.18	108.52
1	B	325	PHE	CA-C-N	6.05	125.53	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	PHE	C-N-CA	6.05	125.53	119.24
1	C	315	TRP	N-CA-C	6.05	119.59	110.64
1	A	29	ASP	CB-CA-C	-6.01	109.66	116.63
1	E	223	GLU	N-CA-C	-6.01	101.89	111.02
1	C	721	ASN	N-CA-C	-5.96	103.66	113.50
1	D	256	ARG	N-CA-C	-5.90	104.97	111.82
1	A	482	ASP	N-CA-C	5.90	118.78	108.52
1	D	321	ASP	CA-C-N	5.90	125.77	119.28
1	D	321	ASP	C-N-CA	5.90	125.77	119.28
1	E	174	ARG	N-CA-C	5.84	117.65	111.28
1	A	589	ARG	N-CA-C	5.82	118.89	109.40
1	E	590	ALA	N-CA-C	-5.78	102.36	110.50
1	D	550	ALA	N-CA-C	-5.76	105.51	112.54
1	F	325	PHE	CA-C-N	5.74	125.42	119.05
1	F	325	PHE	C-N-CA	5.74	125.42	119.05
1	E	325	PHE	CA-C-N	5.71	125.83	119.32
1	E	325	PHE	C-N-CA	5.71	125.83	119.32
1	A	682	TRP	N-CA-C	5.68	118.41	111.82
1	F	128	ARG	N-CA-C	5.66	117.44	108.67
1	D	640	HIS	N-CA-C	-5.65	106.23	113.23
1	C	341	LYS	N-CA-C	-5.62	101.38	110.32
1	A	520	PRO	N-CA-C	-5.62	102.98	111.41
1	F	70	GLU	N-CA-C	5.62	118.38	109.50
1	E	451	VAL	N-CA-C	-5.61	105.15	110.42
1	A	177	GLN	N-CA-C	5.60	118.70	109.85
1	A	315	TRP	CA-C-N	5.59	132.22	121.54
1	A	315	TRP	C-N-CA	5.59	132.22	121.54
1	A	174	ARG	N-CA-C	5.59	118.14	111.71
1	F	315	TRP	CA-C-N	5.57	132.19	121.54
1	F	315	TRP	C-N-CA	5.57	132.19	121.54
1	D	101	ALA	N-CA-C	-5.57	99.35	108.76
1	C	520	PRO	N-CA-C	-5.56	102.72	111.34
1	C	705	ALA	N-CA-C	-5.53	101.82	110.17
1	E	101	ALA	N-CA-C	-5.52	99.42	108.76
1	C	86	ILE	N-CA-C	5.52	116.06	107.28
1	A	705	ALA	N-CA-C	-5.50	101.83	110.36
1	B	614	VAL	N-CA-C	5.49	116.39	108.48
1	F	155	ASP	N-CA-C	5.48	117.61	110.43
1	B	662	TYR	N-CA-C	5.47	118.74	109.76
1	F	8	TRP	N-CA-C	5.47	120.07	112.90
1	D	29	ASP	CB-CA-C	-5.47	110.29	116.63
1	B	595	PHE	CA-C-N	5.46	125.13	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	595	PHE	C-N-CA	5.46	125.13	119.56
1	E	550	ALA	N-CA-C	-5.46	106.57	113.18
1	B	225	VAL	N-CA-C	5.44	118.68	111.17
1	E	315	TRP	CA-C-N	5.44	131.94	121.54
1	E	315	TRP	C-N-CA	5.44	131.94	121.54
1	B	482	ASP	N-CA-C	5.42	118.20	108.17
1	A	325	PHE	CA-C-N	5.42	125.24	119.28
1	A	325	PHE	C-N-CA	5.42	125.24	119.28
1	A	194	TYR	N-CA-C	-5.40	106.53	113.23
1	E	506	GLY	N-CA-C	5.39	121.35	114.66
1	B	742	VAL	N-CA-C	5.39	115.49	110.42
1	D	614	VAL	N-CA-C	5.38	115.87	108.12
1	F	490	MET	N-CA-C	-5.38	105.31	111.07
1	A	275	THR	N-CA-C	-5.38	106.68	113.18
1	D	378	ASP	N-CA-C	5.38	119.15	112.59
1	D	655	GLY	N-CA-C	-5.37	104.38	112.60
1	E	45	THR	N-CA-C	-5.37	107.28	113.88
1	C	589	ARG	N-CA-C	5.37	117.64	108.90
1	B	101	ALA	N-CA-C	-5.36	99.36	108.26
1	A	211	ASN	N-CA-C	5.36	119.00	110.70
1	E	476	PRO	N-CA-C	5.34	123.47	112.47
1	B	256	ARG	N-CA-C	-5.33	105.64	111.82
1	E	685	GLY	N-CA-C	-5.33	107.86	115.64
1	A	614	VAL	N-CA-C	5.32	115.56	108.11
1	C	101	ALA	N-CA-C	-5.32	99.62	108.34
1	D	307	CYS	N-CA-C	5.32	122.12	110.80
1	F	116	GLU	N-CA-C	5.31	117.07	111.28
1	F	682	TRP	N-CA-C	5.31	117.98	111.82
1	B	721	ASN	N-CA-C	-5.30	106.31	114.16
1	F	337	ALA	N-CA-C	-5.30	106.65	113.01
1	C	476	PRO	N-CA-C	5.28	123.35	112.47
1	E	8	TRP	N-CA-C	5.27	119.84	113.41
1	B	29	ASP	CB-CA-C	-5.24	110.55	116.63
1	C	307	CYS	N-CA-C	5.24	120.02	111.37
1	D	70	GLU	N-CA-C	5.24	117.78	109.50
1	F	223	GLU	N-CA-C	-5.24	103.06	111.02
1	A	464	PHE	N-CA-C	-5.23	97.34	107.44
1	C	602	ASP	N-CA-C	5.22	116.66	111.07
1	E	622	GLU	N-CA-C	-5.21	105.52	111.14
1	C	8	TRP	N-CA-C	5.19	119.70	112.90
1	C	315	TRP	CA-C-N	5.19	131.45	121.54
1	C	315	TRP	C-N-CA	5.19	131.45	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	ASP	CA-C-N	5.19	124.90	119.82
1	C	321	ASP	C-N-CA	5.19	124.90	119.82
1	C	225	VAL	N-CA-C	5.18	117.53	111.05
1	B	390	THR	N-CA-C	-5.18	106.96	113.28
1	E	476	PRO	CA-C-N	5.17	131.28	121.97
1	E	476	PRO	C-N-CA	5.17	131.28	121.97
1	C	177	GLN	N-CA-C	5.17	117.53	109.52
1	E	315	TRP	N-CA-C	5.16	121.78	110.80
1	F	476	PRO	CA-C-N	5.13	131.21	121.97
1	F	476	PRO	C-N-CA	5.13	131.21	121.97
1	A	451	VAL	N-CA-C	-5.12	105.55	110.72
1	A	215	CYS	N-CA-C	5.12	117.58	109.96
1	F	612	ASP	N-CA-C	5.11	116.92	111.36
1	B	612	ASP	N-CA-C	5.08	116.81	111.28
1	B	223	GLU	N-CA-C	-5.07	105.19	112.13
1	C	256	ARG	N-CA-C	-5.07	105.84	111.36
1	F	316	CYS	CA-CB-SG	-5.06	102.77	114.40
1	D	342	ILE	N-CA-C	5.06	115.25	108.17
1	C	342	ILE	N-CA-C	5.04	115.17	108.11
1	C	658	SER	N-CA-C	5.03	116.84	109.24
1	C	316	CYS	N-CA-C	5.03	121.51	110.80
1	F	138	GLY	N-CA-C	5.02	116.81	110.38

There are no chirality outliers.

There are no planarity outliers.

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	204	0
1	B	6226	0	5934	207	0
1	C	6226	0	5934	227	0
1	D	6226	0	5934	220	0
1	E	6226	0	5934	237	0
1	F	6226	0	5934	205	0
2	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	25	0	0	2	0
3	A	10	0	6	2	0
3	B	10	0	6	1	0
3	C	10	0	6	2	0
3	E	10	0	6	2	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	168	0	0	4	0
5	B	114	0	0	6	0
5	C	167	0	0	5	0
5	D	145	0	0	5	0
5	E	122	0	0	4	0
5	F	131	0	0	6	0
All	All	38360	0	35688	1275	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 17.

