



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 12:21 am BST

PDB ID : 3KZS
Title : Crystal structure of glycosyl hydrolase family 5 (NP_809925.1) from BACTEROIDES THETA IOTA MICRON VPI-5482 at 2.10 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2009-12-08
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

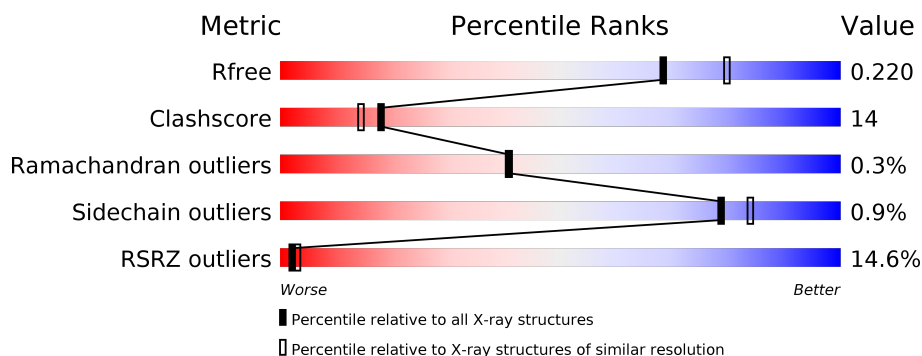
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	463	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
1	B	463	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
1	C	463	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>.</div> </div> </div>
1	D	463	<div> <div>50%</div> <div> <div>40%</div> <div>57%</div> <div>..</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MRD	B	485	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20249 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 glycosyl hydrolase family 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	Se	0	14	0
			3838	2459	649	712	3	15			
1	B	456	Total	C	N	O	S	Se	0	9	0
			3799	2434	643	704	3	15			
1	C	456	Total	C	N	O	S	Se	0	10	0
			3808	2440	645	705	3	15			
1	D	457	Total	C	N	O	S	Se	0	457	0
			7436	4756	1264	1380	6	30			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP Q8A905
B	0	GLY	-	leader sequence	UNP Q8A905
C	0	GLY	-	leader sequence	UNP Q8A905
D	0	GLY	-	leader sequence	UNP Q8A905

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



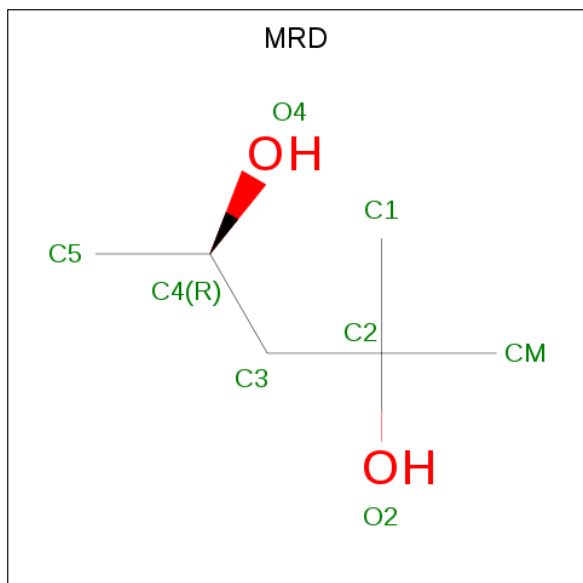
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

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

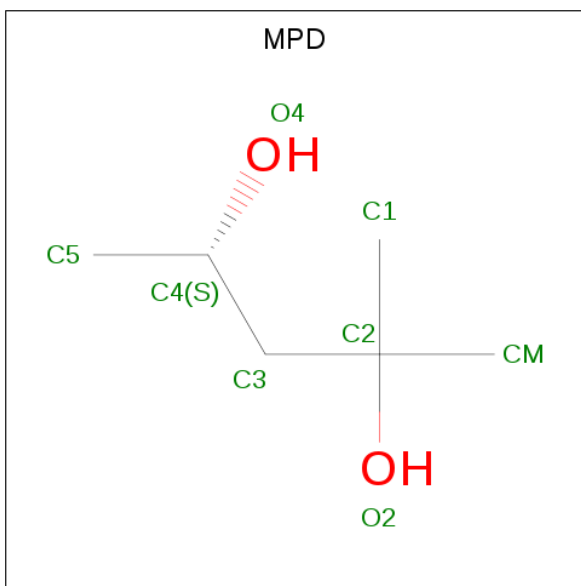
- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:

C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		

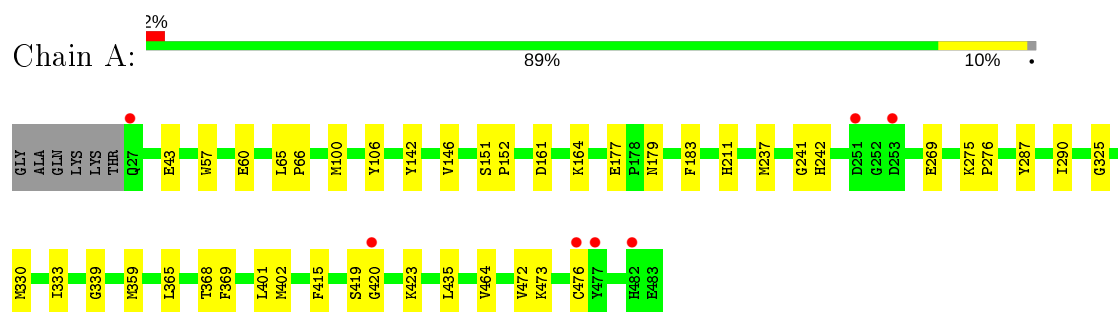
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	404	Total	O	0	0
			404	404		
5	B	352	Total	O	0	0
			352	352		
5	C	411	Total	O	0	0
			411	411		
5	D	41	Total	O	0	0
			41	41		

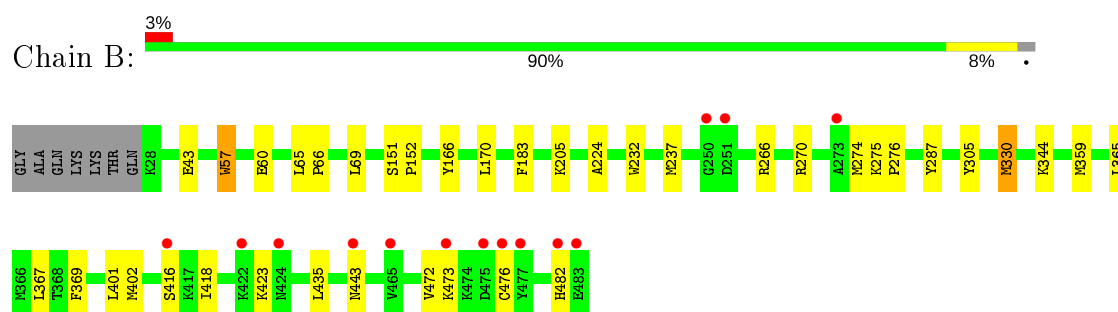
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

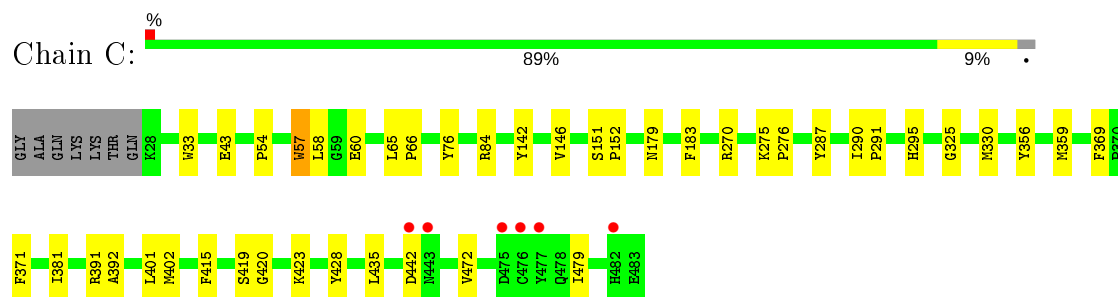
- Molecule 1: glycosyl hydrolase family 5