All (1275) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:565:LEU:HG	1:E:569:MET:HE2	1.22	1.17
1:D:32:MET:HE2	1:D:94:ILE:HG23	1.32	1.12
1:A:274:THR:HG22	1:A:276:SER:H	1.14	1.11
1:E:274:THR:HG22	1:E:276:SER:H	1.00	1.09
1:A:668:LEU:HD21	1:A:714:LEU:HD12	1.39	1.04
1:C:579:ARG:HH11	1:C:579:ARG:HB2	1.21	1.04
1:D:485:ALA:HB1	1:D:519:ALA:HB2	1.40	1.03
1:D:565:LEU:HG	1:D:569:MET:HE2	1.38	1.03
1:C:93:THR:HG22	1:C:104:LYS:HB3	1.40	1.02
1:B:719:THR:HG23	1:B:720:GLY:H	1.23	1.02
1:D:668:LEU:HD21	1:D:714:LEU:HD12	1.39	1.01
1:B:157:GLY:HA3	1:B:204:ARG:HH22	1.25	1.01
1:B:668:LEU:HD21	1:B:714:LEU:HD12	1.40	1.01
1:B:32:MET:HE2	1:B:94:ILE:HG23	1.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:694:GLN:HB2	1:E:697:HIS:HD2	1.27	0.99
1:F:485:ALA:HB1	1:F:519:ALA:HB2	1.41	0.98
1:B:274:THR:HG22	1:B:276:SER:H	1.23	0.97
1:F:463:LEU:O	1:F:477:VAL:HG13	1.65	0.96
1:C:668:LEU:HD21	1:C:714:LEU:HD12	1.46	0.96
1:C:485:ALA:HB1	1:C:519:ALA:HB2	1.46	0.95
1:F:298:LEU:HD23	1:F:560:ARG:HG3	1.48	0.94
1:E:274:THR:HG21	1:E:540:HIS:ND1	1.81	0.94
1:F:274:THR:HG22	1:F:276:SER:H	1.29	0.94
1:A:485:ALA:HB1	1:A:519:ALA:HB2	1.50	0.94
1:E:463:LEU:O	1:E:477:VAL:HG13	1.68	0.93
1:D:381:GLN:HB2	1:D:384:LEU:HD12	1.52	0.91
1:E:274:THR:HG22	1:E:276:SER:N	1.84	0.91
1:B:694:GLN:HB2	1:B:697:HIS:HD2	1.36	0.90
1:C:274:THR:HG21	1:C:540:HIS:ND1	1.86	0.90
1:D:313:PHE:HA	1:D:381:GLN:HE22	1.38	0.89
1:F:668:LEU:HD21	1:F:714:LEU:HD13	1.53	0.88
1:D:280:ASN:HA	1:E:44:ARG:HH21	1.37	0.87
1:D:547:VAL:HG23	1:D:550:ALA:HB2	1.55	0.87
1:E:45:THR:HG23	1:E:46:TRP:HD1	1.39	0.87
1:C:579:ARG:HH11	1:C:579:ARG:CB	1.88	0.87
1:B:463:LEU:O	1:B:477:VAL:HG13	1.74	0.87
1:E:293:MET:HE2	1:E:300:LEU:HD23	1.54	0.86
1:D:766:ASN:C	1:D:768:LEU:H	1.82	0.86
1:E:165:LEU:HD13	1:E:179:VAL:HG11	1.57	0.86
1:A:367:LEU:HG	1:A:425:VAL:HG21	1.59	0.85
1:D:273:LEU:HB2	1:D:300:LEU:HD21	1.59	0.84
1:C:425:VAL:HG22	1:C:426:GLN:N	1.91	0.83
1:E:32:MET:HE3	1:E:94:ILE:HG23	1.60	0.83
1:C:368:LYS:O	1:C:425:VAL:HG23	1.79	0.83
1:F:694:GLN:HB2	1:F:697:HIS:HD2	1.42	0.83
1:E:214:GLN:HG3	1:E:435:LYS:HG2	1.61	0.82
1:F:634:ARG:HH21	1:F:643:GLU:HB3	1.45	0.82
1:A:368:LYS:O	1:A:425:VAL:HG23	1.79	0.82
1:A:463:LEU:O	1:A:477:VAL:HG22	1.81	0.81
1:C:329:GLU:HG3	1:C:408:MET:HG3	1.62	0.81
1:C:525:LYS:HG3	1:C:558:VAL:HG21	1.62	0.81
1:C:32:MET:CE	1:C:94:ILE:HG23	2.12	0.80
1:F:293:MET:HE2	1:F:300:LEU:HD23	1.64	0.80
1:D:540:HIS:C	1:D:546:ARG:HE	1.90	0.79
1:A:525:LYS:HG3	1:A:558:VAL:HG21	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:347:ASN:C	1:F:347:ASN:HD22	1.91	0.79
1:E:179:VAL:HG13	1:E:218:PHE:HB2	1.64	0.79
1:E:382:PRO:HG2	5:E:3048:HOH:O	1.82	0.79
1:B:136:ASN:HD21	1:B:227:LYS:HE3	1.47	0.79
1:F:274:THR:HG21	1:F:540:HIS:ND1	1.97	0.79
1:B:747:LEU:HD23	1:B:748:GLN:N	1.98	0.78
1:D:32:MET:HE1	1:D:102:GLU:O	1.83	0.78
1:A:107:ASN:HD22	1:A:125:ASN:HD21	1.31	0.78
1:B:44:ARG:HA	1:B:47:GLN:HG3	1.65	0.78
1:E:525:LYS:HG2	1:E:558:VAL:HG21	1.64	0.78
1:A:723:ILE:HG12	1:A:770:ILE:HG13	1.65	0.77
1:A:195:LYS:HE2	1:A:478:HIS:HB3	1.66	0.77
1:F:13:GLY:O	1:F:143:THR:HB	1.85	0.77
1:D:280:ASN:HA	1:E:44:ARG:NH2	2.00	0.76
1:D:725:VAL:HB	1:D:768:LEU:HD12	1.67	0.76
1:A:274:THR:HG22	1:A:276:SER:N	1.95	0.76
1:B:719:THR:HG23	1:B:720:GLY:N	1.98	0.76
1:C:762:LYS:HD2	1:C:763:PRO:HD2	1.68	0.76
1:D:541:GLY:HA3	1:D:546:ARG:HH21	1.50	0.75
1:E:723:ILE:HG13	1:E:770:ILE:HB	1.68	0.75
1:E:476:PRO:O	1:E:477:VAL:HG12	1.86	0.75
1:C:32:MET:HE2	1:C:94:ILE:HG23	1.68	0.75
1:E:44:ARG:HG2	1:E:47:GLN:NE2	2.01	0.75
1:A:761:VAL:HG11	1:A:768:LEU:HD21	1.69	0.75
1:F:731:ALA:C	1:F:732:LYS:HD2	2.11	0.75
1:F:273:LEU:HB2	1:F:300:LEU:HD21	1.69	0.75
1:F:300:LEU:HD12	1:F:340:LEU:HD21	1.68	0.75
1:A:522:HIS:CE1	1:A:622:GLU:HG3	2.22	0.74
1:E:673:ASN:HD22	1:E:685:GLY:HA3	1.52	0.74
1:B:157:GLY:HA3	1:B:204:ARG:NH2	2.01	0.74
1:A:635:TRP:CH2	1:A:664:ARG:HG2	2.23	0.74
1:B:332:ILE:HD12	1:B:333:ARG:N	2.01	0.74
1:C:201:MET:HE1	1:C:247:PRO:HB3	1.69	0.74
1:C:579:ARG:HB2	1:C:579:ARG:NH1	2.00	0.74
1:D:293:MET:HE2	1:D:300:LEU:HD23	1.70	0.74
1:D:13:GLY:O	1:D:143:THR:HB	1.87	0.73
1:E:174:ARG:O	1:E:177:GLN:HG2	1.87	0.73
1:E:694:GLN:HB2	1:E:697:HIS:CD2	2.19	0.73
1:B:689:HIS:ND1	1:B:739:ARG:NH1	2.36	0.73
1:C:274:THR:CG2	1:C:540:HIS:HA	2.18	0.73
1:A:174:ARG:O	1:A:177:GLN:HG2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:GLN:NE2	1:D:73:GLN:HG3	2.04	0.73
1:C:755:SER:HB3	1:C:758:GLY:O	1.88	0.73
1:A:750:GLY:HA2	1:A:764:GLN:HG2	1.71	0.72
1:A:588:MET:HE3	5:A:3065:HOH:O	1.90	0.72
1:A:762:LYS:HD2	1:A:763:PRO:HD2	1.72	0.72
1:C:731:ALA:C	1:C:732:LYS:HD2	2.15	0.72
1:B:32:MET:HE1	1:B:102:GLU:C	2.15	0.72
1:A:367:LEU:CG	1:A:425:VAL:HG21	2.19	0.71
1:C:731:ALA:O	1:C:732:LYS:HD2	1.90	0.71
1:E:274:THR:CG2	1:E:276:SER:H	1.92	0.71
1:E:275:THR:O	1:E:276:SER:HB2	1.90	0.71
1:B:694:GLN:HB2	1:B:697:HIS:CD2	2.23	0.71
1:B:275:THR:O	1:B:276:SER:HB2	1.89	0.71
1:D:755:SER:HB3	1:D:758:GLY:O	1.90	0.71
1:C:174:ARG:O	1:C:177:GLN:HG2	1.90	0.71
1:D:377:TRP:HH2	1:D:420:ARG:HD3	1.54	0.71
1:D:731:ALA:C	1:D:732:LYS:HD2	2.16	0.71
1:B:274:THR:HG21	1:B:540:HIS:ND1	2.05	0.71
1:D:730:GLU:HG3	1:D:732:LYS:NZ	2.05	0.71
1:B:201:MET:HE1	1:B:247:PRO:HB3	1.72	0.70
1:C:425:VAL:CG2	1:C:426:GLN:N	2.54	0.70
1:B:343:CYS:HB2	1:B:412:CYS:SG	2.31	0.70
1:A:347:ASN:C	1:A:347:ASN:HD22	1.99	0.70
1:F:694:GLN:HB2	1:F:697:HIS:CD2	2.25	0.70
1:D:522:HIS:CG	1:D:622:GLU:HG3	2.27	0.70
1:F:635:TRP:CH2	1:F:664:ARG:HG2	2.27	0.70
1:D:762:LYS:HD2	1:D:763:PRO:HD2	1.74	0.69
1:A:107:ASN:HD22	1:A:125:ASN:ND2	1.90	0.69
1:A:684:GLU:HG2	1:A:732:LYS:HB2	1.74	0.69
1:A:755:SER:HB3	1:A:758:GLY:O	1.91	0.69
1:D:485:ALA:HB1	1:D:519:ALA:CB	2.20	0.69
1:F:512:ILE:HB	1:F:539:LEU:HD23	1.74	0.69
1:A:742:VAL:HG23	1:A:743:LYS:H	1.57	0.69
1:C:367:LEU:HD11	1:C:425:VAL:HG21	1.74	0.69
1:C:725:VAL:HB	1:C:768:LEU:HB3	1.75	0.69
1:F:382:PRO:HG2	5:F:3046:HOH:O	1.91	0.69
1:B:522:HIS:CG	1:B:622:GLU:HG3	2.27	0.69
1:E:287:ASN:HD21	1:E:334:ARG:NH2	1.90	0.69
1:B:136:ASN:ND2	1:B:227:LYS:HE3	2.08	0.69
1:C:293:MET:HE2	1:C:300:LEU:HD23	1.75	0.68
1:B:693:LEU:HD11	1:B:716:ALA:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:GLN:NE2	1:B:73:GLN:HG3	2.07	0.68
1:B:742:VAL:HG23	1:B:743:LYS:H	1.58	0.68
1:F:311:LYS:HE3	1:F:314:GLN:OE1	1.93	0.68
1:E:165:LEU:CD1	1:E:179:VAL:HG11	2.23	0.68
1:A:548:PRO:HG3	1:A:559:VAL:HG21	1.76	0.67
1:C:367:LEU:CD1	1:C:425:VAL:HG21	2.24	0.67
1:B:459:GLU:CD	1:B:459:GLU:H	2.00	0.67
1:A:165:LEU:HD13	1:A:179:VAL:HG11	1.75	0.67
1:D:742:VAL:HG23	1:D:743:LYS:H	1.59	0.67
1:E:490:MET:HE3	1:E:620:PHE:CD1	2.29	0.67
1:E:673:ASN:ND2	1:E:685:GLY:HA3	2.08	0.67
1:C:133:GLN:HB2	1:C:136:ASN:HD22	1.59	0.67
1:F:347:ASN:ND2	1:F:349:TYR:H	1.93	0.67
1:C:588:MET:HE3	5:C:3030:HOH:O	1.95	0.67
1:D:36:ALA:O	1:D:52:LEU:HD23	1.95	0.67
1:A:341:LYS:C	1:A:342:ILE:HD12	2.20	0.67
1:B:347:ASN:C	1:B:347:ASN:HD22	2.03	0.67
1:D:541:GLY:HA3	1:D:546:ARG:NH2	2.09	0.67
1:A:274:THR:HG21	1:A:540:HIS:ND1	2.09	0.66
1:E:13:GLY:O	1:E:143:THR:HB	1.95	0.66
1:B:174:ARG:O	1:B:177:GLN:HG2	1.95	0.66
1:C:274:THR:HG22	1:C:540:HIS:HA	1.77	0.66
1:B:195:LYS:HE2	1:B:478:HIS:HB3	1.78	0.66
1:C:532:LEU:O	1:C:566:LYS:HD2	1.94	0.66
1:D:730:GLU:HG3	1:D:732:LYS:HZ2	1.61	0.66
1:D:343:CYS:HB2	1:D:412:CYS:SG	2.36	0.66
1:D:566:LYS:HA	1:D:569:MET:HE3	1.78	0.66
1:F:201:MET:HE1	1:F:247:PRO:HB3	1.78	0.66
1:F:763:PRO:HB3	1:F:768:LEU:HD22	1.78	0.66
1:A:201:MET:HE1	1:A:247:PRO:HA	1.77	0.65
1:D:262:ALA:HB3	1:D:476:PRO:HG3	1.79	0.65
1:A:165:LEU:HD12	1:A:174:ARG:HG2	1.78	0.65
1:B:32:MET:HE1	1:B:102:GLU:O	1.95	0.65
1:C:512:ILE:HB	1:C:539:LEU:HD23	1.77	0.65
1:B:719:THR:CG2	1:B:720:GLY:H	2.05	0.65
1:F:705:ALA:HB2	1:F:711:ILE:HB	1.78	0.65
1:D:380:TRP:HA	1:E:49:ASP:OD1	1.97	0.65
1:D:747:LEU:HD23	1:D:748:GLN:N	2.12	0.65
1:F:174:ARG:O	1:F:177:GLN:HG2	1.96	0.65
1:A:500:ILE:HG12	1:A:505:PHE:HB2	1.78	0.65
1:C:347:ASN:C	1:C:347:ASN:HD22	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:ASN:HB3	1:D:153:ARG:HB2	1.79	0.65
1:D:276:SER:HB2	1:D:279:THR:HG23	1.78	0.65
1:E:377:TRP:CZ3	1:E:379:LYS:HD2	2.31	0.65
1:A:16:LEU:HD22	1:A:140:VAL:HG22	1.79	0.65
1:B:123:LEU:N	1:B:123:LEU:HD22	2.11	0.65
1:C:692:ASN:HD22	1:C:692:ASN:H	1.43	0.65
1:D:485:ALA:CB	1:D:519:ALA:HB2	2.23	0.65
1:E:329:GLU:O	1:E:333:ARG:HG2	1.97	0.65
1:C:638:LEU:O	1:C:739:ARG:NH2	2.30	0.65
1:D:540:HIS:CG	1:D:541:GLY:H	2.14	0.65
1:E:417:PHE:HA	1:E:419:GLU:OE2	1.97	0.64
1:C:165:LEU:HD12	1:C:174:ARG:HG2	1.79	0.64
1:F:417:PHE:HA	1:F:419:GLU:OE2	1.97	0.64
1:C:730:GLU:HG3	1:C:732:LYS:NZ	2.13	0.64
1:C:300:LEU:HD13	1:C:301:HIS:N	2.13	0.64
1:C:367:LEU:CG	1:C:425:VAL:HG21	2.27	0.64
1:D:417:PHE:HA	1:D:419:GLU:OE2	1.97	0.64
1:E:476:PRO:O	1:E:477:VAL:CG1	2.45	0.64
1:F:540:HIS:C	1:F:546:ARG:HG3	2.22	0.64
1:F:692:ASN:H	1:F:692:ASN:HD22	1.46	0.64
1:A:274:THR:HG22	1:A:275:THR:N	2.13	0.64
1:B:329:GLU:O	1:B:332:ILE:HG13	1.98	0.64
1:B:681:VAL:HG13	1:B:681:VAL:O	1.97	0.64
1:B:485:ALA:HB1	1:B:519:ALA:HB2	1.78	0.64
1:B:748:GLN:HB2	1:B:769:THR:H	1.62	0.63
1:C:32:MET:HE1	1:C:102:GLU:C	2.23	0.63
1:A:382:PRO:HG2	5:A:3018:HOH:O	1.97	0.63
1:C:31:GLU:OE1	1:C:56:ARG:HD3	1.99	0.63
1:C:692:ASN:HD22	1:C:692:ASN:N	1.96	0.63
1:F:274:THR:HG23	1:F:304:HIS:HD2	1.63	0.63
1:C:153:ARG:HG2	1:C:229:GLN:HB2	1.80	0.63
1:C:367:LEU:HG	1:C:425:VAL:HG21	1.81	0.63
1:C:698:GLU:HG3	1:C:717:ALA:HB2	1.81	0.63
1:D:746:GLY:H	1:D:771:THR:HG23	1.63	0.63
1:B:476:PRO:O	1:B:477:VAL:HG12	1.99	0.63
1:F:476:PRO:O	1:F:477:VAL:HG12	1.99	0.63
1:C:768:LEU:HD13	1:C:769:THR:N	2.14	0.63
1:F:31:GLU:HG2	1:F:58:PHE:HB3	1.82	0.62
1:A:747:LEU:HD22	1:A:750:GLY:O	1.98	0.62
1:B:752:GLN:HB2	1:B:759:LEU:HD11	1.80	0.62
1:A:212:HIS:CE1	1:A:238:GLU:H	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ASN:C	1:A:347:ASN:ND2	2.58	0.62
1:C:82:TYR:HB2	1:C:84:LEU:HD21	1.81	0.62
1:F:447:LEU:C	1:F:447:LEU:HD23	2.24	0.62
1:E:16:LEU:HD22	1:E:140:VAL:HG22	1.80	0.62
1:E:262:ALA:HB3	1:E:476:PRO:HG3	1.81	0.62
1:F:634:ARG:NH2	1:F:643:GLU:HB3	2.14	0.62
1:A:736:LEU:HD13	1:A:736:LEU:C	2.25	0.62
1:D:532:LEU:O	1:D:566:LYS:HD2	2.00	0.62
1:B:521:ALA:HB3	5:B:3120:HOH:O	1.99	0.62
1:F:681:VAL:HG13	1:F:681:VAL:O	2.00	0.62
1:B:274:THR:HG22	1:B:275:THR:N	2.15	0.61
1:C:382:PRO:HG2	5:C:3013:HOH:O	2.00	0.61
1:C:693:LEU:HD11	1:C:716:ALA:O	2.00	0.61
1:D:540:HIS:CG	1:D:541:GLY:N	2.67	0.61
1:D:546:ARG:HA	1:D:546:ARG:HH11	1.66	0.61
1:E:320:TRP:O	1:E:322:PRO:HD3	1.99	0.61
1:A:273:LEU:HD13	1:A:274:THR:N	2.15	0.61
1:C:425:VAL:CG2	1:C:426:GLN:H	2.13	0.61
1:C:579:ARG:HH11	1:C:579:ARG:CG	2.13	0.61
1:E:753:ALA:O	1:E:759:LEU:HD12	2.00	0.61
1:E:18:HIS:O	1:E:38:PRO:HA	2.00	0.61
1:B:307:CYS:HB3	1:B:315:TRP:CZ2	2.36	0.61
1:C:275:THR:O	1:C:276:SER:HB2	2.01	0.61
1:D:459:GLU:H	1:D:459:GLU:CD	2.06	0.61
1:D:744:VAL:HG21	1:D:770:ILE:HG23	1.83	0.61
1:A:425:VAL:HG22	1:A:426:GLN:N	2.14	0.61
1:C:384:LEU:C	1:C:384:LEU:HD23	2.25	0.61
1:D:32:MET:HE1	1:D:102:GLU:C	2.25	0.61
1:F:195:LYS:HE2	1:F:478:HIS:HB3	1.83	0.61
1:C:689:HIS:ND1	1:C:739:ARG:NH1	2.48	0.61
1:D:195:LYS:HE2	1:D:478:HIS:HB3	1.81	0.61
1:D:379:LYS:O	1:D:380:TRP:HB3	2.01	0.61
1:B:766:ASN:O	1:B:767:ALA:HB3	2.00	0.61
1:E:100:TYR:HD2	1:E:113:SER:HA	1.66	0.61
1:C:300:LEU:HD12	1:C:340:LEU:CD2	2.30	0.61
1:F:275:THR:O	1:F:276:SER:HB2	2.01	0.61
1:B:212:HIS:HE1	1:B:238:GLU:H	1.49	0.60
1:F:631:PRO:HD2	1:F:635:TRP:CZ2	2.35	0.60
1:B:690:LEU:HD21	1:B:693:LEU:HD12	1.83	0.60
1:C:522:HIS:CG	1:C:622:GLU:HG3	2.37	0.60
1:A:2:LYS:HE3	1:D:191:GLU:OE2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ASN:C	1:B:347:ASN:ND2	2.59	0.60
1:E:273:LEU:HB2	1:E:300:LEU:HD21	1.82	0.60
1:D:201:MET:HE1	1:D:247:PRO:HB3	1.82	0.60
1:E:21:GLN:NE2	1:E:42:ARG:HG3	2.17	0.60
1:F:579:ARG:HG3	1:F:579:ARG:HH11	1.65	0.60
1:C:417:PHE:HA	1:C:419:GLU:OE2	2.02	0.60
1:B:742:VAL:HG23	1:B:743:LYS:N	2.15	0.60
1:C:547:VAL:HG23	1:C:550:ALA:HB2	1.83	0.60
1:E:772:LEU:HD22	1:E:772:LEU:H	1.65	0.60
1:F:296:ARG:O	1:F:560:ARG:NH1	2.35	0.60
1:F:347:ASN:C	1:F:347:ASN:ND2	2.55	0.60
1:A:290:ILE:CD1	1:A:335:LEU:HD22	2.32	0.60
1:C:459:GLU:CD	1:C:459:GLU:H	2.02	0.60
1:A:770:ILE:HD12	1:A:770:ILE:C	2.27	0.60
1:F:490:MET:HE3	1:F:620:PHE:CD1	2.37	0.60
1:A:368:LYS:O	1:A:425:VAL:CG2	2.50	0.59
1:B:547:VAL:HG23	1:B:550:ALA:HB2	1.82	0.59
1:D:731:ALA:O	1:D:732:LYS:HD2	2.02	0.59
1:E:274:THR:HG21	1:E:540:HIS:CE1	2.36	0.59
1:D:463:LEU:O	1:D:477:VAL:HG13	2.01	0.59
1:B:311:LYS:HE3	1:B:314:GLN:OE1	2.02	0.59
1:F:750:GLY:HA2	1:F:764:GLN:HG2	1.84	0.59
1:C:300:LEU:HD12	1:C:340:LEU:HD22	1.83	0.59
1:C:463:LEU:O	1:C:477:VAL:HB	2.02	0.59
1:C:684:GLU:HG2	1:C:732:LYS:HB2	1.85	0.59
1:D:546:ARG:HH11	1:D:546:ARG:CA	2.15	0.59
1:E:31:GLU:OE1	1:E:56:ARG:HD3	2.02	0.59
1:E:447:LEU:HD23	1:E:447:LEU:C	2.28	0.59
1:F:681:VAL:HG12	2:F:3005:SO4:O3	2.02	0.59
1:A:163:TYR:HB3	1:A:502:LEU:HD13	1.85	0.59
1:B:671:LEU:N	1:B:671:LEU:HD12	2.18	0.59
1:C:347:ASN:C	1:C:347:ASN:ND2	2.61	0.59
1:A:342:ILE:HD12	1:A:342:ILE:N	2.18	0.59
1:B:123:LEU:HA	1:B:127:GLU:O	2.03	0.59
1:F:352:GLN:HA	1:F:357:PHE:CD2	2.37	0.59
1:B:31:GLU:OE1	1:B:56:ARG:HD3	2.02	0.59
1:B:748:GLN:CG	1:B:769:THR:HB	2.32	0.59
1:C:32:MET:HE1	1:C:102:GLU:O	2.03	0.58
1:D:476:PRO:O	1:D:477:VAL:HG13	2.03	0.58
1:A:212:HIS:HE1	1:A:238:GLU:H	1.49	0.58
1:C:343:CYS:HB2	1:C:412:CYS:SG	2.42	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ARG:NH2	1:D:243:ASP:OD1	2.34	0.58
1:E:635:TRP:CH2	1:E:664:ARG:HG2	2.38	0.58
1:B:695:ASP:HA	1:B:718:ARG:HD3	1.85	0.58
1:E:515:PHE:HD1	1:E:516:GLU:HG2	1.68	0.58
1:E:123:LEU:N	1:E:123:LEU:HD22	2.18	0.58
1:C:273:LEU:HD13	1:C:274:THR:N	2.19	0.58
1:C:274:THR:HG21	1:C:540:HIS:HA	1.85	0.58
1:E:520:PRO:O	1:E:521:ALA:HB3	2.03	0.58
1:F:32:MET:HE3	1:F:94:ILE:HG23	1.86	0.58
1:F:123:LEU:N	1:F:123:LEU:HD22	2.17	0.58
1:A:447:LEU:C	1:A:447:LEU:HD23	2.27	0.58
1:C:31:GLU:HG2	1:C:58:PHE:HB3	1.85	0.58
1:F:384:LEU:C	1:F:384:LEU:HD23	2.28	0.58
1:C:631:PRO:O	1:C:646:GLY:HA3	2.03	0.58
1:E:459:GLU:CD	1:E:459:GLU:H	2.12	0.58
1:D:352:GLN:OE1	1:E:73:GLN:N	2.33	0.58
1:D:747:LEU:HD22	1:D:750:GLY:O	2.04	0.58
1:E:536:HIS:HA	5:E:3025:HOH:O	2.04	0.58
1:F:300:LEU:HD12	1:F:340:LEU:CD2	2.34	0.58
1:F:310:MET:SD	1:F:316:CYS:HA	2.44	0.58
1:E:214:GLN:HE22	1:E:232:VAL:CG2	2.17	0.58
1:E:516:GLU:O	1:E:517:ASN:HB2	2.03	0.58
1:F:747:LEU:HD22	1:F:750:GLY:O	2.04	0.58
1:A:134:VAL:O	1:A:135:LYS:HB2	2.04	0.57
1:A:516:GLU:O	1:A:517:ASN:HB2	2.04	0.57
1:B:348:PRO:O	1:B:387:TYR:HD1	1.87	0.57
1:B:714:LEU:HD13	1:B:715:LYS:N	2.20	0.57
1:F:595:PHE:CE1	1:F:631:PRO:HG2	2.39	0.57
1:B:719:THR:HG22	1:B:722:THR:O	2.03	0.57
1:C:447:LEU:C	1:C:447:LEU:HD23	2.28	0.57
1:E:749:ASP:C	1:E:764:GLN:HE22	2.13	0.57
1:C:32:MET:HE3	1:C:94:ILE:HG23	1.85	0.57
1:D:525:LYS:HG2	1:D:558:VAL:HG21	1.86	0.57
1:F:733:ASN:O	1:F:733:ASN:OD1	2.21	0.57
1:D:695:ASP:HA	1:D:718:ARG:HD3	1.86	0.57
1:E:547:VAL:HG23	1:E:550:ALA:HB2	1.86	0.57
1:F:719:THR:HG23	1:F:720:GLY:N	2.20	0.57
1:F:548:PRO:HG3	1:F:559:VAL:HG21	1.86	0.57
1:A:580:ALA:HA	1:A:585:THR:O	2.04	0.57
1:B:28:GLN:NE2	1:B:33:VAL:HG21	2.19	0.57
1:C:123:LEU:N	1:C:123:LEU:HD22	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LEU:HD13	1:C:179:VAL:HG21	1.87	0.57
1:D:736:LEU:HD13	1:D:736:LEU:C	2.29	0.57
1:E:35:TYR:HB3	1:E:52:LEU:HD11	1.87	0.57
1:A:123:LEU:HD13	1:A:128:ARG:HA	1.85	0.57
1:D:298:LEU:CD2	1:D:560:ARG:HB2	2.35	0.57
1:B:278:THR:HG21	1:F:45:THR:HA	1.86	0.56
1:B:384:LEU:C	1:B:384:LEU:HD23	2.31	0.56
1:B:512:ILE:HB	1:B:539:LEU:HD23	1.87	0.56
1:A:153:ARG:HG2	1:A:229:GLN:HB2	1.87	0.56
1:A:377:TRP:CZ3	1:A:379:LYS:HD2	2.41	0.56
1:A:742:VAL:HG23	1:A:743:LYS:N	2.21	0.56
1:C:490:MET:HE2	1:C:620:PHE:CD1	2.39	0.56
1:D:349:TYR:HB3	1:D:384:LEU:HD21	1.87	0.56
1:D:377:TRP:CZ3	1:D:379:LYS:HD2	2.40	0.56
1:D:631:PRO:O	1:D:646:GLY:HA3	2.05	0.56
1:E:204:ARG:HG2	1:E:204:ARG:HH11	1.69	0.56
1:E:476:PRO:C	1:E:477:VAL:HG12	2.29	0.56
1:E:522:HIS:CG	1:E:622:GLU:HG3	2.40	0.56
1:F:204:ARG:O	1:F:204:ARG:HG2	2.05	0.56
1:B:314:GLN:HB3	1:B:354:SER:HB2	1.86	0.56
1:D:174:ARG:O	1:D:177:GLN:HG2	2.04	0.56
1:C:195:LYS:HE2	1:C:478:HIS:HB3	1.87	0.56
1:E:43:GLU:C	1:E:45:THR:H	2.13	0.56
1:C:93:THR:CG2	1:C:104:LYS:HB3	2.25	0.56
1:C:134:VAL:O	1:C:135:LYS:HB2	2.06	0.56
1:C:296:ARG:O	1:C:560:ARG:NH1	2.39	0.56
1:E:174:ARG:HB3	1:E:220:VAL:HG11	1.87	0.56
1:E:539:LEU:HB3	1:E:546:ARG:HB3	1.88	0.56
1:A:275:THR:O	1:A:276:SER:HB2	2.04	0.56
1:B:350:ILE:HD13	1:B:360:LEU:HD12	1.87	0.56
1:C:516:GLU:O	1:C:517:ASN:HB2	2.06	0.56
1:F:137:ASN:HB3	1:F:152:GLU:OE1	2.05	0.56
1:F:485:ALA:HB1	1:F:519:ALA:CB	2.25	0.56
1:E:311:LYS:HE3	1:E:314:GLN:OE1	2.06	0.56
1:B:476:PRO:O	1:B:477:VAL:CG1	2.53	0.56
1:C:290:ILE:CD1	1:C:335:LEU:HD22	2.36	0.56
1:C:591:MET:HE2	1:C:607:GLN:NE2	2.20	0.56
1:F:348:PRO:HG2	1:F:349:TYR:CE1	2.40	0.56
1:A:122:PHE:C	1:A:123:LEU:HD22	2.31	0.56
1:F:155:ASP:OD1	1:F:227:LYS:HE3	2.06	0.56
1:A:48:LEU:HD12	1:A:49:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:HIS:HE1	1:A:237:LEU:HD12	1.70	0.55
1:B:164:GLY:O	1:B:165:LEU:HB2	2.06	0.55
1:A:692:ASN:H	1:A:692:ASN:HD22	1.52	0.55
1:C:18:HIS:O	1:C:38:PRO:HA	2.06	0.55
1:F:165:LEU:HD12	1:F:174:ARG:HG2	1.88	0.55
1:F:476:PRO:O	1:F:477:VAL:CG1	2.54	0.55
1:F:746:GLY:N	1:F:771:THR:HG23	2.21	0.55
1:C:124:ARG:NH2	1:C:243:ASP:OD1	2.38	0.55
1:C:525:LYS:CG	1:C:558:VAL:HG21	2.33	0.55
1:F:767:ALA:O	1:F:768:LEU:C	2.49	0.55
1:B:695:ASP:OD1	1:B:720:GLY:HA2	2.07	0.55
1:D:18:HIS:O	1:D:38:PRO:HA	2.07	0.55
1:D:482:ASP:HB3	1:D:516:GLU:OE1	2.07	0.55
1:A:43:GLU:HB2	1:A:46:TRP:HD1	1.71	0.55
1:E:44:ARG:HG2	1:E:47:GLN:HE22	1.71	0.55
1:B:762:LYS:HD2	1:B:763:PRO:HD2	1.88	0.55
1:E:742:VAL:HG23	1:E:743:LYS:N	2.22	0.55
1:B:500:ILE:HG12	1:B:505:PHE:HB2	1.88	0.55
1:D:672:GLY:HA3	1:D:680:TYR:OH	2.07	0.55
1:D:735:THR:CG2	1:D:736:LEU:N	2.70	0.55
1:E:195:LYS:HE2	1:E:478:HIS:HB3	1.87	0.55
1:B:744:VAL:HG22	1:B:771:THR:O	2.06	0.55
1:D:631:PRO:HD2	1:D:635:TRP:CZ2	2.41	0.55
1:D:765:GLY:C	1:D:767:ALA:H	2.13	0.55
1:B:285:THR:O	1:B:288:SER:HB3	2.07	0.55
1:B:736:LEU:C	1:B:736:LEU:HD13	2.32	0.55
1:C:348:PRO:HG2	1:C:349:TYR:CE1	2.42	0.55
1:B:32:MET:CE	1:B:94:ILE:HG23	2.27	0.54
1:B:730:GLU:HG3	1:B:732:LYS:NZ	2.22	0.54
1:E:565:LEU:CG	1:E:569:MET:HE2	2.15	0.54
1:F:274:THR:HG21	1:F:540:HIS:CE1	2.42	0.54
1:B:648:ARG:HD3	5:C:3115:HOH:O	2.06	0.54
1:B:722:THR:HG23	1:B:769:THR:HG23	1.89	0.54
1:D:136:ASN:ND2	1:D:227:LYS:HE2	2.22	0.54
1:E:718:ARG:HB2	1:E:723:ILE:HG22	1.89	0.54
1:C:261:PRO:HA	1:C:473:GLN:O	2.08	0.54
1:E:133:GLN:HB2	1:E:136:ASN:HD22	1.72	0.54
1:E:479:TRP:CZ2	3:E:804:XYF:H4	2.42	0.54
1:E:500:ILE:HG12	1:E:505:PHE:HB2	1.89	0.54
1:F:744:VAL:HG22	1:F:745:ASN:N	2.22	0.54
1:B:382:PRO:HG2	5:B:3011:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:LEU:HD13	1:B:689:HIS:CD2	2.43	0.54
1:F:273:LEU:HD13	1:F:274:THR:N	2.22	0.54
1:F:331:MET:O	1:F:335:LEU:HG	2.08	0.54
1:A:571:PRO:HB2	1:A:670:ALA:O	2.06	0.54
1:D:700:VAL:HG22	1:D:715:LYS:HG2	1.90	0.54
1:D:766:ASN:C	1:D:768:LEU:N	2.53	0.54
1:E:744:VAL:HG22	1:E:745:ASN:N	2.23	0.54
1:F:350:ILE:HD13	1:F:360:LEU:HD12	1.88	0.54
1:B:13:GLY:O	1:B:143:THR:HB	2.07	0.54
1:E:681:VAL:HG23	1:E:683:HIS:CE1	2.43	0.54
1:F:526:ARG:HD2	1:F:619:VAL:HB	1.90	0.54
1:F:575:ARG:NH2	1:F:579:ARG:HH12	2.05	0.54
1:B:201:MET:CE	1:B:247:PRO:HB3	2.38	0.54
1:C:277:PHE:CD2	1:C:278:THR:HG23	2.42	0.54
1:C:575:ARG:NH1	1:C:579:ARG:HH12	2.05	0.54
1:D:735:THR:CG2	1:D:760:VAL:HG13	2.38	0.54
1:E:522:HIS:CE1	1:E:523:VAL:HG23	2.42	0.54
1:B:479:TRP:HZ2	3:B:802:XYF:H4	1.73	0.54
1:C:20:LEU:HD22	1:C:134:VAL:CG2	2.38	0.54
1:C:136:ASN:HB3	1:C:153:ARG:HB2	1.89	0.54
1:C:291:ASP:O	1:C:295:GLU:HG3	2.08	0.54
1:C:695:ASP:OD1	1:C:719:THR:O	2.25	0.54
1:E:128:ARG:HH22	1:E:131:GLY:HA3	1.72	0.54
1:F:336:LYS:HG2	1:F:342:ILE:CD1	2.37	0.54
1:A:479:TRP:HZ2	3:A:801:XYF:H4	1.73	0.54
1:C:201:MET:CE	1:C:247:PRO:HB3	2.38	0.54
1:E:352:GLN:HA	1:E:357:PHE:CD2	2.43	0.54
1:F:17:ILE:HG12	1:F:139:TYR:HB3	1.90	0.54
1:C:670:ALA:C	1:C:671:LEU:HD12	2.33	0.53
1:C:681:VAL:HG23	1:C:681:VAL:O	2.07	0.53
1:E:736:LEU:C	1:E:736:LEU:HD13	2.33	0.53
1:A:336:LYS:HG2	1:A:342:ILE:HD13	1.90	0.53
1:B:447:LEU:HD23	1:B:447:LEU:C	2.33	0.53
1:C:327:ASP:OD2	1:C:330:GLY:HA3	2.06	0.53
1:D:273:LEU:HD13	1:D:273:LEU:C	2.33	0.53
1:D:483:CYS:SG	1:D:514:GLY:HA2	2.48	0.53
1:A:766:ASN:O	1:A:767:ALA:HB2	2.08	0.53
1:D:772:LEU:H	1:D:772:LEU:HD22	1.72	0.53
1:F:735:THR:HG22	1:F:736:LEU:N	2.23	0.53
1:A:311:LYS:HE3	1:A:314:GLN:OE1	2.08	0.53
1:D:336:LYS:HE3	1:D:411:ASP:OD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:735:THR:CG2	1:E:736:LEU:N	2.72	0.53
1:B:163:TYR:CD2	1:B:592:MET:HE3	2.44	0.53
1:B:310:MET:SD	1:B:316:CYS:HA	2.49	0.53
1:F:267:TRP:CE3	1:F:341:LYS:HG3	2.44	0.53
1:F:497:GLY:O	1:F:500:ILE:HG22	2.09	0.53
1:F:668:LEU:O	1:F:701:CYS:HB2	2.09	0.53
1:A:136:ASN:HB3	1:A:153:ARG:HB2	1.90	0.53
1:E:745:ASN:HB3	1:E:771:THR:O	2.09	0.53
1:F:70:GLU:HB3	1:F:236:TYR:HB2	1.90	0.53
1:A:17:ILE:HG13	1:A:17:ILE:O	2.07	0.53
1:B:315:TRP:HB2	1:B:381:GLN:OE1	2.09	0.53
1:B:352:GLN:HA	1:B:357:PHE:CD2	2.43	0.53
1:B:476:PRO:C	1:B:477:VAL:HG12	2.34	0.53
1:B:332:ILE:HD12	1:B:332:ILE:C	2.34	0.53
1:B:668:LEU:HD13	1:B:690:LEU:HD13	1.91	0.53
1:C:694:GLN:HB2	1:C:697:HIS:CD2	2.44	0.53
1:D:282:ASP:O	1:D:286:VAL:HG23	2.09	0.53
1:D:310:MET:SD	1:D:316:CYS:HA	2.48	0.53
1:E:333:ARG:HH11	1:E:336:LYS:HE3	1.73	0.53
1:E:487:TYR:HD1	1:E:490:MET:HE2	1.73	0.53
1:E:552:ASP:OD1	1:E:555:SER:N	2.38	0.53
1:F:472:ALA:HB1	5:F:3084:HOH:O	2.08	0.53
1:B:16:LEU:HD22	1:B:140:VAL:HG22	1.90	0.53
1:C:540:HIS:C	1:C:546:ARG:HG3	2.34	0.53
1:C:742:VAL:HG23	1:C:743:LYS:N	2.24	0.53
1:D:509:SER:HB3	1:D:536:HIS:HB2	1.91	0.53
1:D:547:VAL:CG2	1:D:550:ALA:HB2	2.34	0.53
1:F:153:ARG:HG2	1:F:229:GLN:HB2	1.91	0.53
1:F:277:PHE:CD2	1:F:278:THR:HG23	2.44	0.53
1:A:343:CYS:HB2	1:A:412:CYS:SG	2.49	0.52
1:F:274:THR:HG22	1:F:275:THR:N	2.25	0.52
1:B:61:GLN:NE2	1:B:87:LEU:HG	2.23	0.52
1:B:262:ALA:HB3	1:B:476:PRO:HG3	1.90	0.52
1:E:742:VAL:HG23	1:E:743:LYS:H	1.74	0.52
1:E:744:VAL:HG21	1:E:770:ILE:CG2	2.39	0.52
1:C:273:LEU:HB2	1:C:300:LEU:HD21	1.91	0.52
1:D:735:THR:HG22	1:D:736:LEU:N	2.24	0.52
1:B:298:LEU:CD2	1:B:560:ARG:HB2	2.39	0.52
1:C:453:LYS:HD2	1:C:458:GLU:OE1	2.09	0.52
1:D:155:ASP:OD1	1:D:227:LYS:HE3	2.09	0.52
1:E:595:PHE:CE1	1:E:631:PRO:HG2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:PHE:HD1	1:C:516:GLU:HG2	1.74	0.52
1:D:766:ASN:O	1:D:768:LEU:N	2.42	0.52
1:E:267:TRP:CE3	1:E:341:LYS:HG3	2.44	0.52
1:F:174:ARG:HB3	1:F:220:VAL:HG11	1.92	0.52
1:F:327:ASP:OD2	1:F:330:GLY:HA3	2.08	0.52
1:F:719:THR:HG23	1:F:720:GLY:H	1.73	0.52
1:B:479:TRP:HA	1:B:509:SER:O	2.10	0.52
1:E:468:ALA:HB1	1:E:472:ALA:HB3	1.91	0.52
1:A:43:GLU:HB3	1:A:45:THR:HG22	1.90	0.52
1:A:212:HIS:CE1	1:A:237:LEU:HD12	2.45	0.52
1:D:540:HIS:C	1:D:546:ARG:NE	2.63	0.52
1:E:290:ILE:CD1	1:E:335:LEU:HD22	2.39	0.52
1:A:80:PRO:HD3	1:A:431:SER:HB3	1.91	0.52
1:A:719:THR:HG23	1:A:720:GLY:H	1.75	0.52
1:F:557:ASP:OD1	1:F:560:ARG:NH2	2.43	0.52
1:D:719:THR:HG22	1:D:722:THR:HB	1.92	0.52
1:E:479:TRP:CH2	3:E:804:XYF:H4	2.45	0.52
1:F:290:ILE:CD1	1:F:335:LEU:HD22	2.39	0.52
1:D:80:PRO:HD3	1:D:431:SER:HB3	1.91	0.52
1:E:744:VAL:HG22	1:E:771:THR:O	2.10	0.52
1:F:516:GLU:O	1:F:517:ASN:HB2	2.09	0.52
1:A:466:ARG:HB2	1:A:479:TRP:CH2	2.44	0.51
1:D:134:VAL:O	1:D:135:LYS:HB2	2.10	0.51
1:D:274:THR:O	1:D:546:ARG:HG3	2.10	0.51
1:D:721:ASN:O	1:D:771:THR:HA	2.10	0.51
1:A:347:ASN:HA	1:A:444:TYR:OH	2.11	0.51
1:C:18:HIS:HB2	1:C:20:LEU:HD21	1.91	0.51
1:D:31:GLU:HG2	1:D:58:PHE:HB3	1.92	0.51
1:E:377:TRP:HE1	1:E:384:LEU:HD22	1.75	0.51
1:A:31:GLU:OE1	1:A:56:ARG:HD3	2.10	0.51
1:B:638:LEU:O	1:B:739:ARG:NH2	2.44	0.51
1:C:306:ASP:O	1:C:309:TRP:HD1	1.94	0.51
1:C:352:GLN:HA	1:C:357:PHE:CD2	2.46	0.51
1:E:282:ASP:HA	1:E:324:THR:CG2	2.40	0.51
1:E:698:GLU:OE1	1:E:715:LYS:HD3	2.09	0.51
1:A:749:ASP:C	1:A:764:GLN:HB2	2.36	0.51
1:B:163:TYR:CE2	1:B:592:MET:HE3	2.46	0.51
1:B:747:LEU:HD22	1:B:750:GLY:O	2.11	0.51
1:D:681:VAL:O	1:D:681:VAL:HG13	2.09	0.51
1:E:463:LEU:O	1:E:477:VAL:CG1	2.52	0.51
1:A:18:HIS:O	1:A:38:PRO:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:689:HIS:ND1	1:D:739:ARG:NE	2.53	0.51
1:E:306:ASP:O	1:E:309:TRP:HD1	1.93	0.51
1:B:31:GLU:HG2	1:B:58:PHE:HB3	1.91	0.51
1:B:744:VAL:HG23	1:B:772:LEU:HA	1.93	0.51
1:A:630:LEU:O	1:A:647:SER:N	2.43	0.51
1:B:17:ILE:HG13	1:B:53:PHE:HZ	1.75	0.51
1:A:635:TRP:CZ3	1:A:664:ARG:HG2	2.46	0.51
1:A:748:GLN:HB2	1:A:769:THR:HG22	1.91	0.51
1:E:150:MET:HB3	1:E:237:LEU:HB2	1.92	0.51
1:E:497:GLY:O	1:E:500:ILE:HG22	2.11	0.51
1:F:134:VAL:O	1:F:135:LYS:HB2	2.11	0.51
1:F:521:ALA:HB3	5:F:3055:HOH:O	2.10	0.51
1:F:652:GLN:NE2	1:F:654:HIS:NE2	2.59	0.51
1:D:547:VAL:HG23	1:D:550:ALA:CB	2.33	0.51
1:E:41:VAL:C	1:E:43:GLU:H	2.18	0.51
1:F:276:SER:HB2	1:F:279:THR:OG1	2.10	0.51
1:A:310:MET:SD	1:A:316:CYS:HA	2.51	0.51
1:B:274:THR:HG23	1:B:304:HIS:HD2	1.76	0.51
1:C:515:PHE:CD1	1:C:516:GLU:HG2	2.46	0.51
1:E:20:LEU:HD12	1:E:38:PRO:O	2.11	0.51
1:E:134:VAL:O	1:E:135:LYS:HB2	2.11	0.51
1:F:214:GLN:HG3	1:F:435:LYS:HG2	1.93	0.51
1:A:273:LEU:HD13	1:A:273:LEU:C	2.36	0.50
1:A:723:ILE:HG13	1:A:723:ILE:O	2.11	0.50
1:E:343:CYS:HB2	1:E:412:CYS:SG	2.52	0.50
1:B:274:THR:CG2	1:B:275:THR:N	2.75	0.50
1:D:165:LEU:HA	1:D:197:ILE:O	2.11	0.50
1:E:287:ASN:HD21	1:E:334:ARG:HH21	1.59	0.50
1:E:681:VAL:O	1:E:681:VAL:HG13	2.09	0.50
1:E:767:ALA:O	1:E:769:THR:HG23	2.12	0.50
1:D:123:LEU:HD23	1:D:128:ARG:HA	1.94	0.50
1:D:296:ARG:HD2	1:D:549:TRP:CE3	2.45	0.50
1:D:380:TRP:H	1:E:49:ASP:HA	1.75	0.50
1:D:476:PRO:O	1:D:477:VAL:CG1	2.60	0.50
1:D:670:ALA:HB2	1:D:701:CYS:SG	2.51	0.50
1:A:274:THR:CG2	1:A:275:THR:N	2.74	0.50
1:D:201:MET:CE	1:D:247:PRO:HB3	2.42	0.50
1:D:630:LEU:HG	1:D:635:TRP:CD1	2.46	0.50
1:E:668:LEU:O	1:E:701:CYS:HB2	2.12	0.50
1:A:735:THR:CG2	1:A:760:VAL:HG13	2.41	0.50
1:B:671:LEU:HD13	1:B:689:HIS:HD2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:723:ILE:HG13	1:B:723:ILE:O	2.10	0.50
1:D:378:ASP:HA	1:D:381:GLN:O	2.11	0.50
1:F:429:ASP:CG	1:F:431:SER:HG	2.19	0.50
1:A:380:TRP:CD1	1:A:381:GLN:HG2	2.47	0.50
1:B:332:ILE:HG12	1:B:408:MET:O	2.12	0.50
1:B:379:LYS:O	1:B:380:TRP:HB3	2.11	0.50
1:C:133:GLN:HB2	1:C:136:ASN:ND2	2.26	0.50
1:B:20:LEU:HD12	1:B:38:PRO:O	2.11	0.50
1:C:725:VAL:CG2	1:C:768:LEU:HD12	2.42	0.50
1:C:736:LEU:HD13	1:C:736:LEU:C	2.37	0.50
1:F:748:GLN:O	1:F:768:LEU:HA	2.12	0.50
1:A:61:GLN:HB2	1:A:64:ILE:HD12	1.94	0.50
1:A:273:LEU:HD12	1:A:303:PHE:CE1	2.47	0.50
1:B:417:PHE:HA	1:B:419:GLU:OE2	2.12	0.50
1:B:548:PRO:HG3	1:B:559:VAL:HG21	1.94	0.50
1:C:654:HIS:ND1	1:C:658:SER:OG	2.35	0.50
1:D:447:LEU:C	1:D:447:LEU:HD23	2.37	0.50
1:B:45:THR:HG23	1:B:46:TRP:CD1	2.47	0.50
1:D:500:ILE:HG12	1:D:505:PHE:HB2	1.94	0.50
1:E:201:MET:HE1	1:E:247:PRO:HA	1.94	0.50
1:E:214:GLN:NE2	1:E:232:VAL:CG2	2.75	0.50
1:F:476:PRO:C	1:F:477:VAL:HG12	2.37	0.50
1:F:554:GLU:O	1:F:558:VAL:HG23	2.12	0.50
1:F:692:ASN:HD22	1:F:692:ASN:N	2.06	0.50
1:A:16:LEU:CD2	1:A:140:VAL:HG22	2.40	0.49
1:A:695:ASP:OD1	1:A:719:THR:O	2.29	0.49
1:A:731:ALA:C	1:A:732:LYS:HD2	2.37	0.49
1:C:17:ILE:HG13	1:C:53:PHE:HZ	1.76	0.49
1:D:693:LEU:HD13	1:D:718:ARG:HB2	1.94	0.49
1:E:38:PRO:HG2	1:E:51:PRO:HB2	1.94	0.49
1:E:566:LYS:HA	1:E:569:MET:HE3	1.94	0.49
1:F:329:GLU:H	1:F:329:GLU:CD	2.20	0.49
1:A:767:ALA:O	1:A:768:LEU:C	2.54	0.49
1:C:747:LEU:HD22	1:C:750:GLY:O	2.12	0.49
1:D:546:ARG:HH11	1:D:546:ARG:N	2.09	0.49
1:D:733:ASN:OD1	1:D:733:ASN:O	2.29	0.49
1:E:489:SER:O	1:E:492:GLU:HG2	2.12	0.49
1:E:588:MET:HE3	5:E:3008:HOH:O	2.12	0.49
1:F:17:ILE:CG1	1:F:139:TYR:HB3	2.42	0.49
1:A:182:TRP:CE3	1:A:215:CYS:HB2	2.48	0.49
1:C:70:GLU:HG2	5:C:3100:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:TYR:HB3	1:C:502:LEU:HD13	1.94	0.49
1:C:347:ASN:HA	1:C:444:TYR:OH	2.12	0.49
1:D:160:GLU:HG3	1:D:204:ARG:HG2	1.94	0.49
1:D:770:ILE:N	1:D:770:ILE:HD12	2.28	0.49
1:E:196:ASN:C	1:E:197:ILE:HG12	2.37	0.49
1:F:487:TYR:HD1	1:F:490:MET:HE2	1.76	0.49
1:F:579:ARG:HG3	1:F:579:ARG:NH1	2.27	0.49
1:B:525:LYS:HG2	1:B:558:VAL:HG21	1.94	0.49
1:C:123:LEU:HD13	1:C:128:ARG:HA	1.94	0.49
1:C:273:LEU:HD13	1:C:273:LEU:C	2.37	0.49