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S467	Y404	G339	A278	L212	P152	R84	GLY
S468		A340	M274	M213	V153	G85	ALA
K469	T407	Y341	K276	T214	S154	H86	GLN
D470		G342	P276	F215	H155	N87	LYS
Y471	N411	A343	M277	H216	G156	V88	LYS
Y472	E412		K278	R217	E157	I89	THR
K473	N413	P346	P279	R218	M158	G90	Q27
K474	N347	M347	V280	G219	N159	N91	K28
D475	Y348	Y348	I281	R220	V160	G92	T29
C476	D349	D349	D282	T221	Q162	T93	Y30
Y477	A350	G283	G283	T222	Q162	L94	I31
Q478	L351	E284	E284	S223	A163	N95	P32
I479	N352	P285	P285	A224	K164	N96	K33
D480	D353	I286	I286	T225	A165	N97	S34
T481	P354	Y287	Y287	W226	Y166	P98	N35
H482	G355	E288	E288	F227	G167	S99	G36
E483	Y356	E289	E289	N228	K168	M100	K37
	N357	I290	I290	N229	F169	N101	L38
	Q358	P291	P291	A230	L170	I102	V39
	K360	H292	H292	P231	A171	Y103	V40
	Y361	G293	G293	W232	E172	G104	S41
	L362	L294	L294	L233	R173	Q105	E42
	K363	H295	H295	D234	Y174	Y106	E43
	N364	D296	D296	F235	K175	G44	G44
	L365	E297	E297	N236	D176	R45	R45
	M366	M298	M298	M237	E177	Y46	Y46
	K367	E299	E299	F238	P178	L47	L47
	L368	L300	L300		M113	K48	K48
	T368	L301	L301	G241	N179	H49	H49
	F369	M302	M302	H242	I180	E50	E50
	P370	K302	K302	R243	W182	M51	M51
	F371	Y305	Y305	R244	F183	G52	G52
	F372	D306	D306	Y245	I184	T53	T53
	E373	V307	V307	G246	G185	P54	P54
	R374	R308	R308	Q247	G186	F55	F55
	V375	R309	R309	R248	D187	F56	F56
	D377	A310	A310	F249	I188	W57	W57
	Q378	Y312	Y312	G250	W126	L58	L58
	S379	W313	W313	D251	D127	G59	G59
	V380	S314	S314	Y254	M129	E60	E60
	I381	V315	V315	D253	D130	T61	T61
	A382	F316	F316	P255	Y131	W63	W63
	G383	F320	F320	L256	T194	L64	L64
	Q384	G321	G321	E257	E196	L65	L65
	N385			N259	W197	P66	P66
	Y389	Y324	Y324	T260	E198	E67	E67
	A392	G325	G325	E261	A199	R68	R68
	A394	H326	H326	E262	L200	L69	L69
		N327	N327	D263	A201	N70	N70
		I329	I329	N264	T202	E73	E73
	G397	M330	M330	W265	S203	Y76	Y76
	D399	Q331	Q331	R266	L204	G144	G144
	Y400	F332	F332	V267	K205	M145	M145
	L401	I333	I333	V268	A206	V146	V146
	M402			E269	C147	C147	C147
	V403	V337	V337	R270	D208	I148	I148
		G338	G338	S271	K209	G149	G149
				M272	N210	R82	R82
					S151	R83	R83

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	261.33Å 261.33Å 183.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.18 – 2.10 85.18 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (85.18-2.10) 100.0 (85.18-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0053	Depositor
R, R_{free}	0.185 , 0.222 0.186 , 0.220	Depositor DCC
R_{free} test set	6991 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20249	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/3982	0.48	0/5363
1	B	0.67	1/3929 (0.0%)	0.47	0/5295
1	C	0.68	0/3941	0.49	0/5310
1	D	0.41	0/7634	0.39	0/10294
All	All	0.59	1/19486 (0.0%)	0.45	0/26262

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	330	MSE	CB-CG	-5.14	1.37	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3838	0	3621	33	0
1	B	3799	0	3573	29	0
1	C	3808	0	3586	29	0
1	D	7436	0	6920	394	0
2	A	30	0	0	0	0
2	B	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	25	0	0	1	0
3	A	24	0	42	5	0
3	B	24	0	42	7	0
3	C	16	0	28	4	0
4	C	16	0	28	5	0
5	A	404	0	0	2	0
5	B	352	0	0	0	0
5	C	411	0	0	2	0
5	D	41	0	0	6	0
All	All	20249	0	17840	498	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 14.

All (498) 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)
3:A:485:MRD:C5	3:A:485:MRD:HMC2	1.50	1.40
3:A:485:MRD:H5C3	3:A:485:MRD:CM	1.51	1.36
1:D:42[A]:GLU:OE1	1:D:43[A]:GLU:N	1.63	1.32
1:D:65[A]:LEU:HD13	1:D:69[A]:LEU:HD12	1.31	1.12
1:D:65[A]:LEU:CD1	1:D:69[A]:LEU:HD12	1.81	1.10
1:D:359[A]:MSE:HA	1:D:359[A]:MSE:HE2	1.37	1.01
1:D:401[B]:LEU:HD11	1:D:464[B]:VAL:HB	1.42	1.01
1:D:435[A]:LEU:HD21	1:D:472[A]:VAL:HG11	1.42	0.99
1:D:359[B]:MSE:HE2	1:D:359[B]:MSE:HA	1.47	0.95
1:D:42[A]:GLU:C	1:D:42[A]:GLU:OE1	2.04	0.95
1:D:42[A]:GLU:OE1	1:D:43[A]:GLU:CA	2.15	0.94
1:D:370[A]:PRO:HB3	1:D:373[A]:GLU:OE2	1.70	0.92
1:D:185[B]:GLY:HA2	1:D:197[B]:TRP:CH2	2.05	0.92
1:B:344:LYS:HE3	3:C:484:MRD:HMC1	1.53	0.91
1:D:369[A]:PHE:CD1	1:D:402[A]:MSE:CE	2.54	0.91
1:D:401[A]:LEU:O	1:D:401[A]:LEU:HD12	1.72	0.90
1:D:354[A]:PRO:O	1:D:358[A]:GLN:HG3	1.74	0.88
1:D:401[B]:LEU:CD1	1:D:464[B]:VAL:HB	2.03	0.88
1:D:129[A]:MSE:HE3	1:D:129[A]:MSE:HA	1.55	0.88
1:D:168[A]:LYS:O	1:D:172[A]:GLU:HG2	1.75	0.87
1:D:477[A]:TYR:O	1:D:478[A]:GLN:HB3	1.75	0.86
1:D:149[A]:TRP:O	1:D:152[A]:PRO:HD2	1.77	0.85
1:D:369[B]:PHE:CD1	1:D:402[B]:MSE:CE	2.59	0.85
1:D:58[B]:LEU:HD11	1:D:359[B]:MSE:HB3	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369[B]:PHE:CE1	1:D:402[B]:MSE:CE	2.60	0.83
1:D:129[B]:MSE:HE3	1:D:129[B]:MSE:HA	1.59	0.83
1:D:253[B]:ASP:OD1	1:D:254[B]:TYR:N	2.13	0.81
1:D:333[B]:ILE:HD11	1:D:339[B]:GLY:HA2	1.62	0.81
1:D:435[A]:LEU:O	1:D:477[A]:TYR:HA	1.81	0.80
1:D:286[B]:ILE:HD13	1:D:310[B]:TYR:CE1	2.17	0.79
1:D:364[A]:ASN:HA	1:D:482[A]:HIS:CB	2.12	0.79
1:D:171[B]:ALA:O	1:D:175[B]:LYS:HB3	1.82	0.79
1:B:305:TYR:CE2	3:B:485:MRD:H1C1	2.18	0.78
1:D:41[A]:SER:HB3	1:D:43[A]:GLU:OE2	1.83	0.78
4:C:17:MPD:H52	4:C:17:MPD:HM1	1.64	0.78
1:D:435[A]:LEU:HD21	1:D:472[A]:VAL:CG1	2.14	0.78
1:D:369[B]:PHE:CD1	1:D:402[B]:MSE:HE3	2.19	0.77
3:A:485:MRD:H5C3	3:A:485:MRD:HMC2	0.78	0.77
1:D:65[A]:LEU:HD12	1:D:69[A]:LEU:HD12	1.68	0.76
1:D:477[B]:TYR:C	1:D:478[B]:GLN:HG2	2.05	0.76
1:D:185[B]:GLY:HA2	1:D:197[B]:TRP:CZ3	2.20	0.76
1:D:275[B]:LYS:HA	1:D:276[B]:PRO:C	2.06	0.75
1:D:233[B]:LEU:HD23	1:D:233[B]:LEU:C	2.08	0.73
1:D:212[B]:LEU:HA	1:D:234[B]:ASP:OD2	1.89	0.73
1:D:369[B]:PHE:CE1	1:D:402[B]:MSE:HE2	2.24	0.73
1:D:42[A]:GLU:OE1	1:D:43[A]:GLU:HA	1.87	0.73
1:A:269:GLU:HG3	5:A:487:HOH:O	1.87	0.73
1:A:100:MSE:HE1	1:A:106:TYR:CE1	2.24	0.73
1:D:370[B]:PRO:HB3	1:D:373[B]:GLU:OE2	1.89	0.73
1:D:369[A]:PHE:CE1	1:D:402[A]:MSE:HE2	2.24	0.73
1:D:473[A]:LYS:HB2	1:D:476[A]:CYS:HB2	1.70	0.72
1:D:65[B]:LEU:CD1	1:D:69[B]:LEU:HD12	2.19	0.72
1:C:270:ARG:NH1	5:C:1146:HOH:O	2.23	0.72
1:D:159[A]:ASN:OD1	1:D:162[A]:GLN:HG3	1.90	0.72
1:D:435[B]:LEU:HD21	1:D:472[B]:VAL:HG11	1.71	0.71
1:C:419:SER:O	1:C:423:LYS:HE2	1.91	0.71
1:D:455[B]:SER:HA	5:D:484:HOH:O	1.90	0.71
1:D:477[B]:TYR:O	1:D:478[B]:GLN:CB	2.39	0.71
1:D:292[B]:HIS:HD2	1:D:300[B]:LEU:O	1.74	0.71
1:C:415:PHE:O	1:C:423:LYS:NZ	2.24	0.71
1:D:183[B]:PHE:CE2	1:D:237[B]:MSE:HE1	2.24	0.71
1:D:435[B]:LEU:HD21	1:D:472[B]:VAL:CG1	2.21	0.70
1:D:401[B]:LEU:HD11	1:D:464[B]:VAL:CB	2.21	0.70
1:D:333[B]:ILE:CD1	1:D:339[B]:GLY:HA2	2.21	0.70
1:D:427[A]:TRP:NE1	1:D:438[A]:ILE:HD11	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359[A]:MSE:HA	1:D:359[A]:MSE:CE	2.18	0.69
1:D:63[B]:TRP:HZ3	1:D:146[B]:VAL:HG21	1.57	0.69
1:D:270[A]:ARG:O	1:D:274[A]:MSE:HE3	1.91	0.69
1:D:282[B]:ASP:OD2	1:D:285[B]:PRO:HB3	1.93	0.68
1:D:287[A]:TYR:CD1	1:D:325[A]:GLY:HA3	2.29	0.68
1:D:233[A]:LEU:HD23	1:D:233[A]:LEU:C	2.13	0.68
1:D:233[B]:LEU:HD21	1:D:235[B]:PHE:C	2.14	0.68
1:D:196[A]:GLU:N	1:D:196[A]:GLU:OE1	2.25	0.68
1:D:427[A]:TRP:CD1	1:D:438[A]:ILE:HD11	2.28	0.68
1:D:69[A]:LEU:HD11	1:D:332[A]:PHE:CE1	2.29	0.67
1:D:369[A]:PHE:CE1	1:D:402[A]:MSE:CE	2.78	0.67
1:D:401[A]:LEU:C	1:D:401[A]:LEU:HD12	2.14	0.67
1:D:381[A]:ILE:HD13	1:D:392[A]:ALA:HB3	1.76	0.67
1:D:100[B]:MSE:HE1	1:D:106[B]:TYR:CE1	2.31	0.66
1:D:228[B]:ASN:ND2	1:D:274[B]:MSE:CB	2.59	0.66
1:A:415:PHE:O	1:A:423:LYS:NZ	2.28	0.66
1:D:161[A]:ASP:HA	1:D:164[A]:LYS:HE2	1.77	0.66
1:D:364[A]:ASN:ND2	1:D:481[A]:THR:HA	2.11	0.66
1:D:477[B]:TYR:O	1:D:478[B]:GLN:CG	2.44	0.65
1:D:219[A]:GLY:O	1:D:220[A]:ARG:HB2	1.96	0.65
1:D:288[A]:GLU:HG2	1:D:289[A]:GLU:HG2	1.77	0.65
1:D:194[B]:THR:O	1:D:198[B]:GLU:HG2	1.96	0.65
1:D:477[A]:TYR:O	1:D:478[A]:GLN:CB	2.45	0.65
1:D:200[A]:LEU:O	1:D:204[A]:ILE:HG13	1.97	0.64
1:D:133[B]:ILE:HD12	1:D:174[B]:TYR:CE1	2.32	0.64
1:D:172[A]:GLU:OE2	1:D:207[A]:ILE:HD13	1.97	0.64
1:D:142[A]:TYR:HA	1:D:179[A]:ASN:HB2	1.79	0.64
1:D:477[B]:TYR:O	1:D:478[B]:GLN:HG2	1.98	0.64
1:B:367:LEU:HD13	1:B:482[A]:HIS:ND1	2.13	0.64
1:D:291[A]:PRO:HA	1:D:301[A]:LEU:HD23	1.79	0.64
1:D:84[A]:ARG:HD2	1:D:356[A]:TYR:CE2	2.32	0.64
1:D:205[B]:LYS:NZ	1:D:232[B]:TRP:O	2.27	0.64
1:D:286[A]:ILE:HD13	1:D:310[A]:TYR:CE1	2.32	0.64
1:D:228[B]:ASN:ND2	1:D:274[B]:MSE:HB3	2.12	0.64
1:D:35[B]:ASN:ND2	1:D:53[B]:THR:HG21	2.13	0.63
1:D:130[A]:ASP:OD2	1:D:173[A]:ARG:NH2	2.31	0.63
1:D:86[A]:TYR:O	1:D:141[A]:LEU:CD2	2.46	0.63
1:D:290[B]:ILE:CD1	1:D:294[B]:LEU:CD2	2.77	0.62
1:D:60[B]:GLU:OE2	1:D:61[B]:THR:N	2.29	0.62
1:D:359[B]:MSE:HA	1:D:359[B]:MSE:CE	2.28	0.62
1:D:377[A]:ASP:OD1	1:D:379[A]:SER:OG	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:LEU:HD21	1:A:472:VAL:HG11	1.80	0.62
3:A:485:MRD:H5C2	3:A:485:MRD:HMC2	1.71	0.62
1:D:369[A]:PHE:CD1	1:D:402[A]:MSE:HE3	2.32	0.62
1:D:65[B]:LEU:HB3	1:D:66[B]:PRO:HD3	1.80	0.62
3:A:485:MRD:H5C3	3:A:485:MRD:HMC1	1.71	0.62
1:D:149[B]:TRP:CZ2	1:D:187[B]:ASP:HB2	2.34	0.62
1:D:437[B]:TYR:CZ	1:D:439[B]:GLY:HA2	2.35	0.62
1:D:363[A]:LYS:HE2	1:D:482[A]:HIS:O	2.00	0.62
1:D:149[A]:TRP:CZ2	1:D:187[A]:ASP:CB	2.83	0.62
1:D:172[B]:GLU:OE2	1:D:207[B]:ILE:HD13	2.00	0.62
1:B:65:LEU:HD13	1:B:69:LEU:HD12	1.82	0.61
1:D:286[B]:ILE:CD1	1:D:310[B]:TYR:CE1	2.82	0.61
1:D:333[A]:ILE:HG13	1:D:343[A]:ALA:HB1	1.80	0.61
1:A:365:LEU:HD11	1:A:402:MSE:HE2	1.81	0.61
1:B:369:PHE:CE1	1:B:402:MSE:CE	2.82	0.61
1:D:475[B]:ASP:O	1:D:475[B]:ASP:OD1	2.17	0.61
1:D:362[A]:LEU:O	1:D:366[A]:MSE:HG2	2.00	0.61