1:C:274:THR:HG21	1:C:540:HIS:CG	2.48	0.49
1:C:298:LEU:HD23	1:C:560:ARG:HG3	1.93	0.49
1:C:479:TRP:CZ2	3:C:803:XYF:H4	2.48	0.49
1:D:382:PRO:HG2	5:D:3059:HOH:O	2.11	0.49
1:D:576:GLU:O	1:D:579:ARG:HB2	2.13	0.49
1:D:738:LEU:HB2	1:D:741:VAL:HB	1.94	0.49
1:D:749:ASP:OD2	1:D:767:ALA:HB3	2.12	0.49
1:E:305:PHE:HB2	1:E:344:VAL:HG12	1.95	0.49
1:E:748:GLN:HB2	1:E:769:THR:OG1	2.13	0.49
1:F:219:GLU:HB2	1:F:229:GLN:HB3	1.93	0.49
1:B:723:ILE:CG1	1:B:770:ILE:HB	2.42	0.49
1:B:747:LEU:HD23	1:B:748:GLN:H	1.76	0.49
1:E:548:PRO:HG3	1:E:559:VAL:HG21	1.95	0.49
1:F:18:HIS:O	1:F:38:PRO:HA	2.13	0.49
1:F:414:LYS:NZ	1:F:538:ARG:HH22	2.10	0.49
1:A:107:ASN:ND2	1:A:125:ASN:HD21	2.05	0.49
1:A:124:ARG:NH2	1:A:243:ASP:OD1	2.43	0.49
1:E:731:ALA:C	1:E:732:LYS:HD2	2.37	0.49
1:A:290:ILE:HD12	1:A:335:LEU:HD22	1.95	0.49
1:A:576:GLU:HG3	1:A:611:GLY:HA3	1.93	0.49
1:E:772:LEU:HD22	1:E:772:LEU:N	2.28	0.49
1:F:438:ASN:HB3	5:F:3119:HOH:O	2.12	0.49
1:B:152:GLU:HB3	1:B:230:PHE:CE1	2.48	0.49
1:B:273:LEU:HD12	1:B:303:PHE:HE1	1.78	0.49
1:E:124:ARG:NH2	1:E:243:ASP:OD1	2.46	0.49
1:E:747:LEU:HD22	1:E:750:GLY:O	2.13	0.49
1:A:262:ALA:HB3	1:A:476:PRO:HG3	1.94	0.49
1:A:417:PHE:HA	1:A:419:GLU:OE2	2.12	0.49
1:B:332:ILE:O	1:B:336:LYS:HG3	2.13	0.49
1:D:698:GLU:OE1	1:D:715:LYS:HD3	2.13	0.49
1:F:134:VAL:HG22	1:F:135:LYS:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LYS:HG3	1:A:458:GLU:HG3	1.93	0.49
1:C:668:LEU:CD2	1:C:714:LEU:HD12	2.32	0.49
1:D:341:LYS:C	1:D:342:ILE:HD12	2.38	0.49
1:D:749:ASP:CG	1:D:767:ALA:HB3	2.38	0.49
1:F:82:TYR:HB3	1:F:84:LEU:HD13	1.95	0.49
1:A:58:PHE:N	1:A:58:PHE:CD1	2.81	0.48
1:C:356:VAL:HG11	1:C:397:TRP:CH2	2.48	0.48
1:C:652:GLN:NE2	1:C:654:HIS:NE2	2.60	0.48
1:D:145:ASN:OD1	1:D:147:ARG:HB2	2.13	0.48
1:F:719:THR:HG22	5:F:3140:HOH:O	2.13	0.48
1:A:498:LEU:HD21	1:A:608:TYR:HB3	1.95	0.48
1:B:204:ARG:HD2	1:B:206:TYR:HE2	1.79	0.48
1:C:82:TYR:HB2	1:C:84:LEU:CD2	2.42	0.48
1:D:32:MET:CE	1:D:94:ILE:HG23	2.23	0.48
1:E:723:ILE:CG1	1:E:770:ILE:HB	2.41	0.48
1:A:749:ASP:HB3	1:A:764:GLN:O	2.13	0.48
1:B:16:LEU:CD2	1:B:140:VAL:HG22	2.43	0.48
1:B:98:GLU:H	1:B:98:GLU:CD	2.21	0.48
1:B:748:GLN:HG3	1:B:769:THR:HB	1.94	0.48
1:D:273:LEU:HD12	1:D:303:PHE:HD1	1.77	0.48
1:D:723:ILE:CG1	1:D:770:ILE:HB	2.43	0.48
1:E:277:PHE:CD2	1:E:278:THR:HG23	2.48	0.48
1:B:134:VAL:O	1:B:135:LYS:HB2	2.13	0.48
1:B:432:ASP:OD2	1:B:435:LYS:HG3	2.13	0.48
1:C:122:PHE:C	1:C:123:LEU:HD22	2.39	0.48
1:E:201:MET:CE	1:E:247:PRO:HA	2.43	0.48
1:E:763:PRO:O	1:E:764:GLN:HB3	2.12	0.48
1:B:347:ASN:HA	1:B:444:TYR:OH	2.14	0.48
1:C:2:LYS:HA	1:C:223:GLU:OE1	2.13	0.48
1:C:167:GLU:OE2	1:C:195:LYS:NZ	2.43	0.48
1:C:208:VAL:HA	1:C:240:PHE:O	2.13	0.48
1:E:634:ARG:HG3	1:E:634:ARG:NH2	2.28	0.48
1:F:280:ASN:HB3	5:F:3086:HOH:O	2.13	0.48
1:F:336:LYS:HG2	1:F:342:ILE:HD13	1.94	0.48
1:A:201:MET:HE1	1:A:247:PRO:CA	2.42	0.48
1:A:476:PRO:C	1:A:477:VAL:HG13	2.39	0.48
1:B:730:GLU:HG3	1:B:732:LYS:HZ2	1.77	0.48
1:C:500:ILE:HG12	1:C:505:PHE:HB2	1.95	0.48
1:D:515:PHE:CD1	1:D:542:SER:HB2	2.49	0.48
1:D:719:THR:CG2	1:D:722:THR:HB	2.44	0.48
1:E:208:VAL:HA	1:E:240:PHE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:489:SER:HA	1:E:492:GLU:CD	2.38	0.48
1:F:522:HIS:CB	1:F:622:GLU:HG3	2.44	0.48
1:A:405:LEU:O	1:A:408:MET:HB3	2.14	0.48
1:B:296:ARG:HD3	1:B:556:CYS:SG	2.53	0.48
1:B:672:GLY:HA3	1:B:680:TYR:OH	2.13	0.48
1:C:11:GLN:HB2	1:C:14:LEU:HD12	1.96	0.48
1:D:274:THR:OG1	1:D:304:HIS:HB3	2.14	0.48
1:D:315:TRP:CE3	1:D:381:GLN:NE2	2.82	0.48
1:D:580:ALA:HA	1:D:585:THR:O	2.14	0.48
1:E:282:ASP:HB3	1:E:324:THR:HG23	1.94	0.48
1:E:300:LEU:HD13	1:E:301:HIS:N	2.28	0.48
1:F:136:ASN:HB3	1:F:153:ARG:HB2	1.96	0.48
1:A:121:ASP:OD1	1:A:128:ARG:HD2	2.14	0.48
1:D:164:GLY:O	1:D:165:LEU:HB2	2.14	0.48
1:D:327:ASP:OD2	1:D:330:GLY:HA3	2.14	0.48
1:D:588:MET:HE3	5:D:3075:HOH:O	2.13	0.48
1:D:725:VAL:CB	1:D:768:LEU:HD12	2.40	0.48
1:E:274:THR:CG2	1:E:275:THR:N	2.77	0.48
1:F:332:ILE:O	1:F:336:LYS:HG3	2.13	0.48
1:F:333:ARG:HG2	1:F:333:ARG:HH11	1.78	0.48
1:F:515:PHE:CD1	1:F:542:SER:HB2	2.49	0.48
1:A:31:GLU:HG2	1:A:58:PHE:HB3	1.94	0.48
1:B:670:ALA:HB2	1:B:701:CYS:SG	2.54	0.48
1:C:272:TRP:HB2	1:C:538:ARG:HG3	1.94	0.48
1:C:272:TRP:CB	1:C:538:ARG:HG3	2.44	0.48
1:D:136:ASN:HD21	1:D:227:LYS:HE2	1.77	0.48
1:E:466:ARG:HB2	1:E:479:TRP:CZ3	2.48	0.48
1:F:277:PHE:HB3	1:F:542:SER:O	2.14	0.48
1:B:341:LYS:C	1:B:342:ILE:HD12	2.38	0.48
1:D:698:GLU:HG3	1:D:717:ALA:HB2	1.95	0.48
1:E:100:TYR:CD2	1:E:113:SER:HA	2.49	0.48
1:F:262:ALA:HB3	1:F:476:PRO:HG3	1.95	0.48
1:B:521:ALA:O	1:B:525:LYS:HD3	2.13	0.47
1:B:693:LEU:HD21	1:B:697:HIS:O	2.14	0.47
1:C:579:ARG:NH1	1:C:579:ARG:CG	2.76	0.47
1:C:772:LEU:N	1:C:772:LEU:HD22	2.29	0.47
1:D:273:LEU:HD12	1:D:303:PHE:CD1	2.49	0.47
1:D:748:GLN:O	1:D:768:LEU:HA	2.14	0.47
1:E:588:MET:HG3	1:E:608:TYR:CD1	2.48	0.47
1:F:290:ILE:HD11	1:F:335:LEU:HD22	1.96	0.47
1:F:479:TRP:HE1	1:F:511:ASP:CG	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:488:GLU:H	1:F:488:GLU:CD	2.22	0.47
1:A:384:LEU:C	1:A:384:LEU:HD23	2.38	0.47
1:B:766:ASN:O	1:B:767:ALA:CB	2.62	0.47
1:D:163:TYR:CE2	1:D:592:MET:HE3	2.49	0.47
1:E:283:GLU:OE2	1:E:331:MET:HB2	2.14	0.47
1:A:167:GLU:OE2	1:A:195:LYS:NZ	2.45	0.47
1:A:267:TRP:CE3	1:A:341:LYS:HG3	2.49	0.47
1:B:753:ALA:O	1:B:759:LEU:HD12	2.13	0.47
1:E:43:GLU:HB3	1:E:45:THR:HG22	1.96	0.47
1:E:133:GLN:HB2	1:E:136:ASN:ND2	2.29	0.47
1:C:274:THR:HG23	1:C:276:SER:H	1.79	0.47
1:E:731:ALA:O	1:E:732:LYS:HD2	2.15	0.47
1:F:17:ILE:HG13	1:F:53:PHE:HZ	1.80	0.47
1:A:191:GLU:HB3	1:D:222:SER:O	2.15	0.47
1:B:273:LEU:HB2	1:B:300:LEU:HD11	1.95	0.47
1:D:490:MET:HE3	1:D:620:PHE:CD1	2.50	0.47
1:F:515:PHE:HE2	1:F:540:HIS:HE2	1.63	0.47
1:A:261:PRO:HA	1:A:473:GLN:O	2.14	0.47
1:A:479:TRP:CZ2	3:A:801:XYF:H4	2.48	0.47
1:A:692:ASN:HD22	1:A:692:ASN:N	2.10	0.47
1:B:277:PHE:HB3	1:B:542:SER:O	2.15	0.47
1:C:20:LEU:HD22	1:C:134:VAL:HG22	1.97	0.47
1:D:405:LEU:O	1:D:408:MET:HB3	2.15	0.47
1:D:437:HIS:HB3	5:D:3049:HOH:O	2.13	0.47
1:D:746:GLY:N	1:D:771:THR:HG23	2.30	0.47
1:E:298:LEU:HD13	1:E:548:PRO:HG2	1.96	0.47
1:F:659:LEU:O	1:F:661:VAL:HG23	2.14	0.47
1:F:735:THR:CG2	1:F:760:VAL:HG13	2.45	0.47
1:A:201:MET:CE	1:A:247:PRO:HA	2.45	0.47
1:A:512:ILE:HA	1:A:527:TRP:CD1	2.50	0.47
1:B:509:SER:HB2	1:B:536:HIS:HB2	1.97	0.47
1:D:293:MET:CE	1:D:300:LEU:HD23	2.41	0.47
1:D:476:PRO:C	1:D:477:VAL:CG1	2.88	0.47
1:E:191:GLU:HB3	1:F:222:SER:O	2.14	0.47
1:A:497:GLY:O	1:A:500:ILE:HG22	2.14	0.47
1:A:692:ASN:H	1:A:692:ASN:ND2	2.13	0.47
1:B:274:THR:HG21	1:B:540:HIS:CE1	2.49	0.47
1:C:267:TRP:CE3	1:C:341:LYS:HG3	2.49	0.47
1:D:356:VAL:HG12	1:D:360:LEU:HG	1.96	0.47
1:D:772:LEU:HD22	1:D:772:LEU:N	2.30	0.47
1:F:691:PHE:O	1:F:692:ASN:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:LEU:HD12	1:B:303:PHE:CE1	2.50	0.47
1:C:341:LYS:C	1:C:342:ILE:HD12	2.40	0.47
1:C:772:LEU:HD22	1:C:772:LEU:H	1.80	0.47
1:E:80:PRO:HD3	1:E:431:SER:HB3	1.96	0.47
1:E:290:ILE:HD12	1:E:335:LEU:HD22	1.96	0.47
1:F:273:LEU:HD13	1:F:273:LEU:C	2.40	0.47
1:B:64:ILE:HG12	1:B:242:ILE:HG23	1.97	0.46
1:C:747:LEU:HD23	1:C:748:GLN:N	2.29	0.46
1:E:670:ALA:C	1:E:671:LEU:HD12	2.40	0.46
1:F:201:MET:HE2	1:F:502:LEU:CD2	2.45	0.46
1:F:311:LYS:HE3	1:F:314:GLN:CD	2.40	0.46
1:C:510:HIS:N	1:C:510:HIS:CD2	2.82	0.46
1:C:770:ILE:HD12	1:C:770:ILE:C	2.40	0.46
1:D:634:ARG:HH21	1:D:634:ARG:HG3	1.80	0.46
1:F:687:ALA:O	1:F:689:HIS:HD2	1.98	0.46
1:A:123:LEU:HD22	1:A:123:LEU:N	2.31	0.46
1:A:747:LEU:C	1:A:747:LEU:HD23	2.40	0.46
1:B:364:GLY:HA2	5:B:3104:HOH:O	2.15	0.46
1:D:560:ARG:O	1:D:564:GLN:HG3	2.16	0.46
1:E:296:ARG:HH11	1:E:296:ARG:HG3	1.80	0.46
1:E:634:ARG:HG3	1:E:634:ARG:HH21	1.79	0.46
1:A:352:GLN:HA	1:A:357:PHE:CD2	2.50	0.46
1:B:610:LEU:O	1:B:614:VAL:HG13	2.15	0.46
1:B:768:LEU:HD23	1:B:768:LEU:C	2.41	0.46
1:C:745:ASN:HB3	1:C:771:THR:O	2.16	0.46
1:E:300:LEU:HD12	1:E:340:LEU:HD22	1.97	0.46
1:E:472:ALA:HB1	5:E:3063:HOH:O	2.15	0.46
1:F:419:GLU:CD	1:F:419:GLU:H	2.23	0.46
1:A:70:GLU:HG3	5:A:3171:HOH:O	2.16	0.46
1:A:163:TYR:CE2	1:A:592:MET:HE3	2.51	0.46
1:A:761:VAL:CG1	1:A:768:LEU:HD21	2.43	0.46
1:B:44:ARG:HA	1:B:47:GLN:CG	2.42	0.46
1:B:592:MET:SD	1:B:592:MET:C	2.98	0.46
1:C:766:ASN:O	1:C:767:ALA:HB2	2.15	0.46
1:D:389:PHE:O	1:D:395:CYS:SG	2.73	0.46
1:F:735:THR:CG2	1:F:736:LEU:N	2.78	0.46
1:C:17:ILE:HG13	1:C:17:ILE:O	2.14	0.46
1:F:747:LEU:HD23	1:F:748:GLN:N	2.31	0.46
1:B:341:LYS:O	1:B:342:ILE:HD12	2.15	0.46
1:B:525:LYS:O	1:B:528:CYS:HB2	2.16	0.46
1:D:278:THR:CG2	1:E:45:THR:HA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:THR:O	1:F:276:SER:CB	2.62	0.46
1:A:693:LEU:HD22	1:A:718:ARG:HB3	1.97	0.46
1:B:82:TYR:CD1	1:B:470:VAL:HB	2.50	0.46
1:D:479:TRP:CZ3	1:D:481:GLY:HA2	2.51	0.46
1:A:290:ILE:HD13	1:A:340:LEU:CD1	2.46	0.46
1:C:452:LEU:HD12	1:C:452:LEU:HA	1.76	0.46
1:D:738:LEU:CB	1:D:741:VAL:HB	2.46	0.46
1:F:525:LYS:HD3	1:F:656:PHE:CG	2.51	0.46
1:C:44:ARG:HB3	1:E:308:PHE:CZ	2.51	0.46
1:C:693:LEU:HD13	1:C:718:ARG:HB2	1.98	0.46
1:C:730:GLU:HG3	1:C:732:LYS:HZ3	1.79	0.46
1:E:129:ILE:O	1:E:130:THR:HB	2.15	0.46
1:B:137:ASN:HB3	1:B:152:GLU:OE1	2.15	0.45
1:B:331:MET:O	1:B:335:LEU:HG	2.16	0.45
1:B:670:ALA:C	1:B:671:LEU:HD12	2.41	0.45
1:C:84:LEU:N	1:C:84:LEU:HD22	2.31	0.45
1:C:262:ALA:HB3	1:C:476:PRO:HG3	1.97	0.45
1:E:248:LYS:HB2	2:E:3006:SO4:O4	2.16	0.45
1:E:287:ASN:ND2	1:E:334:ARG:HH21	2.14	0.45
1:F:569:MET:CB	1:F:573:LEU:HD22	2.46	0.45
1:A:414:LYS:NZ	1:A:538:ARG:HH12	2.15	0.45
1:A:490:MET:HE2	1:A:620:PHE:CD1	2.52	0.45
1:A:719:THR:HG23	1:A:720:GLY:N	2.31	0.45
1:B:304:HIS:HA	1:B:343:CYS:O	2.17	0.45
1:B:717:ALA:O	1:B:723:ILE:HA	2.15	0.45
1:D:269:PHE:O	1:D:566:LYS:HE2	2.15	0.45
1:D:297:ASN:O	1:D:299:PRO:HD3	2.16	0.45
1:E:48:LEU:HD12	1:E:49:ASP:OD2	2.16	0.45
1:E:129:ILE:HG22	1:E:204:ARG:NH1	2.30	0.45
1:E:348:PRO:HG2	1:E:349:TYR:CE1	2.51	0.45
1:F:289:PHE:CD1	1:F:547:VAL:HG11	2.51	0.45
1:F:513:GLY:H	1:F:527:TRP:CG	2.34	0.45
1:A:176:GLY:O	1:D:177:GLN:HB3	2.16	0.45
1:A:615:MET:SD	1:A:615:MET:C	3.00	0.45
1:C:425:VAL:HG22	1:C:426:GLN:H	1.68	0.45
1:D:205:GLY:HA3	1:D:245:PRO:O	2.15	0.45
1:D:719:THR:HG23	1:D:720:GLY:N	2.32	0.45
1:E:136:ASN:HB3	1:E:153:ARG:HB2	1.98	0.45
1:F:500:ILE:HG12	1:F:505:PHE:HB2	1.98	0.45
1:F:746:GLY:H	1:F:771:THR:HG23	1.82	0.45
1:A:267:TRP:CD2	1:A:341:LYS:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:LEU:N	1:C:48:LEU:HD23	2.31	0.45
1:C:267:TRP:CD2	1:C:341:LYS:HG3	2.52	0.45
1:C:525:LYS:HD2	1:C:555:SER:HA	1.99	0.45
1:D:153:ARG:HG2	1:D:229:GLN:HB2	1.99	0.45
1:D:262:ALA:HB3	1:D:476:PRO:CG	2.44	0.45
1:E:165:LEU:HD13	1:E:179:VAL:CG1	2.38	0.45
1:E:282:ASP:HA	1:E:324:THR:HG23	1.98	0.45
1:F:732:LYS:HD2	1:F:732:LYS:N	2.30	0.45
1:A:681:VAL:HG22	1:A:681:VAL:O	2.17	0.45
1:A:735:THR:HG23	1:A:760:VAL:HG13	1.97	0.45
1:C:137:ASN:HB3	1:C:152:GLU:OE1	2.17	0.45
1:C:277:PHE:CZ	1:D:48:LEU:HD22	2.52	0.45
1:D:549:TRP:HB3	1:D:556:CYS:SG	2.56	0.45
1:E:291:ASP:O	1:E:295:GLU:HG3	2.17	0.45
1:E:654:HIS:N	1:E:654:HIS:CD2	2.85	0.45
1:F:60:PRO:O	1:F:61:GLN:HG3	2.16	0.45
1:F:570:MET:HG3	1:F:678:PRO:HA	1.97	0.45
1:A:123:LEU:HD13	1:A:128:ARG:CA	2.47	0.45
1:A:425:VAL:CG2	1:A:426:GLN:N	2.79	0.45
1:B:327:ASP:OD2	1:B:330:GLY:HA3	2.17	0.45
1:C:671:LEU:HD12	1:C:671:LEU:N	2.32	0.45
1:F:749:ASP:CG	1:F:767:ALA:HB3	2.41	0.45
1:A:155:ASP:OD1	1:A:227:LYS:HE3	2.16	0.45
1:A:264:PRO:HD3	1:A:507:PHE:CE2	2.52	0.45
1:A:274:THR:CG2	1:A:276:SER:H	2.05	0.45
1:A:723:ILE:O	1:A:723:ILE:CG1	2.65	0.45
1:B:671:LEU:N	1:B:671:LEU:CD1	2.80	0.45
1:D:163:TYR:HB3	1:D:502:LEU:HD13	1.98	0.45
1:D:736:LEU:HD13	1:D:737:CYS:N	2.31	0.45
1:E:45:THR:HG23	1:E:46:TRP:CD1	2.32	0.45
1:E:190:THR:HA	1:F:223:GLU:O	2.16	0.45
1:E:752:GLN:HB2	1:E:759:LEU:HD11	1.98	0.45
1:F:379:LYS:O	1:F:380:TRP:HB3	2.16	0.45
1:A:689:HIS:CE1	1:A:739:ARG:HH21	2.35	0.45
1:B:466:ARG:HB2	1:B:479:TRP:CH2	2.52	0.45
1:D:487:TYR:HD1	1:D:490:MET:HE2	1.81	0.45
1:F:510:HIS:N	1:F:510:HIS:CD2	2.83	0.45
1:A:693:LEU:HD11	1:A:716:ALA:O	2.17	0.45
1:B:277:PHE:CD2	1:B:278:THR:HG23	2.52	0.45
1:C:201:MET:HE1	1:C:247:PRO:CB	2.42	0.45
1:E:718:ARG:HB2	1:E:723:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:538:ARG:NH2	1:F:540:HIS:CD2	2.85	0.45
1:F:692:ASN:N	1:F:692:ASN:ND2	2.64	0.45
1:A:290:ILE:HD13	1:A:340:LEU:HD11	1.98	0.45
1:B:703:VAL:O	1:B:711:ILE:HG22	2.17	0.45
1:C:347:ASN:ND2	1:C:349:TYR:H	2.14	0.45
1:C:466:ARG:HB2	1:C:479:TRP:CH2	2.52	0.45
1:C:692:ASN:ND2	5:C:3050:HOH:O	2.48	0.45
1:E:297:ASN:O	1:E:299:PRO:HD3	2.16	0.45
1:F:690:LEU:HD21	1:F:693:LEU:HD12	1.99	0.45
1:A:476:PRO:O	1:A:477:VAL:HG13	2.17	0.44
1:C:630:LEU:O	1:C:647:SER:N	2.50	0.44
1:D:38:PRO:HG2	1:D:51:PRO:HD2	1.98	0.44
1:D:276:SER:HB2	1:D:279:THR:CG2	2.47	0.44
1:F:82:TYR:CD1	1:F:470:VAL:HB	2.52	0.44
1:F:634:ARG:NH2	1:F:643:GLU:CB	2.80	0.44
1:B:272:TRP:HB2	1:B:538:ARG:HA	1.98	0.44
1:C:277:PHE:HZ	1:D:48:LEU:HD22	1.81	0.44
1:D:278:THR:HG21	1:E:45:THR:HA	1.98	0.44
1:E:262:ALA:HB3	1:E:476:PRO:CG	2.47	0.44
1:E:469:SER:O	1:E:470:VAL:C	2.60	0.44
1:B:118:TRP:CD1	1:B:118:TRP:C	2.95	0.44
1:B:247:PRO:HD2	5:B:3046:HOH:O	2.16	0.44
1:C:24:GLU:HA	2:C:3011:SO4:O1	2.17	0.44
1:C:279:THR:HG22	1:C:543:LYS:O	2.17	0.44
1:C:498:LEU:HD21	1:C:608:TYR:HB3	1.99	0.44
1:F:89:ASP:OD1	1:F:89:ASP:N	2.49	0.44
1:A:352:GLN:CD	1:B:73:GLN:HG3	2.42	0.44
1:B:479:TRP:CD1	1:B:481:GLY:H	2.36	0.44
1:B:631:PRO:HD2	1:B:635:TRP:CZ2	2.52	0.44
1:C:482:ASP:OD1	3:C:803:XYF:O4	2.33	0.44
1:D:275:THR:HG23	1:D:275:THR:O	2.17	0.44
1:B:191:GLU:HB3	1:C:222:SER:O	2.17	0.44
1:B:635:TRP:CZ3	1:B:664:ARG:HG2	2.53	0.44
1:C:576:GLU:O	1:C:579:ARG:HB3	2.16	0.44
1:D:635:TRP:CH2	1:D:664:ARG:HG2	2.52	0.44
1:D:769:THR:C	1:D:770:ILE:HD12	2.43	0.44
1:F:252:ASP:HA	1:F:583:ARG:O	2.17	0.44
1:F:342:ILE:HD12	1:F:342:ILE:N	2.33	0.44
1:F:353:LYS:O	1:F:353:LYS:HG2	2.17	0.44
1:F:551:TYR:O	1:F:552:ASP:HB3	2.18	0.44
1:F:619:VAL:HG11	1:F:624:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:GLN:O	1:A:749:ASP:HB2	2.17	0.44
1:C:100:TYR:CD1	1:C:111:ARG:HD2	2.53	0.44
1:D:348:PRO:HG2	1:D:349:TYR:CE1	2.53	0.44
1:D:744:VAL:HG21	1:D:770:ILE:CG2	2.47	0.44