1:D:113[B]:ASN:OD1	1:D:115[B]:LYS:CG	2.48	0.61
1:D:450[A]:HIS:CE1	1:D:452[A]:SER:HB3	2.36	0.61
1:D:171[A]:ALA:O	1:D:175[A]:LYS:HB3	2.01	0.61
3:B:18:MRD:H1C1	3:B:18:MRD:H5C3	1.82	0.60
1:D:60[A]:GLU:OE2	1:D:61[A]:THR:N	2.34	0.60
1:D:228[B]:ASN:HD22	1:D:274[B]:MSE:HB3	1.65	0.60
1:D:290[B]:ILE:HD11	1:D:294[B]:LEU:CD2	2.31	0.60
1:D:477[B]:TYR:O	1:D:478[B]:GLN:HB3	2.01	0.60
1:C:391:ARG:HH21	4:C:485:MPD:H53	1.65	0.60
1:D:238[B]:PHE:CE1	1:D:282[B]:ASP:CB	2.85	0.60
1:D:424[A]:ASN:ND2	1:D:474[A]:LYS:HE2	2.17	0.60
1:D:149[A]:TRP:CZ2	1:D:187[A]:ASP:HB2	2.37	0.60
1:D:63[B]:TRP:HB3	1:D:92[B]:GLN:HG3	1.83	0.60
1:D:65[A]:LEU:N	1:D:66[A]:PRO:CD	2.64	0.60
1:A:435:LEU:HD21	1:A:472:VAL:CG1	2.31	0.60
1:D:414[B]:ASP:OD1	1:D:416[B]:SER:OG	2.18	0.60
1:D:369[A]:PHE:CD1	1:D:402[A]:MSE:HE1	2.36	0.59
1:C:369:PHE:CD1	1:C:402:MSE:CE	2.85	0.59
1:D:46[B]:TYR:HE1	1:D:374[B]:ARG:NH2	2.00	0.59
1:D:142[B]:TYR:HA	1:D:179[B]:ASN:HB2	1.83	0.59
1:D:214[A]:THR:HB	1:D:235[A]:PHE:CZ	2.37	0.59
1:C:76:TYR:OH	3:C:484:MRD:H1C1	2.03	0.59
1:D:238[B]:PHE:CE1	1:D:282[B]:ASP:CG	2.76	0.59
1:D:381[B]:ILE:HD13	1:D:392[B]:ALA:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63[A]:TRP:HB3	1:D:92[A]:GLN:HG3	1.85	0.58
1:C:391:ARG:HE	4:C:485:MPD:H31	1.67	0.58
1:D:401[B]:LEU:O	1:D:401[B]:LEU:HD12	2.04	0.58
1:B:275:LYS:HA	1:B:276:PRO:C	2.24	0.58
1:D:84[B]:ARG:CD	1:D:356[B]:TYR:CE2	2.86	0.58
1:D:236[B]:ASN:ND2	5:D:584:HOH:O	2.35	0.57
1:D:65[B]:LEU:HD12	1:D:69[B]:LEU:HD12	1.85	0.57
1:D:180[A]:ILE:HB	1:D:211[A]:HIS:CD2	2.40	0.57
1:D:149[A]:TRP:O	1:D:152[A]:PRO:CD	2.51	0.56
1:D:185[B]:GLY:HA2	1:D:197[B]:TRP:CZ2	2.40	0.56
1:D:151[B]:SER:HB2	1:D:152[B]:PRO:CD	2.35	0.56
1:D:149[A]:TRP:CZ2	1:D:187[A]:ASP:HB3	2.41	0.56
1:D:228[B]:ASN:ND2	1:D:274[B]:MSE:HB2	2.21	0.56
1:D:275[A]:LYS:HA	1:D:276[A]:PRO:C	2.24	0.56
1:D:435[A]:LEU:CD2	1:D:472[A]:VAL:CG1	2.83	0.56
1:A:369:PHE:CE1	1:A:402:MSE:CE	2.88	0.56
1:B:65:LEU:HB3	1:B:66:PRO:HD3	1.88	0.56
1:D:238[B]:PHE:CZ	1:D:282[B]:ASP:HB2	2.40	0.56
1:D:309[B]:ARG:O	1:D:313[B]:TRP:HB2	2.04	0.56
1:D:399[A]:ASP:OD2	1:D:469[A]:LYS:HG3	2.06	0.56
1:D:63[B]:TRP:CZ3	1:D:146[B]:VAL:HG21	2.38	0.56
1:B:369:PHE:CD1	1:B:402:MSE:CE	2.89	0.56
1:D:401[A]:LEU:HG	1:D:418[A]:ILE:HD13	1.88	0.56
1:D:168[A]:LYS:O	1:D:172[A]:GLU:CG	2.51	0.56
1:D:224[B]:ALA:O	1:D:228[B]:ASN:HB2	2.06	0.56
1:D:399[B]:ASP:OD2	1:D:471[B]:TYR:OH	2.23	0.55
1:B:305:TYR:CZ	3:B:485:MRD:H1C1	2.41	0.55
1:D:89[B]:ILE:HG22	1:D:91[B]:VAL:HG13	1.89	0.55
1:D:129[A]:MSE:HE3	1:D:132[A]:ILE:HD12	1.87	0.55
1:D:264[B]:ASN:HA	1:D:267[B]:PHE:CD2	2.42	0.55
4:C:485:MPD:HM1	4:C:485:MPD:H52	1.87	0.55
1:D:117[A]:ILE:HG23	1:D:118[A]:ASN:OD1	2.06	0.55
1:D:40[A]:VAL:HG23	5:D:756:HOH:O	2.06	0.55
4:C:17:MPD:H52	4:C:17:MPD:CM	2.35	0.55
1:D:70[A]:ASN:HB3	1:D:102[A]:ILE:HD13	1.89	0.55
1:D:308[B]:ARG:HE	1:D:459[B]:ASP:CG	2.10	0.55
1:D:258[A]:GLU:O	1:D:259[A]:ASN:HB2	2.06	0.55
1:D:333[B]:ILE:CD1	1:D:339[B]:GLY:CA	2.84	0.55
1:A:65:LEU:HB3	1:A:66:PRO:HD3	1.89	0.55
1:D:146[A]:VAL:HA	1:D:183[A]:PHE:HB2	1.89	0.54
1:A:275:LYS:HA	1:A:276:PRO:C	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:LEU:HD21	1:C:472:VAL:HG11	1.89	0.54
1:C:275:LYS:HA	1:C:276:PRO:C	2.28	0.54
1:D:100[A]:MSE:HE1	1:D:106[A]:TYR:CE1	2.42	0.54
1:D:287[B]:TYR:CD1	1:D:325[B]:GLY:HA3	2.41	0.54
1:D:459[B]:ASP:N	1:D:459[B]:ASP:OD1	2.41	0.54
1:A:419:SER:O	1:A:423:LYS:HE2	2.08	0.54
1:C:420:GLY:O	1:C:423:LYS:HE3	2.07	0.54
1:D:46[B]:TYR:HE1	1:D:374[B]:ARG:HH21	1.56	0.54
1:D:290[B]:ILE:HD11	1:D:294[B]:LEU:HD22	1.90	0.54
1:D:290[A]:ILE:HG12	1:D:291[A]:PRO:HD2	1.89	0.54
1:D:129[A]:MSE:HA	1:D:129[A]:MSE:CE	2.32	0.54
1:D:287[B]:TYR:O	1:D:290[B]:ILE:HG22	2.07	0.53
1:D:466[B]:ASP:HB3	1:D:469[B]:LYS:HG2	1.90	0.53
1:D:84[B]:ARG:HD2	1:D:356[B]:TYR:CE2	2.44	0.53
1:D:146[A]:VAL:HG22	1:D:183[A]:PHE:HB3	1.90	0.53
1:D:370[B]:PRO:HD3	1:D:471[B]:TYR:CE1	2.43	0.53
1:D:292[B]:HIS:CD2	1:D:300[B]:LEU:HB2	2.43	0.53
1:D:245[B]:TYR:HA	1:D:261[B]:GLU:OE1	2.09	0.53
1:D:394[A]:ALA:HB2	1:D:403[A]:VAL:HG22	1.91	0.53
1:D:92[B]:GLN:HA	1:D:146[B]:VAL:HB	1.91	0.53
1:D:403[A]:VAL:HG11	1:D:411[A]:MSE:SE	2.59	0.53
1:A:359:MSE:HE2	1:A:359:MSE:HA	1.91	0.52
1:A:473:LYS:HB2	1:A:476:CYS:HB2	1.91	0.52
1:D:185[B]:GLY:CA	1:D:197[B]:TRP:CZ3	2.92	0.52
1:D:359[B]:MSE:HE2	1:D:359[B]:MSE:CA	2.31	0.52
1:D:466[A]:ASP:HB3	1:D:469[A]:LYS:HG2	1.91	0.52
1:D:79[A]:GLU:O	1:D:83[A]:ARG:HG3	2.09	0.52
1:D:401[A]:LEU:HD11	1:D:464[A]:VAL:HB	1.90	0.52
1:D:57[B]:TRP:CZ2	1:D:88[B]:VAL:HG11	2.44	0.52
1:D:389[B]:TYR:O	1:D:407[B]:THR:HG23	2.10	0.52
1:D:41[B]:SER:HB3	1:D:43[B]:GLU:OE2	2.09	0.52
1:C:65:LEU:HB3	1:C:66:PRO:HD3	1.92	0.52
1:D:228[B]:ASN:ND2	5:D:1115:HOH:O	2.42	0.52
1:D:205[A]:LYS:HE3	1:D:213[A]:MSE:HE3	1.92	0.52
1:D:84[A]:ARG:CD	1:D:356[A]:TYR:CE2	2.92	0.52
1:B:435:LEU:HD21	1:B:472:VAL:HG11	1.91	0.52
1:D:233[B]:LEU:HD23	1:D:235[B]:PHE:N	2.25	0.52
1:D:242[A]:HIS:ND1	1:D:286[A]:ILE:HA	2.25	0.51
1:D:42[A]:GLU:C	1:D:42[A]:GLU:CD	2.69	0.51
1:D:89[A]:ILE:HB	1:D:143[A]:ILE:HD13	1.93	0.51
1:D:87[B]:ASN:HA	1:D:141[B]:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:MSE:HE1	1:A:106:TYR:CD1	2.45	0.51
1:D:171[B]:ALA:HB1	1:D:207[B]:ILE:HB	1.93	0.51
1:B:359:MSE:HE2	1:B:359:MSE:HA	1.93	0.51
1:D:427[B]:TRP:HB2	1:D:436[B]:GLU:HB3	1.92	0.51
1:D:57[A]:TRP:C	1:D:57[A]:TRP:CD1	2.85	0.51
1:D:67[A]:GLU:OE2	1:D:92[A]:GLN:O	2.29	0.51
1:D:146[A]:VAL:HG22	1:D:183[A]:PHE:CB	2.41	0.50
1:D:377[B]:ASP:OD1	1:D:379[B]:SER:OG	2.26	0.50
1:D:401[A]:LEU:CD1	1:D:401[A]:LEU:C	2.79	0.50
1:C:369:PHE:CE1	1:C:402:MSE:CE	2.94	0.50
1:D:40[B]:VAL:O	1:D:41[B]:SER:O	2.28	0.50
1:D:364[A]:ASN:CG	1:D:481[A]:THR:HA	2.31	0.50
1:D:57[B]:TRP:CD1	1:D:57[B]:TRP:C	2.85	0.50
1:D:233[B]:LEU:C	1:D:233[B]:LEU:CD2	2.79	0.50
1:D:333[B]:ILE:HD11	1:D:339[B]:GLY:CA	2.35	0.50
1:D:456[A]:SER:OG	1:D:458[A]:ASN:ND2	2.40	0.50
1:D:64[B]:LEU:HA	1:D:67[B]:GLU:OE1	2.10	0.50
1:D:63[B]:TRP:HB3	1:D:92[B]:GLN:NE2	2.27	0.50
1:D:186[B]:GLY:H	1:D:188[B]:ILE:HG22	1.75	0.50
1:D:331[B]:GLN:HG3	1:D:333[B]:ILE:HG12	1.94	0.50
1:D:58[A]:LEU:HD11	1:D:359[A]:MSE:HB3	1.92	0.50
1:B:369:PHE:CD1	1:B:402:MSE:HE3	2.47	0.50
1:D:293[B]:GLY:O	1:D:294[B]:LEU:HB2	2.12	0.50
1:D:369[B]:PHE:CD1	1:D:402[B]:MSE:HE1	2.43	0.50
1:D:86[A]:TYR:O	1:D:141[A]:LEU:HD22	2.11	0.50
1:D:190[A]:GLY:HA3	1:D:226[A]:TRP:CD2	2.47	0.49
1:D:264[B]:ASN:HA	1:D:267[B]:PHE:HD2	1.76	0.49
1:D:427[B]:TRP:CD2	1:D:450[B]:HIS:HD2	2.30	0.49
1:D:233[B]:LEU:HD21	1:D:235[B]:PHE:O	2.11	0.49
1:D:292[B]:HIS:CD2	1:D:300[B]:LEU:O	2.60	0.49
1:A:287:TYR:CD1	1:A:325:GLY:HA3	2.48	0.49
1:D:192[B]:VAL:O	1:D:193[B]:LYS:HB2	2.12	0.49
1:D:214[A]:THR:HB	1:D:235[A]:PHE:CE2	2.47	0.49
1:D:95[A]:ASN:O	1:D:96[A]:ASN:ND2	2.45	0.49
1:D:456[B]:SER:OG	1:D:458[B]:ASN:ND2	2.45	0.49
1:D:164[B]:LYS:O	1:D:168[B]:LYS:HG3	2.13	0.49
1:D:346[A]:PRO:HB3	1:D:348[A]:TYR:CZ	2.48	0.49
1:D:333[A]:ILE:CD1	1:D:339[A]:GLY:HA3	2.43	0.49
1:A:420:GLY:O	1:A:423:LYS:HE3	2.13	0.49
1:D:189[A]:ARG:HB2	1:D:192[A]:VAL:HG23	1.94	0.49
1:D:333[A]:ILE:HD12	1:D:339[A]:GLY:HA3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ALA:HB1	1:B:274:MSE:HE3	1.95	0.48
1:B:57:TRP:C	1:B:57:TRP:CD1	2.86	0.48
1:D:238[B]:PHE:CE1	1:D:282[B]:ASP:HB2	2.48	0.48
1:D:364[A]:ASN:OD1	1:D:482[A]:HIS:N	2.30	0.48
1:D:184[B]:ILE:HG22	1:D:185[B]:GLY:N	2.27	0.48
1:D:373[B]:GLU:OE1	1:D:373[B]:GLU:N	2.47	0.48
1:D:76[B]:TYR:CE1	1:D:80[B]:GLN:NE2	2.82	0.48
1:D:153[B]:VAL:O	1:D:156[B]:GLY:N	2.44	0.48
1:D:40[B]:VAL:O	1:D:41[B]:SER:C	2.51	0.48
1:D:238[B]:PHE:HE1	1:D:282[B]:ASP:CG	2.16	0.48
1:C:369:PHE:CE1	1:C:402:MSE:HE2	2.49	0.48
1:D:213[A]:MSE:N	1:D:234[A]:ASP:OD2	2.46	0.48
1:D:227[A]:PHE:HB2	1:D:233[A]:LEU:CD1	2.44	0.48
1:B:435:LEU:HD21	1:B:472:VAL:CG1	2.44	0.48
1:C:442:ASP:OD1	1:C:442:ASP:C	2.52	0.48
1:D:112[B]:TYR:OH	1:D:157[B]:GLU:O	2.23	0.48
1:D:94[B]:LEU:HD12	1:D:166[B]:TYR:CZ	2.49	0.48
1:D:324[A]:TYR:CG	1:D:325[A]:GLY:N	2.81	0.48
1:D:359[A]:MSE:CA	1:D:359[A]:MSE:HE2	2.27	0.48
1:D:331[A]:GLN:CD	1:D:333[A]:ILE:HD11	2.34	0.48
1:D:401[B]:LEU:HD12	1:D:401[B]:LEU:C	2.35	0.48
1:D:435[A]:LEU:HB3	1:D:478[A]:GLN:N	2.29	0.48
1:D:254[A]:TYR:CE2	1:D:256[A]:ILE:HG13	2.49	0.47
1:D:65[A]:LEU:N	1:D:66[A]:PRO:HD3	2.29	0.47
1:D:369[A]:PHE:O	1:D:370[A]:PRO:C	2.53	0.47
1:D:412[A]:GLU:HG2	1:D:447[A]:LYS:HB2	1.97	0.47
1:D:248[A]:ARG:CD	1:D:254[A]:TYR:CE1	2.97	0.47
1:D:42[B]:GLU:C	1:D:42[B]:GLU:CD	2.72	0.47
1:D:194[B]:THR:O	1:D:198[B]:GLU:CG	2.62	0.47
1:D:33[B]:TRP:CH2	1:D:179[B]:ASN:HB3	2.50	0.47
1:D:373[A]:GLU:OE1	1:D:373[A]:GLU:N	2.45	0.47
1:D:437[B]:TYR:CE2	1:D:439[B]:GLY:HA2	2.49	0.47
1:D:233[A]:LEU:C	1:D:233[A]:LEU:CD2	2.83	0.47
1:D:432[B]:ASP:OD2	1:D:434[B]:LYS:HD2	2.14	0.47
1:D:326[B]:HIS:CE1	1:D:350[B]:ALA:HB1	2.50	0.47
1:D:369[B]:PHE:O	1:D:370[B]:PRO:C	2.53	0.47
1:D:84[A]:ARG:O	1:D:360[A]:LYS:HB3	2.14	0.47
1:D:233[A]:LEU:HD21	1:D:235[A]:PHE:C	2.35	0.47
1:A:142:TYR:HA	1:A:179:ASN:HB2	1.97	0.47
1:D:129[B]:MSE:CE	1:D:129[B]:MSE:HA	2.39	0.47
1:D:172[B]:GLU:OE1	1:D:172[B]:GLU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63[B]:TRP:HA	1:D:91[B]:VAL:HA	1.96	0.47
1:D:33[B]:TRP:CZ3	1:D:179[B]:ASN:HB3	2.50	0.47
1:D:251[B]:ASP:OD1	1:D:251[B]:ASP:O	2.33	0.46
1:D:84[B]:ARG:NE	1:D:357[B]:ASN:OD1	2.39	0.46
1:C:381:ILE:HD13	1:C:392:ALA:HB3	1.98	0.46
1:D:415[B]:PHE:CZ	1:D:448[B]:PHE:CZ	3.04	0.46
1:D:151[A]:SER:N	1:D:152[A]:PRO:HD2	2.31	0.46
1:D:177[A]:GLU:O	1:D:211[A]:HIS:NE2	2.48	0.46
1:D:286[B]:ILE:CD1	1:D:310[B]:TYR:CD1	2.99	0.46
1:C:33:TRP:CH2	1:C:179:ASN:HB3	2.51	0.46
1:D:290[B]:ILE:HG12	1:D:291[B]:PRO:HD2	1.98	0.46
1:D:427[A]:TRP:CE2	1:D:438[A]:ILE:HD11	2.50	0.46
1:D:65[A]:LEU:HB3	1:D:66[A]:PRO:HD3	1.98	0.46
1:D:130[A]:ASP:OD1	1:D:174[A]:TYR:HE1	1.99	0.46
1:D:293[A]:GLY:O	1:D:294[A]:LEU:HB2	2.16	0.46
1:D:280[A]:VAL:HG22	1:D:281[A]:ILE:N	2.30	0.46
1:D:308[B]:ARG:NH2	1:D:457[B]:GLY:O	2.49	0.46
1:D:173[B]:ARG:HD3	1:D:174[B]:TYR:CE2	2.51	0.46
1:D:295[B]:HIS:O	1:D:296[B]:ASP:C	2.54	0.46
1:D:312[A]:TYR:CE2	1:D:362[A]:LEU:HD13	2.51	0.46
1:D:65[A]:LEU:HD12	1:D:69[A]:LEU:HB2	1.98	0.46
1:D:153[B]:VAL:HG12	1:D:193[B]:LYS:HG3	1.97	0.46
1:D:164[A]:LYS:O	1:D:168[A]:LYS:HG3	2.16	0.46
1:D:265[A]:TRP:CZ3	1:D:269[A]:GLU:OE2	2.69	0.46
1:D:70[A]:ASN:OD1	1:D:73[A]:GLU:HG3	2.15	0.46
1:D:288[A]:GLU:O	1:D:289[A]:GLU:HB2	2.16	0.45
1:D:45[B]:ARG:NH1	5:D:1186:HOH:O	2.27	0.45
1:D:76[B]:TYR:O	1:D:80[B]:GLN:HG2	2.15	0.45
1:A:161:ASP:HA	1:A:164[A]:LYS:CE	2.47	0.45
1:C:435:LEU:HD21	1:C:472:VAL:CG1	2.45	0.45
1:A:369:PHE:CE1	1:A:402:MSE:HE3	2.51	0.45
1:D:290[B]:ILE:HD13	1:D:294[B]:LEU:HD21	1.98	0.45
1:D:65[A]:LEU:HD13	1:D:69[A]:LEU:CD1	2.22	0.45
1:D:238[B]:PHE:CE1	1:D:282[B]:ASP:OD1	2.70	0.45
1:D:288[A]:GLU:HB2	1:D:307[A]:VAL:HG21	1.97	0.45
1:D:297[B]:GLU:HG3	1:D:342[B]:GLY:HA3	1.99	0.45
1:D:59[B]:GLY:HA2	1:D:88[B]:VAL:O	2.16	0.45
1:D:248[B]:ARG:CZ	1:D:254[B]:TYR:CD1	3.00	0.45
1:D:246[B]:GLY:N	1:D:261[B]:GLU:OE1	2.45	0.45
1:A:183:PHE:CE2	1:A:237:MSE:HE1	2.52	0.45
1:A:333:ILE:HD11	1:A:339:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:SER:HB2	1:C:152:PRO:CD	2.47	0.45
1:D:133[A]:ILE:HG21	1:D:180[A]:ILE:HD11	1.99	0.45
1:D:170[B]:LEU:HB3	1:D:182[B]:TRP:CH2	2.52	0.45
5:A:739:HOH:O	3:B:485:MRD:H5C1	2.16	0.45
1:C:84:ARG:CD	1:C:356:TYR:CE2	3.00	0.44
1:D:248[B]:ARG:HD3	1:D:254[B]:TYR:CZ	2.52	0.44
1:D:97[A]:VAL:HB	1:D:157[A]:GLU:OE1	2.17	0.44
1:B:344:LYS:CE	3:C:484:MRD:HMC1	2.35	0.44
1:D:369[A]:PHE:HD1	1:D:402[A]:MSE:HE1	1.80	0.44
1:D:41[A]:SER:CB	1:D:43[A]:GLU:OE2	2.59	0.44
1:C:401:LEU:C	1:C:401:LEU:HD12	2.38	0.44
1:D:180[A]:ILE:HB	1:D:211[A]:HIS:NE2	2.33	0.44
1:D:183[A]:PHE:CE2	1:D:237[A]:MSE:HE1	2.53	0.44
1:B:401:LEU:HD12	1:B:401:LEU:C	2.38	0.44
1:D:238[B]:PHE:CE1	1:D:282[B]:ASP:HA	2.53	0.44
1:D:46[A]:TYR:OH	1:D:374[A]:ARG:O	2.25	0.44
1:D:450[A]:HIS:ND1	1:D:452[A]:SER:OG	2.30	0.44
1:A:146:VAL:HA	1:A:183:PHE:HB2	2.00	0.44
1:C:58:LEU:HD11	1:C:359:MSE:HB3	2.00	0.44
1:D:149[B]:TRP:O	1:D:152[B]:PRO:HG2	2.18	0.44
1:D:370[B]:PRO:HB2	1:D:400[B]:TYR:HE1	1.83	0.44
1:D:86[A]:TYR:O	1:D:141[A]:LEU:HD21	2.18	0.44
1:D:296[B]:ASP:HB3	1:D:299[B]:GLU:HG2	1.99	0.44
1:B:416:SER:HA	1:B:443:ASN:OD1	2.18	0.44
1:D:146[A]:VAL:O	1:D:147[A]:CYS:C	2.56	0.44