1:F:45:THR:HG23	1:F:46:TRP:CD1	2.53	0.44
1:F:692:ASN:H	1:F:692:ASN:ND2	2.12	0.44
1:A:38:PRO:HG2	1:A:51:PRO:HD2	1.99	0.44
1:A:137:ASN:HB3	1:A:152:GLU:OE1	2.17	0.44
1:B:668:LEU:O	1:B:701:CYS:HB2	2.18	0.44
1:B:751:SER:OG	1:B:762:LYS:HB3	2.18	0.44
1:D:488:GLU:O	1:D:492:GLU:HG3	2.16	0.44
1:A:11:GLN:HB2	1:A:14:LEU:HD12	2.00	0.44
1:A:711:ILE:HG12	1:A:711:ILE:O	2.17	0.44
1:B:2:LYS:HA	1:B:223:GLU:OE1	2.18	0.44
1:D:452:LEU:N	1:D:452:LEU:HD12	2.33	0.44
1:D:610:LEU:O	1:D:614:VAL:HG13	2.17	0.44
1:F:347:ASN:HA	1:F:444:TYR:OH	2.18	0.44
1:A:290:ILE:HD12	1:A:335:LEU:CD2	2.48	0.44
1:C:156:LEU:HD11	1:C:228:VAL:HG23	1.98	0.44
1:D:300:LEU:HD13	1:D:301:HIS:H	1.82	0.44
1:E:744:VAL:HG23	1:E:772:LEU:HA	2.00	0.44
1:B:380:TRP:CD1	1:B:381:GLN:HG2	2.53	0.43
1:E:631:PRO:HD2	1:E:635:TRP:CZ2	2.53	0.43
1:A:273:LEU:HB2	1:A:300:LEU:HD21	2.00	0.43
1:A:744:VAL:HG22	1:A:745:ASN:N	2.32	0.43
1:B:25:VAL:HG21	1:B:114:LYS:HE2	2.00	0.43
1:B:635:TRP:CH2	1:B:664:ARG:HG2	2.53	0.43
1:C:692:ASN:N	1:C:692:ASN:ND2	2.61	0.43
1:D:735:THR:HG21	1:D:760:VAL:HG13	1.99	0.43
1:E:174:ARG:O	1:E:175:ASN:C	2.61	0.43
1:E:734:TRP:CH2	1:E:763:PRO:HG3	2.53	0.43
1:F:202:THR:C	1:F:204:ARG:H	2.26	0.43
1:F:214:GLN:HG3	1:F:435:LYS:CG	2.48	0.43
1:A:763:PRO:HB3	1:A:768:LEU:HD12	1.99	0.43
1:C:11:GLN:HB2	1:C:14:LEU:CD1	2.48	0.43
1:C:325:PHE:N	1:C:326:PRO:HD3	2.33	0.43
1:C:436:MET:O	1:C:437:HIS:C	2.62	0.43
1:E:163:TYR:HB3	1:E:502:LEU:HD13	2.01	0.43
1:E:554:GLU:O	1:E:558:VAL:HG23	2.17	0.43
1:F:82:TYR:CB	1:F:84:LEU:HD13	2.47	0.43
1:A:25:VAL:HG21	1:A:114:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ASP:OD2	1:A:330:GLY:HA3	2.19	0.43
1:A:390:THR:HB	1:A:429:ASP:CG	2.43	0.43
1:B:532:LEU:O	1:B:566:LYS:HD2	2.18	0.43
1:D:419:GLU:CD	1:D:466:ARG:HH21	2.26	0.43
1:F:359:GLU:OE2	1:F:363:LYS:NZ	2.49	0.43
1:A:300:LEU:HD12	1:A:340:LEU:CD2	2.48	0.43
1:A:347:ASN:ND2	1:A:349:TYR:H	2.16	0.43
1:B:575:ARG:O	1:B:578:ALA:HB3	2.18	0.43
1:C:89:ASP:OD1	1:C:89:ASP:N	2.51	0.43
1:C:165:LEU:HD13	1:C:179:VAL:CG2	2.48	0.43
1:D:522:HIS:CD2	1:D:622:GLU:HG3	2.53	0.43
1:A:425:VAL:HG22	1:A:426:GLN:H	1.81	0.43
1:D:311:LYS:HE3	1:D:314:GLN:OE1	2.18	0.43
1:E:17:ILE:O	1:E:17:ILE:HG13	2.19	0.43
1:F:615:MET:SD	1:F:615:MET:C	3.02	0.43
1:B:516:GLU:O	1:B:517:ASN:HB2	2.19	0.43
1:C:575:ARG:CZ	1:C:579:ARG:HH12	2.31	0.43
1:C:768:LEU:HD13	1:C:768:LEU:C	2.43	0.43
1:D:290:ILE:CD1	1:D:335:LEU:HD22	2.49	0.43
1:E:128:ARG:HH22	1:E:131:GLY:CA	2.31	0.43
1:E:165:LEU:HA	1:E:197:ILE:O	2.18	0.43
1:E:749:ASP:C	1:E:764:GLN:NE2	2.76	0.43
1:F:432:ASP:OD1	1:F:432:ASP:C	2.61	0.43
1:F:509:SER:HB2	1:F:536:HIS:HB2	2.00	0.43
1:A:262:ALA:HB3	1:A:476:PRO:CD	2.49	0.43
1:A:429:ASP:OD1	1:A:431:SER:OG	2.30	0.43
1:A:525:LYS:CG	1:A:558:VAL:HG21	2.42	0.43
1:A:547:VAL:HA	1:A:548:PRO:HD3	1.91	0.43
1:A:751:SER:OG	1:A:762:LYS:HB3	2.19	0.43
1:B:732:LYS:O	1:B:733:ASN:C	2.61	0.43
1:C:48:LEU:HD13	1:E:277:PHE:HZ	1.83	0.43
1:C:70:GLU:HB3	1:C:236:TYR:HB2	2.01	0.43
1:E:533:LEU:CD2	1:E:569:MET:HE1	2.49	0.43
1:F:164:GLY:O	1:F:165:LEU:HB2	2.18	0.43
1:F:275:THR:HG22	1:F:303:PHE:HZ	1.83	0.43
1:C:226:SER:O	1:C:227:LYS:HG3	2.19	0.43
1:E:164:GLY:O	1:E:165:LEU:HB2	2.18	0.43
1:E:287:ASN:ND2	1:E:334:ARG:NH2	2.64	0.43
1:E:302:VAL:HG22	1:E:341:LYS:HB2	2.00	0.43
1:E:476:PRO:C	1:E:477:VAL:CG1	2.92	0.43
1:A:515:PHE:HD1	1:A:516:GLU:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ALA:HB2	1:A:701:CYS:SG	2.59	0.43
1:B:738:LEU:HD11	1:B:770:ILE:HD13	2.01	0.43
1:C:290:ILE:HD13	1:C:340:LEU:CD1	2.49	0.43
1:C:314:GLN:HB3	1:C:354:SER:HB2	2.00	0.43
1:C:525:LYS:HB3	1:C:656:PHE:CD1	2.54	0.43
1:D:576:GLU:OE2	1:D:579:ARG:NH1	2.52	0.43
1:D:765:GLY:O	1:D:767:ALA:N	2.50	0.43
1:E:310:MET:SD	1:E:316:CYS:HA	2.59	0.43
1:E:432:ASP:OD1	1:E:432:ASP:C	2.62	0.43
1:B:262:ALA:O	1:B:264:PRO:HD3	2.19	0.42
1:D:191:GLU:OE1	1:D:191:GLU:N	2.48	0.42
1:D:358:LYS:HE2	1:D:362:GLU:OE2	2.19	0.42
1:F:167:GLU:OE2	1:F:195:LYS:NZ	2.38	0.42
1:F:459:GLU:CD	1:F:459:GLU:H	2.26	0.42
1:F:592:MET:C	1:F:592:MET:SD	3.02	0.42
1:F:723:ILE:N	1:F:723:ILE:HD12	2.34	0.42
1:A:652:GLN:NE2	1:A:654:HIS:NE2	2.66	0.42
1:A:736:LEU:C	1:A:736:LEU:CD1	2.90	0.42
1:C:45:THR:HG23	1:C:46:TRP:CD1	2.53	0.42
1:C:70:GLU:OE1	1:C:73:GLN:HG2	2.18	0.42
1:D:264:PRO:HD3	1:D:507:PHE:CE2	2.54	0.42
1:D:354:SER:HA	1:D:355:PRO:HD3	1.91	0.42
1:E:318:PHE:HB2	1:E:401:LYS:HD2	2.00	0.42
1:F:98:GLU:O	1:F:98:GLU:HG3	2.19	0.42
1:F:406:VAL:HG11	1:F:455:THR:HB	2.01	0.42
1:F:681:VAL:HG12	2:F:3005:SO4:S	2.60	0.42
1:F:770:ILE:C	1:F:770:ILE:HD12	2.44	0.42
1:A:692:ASN:N	1:A:692:ASN:ND2	2.67	0.42
1:C:31:GLU:HG2	1:C:58:PHE:CB	2.49	0.42
1:C:274:THR:HG23	1:C:276:SER:N	2.34	0.42
1:D:273:LEU:HD13	1:D:274:THR:N	2.34	0.42
1:E:204:ARG:HG2	1:E:204:ARG:NH1	2.33	0.42
1:E:488:GLU:CD	1:E:488:GLU:H	2.27	0.42
1:F:157:GLY:HA3	1:F:204:ARG:NH2	2.33	0.42
1:A:300:LEU:HD12	1:A:340:LEU:HD21	2.02	0.42
1:A:367:LEU:CD1	1:A:425:VAL:HG21	2.49	0.42
1:A:544:SER:O	1:A:546:ARG:NH1	2.53	0.42
1:C:123:LEU:HA	1:C:127:GLU:O	2.19	0.42
1:C:212:HIS:HA	1:C:213:PRO:HD3	1.88	0.42
1:C:342:ILE:HD12	1:C:342:ILE:N	2.34	0.42
1:C:475:PHE:HA	1:C:476:PRO:HD2	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:748:GLN:HB2	1:C:769:THR:HB	2.01	0.42
1:D:540:HIS:CA	1:D:546:ARG:HD2	2.50	0.42
1:E:358:LYS:HG2	1:E:362:GLU:OE2	2.19	0.42
1:E:379:LYS:O	1:E:380:TRP:HB3	2.19	0.42
1:E:683:HIS:HD2	1:E:730:GLU:HG2	1.84	0.42
1:F:273:LEU:HD22	1:F:274:THR:H	1.83	0.42
5:A:3014:HOH:O	1:F:381:GLN:C	2.62	0.42
1:C:356:VAL:HG11	1:C:397:TRP:HH2	1.85	0.42
1:D:384:LEU:C	1:D:384:LEU:HD23	2.45	0.42
1:D:526:ARG:HD2	1:D:619:VAL:HB	2.00	0.42
1:A:37:ALA:HA	1:A:38:PRO:HD3	1.79	0.42
1:A:354:SER:HA	1:A:355:PRO:HD3	1.89	0.42
1:C:43:GLU:HB3	1:C:45:THR:HG22	2.01	0.42
1:C:635:TRP:CH2	1:C:664:ARG:HB3	2.55	0.42
1:E:320:TRP:CE2	1:E:328:PRO:HB3	2.55	0.42
1:E:520:PRO:O	1:E:521:ALA:CB	2.67	0.42
1:F:693:LEU:HD11	1:F:716:ALA:O	2.18	0.42
1:A:320:TRP:O	1:A:322:PRO:HD3	2.20	0.42
1:A:528:CYS:O	1:A:532:LEU:HD23	2.19	0.42
1:B:123:LEU:N	1:B:123:LEU:CD2	2.82	0.42
1:B:668:LEU:CD2	1:B:714:LEU:HD12	2.29	0.42
1:C:164:GLY:O	1:C:165:LEU:HB2	2.20	0.42
1:D:58:PHE:CD1	1:D:58:PHE:N	2.88	0.42
1:D:69:ILE:HG12	1:D:150:MET:CE	2.50	0.42
1:D:619:VAL:HG11	1:D:624:GLY:HA2	2.01	0.42
1:E:58:PHE:CD1	1:E:58:PHE:N	2.88	0.42
1:E:735:THR:HG23	1:E:736:LEU:N	2.34	0.42
1:E:764:GLN:NE2	1:E:764:GLN:O	2.53	0.42
1:F:668:LEU:HD21	1:F:714:LEU:CD1	2.36	0.42
1:F:753:ALA:O	1:F:759:LEU:HD12	2.20	0.42
1:A:164:GLY:O	1:A:165:LEU:HB2	2.20	0.42
1:A:424:ASP:OD2	1:A:424:ASP:N	2.50	0.42
1:A:735:THR:CG2	1:A:736:LEU:N	2.81	0.42
1:B:744:VAL:CG2	1:B:772:LEU:HA	2.50	0.42
1:D:497:GLY:O	1:D:500:ILE:HG22	2.20	0.42
1:C:300:LEU:HD13	1:C:300:LEU:C	2.44	0.42
1:C:736:LEU:CD1	1:C:738:LEU:HD23	2.50	0.42
1:D:736:LEU:C	1:D:736:LEU:CD1	2.93	0.42
1:E:406:VAL:C	1:E:408:MET:H	2.27	0.42
1:F:80:PRO:HD3	1:F:431:SER:HB3	2.01	0.42
1:F:341:LYS:C	1:F:342:ILE:HD12	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:GLY:O	1:B:500:ILE:HG22	2.20	0.42
1:C:182:TRP:CE3	1:C:215:CYS:HB2	2.55	0.42
1:D:344:VAL:HG22	1:D:410:VAL:HG11	2.02	0.42
1:D:588:MET:HG3	1:D:608:TYR:CD1	2.54	0.42
1:E:17:ILE:HG12	1:E:139:TYR:HB3	2.02	0.42
1:E:334:ARG:O	1:E:337:ALA:HB3	2.20	0.42
1:E:565:LEU:O	1:E:569:MET:HG3	2.19	0.42
1:A:752:GLN:OE1	1:A:759:LEU:HD21	2.20	0.41
1:B:145:ASN:OD1	1:B:147:ARG:HB2	2.19	0.41
1:B:195:LYS:HB3	1:B:468:ALA:HB3	2.00	0.41
1:B:405:LEU:O	1:B:410:VAL:HG23	2.20	0.41
1:B:485:ALA:HB1	1:B:519:ALA:CB	2.48	0.41
1:C:171:ALA:O	1:C:174:ARG:NH2	2.39	0.41
1:D:262:ALA:HB3	1:D:476:PRO:CD	2.50	0.41
1:D:634:ARG:CZ	1:D:645:ASP:OD1	2.67	0.41
1:E:37:ALA:HA	1:E:38:PRO:HD3	1.87	0.41
1:E:43:GLU:C	1:E:45:THR:N	2.78	0.41
1:E:214:GLN:HE22	1:E:232:VAL:HG21	1.85	0.41
1:E:314:GLN:HB3	1:E:317:ASP:OD2	2.19	0.41
1:F:634:ARG:HH21	1:F:643:GLU:CB	2.24	0.41
1:A:191:GLU:OE1	1:D:223:GLU:HA	2.21	0.41
1:A:300:LEU:CD1	1:A:340:LEU:HD22	2.51	0.41
1:B:182:TRP:CE3	1:B:215:CYS:HB2	2.55	0.41
1:B:540:HIS:C	1:B:546:ARG:HG3	2.45	0.41
1:B:764:GLN:HG3	1:B:764:GLN:O	2.20	0.41
1:C:367:LEU:HD11	1:C:425:VAL:CG2	2.46	0.41
1:C:580:ALA:HA	1:C:585:THR:O	2.19	0.41
1:B:208:VAL:HA	1:B:240:PHE:O	2.20	0.41
1:B:634:ARG:HG2	1:B:692:ASN:OD1	2.20	0.41
1:C:17:ILE:HG12	1:C:139:TYR:HB3	2.02	0.41
1:C:36:ALA:O	1:C:52:LEU:HD22	2.20	0.41
1:D:21:GLN:HE22	1:D:41:VAL:H	1.68	0.41
1:E:17:ILE:CG1	1:E:139:TYR:HB3	2.51	0.41
1:F:108:LEU:HD22	1:F:243:ASP:HB2	2.02	0.41
1:F:201:MET:CE	1:F:247:PRO:HB3	2.47	0.41
1:F:273:LEU:HD12	1:F:303:PHE:HE1	1.85	0.41
1:F:522:HIS:CG	1:F:622:GLU:HG3	2.56	0.41
1:B:190:THR:HA	1:C:223:GLU:O	2.21	0.41
1:D:39:ARG:HD2	5:D:3056:HOH:O	2.20	0.41
1:D:476:PRO:C	1:D:477:VAL:HG12	2.46	0.41
1:E:296:ARG:O	1:E:560:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:547:VAL:CG2	1:E:550:ALA:HB2	2.50	0.41
1:E:569:MET:CB	1:E:573:LEU:HD22	2.50	0.41
1:E:634:ARG:HH21	1:E:643:GLU:HB3	1.86	0.41
1:A:273:LEU:HD12	1:A:303:PHE:HE1	1.85	0.41
1:A:307:CYS:HB3	1:A:315:TRP:CZ2	2.56	0.41
1:A:308:PHE:CZ	1:B:44:ARG:HB3	2.55	0.41
1:A:731:ALA:O	1:A:732:LYS:HD2	2.20	0.41
1:B:200:TYR:CE2	1:B:208:VAL:HG22	2.55	0.41
1:B:222:SER:O	1:C:191:GLU:HB3	2.19	0.41
1:C:526:ARG:NH2	1:C:624:GLY:HA2	2.35	0.41
1:D:745:ASN:HB3	1:D:771:THR:O	2.20	0.41
1:E:82:TYR:CD1	1:E:470:VAL:HB	2.55	0.41
1:E:173:VAL:HG21	1:E:603:TYR:CD1	2.56	0.41
1:A:336:LYS:CG	1:A:342:ILE:HD13	2.50	0.41
1:A:681:VAL:HG23	1:A:683:HIS:CE1	2.56	0.41
1:A:770:ILE:HD11	1:A:772:LEU:CD2	2.50	0.41
1:B:472:ALA:HB1	5:B:3074:HOH:O	2.21	0.41
1:B:552:ASP:OD1	1:B:555:SER:N	2.38	0.41
1:C:143:THR:O	1:C:143:THR:HG22	2.20	0.41
1:C:453:LYS:HG3	1:C:458:GLU:HA	2.02	0.41
1:C:591:MET:HE2	1:C:607:GLN:HE21	1.86	0.41
1:C:635:TRP:CZ3	1:C:664:ARG:HB3	2.55	0.41
1:E:182:TRP:CE3	1:E:215:CYS:HB2	2.56	0.41
1:E:333:ARG:NH1	1:E:336:LYS:HE3	2.36	0.41
1:E:345:TRP:O	1:E:346:ILE:CG2	2.69	0.41
1:A:167:GLU:CD	1:A:195:LYS:HZ2	2.29	0.41
1:A:321:ASP:OD1	1:A:321:ASP:C	2.64	0.41
1:A:548:PRO:CG	1:A:559:VAL:HG21	2.48	0.41
1:B:252:ASP:HA	1:B:583:ARG:O	2.21	0.41
1:B:293:MET:HE2	1:B:300:LEU:HD13	2.03	0.41
1:B:439:HIS:NE2	1:B:443:ILE:HD11	2.34	0.41
1:B:635:TRP:HB3	1:B:662:TYR:HB3	2.03	0.41
1:C:730:GLU:HG3	1:C:732:LYS:HZ2	1.86	0.41
1:E:32:MET:HE1	1:E:102:GLU:N	2.36	0.41
1:E:80:PRO:HD2	1:E:435:LYS:HB2	2.01	0.41
1:E:277:PHE:HB3	1:E:542:SER:HA	2.02	0.41
1:F:770:ILE:HD11	1:F:772:LEU:HD23	2.02	0.41
1:B:583:ARG:HD3	5:B:3057:HOH:O	2.19	0.41
1:B:639:TRP:HE1	1:B:640:HIS:CE1	2.38	0.41
1:B:718:ARG:CB	1:B:723:ILE:HG22	2.51	0.41
1:D:67:VAL:O	1:D:238:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ALA:O	1:D:174:ARG:NH2	2.43	0.41
1:D:533:LEU:HD12	1:D:533:LEU:HA	1.94	0.41
1:E:275:THR:HG22	1:E:303:PHE:HZ	1.86	0.41
1:F:485:ALA:CB	1:F:519:ALA:HB2	2.31	0.41
1:A:521:ALA:O	1:A:525:LYS:HE3	2.20	0.41
1:A:691:PHE:O	1:A:692:ASN:C	2.64	0.41
1:A:693:LEU:HD23	1:A:693:LEU:C	2.46	0.41
1:C:11:GLN:HA	1:C:12:PRO:HD3	1.97	0.41
1:C:408:MET:HE3	1:C:408:MET:HB2	1.99	0.41
1:D:287:ASN:C	1:D:289:PHE:N	2.79	0.41
1:E:314:GLN:HB3	1:E:354:SER:HB2	2.01	0.41
1:E:570:MET:HG3	1:E:678:PRO:HA	2.03	0.41
1:F:37:ALA:HA	1:F:38:PRO:HD3	1.81	0.41
1:F:82:TYR:CE1	1:F:470:VAL:HB	2.56	0.41
1:F:212:HIS:HA	1:F:213:PRO:HD3	1.90	0.41
1:F:547:VAL:HA	1:F:548:PRO:HD3	1.96	0.41
1:F:631:PRO:O	1:F:646:GLY:HA3	2.20	0.41
1:A:306:ASP:O	1:A:309:TRP:HD1	2.04	0.41
1:B:633:GLY:O	1:B:646:GLY:N	2.53	0.41
1:C:37:ALA:HA	1:C:38:PRO:HD3	1.78	0.41
1:C:509:SER:OG	1:C:510:HIS:N	2.54	0.41
1:D:155:ASP:HB3	5:D:3094:HOH:O	2.21	0.41
1:E:153:ARG:HG2	1:E:229:GLN:HB2	2.02	0.41
1:E:327:ASP:OD2	1:E:330:GLY:HA3	2.20	0.41
1:E:447:LEU:O	1:E:451:VAL:HG23	2.20	0.41
1:E:716:ALA:HA	1:E:724:THR:O	2.21	0.41
1:A:11:GLN:HB2	1:A:14:LEU:CD1	2.51	0.40
1:B:120:LEU:HD23	1:B:121:ASP:N	2.36	0.40
1:C:712:PHE:CG	1:C:731:ALA:HB2	2.55	0.40
1:D:261:PRO:O	1:D:581:ASN:HA	2.21	0.40
1:D:681:VAL:HG23	1:D:683:HIS:CE1	2.56	0.40
1:B:122:PHE:CE1	1:B:241:VAL:HG21	2.56	0.40
1:B:601:CYS:HA	1:B:604:LEU:HG	2.03	0.40
1:C:349:TYR:HB3	1:C:384:LEU:HD21	2.03	0.40
1:D:277:PHE:CD2	1:D:278:THR:HG23	2.56	0.40
1:D:308:PHE:CE1	1:D:315:TRP:HZ2	2.40	0.40
1:E:273:LEU:CB	1:E:300:LEU:HD21	2.48	0.40
1:E:287:ASN:CG	1:E:334:ARG:HH21	2.28	0.40
1:E:384:LEU:HD23	1:E:384:LEU:C	2.47	0.40
1:E:516:GLU:O	1:E:517:ASN:CB	2.68	0.40
1:E:610:LEU:O	1:E:614:VAL:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:719:THR:HG22	1:E:722:THR:O	2.22	0.40
1:F:67:VAL:O	1:F:238:GLU:HA	2.21	0.40
1:F:635:TRP:CZ3	1:F:664:ARG:HG2	2.56	0.40
1:F:761:VAL:HG11	1:F:768:LEU:HD11	2.03	0.40
1:A:747:LEU:HD11	1:A:761:VAL:HG13	2.02	0.40
1:B:690:LEU:O	1:B:739:ARG:HB2	2.21	0.40
1:B:718:ARG:HH21	1:B:772:LEU:HD12	1.86	0.40
1:C:18:HIS:HB2	1:C:20:LEU:CD2	2.51	0.40
1:C:310:MET:SD	1:C:316:CYS:HA	2.61	0.40
1:D:315:TRP:HE3	1:D:381:GLN:CD	2.30	0.40
1:D:772:LEU:H	1:D:772:LEU:CD2	2.34	0.40
1:E:202:THR:C	1:E:204:ARG:H	2.28	0.40
1:E:300:LEU:HD12	1:E:340:LEU:CD2	2.52	0.40
1:E:512:ILE:HB	1:E:539:LEU:HD23	2.02	0.40
1:E:540:HIS:C	1:E:546:ARG:HG3	2.45	0.40
1:B:381:GLN:O	1:B:384:LEU:HB2	2.21	0.40
1:C:274:THR:HG22	1:C:539:LEU:O	2.21	0.40
1:C:419:GLU:H	1:C:419:GLU:CD	2.29	0.40
1:C:598:ASP:HA	1:C:599:PRO:HD2	1.94	0.40
1:D:282:ASP:HA	1:D:324:THR:HG23	2.04	0.40
1:D:634:ARG:HG3	1:D:634:ARG:NH2	2.35	0.40
1:F:533:LEU:HD23	1:F:659:LEU:HD11	2.03	0.40
1:F:670:ALA:HB2	1:F:701:CYS:SG	2.61	0.40
1:A:202:THR:C	1:A:204:ARG:H	2.30	0.40
1:A:635:TRP:HB3	1:A:662:TYR:HB3	2.03	0.40
1:C:84:LEU:HD22	1:C:84:LEU:H	1.84	0.40
1:C:479:TRP:CD1	1:C:481:GLY:H	2.40	0.40
1:D:635:TRP:O	1:D:643:GLU:HA	2.22	0.40
1:E:324:THR:HG22	1:E:325:PHE:CE2	2.56	0.40
1:F:31:GLU:OE1	1:F:56:ARG:HD3	2.22	0.40
1:F:273:LEU:CB	1:F:300:LEU:HD21	2.45	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%)	716 (93%)	45 (6%)	10 (1%)	9	8
1	B	771/778 (99%)	712 (92%)	44 (6%)	15 (2%)	6	4
1	C	771/778 (99%)	716 (93%)	47 (6%)	8 (1%)	12	11
1	D	771/778 (99%)	709 (92%)	47 (6%)	15 (2%)	6	4
1	E	771/778 (99%)	709 (92%)	52 (7%)	10 (1%)	9	8
1	F	771/778 (99%)	709 (92%)	51 (7%)	11 (1%)	9	7
All	All	4626/4668 (99%)	4271 (92%)	286 (6%)	69 (2%)	8	6