1:C:146:VAL:HA	1:C:183:PHE:HB2	1.99	0.44
1:C:295:HIS:NE2	2:C:1:SO4:O3	2.50	0.44
1:A:151:SER:HB2	1:A:152:PRO:CD	2.48	0.43
1:B:65:LEU:CD1	1:B:69:LEU:HD12	2.46	0.43
1:D:241[A]:GLY:HA2	1:D:242[A]:HIS:HA	1.73	0.43
1:D:268[B]:VAL:O	1:D:272[B]:MSE:HG3	2.17	0.43
1:D:288[B]:GLU:HG2	1:D:289[B]:GLU:HG2	2.00	0.43
1:D:290[B]:ILE:CD1	1:D:294[B]:LEU:HD21	2.48	0.43
3:B:485:MRD:H5C3	3:B:485:MRD:HMC1	2.00	0.43
1:D:44[B]:GLY:O	1:D:277[B]:MSE:HE3	2.19	0.43
1:D:97[A]:VAL:HA	1:D:98[A]:PRO:HA	1.73	0.43
1:D:87[B]:ASN:HA	1:D:141[B]:LEU:CD2	2.48	0.43
1:D:130[A]:ASP:OD1	1:D:174[A]:TYR:CE1	2.72	0.43
1:D:177[B]:GLU:O	1:D:211[B]:HIS:NE2	2.50	0.43
1:D:189[B]:ARG:NH2	1:D:191[B]:ASP:OD2	2.43	0.43
1:D:280[B]:VAL:HG22	1:D:281[B]:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:PRO:HB3	1:C:371:PHE:CD2	2.53	0.43
1:D:254[A]:TYR:CE2	1:D:256[A]:ILE:CG1	3.02	0.43
1:A:368:THR:O	1:A:368:THR:HG22	2.18	0.43
1:D:65[B]:LEU:N	1:D:66[B]:PRO:CD	2.81	0.43
1:A:100:MSE:HE2	1:A:100:MSE:HB2	1.75	0.43
1:D:146[B]:VAL:HA	1:D:183[B]:PHE:HB2	2.01	0.43
1:D:327[B]:ASN:O	1:D:331[B]:GLN:HG2	2.19	0.43
1:D:370[A]:PRO:HB2	1:D:400[A]:TYR:HE1	1.84	0.43
1:D:374[B]:ARG:HB2	1:D:400[B]:TYR:OH	2.18	0.43
1:D:459[A]:ASP:OD1	1:D:459[A]:ASP:N	2.51	0.43
1:B:166:TYR:CZ	1:B:170:LEU:HD11	2.54	0.43
1:B:183:PHE:CE2	1:B:237:MSE:HE1	2.53	0.43
1:A:57:TRP:C	1:A:57:TRP:CD1	2.92	0.43
1:D:227[A]:PHE:HB2	1:D:233[A]:LEU:HD12	2.01	0.43
1:D:380[B]:VAL:HB	1:D:394[B]:ALA:CB	2.49	0.43
1:D:151[B]:SER:HB2	1:D:152[B]:PRO:HD3	2.00	0.43
1:D:166[B]:TYR:CE2	1:D:170[B]:LEU:HD11	2.54	0.43
1:A:177:GLU:O	1:A:211:HIS:NE2	2.52	0.42
3:B:485:MRD:C5	3:B:485:MRD:HMC1	2.49	0.42
1:C:428:TYR:CE1	1:C:479:ILE:HD12	2.54	0.42
1:D:63[A]:TRP:HZ3	1:D:146[A]:VAL:HG21	1.85	0.42
1:D:97[B]:VAL:HA	1:D:98[B]:PRO:HA	1.76	0.42
1:A:241:GLY:HA2	1:A:242:HIS:HA	1.89	0.42
1:D:128[A]:HIS:O	1:D:132[A]:ILE:HG13	2.20	0.42
1:D:149[A]:TRP:O	1:D:152[A]:PRO:CG	2.67	0.42
1:D:243[A]:ARG:HD3	1:D:247[A]:GLN:O	2.19	0.42
1:D:296[A]:ASP:HB3	1:D:299[A]:GLU:CG	2.49	0.42
1:D:179[B]:ASN:O	1:D:180[B]:ILE:HD13	2.19	0.42
1:D:426[A]:TRP:CD1	1:D:437[A]:TYR:HA	2.55	0.42
1:D:56[B]:PHE:CE1	1:D:366[B]:MSE:HG3	2.54	0.42
1:D:95[B]:ASN:O	1:D:96[B]:ASN:ND2	2.52	0.42
1:C:287:TYR:CD1	1:C:325:GLY:HA3	2.55	0.42
1:D:311[B]:ALA:HB1	1:D:362[B]:LEU:HD22	2.02	0.42
1:D:315[A]:VAL:HG21	1:D:362[A]:LEU:HD21	2.00	0.42
1:B:205:LYS:NZ	1:B:232:TRP:O	2.50	0.42
1:B:418:ILE:O	1:B:423:LYS:NZ	2.53	0.42
1:C:57:TRP:CD1	1:C:57:TRP:C	2.93	0.42
1:D:333[B]:ILE:HD12	1:D:339[B]:GLY:CA	2.50	0.42
1:D:39[B]:VAL:HG12	1:D:40[B]:VAL:N	2.35	0.42
1:D:401[B]:LEU:HD11	1:D:464[B]:VAL:CG2	2.50	0.42
1:A:369:PHE:CD1	1:A:402:MSE:HE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:LYS:HB2	1:B:476:CYS:SG	2.60	0.42
1:D:161[B]:ASP:HA	1:D:164[B]:LYS:HE2	2.02	0.42
1:D:415[B]:PHE:HZ	1:D:448[B]:PHE:CZ	2.38	0.42
1:C:290:ILE:HG12	1:C:291:PRO:HD2	2.01	0.42
1:D:361[B]:TYR:CD1	1:D:433[B]:GLY:HA3	2.54	0.42
1:D:230[B]:ALA:HA	1:D:231[B]:PRO:HD3	1.87	0.41
1:D:455[B]:SER:CA	5:D:484:HOH:O	2.60	0.41
1:D:275[B]:LYS:CA	1:D:276[B]:PRO:C	2.84	0.41
1:D:324[B]:TYR:CG	1:D:325[B]:GLY:N	2.89	0.41
1:D:354[A]:PRO:O	1:D:358[A]:GLN:CG	2.57	0.41
1:D:30[B]:TYR:CG	1:D:483[B]:GLU:HB2	2.55	0.41
1:D:62[B]:GLY:O	1:D:91[B]:VAL:HG12	2.20	0.41
1:D:130[B]:ASP:OD1	1:D:174[B]:TYR:OH	2.30	0.41
1:D:149[A]:TRP:CH2	1:D:187[A]:ASP:HB2	2.54	0.41
1:D:212[B]:LEU:CA	1:D:234[B]:ASP:OD2	2.64	0.41
1:D:308[B]:ARG:NH2	1:D:459[B]:ASP:OD1	2.53	0.41
1:D:60[A]:GLU:HG3	1:D:81[A]:CYS:SG	2.60	0.41
1:D:130[B]:ASP:OD2	1:D:173[B]:ARG:NH2	2.51	0.41
1:A:401:LEU:HG	1:A:464:VAL:HB	2.03	0.41
1:B:266:ARG:O	1:B:270:ARG:HG3	2.21	0.41
1:B:365:LEU:HD11	1:B:402:MSE:HE2	2.02	0.41
1:D:247[B]:GLN:NE2	1:D:292[B]:HIS:O	2.39	0.41
1:D:31[A]:ILE:HA	1:D:32[A]:PRO:HD3	1.92	0.41
1:D:117[B]:ILE:HG23	1:D:118[B]:ASN:N	2.36	0.41
1:D:172[B]:GLU:CD	1:D:207[B]:ILE:HG21	2.41	0.41
1:D:414[B]:ASP:C	1:D:414[B]:ASP:OD1	2.58	0.41
1:B:305:TYR:CD2	3:B:485:MRD:H1C1	2.55	0.41
1:D:190[B]:GLY:O	1:D:194[B]:THR:OG1	2.20	0.41
1:D:245[B]:TYR:CZ	1:D:262[B]:GLU:HB2	2.56	0.41
1:D:437[A]:TYR:CZ	1:D:439[A]:GLY:HA2	2.55	0.41
1:A:365:LEU:HD11	1:A:402:MSE:CE	2.49	0.41
1:C:142:TYR:HA	1:C:179:ASN:HB2	2.03	0.41
1:D:296[A]:ASP:HB3	1:D:299[A]:GLU:HG2	2.02	0.41
1:A:369:PHE:CD1	1:A:402:MSE:CE	3.04	0.41
3:C:20:MRD:H3C1	5:C:1059:HOH:O	2.21	0.41
1:D:177[B]:GLU:HA	1:D:178[B]:PRO:HD2	1.88	0.41
1:D:69[B]:LEU:HD22	1:D:73[B]:GLU:HB3	2.03	0.41
1:D:241[B]:GLY:HA2	1:D:242[B]:HIS:HA	1.82	0.41
1:D:393[A]:ILE:CG2	1:D:404[A]:TYR:HB3	2.51	0.41
1:D:393[A]:ILE:HG22	1:D:404[A]:TYR:HB3	2.02	0.41
1:D:393[A]:ILE:O	1:D:393[A]:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41[B]:SER:OG	1:D:43[B]:GLU:OE1	2.24	0.41
1:D:164[A]:LYS:HB2	1:D:164[A]:LYS:HE3	1.88	0.40
1:D:45[A]:ARG:O	1:D:279[A]:PRO:HB3	2.21	0.40
1:D:414[B]:ASP:CG	1:D:416[B]:SER:HG	2.20	0.40
1:D:311[B]:ALA:O	1:D:315[B]:VAL:HG23	2.22	0.40
1:A:333:ILE:HD11	1:A:339:GLY:CA	2.51	0.40
1:B:151:SER:HB2	1:B:152:PRO:CD	2.52	0.40
1:B:287:TYR:CE2	1:B:330:MSE:HG3	2.56	0.40
1:D:168[B]:LYS:O	1:D:172[B]:GLU:HG2	2.21	0.40
1:D:248[B]:ARG:CD	1:D:254[B]:TYR:CZ	3.04	0.40
1:D:37[B]:LYS:O	1:D:49[B]:HIS:HA	2.22	0.40
1:D:248[A]:ARG:CZ	1:D:254[A]:TYR:CD1	3.04	0.40
1:D:331[A]:GLN:OE1	1:D:333[A]:ILE:HD11	2.22	0.40
1:D:414[A]:ASP:OD1	1:D:416[A]:SER:OG	2.26	0.40
1:D:415[B]:PHE:CD2	1:D:464[B]:VAL:HG11	2.57	0.40
1:D:429[A]:THR:OG1	1:D:432[A]:ASP:OD1	2.23	0.40
1:A:287:TYR:O	1:A:290:ILE:HG22	2.22	0.40
1:D:368[A]:THR:HG22	1:D:368[A]:THR:O	2.22	0.40
1:D:54[A]:PRO:HG3	1:D:372[A]:PHE:CE2	2.56	0.40
1:D:370[A]:PRO:CB	1:D:373[A]:GLU:OE2	2.56	0.40
1:D:37[A]:LYS:HG2	1:D:50[A]:GLU:OE1	2.22	0.40
1:D:424[A]:ASN:O	1:D:464[A]:VAL:HG13	2.22	0.40
1:D:65[B]:LEU:HD13	1:D:69[B]:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	469/463 (101%)	452 (96%)	17 (4%)	0	100	100
1	B	463/463 (100%)	444 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	464/463 (100%)	444 (96%)	20 (4%)	0	100	100
1	D	910/463 (196%)	834 (92%)	66 (7%)	10 (1%)	14	9
All	All	2306/1852 (124%)	2174 (94%)	122 (5%)	10 (0%)	41	32