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	767	ALA
1	B	764	GLN
1	B	766	ASN
1	C	766	ASN
1	C	767	ALA
1	D	517	ASN
1	D	764	GLN
1	A	480	GLY
1	A	681	VAL
1	B	276	SER
1	B	307	CYS
1	B	308	PHE
1	B	733	ASN
1	B	772	LEU
1	C	480	GLY
1	D	276	SER
1	D	546	ARG
1	D	720	GLY
1	D	772	LEU
1	E	720	GLY
1	E	764	GLN
1	E	767	ALA
1	F	77	ASN
1	F	767	ALA
1	F	768	LEU
1	A	692	ASN
1	A	768	LEU

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Mol	Chain	Res	Type
1	B	476	PRO
1	C	431	SER
1	D	307	CYS
1	D	476	PRO
1	D	733	ASN
1	D	767	ALA
1	E	44	ARG
1	E	316	CYS
1	F	308	PHE
1	F	552	ASP
1	A	277	PHE
1	A	476	PRO
1	B	214	GLN
1	B	316	CYS
1	B	431	SER
1	B	745	ASN
1	C	316	CYS
1	C	477	VAL
1	C	764	GLN
1	D	745	ASN
1	F	276	SER
1	F	692	ASN
1	A	308	PHE
1	A	316	CYS
1	A	477	VAL
1	B	477	VAL
1	B	480	GLY
1	C	308	PHE
1	D	380	TRP
1	D	477	VAL
1	E	417	PHE
1	E	477	VAL
1	E	766	ASN
1	F	316	CYS
1	E	277	PHE
1	F	476	PRO
1	F	477	VAL
1	D	328	PRO
1	F	720	GLY
1	D	742	VAL
1	E	476	PRO
1	B	328	PRO

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%)	629 (95%)	30 (5%)	24	32
1	B	659/665 (99%)	639 (97%)	20 (3%)	36	49
1	C	659/665 (99%)	629 (95%)	30 (5%)	24	32
1	D	659/665 (99%)	632 (96%)	27 (4%)	27	37
1	E	659/665 (99%)	632 (96%)	27 (4%)	27	37
1	F	659/665 (99%)	628 (95%)	31 (5%)	23	31
All	All	3954/3990 (99%)	3789 (96%)	165 (4%)	26	36

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	52	LEU
1	A	120	LEU
1	A	123	LEU
1	A	174	ARG
1	A	179	VAL
1	A	208	VAL
1	A	316	CYS
1	A	347	ASN
1	A	348	PRO
1	A	356	VAL
1	A	419	GLU
1	A	452	LEU
1	A	464	PHE
1	A	477	VAL
1	A	479	TRP
1	A	510	HIS
1	A	525	LYS
1	A	533	LEU
1	A	573	LEU
1	A	614	VAL
1	A	616	VAL

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Mol	Chain	Res	Type
1	A	630	LEU
1	A	657	LEU
1	A	671	LEU
1	A	681	VAL
1	A	733	ASN
1	A	735	THR
1	A	768	LEU
1	A	770	ILE
1	B	84	LEU
1	B	120	LEU
1	B	123	LEU
1	B	146	GLN
1	B	179	VAL
1	B	208	VAL
1	B	285	THR
1	B	316	CYS
1	B	347	ASN
1	B	459	GLU
1	B	464	PHE
1	B	510	HIS
1	B	533	LEU
1	B	573	LEU
1	B	614	VAL
1	B	616	VAL
1	B	630	LEU
1	B	657	LEU
1	B	686	THR
1	B	693	LEU
1	C	93	THR
1	C	120	LEU
1	C	123	LEU
1	C	174	ARG
1	C	179	VAL
1	C	208	VAL
1	C	276	SER
1	C	285	THR
1	C	306	ASP
1	C	316	CYS
1	C	347	ASN
1	C	348	PRO
1	C	419	GLU
1	C	452	LEU

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Mol	Chain	Res	Type
1	C	459	GLU
1	C	464	PHE
1	C	479	TRP
1	C	510	HIS
1	C	525	LYS
1	C	533	LEU
1	C	573	LEU
1	C	579	ARG
1	C	592	MET
1	C	614	VAL
1	C	616	VAL
1	C	657	LEU
1	C	692	ASN
1	C	693	LEU
1	C	721	ASN
1	C	770	ILE
1	D	52	LEU
1	D	69	ILE
1	D	143	THR
1	D	174	ARG
1	D	178	THR
1	D	179	VAL
1	D	208	VAL
1	D	300	LEU
1	D	306	ASP
1	D	316	CYS
1	D	348	PRO
1	D	352	GLN
1	D	419	GLU
1	D	459	GLU
1	D	464	PHE
1	D	477	VAL
1	D	510	HIS
1	D	533	LEU
1	D	537	SER
1	D	546	ARG
1	D	573	LEU
1	D	614	VAL
1	D	616	VAL
1	D	630	LEU
1	D	693	LEU
1	D	742	VAL

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Mol	Chain	Res	Type
1	D	771	THR
1	E	45	THR
1	E	48	LEU
1	E	120	LEU
1	E	123	LEU
1	E	143	THR
1	E	174	ARG
1	E	179	VAL
1	E	208	VAL
1	E	214	GLN
1	E	282	ASP
1	E	300	LEU
1	E	316	CYS
1	E	452	LEU
1	E	459	GLU
1	E	464	PHE
1	E	479	TRP
1	E	537	SER
1	E	573	LEU
1	E	614	VAL
1	E	616	VAL
1	E	630	LEU
1	E	653	GLN
1	E	693	LEU
1	E	723	ILE
1	E	735	THR
1	E	756	GLU
1	E	772	LEU
1	F	120	LEU
1	F	123	LEU
1	F	143	THR
1	F	174	ARG
1	F	178	THR
1	F	179	VAL
1	F	189	SER
1	F	208	VAL
1	F	214	GLN
1	F	300	LEU
1	F	306	ASP
1	F	316	CYS
1	F	329	GLU
1	F	347	ASN

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Mol	Chain	Res	Type
1	F	348	PRO
1	F	419	GLU
1	F	452	LEU
1	F	459	GLU
1	F	464	PHE
1	F	510	HIS
1	F	533	LEU
1	F	537	SER
1	F	573	LEU
1	F	579	ARG
1	F	614	VAL
1	F	616	VAL
1	F	630	LEU
1	F	693	LEU
1	F	714	LEU
1	F	770	ILE
1	F	771	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	18	HIS
1	A	27	GLN
1	A	73	GLN
1	A	77	ASN
1	A	107	ASN
1	A	125	ASN
1	A	133	GLN
1	A	212	HIS
1	A	287	ASN
1	A	347	ASN
1	A	445	ASN
1	A	564	GLN
1	A	652	GLN
1	A	692	ASN
1	A	697	HIS
1	B	7	ASN
1	B	11	GLN
1	B	27	GLN
1	B	28	GLN
1	B	47	GLN

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Mol	Chain	Res	Type
1	B	125	ASN
1	B	141	GLN
1	B	146	GLN
1	B	212	HIS
1	B	347	ASN
1	B	450	ASN
1	B	564	GLN
1	B	650	HIS
1	B	652	GLN
1	B	692	ASN
1	B	697	HIS
1	B	740	ASN
1	B	745	ASN
1	B	764	GLN
1	C	11	GLN
1	C	27	GLN
1	C	77	ASN
1	C	107	ASN
1	C	133	GLN
1	C	146	GLN
1	C	347	ASN
1	C	361	GLN
1	C	517	ASN
1	C	564	GLN
1	C	652	GLN
1	C	653	GLN
1	C	692	ASN
1	C	697	HIS
1	D	7	ASN
1	D	15	ASN
1	D	27	GLN
1	D	107	ASN
1	D	133	GLN
1	D	141	GLN
1	D	146	GLN
1	D	381	GLN
1	D	445	ASN
1	D	613	ASN
1	D	697	HIS
1	D	721	ASN
1	D	733	ASN
1	E	11	GLN

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Mol	Chain	Res	Type
1	E	21	GLN
1	E	27	GLN
1	E	47	GLN
1	E	73	GLN
1	E	77	ASN
1	E	107	ASN
1	E	133	GLN
1	E	146	GLN
1	E	192	GLN
1	E	214	GLN
1	E	280	ASN
1	E	652	GLN
1	E	697	HIS
1	E	733	ASN
1	E	752	GLN
1	E	764	GLN
1	F	21	GLN
1	F	27	GLN
1	F	73	GLN
1	F	77	ASN
1	F	81	HIS
1	F	107	ASN
1	F	133	GLN
1	F	280	ASN
1	F	347	ASN
1	F	613	ASN
1	F	650	HIS
1	F	652	GLN
1	F	692	ASN
1	F	697	HIS
1	F	733	ASN
1	F	764	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

21 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	A	3012	-	4,4,4	1.86	2 (50%)	6,6,6	0.81	0
4	MPO	C	2002	-	13,13,13	2.11	2 (15%)	17,17,17	2.14	6 (35%)
2	SO4	F	3005	-	4,4,4	1.85	2 (50%)	6,6,6	0.82	0
2	SO4	F	3009	-	4,4,4	1.87	2 (50%)	6,6,6	0.84	0
2	SO4	C	3007	-	4,4,4	1.84	2 (50%)	6,6,6	0.84	0
3	XYF	A	801	1	10,10,11	1.62	3 (30%)	14,14,16	0.63	0
2	SO4	F	3001	-	4,4,4	1.85	2 (50%)	6,6,6	0.81	0
4	MPO	B	2001	-	13,13,13	2.01	2 (15%)	17,17,17	2.19	6 (35%)
2	SO4	B	3010	-	4,4,4	1.87	2 (50%)	6,6,6	0.84	0
2	SO4	D	3004	-	4,4,4	1.90	2 (50%)	6,6,6	0.83	0
2	SO4	F	3003	-	4,4,4	1.88	2 (50%)	6,6,6	0.85	0
2	SO4	B	3008	-	4,4,4	1.85	2 (50%)	6,6,6	0.84	0
2	SO4	A	3013	-	4,4,4	1.87	2 (50%)	6,6,6	0.82	0
2	SO4	E	3006	-	4,4,4	1.87	2 (50%)	6,6,6	0.83	0
4	MPO	D	2003	-	13,13,13	1.95	2 (15%)	17,17,17	2.21	6 (35%)
3	XYF	E	804	1	10,10,11	1.59	3 (30%)	14,14,16	0.60	0
4	MPO	E	2004	-	13,13,13	1.94	2 (15%)	17,17,17	2.18	6 (35%)
2	SO4	C	3011	-	4,4,4	1.82	2 (50%)	6,6,6	0.84	0
2	SO4	F	3002	-	4,4,4	1.85	2 (50%)	6,6,6	0.83	0
3	XYF	B	802	1	10,10,11	1.59	3 (30%)	14,14,16	0.66	0
3	XYF	C	803	1	10,10,11	1.61	3 (30%)	14,14,16	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	XYF	A	801	1	-	-	0/1/1/1
4	MPO	C	2002	-	-	5/7/15/15	0/1/1/1
4	MPO	B	2001	-	-	3/7/15/15	0/1/1/1
4	MPO	D	2003	-	-	3/7/15/15	0/1/1/1
3	XYF	B	802	1	-	-	0/1/1/1
3	XYF	E	804	1	-	-	0/1/1/1
4	MPO	E	2004	-	-	2/7/15/15	0/1/1/1
3	XYF	C	803	1	-	-	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2002	MPO	C1-S1	6.27	1.86	1.77
4	B	2001	MPO	C1-S1	5.87	1.85	1.77
4	D	2003	MPO	C1-S1	5.62	1.85	1.77
4	E	2004	MPO	C1-S1	5.51	1.85	1.77
3	B	802	XYF	O5-C1	3.42	1.44	1.39
3	C	803	XYF	O5-C1	3.41	1.44	1.39
3	A	801	XYF	O5-C1	3.38	1.44	1.39
3	E	804	XYF	O5-C1	3.36	1.44	1.39
2	D	3004	SO4	O1-S	3.10	1.63	1.44
2	A	3013	SO4	O1-S	3.07	1.63	1.44
2	F	3009	SO4	O1-S	3.06	1.63	1.44
2	B	3010	SO4	O1-S	3.06	1.63	1.44
2	F	3003	SO4	O1-S	3.05	1.63	1.44
2	A	3012	SO4	O1-S	3.05	1.62	1.44
2	E	3006	SO4	O1-S	3.04	1.62	1.44
2	B	3008	SO4	O1-S	3.03	1.62	1.44
2	F	3002	SO4	O1-S	3.03	1.62	1.44
2	F	3001	SO4	O1-S	3.02	1.62	1.44
2	F	3005	SO4	O1-S	3.02	1.62	1.44
2	C	3007	SO4	O1-S	2.99	1.62	1.44
2	C	3011	SO4	O1-S	2.95	1.62	1.44
3	A	801	XYF	C2-C1	2.67	1.53	1.52
3	E	804	XYF	F5-C1	-2.60	1.35	1.39
3	C	803	XYF	F5-C1	-2.57	1.35	1.39
3	A	801	XYF	F5-C1	-2.56	1.35	1.39
3	B	802	XYF	F5-C1	-2.55	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	803	XYF	C2-C1	2.52	1.53	1.52
3	E	804	XYF	C2-C1	2.46	1.53	1.52
3	B	802	XYF	C2-C1	2.39	1.53	1.52
4	B	2001	MPO	C4-N1	2.34	1.53	1.46
4	E	2004	MPO	C4-N1	2.31	1.53	1.46
4	C	2002	MPO	C4-N1	2.30	1.53	1.46
4	D	2003	MPO	C4-N1	2.19	1.52	1.46
2	F	3003	SO4	O3-S	-2.16	1.30	1.48
2	D	3004	SO4	O3-S	-2.14	1.30	1.48
2	E	3006	SO4	O3-S	-2.11	1.30	1.48
2	B	3010	SO4	O3-S	-2.11	1.30	1.48
2	A	3013	SO4	O3-S	-2.10	1.30	1.48
2	F	3005	SO4	O3-S	-2.10	1.30	1.48
2	F	3009	SO4	O3-S	-2.09	1.31	1.48
2	F	3001	SO4	O3-S	-2.09	1.31	1.48
2	F	3002	SO4	O3-S	-2.08	1.31	1.48
2	C	3007	SO4	O3-S	-2.08	1.31	1.48
2	A	3012	SO4	O3-S	-2.08	1.31	1.48
2	C	3011	SO4	O3-S	-2.08	1.31	1.48
2	B	3008	SO4	O3-S	-2.05	1.31	1.48