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	41[A]	SER
1	D	41[B]	SER
1	D	295[A]	HIS
1	D	295[B]	HIS
1	D	478[A]	GLN
1	D	478[B]	GLN
1	D	253[A]	ASP
1	D	253[B]	ASP
1	D	442[A]	ASP
1	D	442[B]	ASP

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	401/380 (106%)	398 (99%)	3 (1%)	84	88
1	B	395/380 (104%)	392 (99%)	3 (1%)	81	86
1	C	396/380 (104%)	392 (99%)	4 (1%)	76	82
1	D	758/380 (200%)	750 (99%)	8 (1%)	73	79
All	All	1950/1520 (128%)	1932 (99%)	18 (1%)	78	84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	60	GLU

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Mol	Chain	Res	Type
1	A	330	MSE
1	B	43	GLU
1	B	57	TRP
1	B	60	GLU
1	C	43	GLU
1	C	57	TRP
1	C	60	GLU
1	C	330	MSE
1	D	57[A]	TRP
1	D	57[B]	TRP
1	D	60[A]	GLU
1	D	60[B]	GLU
1	D	129[A]	MSE
1	D	129[B]	MSE
1	D	330[A]	MSE
1	D	330[B]	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	295	HIS
1	B	116	ASN
1	C	116	ASN
1	C	298	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