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2003	MPO	C2-C1-S1	-6.57	103.17	113.25
4	E	2004	MPO	C2-C1-S1	-6.42	103.41	113.25
4	B	2001	MPO	C2-C1-S1	-6.32	103.56	113.25
4	C	2002	MPO	C2-C1-S1	-6.06	103.95	113.25
4	B	2001	MPO	O1-S1-C1	2.96	111.19	106.73
4	C	2002	MPO	O1-S1-C1	2.83	111.01	106.73
4	E	2004	MPO	O1-S1-C1	2.66	110.75	106.73
4	D	2003	MPO	O1-S1-C1	2.61	110.67	106.73
4	B	2001	MPO	C3-C2-C1	-2.45	104.76	113.02
4	E	2004	MPO	O2-S1-C1	2.41	110.38	106.73
4	C	2002	MPO	O2-S1-C1	2.40	110.36	106.73
4	E	2004	MPO	C3-C2-C1	-2.39	104.96	113.02
4	D	2003	MPO	C5-C4-N1	-2.38	106.51	110.12
4	D	2003	MPO	C3-C2-C1	-2.36	105.06	113.02
4	B	2001	MPO	O2-S1-C1	2.36	110.29	106.73
4	C	2002	MPO	C5-C4-N1	-2.33	106.57	110.12
4	C	2002	MPO	C3-C2-C1	-2.33	105.17	113.02
4	D	2003	MPO	O2-S1-C1	2.31	110.22	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	MPO	C5-C4-N1	-2.20	106.78	110.12
4	E	2004	MPO	C5-C4-N1	-2.20	106.78	110.12
4	E	2004	MPO	C2-C3-N1	-2.10	108.04	113.93
4	D	2003	MPO	C2-C3-N1	-2.09	108.06	113.93
4	B	2001	MPO	C2-C3-N1	-2.08	108.08	113.93
4	C	2002	MPO	C2-C3-N1	-2.02	108.27	113.93

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2001	MPO	C1-C2-C3-N1
4	C	2002	MPO	C1-C2-C3-N1
4	D	2003	MPO	C2-C3-N1-C7
4	B	2001	MPO	C2-C3-N1-C4
4	D	2003	MPO	C2-C3-N1-C4
4	E	2004	MPO	C2-C3-N1-C4
4	C	2002	MPO	C2-C3-N1-C4
4	C	2002	MPO	C2-C3-N1-C7
4	B	2001	MPO	C2-C3-N1-C7
4	E	2004	MPO	C2-C3-N1-C7
4	C	2002	MPO	C2-C1-S1-O2
4	C	2002	MPO	C2-C1-S1-O3
4	D	2003	MPO	C1-C2-C3-N1

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3005	SO4	2	0
3	A	801	XYF	2	0
2	E	3006	SO4	1	0
3	E	804	XYF	2	0
2	C	3011	SO4	1	0
3	B	802	XYF	1	0
3	C	803	XYF	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.26	38 (4%)	35 31	16, 28, 48, 76	0
1	B	773/778 (99%)	0.67	68 (8%)	15 13	20, 36, 61, 82	0
1	C	773/778 (99%)	0.32	30 (3%)	43 40	17, 29, 50, 72	0
1	D	773/778 (99%)	0.59	86 (11%)	10 8	17, 31, 63, 84	0
1	E	773/778 (99%)	0.50	63 (8%)	17 15	18, 32, 55, 90	0
1	F	773/778 (99%)	0.40	52 (6%)	24 21	19, 30, 55, 77	0
All	All	4638/4668 (99%)	0.46	337 (7%)	21 18	16, 31, 56, 90	0

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	281	TYR	7.3
1	D	541	GLY	7.0
1	D	277	PHE	6.6
1	E	46	TRP	6.6
1	D	540	HIS	6.6
1	D	380	TRP	6.4
1	D	545	TYR	6.3
1	D	279	THR	6.2
1	D	278	THR	6.2
1	D	382	PRO	6.0
1	B	767	ALA	5.9
1	B	766	ASN	5.8
1	D	276	SER	5.8
1	D	275	THR	5.7
1	A	768	LEU	5.3
1	D	546	ARG	5.3
1	D	306	ASP	5.2
1	D	280	ASN	5.1
1	F	766	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	47	GLN	5.1
1	D	773	HIS	5.1
1	B	765	GLY	5.0
1	C	767	ALA	5.0
1	B	773	HIS	4.9
1	F	773	HIS	4.9
1	D	542	SER	4.9
1	C	773	HIS	4.9
1	E	766	ASN	4.9
1	D	377	TRP	4.9
1	E	477	VAL	4.9
1	C	766	ASN	4.8
1	D	513	GLY	4.7
1	D	514	GLY	4.7
1	F	719	THR	4.7
1	E	117	PHE	4.7
1	D	544	SER	4.7
1	D	766	ASN	4.6
1	D	543	LYS	4.5
1	E	40	ASP	4.5
1	D	477	VAL	4.5
1	F	550	ALA	4.3
1	B	768	LEU	4.3
1	E	49	ASP	4.3
1	A	719	THR	4.3
1	A	477	VAL	4.2
1	E	43	GLU	4.2
1	A	773	HIS	4.2
1	D	289	PHE	4.2
1	D	379	LYS	4.1
1	D	381	GLN	4.1
1	F	765	GLY	4.0
1	E	48	LEU	4.0
1	A	766	ASN	4.0
1	E	773	HIS	3.9
1	A	767	ALA	3.9
1	E	44	ARG	3.9
1	D	747	LEU	3.9
1	E	540	HIS	3.9
1	E	50	THR	3.8
1	A	765	GLY	3.8
1	D	517	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	723	ILE	3.8
1	E	42	ARG	3.8
1	A	46	TRP	3.7
1	D	383	GLY	3.7
1	A	723	ILE	3.7
1	A	720	GLY	3.6
1	D	282	ASP	3.6
1	B	476	PRO	3.6
1	B	332	ILE	3.6
1	D	519	ALA	3.6
1	F	545	TYR	3.6
1	E	45	THR	3.6
1	F	540	HIS	3.6
1	D	765	GLY	3.5
1	D	378	ASP	3.5
1	D	333	ARG	3.5
1	C	765	GLY	3.5
1	D	768	LEU	3.5
1	F	747	LEU	3.5
1	B	337	ALA	3.4
1	B	333	ARG	3.4
1	D	723	ILE	3.4
1	F	277	PHE	3.4
1	B	477	VAL	3.4
1	F	547	VAL	3.4
1	B	772	LEU	3.4
1	D	307	CYS	3.4
1	D	515	PHE	3.3
1	B	699	ALA	3.3
1	B	770	ILE	3.3
1	B	681	VAL	3.3
1	F	767	ALA	3.3
1	E	551	TYR	3.3
1	B	742	VAL	3.3
1	E	767	ALA	3.2
1	C	770	ILE	3.2
1	C	719	THR	3.2
1	B	723	ILE	3.2
1	A	744	VAL	3.2
1	A	753	ALA	3.2
1	D	742	VAL	3.2
1	D	764	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	477	VAL	3.2
1	C	46	TRP	3.2
1	B	204	ARG	3.1
1	D	746	GLY	3.1
1	F	748	GLN	3.1
1	F	762	LYS	3.1
1	F	517	ASN	3.1
1	B	744	VAL	3.1
1	E	41	VAL	3.1
1	D	719	THR	3.1
1	D	720	GLY	3.1
1	D	772	LEU	3.1
1	B	722	THR	3.1
1	B	339	GLY	3.1
1	C	748	GLN	3.1
1	D	424	ASP	3.1
1	B	736	LEU	3.1
1	D	300	LEU	3.1
1	F	289	PHE	3.0
1	F	695	ASP	3.0
1	E	52	LEU	3.0
1	C	98	GLU	3.0
1	B	545	TYR	3.0
1	B	719	THR	3.0
1	E	541	GLY	3.0
1	F	519	ALA	3.0
1	B	761	VAL	3.0
1	E	76	LEU	3.0
1	D	100	TYR	3.0
1	F	551	TYR	3.0
1	E	316	CYS	2.9
1	F	315	TRP	2.9
1	B	323	LEU	2.9
1	D	483	CYS	2.9
1	F	278	THR	2.9
1	E	720	GLY	2.9
1	E	544	SER	2.9
1	E	281	TYR	2.9
1	A	476	PRO	2.9
1	B	763	PRO	2.9
1	B	759	LEU	2.9
1	F	477	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	743	LYS	2.8
1	D	743	LYS	2.8
1	D	476	PRO	2.8
1	E	289	PHE	2.8
1	E	520	PRO	2.8
1	B	88	GLN	2.8
1	A	770	ILE	2.8
1	E	719	THR	2.8
1	E	722	THR	2.8
1	F	516	GLU	2.8
1	D	753	ALA	2.8
1	F	515	PHE	2.8
1	B	286	VAL	2.8
1	A	76	LEU	2.7
1	A	281	TYR	2.7
1	F	770	ILE	2.7
1	A	117	PHE	2.7
1	F	88	GLN	2.7
1	E	517	ASN	2.7
1	E	17	ILE	2.7
1	E	765	GLY	2.7
1	C	744	VAL	2.6
1	F	733	ASN	2.6
1	C	755	SER	2.6
1	D	763	PRO	2.6
1	F	544	SER	2.6
1	E	77	ASN	2.6
1	E	277	PHE	2.6
1	C	204	ARG	2.6
1	E	39	ARG	2.6
1	E	545	TYR	2.6
1	F	281	TYR	2.6
1	B	724	THR	2.6
1	F	763	PRO	2.6
1	D	98	GLU	2.6
1	D	767	ALA	2.6
1	F	518	THR	2.6
1	A	762	LYS	2.6
1	C	127	GLU	2.6
1	D	516	GLU	2.6
1	F	634	ARG	2.6
1	E	733	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	745	ASN	2.6
1	D	547	VAL	2.6
1	C	100	TYR	2.6
1	D	756	GLU	2.5
1	A	316	CYS	2.5
1	B	731	ALA	2.5
1	D	749	ASP	2.5
1	D	274	THR	2.5
1	D	681	VAL	2.5
1	A	459	GLU	2.5
1	C	768	LEU	2.5
1	B	729	GLY	2.5
1	B	711	ILE	2.5
1	D	315	TRP	2.5
1	D	319	GLU	2.5
1	D	760	VAL	2.5
1	F	754	GLU	2.5
1	A	100	TYR	2.5
1	E	115	GLY	2.5
1	F	720	GLY	2.5
1	A	99	ARG	2.4
1	A	127	GLU	2.4
1	E	98	GLU	2.4
1	B	732	LYS	2.4
1	C	88	GLN	2.4
1	C	746	GLY	2.4
1	E	116	GLU	2.4
1	A	769	THR	2.4
1	D	744	VAL	2.4
1	C	762	LYS	2.4
1	F	543	LYS	2.4
1	F	539	LEU	2.4
1	A	733	ASN	2.4
1	C	29	ASP	2.4
1	B	407	ALA	2.4
1	D	284	ALA	2.4
1	E	279	THR	2.4
1	F	549	TRP	2.4
1	E	764	GLN	2.4
1	F	424	ASP	2.4
1	A	746	GLY	2.4
1	E	513	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	274	THR	2.4
1	B	738	LEU	2.4
1	F	730	GLU	2.4
1	A	749	ASP	2.3
1	D	750	GLY	2.3
1	B	771	THR	2.3
1	B	90	VAL	2.3
1	B	316	CYS	2.3
1	B	714	LEU	2.3
1	E	748	GLN	2.3
1	C	733	ASN	2.3
1	C	735	THR	2.3
1	D	722	THR	2.3
1	E	295	GLU	2.3
1	A	743	LYS	2.3
1	F	721	ASN	2.3
1	B	319	GLU	2.3
1	B	764	GLN	2.3
1	A	772	LEU	2.3
1	B	452	LEU	2.3
1	E	768	LEU	2.3
1	D	721	ASN	2.3
1	D	733	ASN	2.3
1	C	45	THR	2.3
1	B	98	GLU	2.3
1	B	295	GLU	2.3
1	D	88	GLN	2.3
1	C	772	LEU	2.2
1	F	768	LEU	2.2
1	B	749	ASP	2.2
1	F	89	ASP	2.2
1	D	518	THR	2.2
1	E	476	PRO	2.2
1	F	476	PRO	2.2
1	A	722	THR	2.2
1	B	519	ALA	2.2
1	C	550	ALA	2.2
1	D	717	ALA	2.2
1	D	290	ILE	2.2
1	E	669	LEU	2.2
1	B	77	ASN	2.2
1	C	625	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	29	ASP	2.2
1	F	548	PRO	2.2
1	F	750	GLY	2.2
1	C	764	GLN	2.2
1	E	88	GLN	2.2
1	B	753	ALA	2.2
1	C	278	THR	2.2
1	B	741	VAL	2.2
1	E	547	VAL	2.2
1	F	744	VAL	2.2
1	B	325	PHE	2.2
1	F	117	PHE	2.2
1	F	95	GLU	2.2
1	D	99	ARG	2.1
1	B	46	TRP	2.1
1	B	734	TRP	2.1
1	B	89	ASP	2.1
1	D	293	MET	2.1
1	B	277	PHE	2.1
1	B	762	LYS	2.1
1	F	127	GLU	2.1
1	F	756	GLU	2.1
1	F	316	CYS	2.1
1	D	706	ALA	2.1
1	E	706	ALA	2.1
1	F	771	THR	2.1
1	E	770	ILE	2.1
1	A	29	ASP	2.1
1	A	77	ASN	2.1
1	D	748	GLN	2.1
1	E	51	PRO	2.1
1	E	334	ARG	2.1
1	E	519	ALA	2.1
1	C	732	LYS	2.1
1	A	48	LEU	2.1
1	B	730	GLU	2.1
1	C	43	GLU	2.1
1	A	742	VAL	2.1
1	D	308	PHE	2.1
1	E	479	TRP	2.1
1	E	516	GLU	2.1
1	B	671	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	30	ASN	2.1
1	B	29	ASP	2.1
1	B	721	ASN	2.1
1	F	479	TRP	2.1
1	D	91	LYS	2.0
1	E	285	THR	2.0
1	B	550	ALA	2.0
1	A	747	LEU	2.0
1	E	280	ASN	2.0
1	E	742	VAL	2.0
1	A	115	GLY	2.0
1	E	743	LYS	2.0
1	B	549	TRP	2.0
1	B	756	GLU	2.0
1	D	127	GLU	2.0
1	D	285	THR	2.0
1	D	288	SER	2.0
1	D	632	GLU	2.0
1	B	716	ALA	2.0
1	A	748	GLN	2.0
1	B	540	HIS	2.0
1	B	701	CYS	2.0
1	D	745	ASN	2.0
1	D	762	LYS	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	A	3012	5/5	0.65	0.17	87,87,88,88	0
2	SO4	C	3011	5/5	0.72	0.20	105,106,106,106	0
2	SO4	F	3009	5/5	0.74	0.13	91,91,92,92	0
2	SO4	B	3010	5/5	0.76	0.14	88,89,89,90	0
4	MPO	B	2001	13/13	0.79	0.20	68,68,69,69	0
2	SO4	F	3003	5/5	0.81	0.18	67,68,69,69	0
2	SO4	F	3005	5/5	0.81	0.16	58,58,59,59	0
4	MPO	C	2002	13/13	0.82	0.17	52,57,61,62	0
2	SO4	F	3001	5/5	0.83	0.16	91,91,91,92	0
3	XYF	E	804	10/11	0.84	0.18	25,26,27,29	10
3	XYF	C	803	10/11	0.85	0.11	33,36,38,40	0
2	SO4	E	3006	5/5	0.86	0.15	84,84,85,85	0
4	MPO	E	2004	13/13	0.86	0.17	53,55,57,58	0
2	SO4	B	3008	5/5	0.87	0.12	72,72,72,73	0
2	SO4	F	3002	5/5	0.87	0.13	76,77,77,78	0
3	XYF	B	802	10/11	0.88	0.10	37,41,43,45	0
4	MPO	D	2003	13/13	0.88	0.14	53,57,63,63	0
2	SO4	C	3007	5/5	0.88	0.14	75,76,76,77	0
2	SO4	D	3004	5/5	0.89	0.14	75,75,75,75	0
2	SO4	A	3013	5/5	0.90	0.14	77,77,78,78	0
3	XYF	A	801	10/11	0.92	0.08	35,36,38,39	0

6.5 Other polymers

There are no such residues in this entry.