26 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	6	-	4,4,4	0.12	0	6,6,6	0.11	0
2	SO4	C	1	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	A	5	-	4,4,4	0.18	0	6,6,6	0.08	0
2	SO4	A	15	-	4,4,4	1.34	0	6,6,6	0.33	0
3	MRD	C	484	-	7,7,7	0.26	0	9,10,10	0.32	0
4	MPD	C	17	-	7,7,7	0.39	0	9,10,10	0.29	0
3	MRD	C	20	-	7,7,7	0.54	0	9,10,10	0.25	0
2	SO4	A	9	-	4,4,4	0.18	0	6,6,6	0.14	0
3	MRD	B	485	-	7,7,7	0.34	0	9,10,10	0.20	0
3	MRD	A	485	-	7,7,7	0.46	0	9,10,10	0.20	0
2	SO4	B	16	-	4,4,4	0.19	0	6,6,6	0.10	0
2	SO4	A	12	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	13	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	C	4	-	4,4,4	0.21	0	6,6,6	0.11	0
2	SO4	C	11	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	B	7	-	4,4,4	0.16	0	6,6,6	0.08	0
2	SO4	C	14	-	4,4,4	0.17	0	6,6,6	0.09	0
4	MPD	C	485	-	7,7,7	0.42	0	9,10,10	0.16	0
3	MRD	A	19	-	7,7,7	0.47	0	9,10,10	0.17	0
2	SO4	C	8	-	4,4,4	0.17	0	6,6,6	0.14	0
2	SO4	B	10	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	B	2	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	A	3	-	4,4,4	0.17	0	6,6,6	0.13	0
3	MRD	B	18	-	7,7,7	0.46	0	9,10,10	0.32	0
3	MRD	A	484	-	7,7,7	0.41	0	9,10,10	0.15	0
3	MRD	B	484	-	7,7,7	0.35	0	9,10,10	0.25	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	MRD	A	485	-	-	5/5/5/5	-
3	MRD	A	19	-	-	2/5/5/5	-
3	MRD	B	485	-	-	3/5/5/5	-
4	MPD	C	485	-	-	4/5/5/5	-
3	MRD	C	484	-	-	2/5/5/5	-
4	MPD	C	17	-	-	4/5/5/5	-
3	MRD	C	20	-	-	0/5/5/5	-
3	MRD	B	18	-	-	2/5/5/5	-
3	MRD	A	484	-	-	0/5/5/5	-
3	MRD	B	484	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	484	MRD	C2-C3-C4-O4
4	C	17	MPD	CM-C2-C3-C4
4	C	17	MPD	C2-C3-C4-O4
3	A	485	MRD	CM-C2-C3-C4
3	A	485	MRD	C2-C3-C4-O4
3	A	485	MRD	C2-C3-C4-C5
4	C	485	MPD	C2-C3-C4-O4
3	B	18	MRD	C2-C3-C4-O4
4	C	17	MPD	O2-C2-C3-C4
3	A	485	MRD	O2-C2-C3-C4
3	C	484	MRD	C2-C3-C4-C5
3	A	19	MRD	C2-C3-C4-C5
4	C	17	MPD	C1-C2-C3-C4
3	B	485	MRD	C1-C2-C3-C4
3	A	485	MRD	C1-C2-C3-C4
4	C	485	MPD	CM-C2-C3-C4
3	A	19	MRD	CM-C2-C3-C4
3	B	485	MRD	O2-C2-C3-C4
4	C	485	MPD	O2-C2-C3-C4
3	B	18	MRD	O2-C2-C3-C4
3	B	485	MRD	C2-C3-C4-C5
4	C	485	MPD	C2-C3-C4-C5

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	SO4	1	0
3	C	484	MRD	3	0
4	C	17	MPD	2	0
3	C	20	MRD	1	0
3	B	485	MRD	6	0
3	A	485	MRD	5	0
4	C	485	MPD	3	0
3	B	18	MRD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	442/463 (95%)	-0.07	7 (1%) 72 75	11, 20, 38, 55	0
1	B	441/463 (95%)	0.01	14 (3%) 47 54	14, 24, 42, 60	0
1	C	441/463 (95%)	-0.15	6 (1%) 75 78	13, 20, 36, 57	0
1	D	442/463 (95%)	2.24	230 (52%) 0 0	26, 32, 42, 59	0
All	All	1766/1852 (95%)	0.51	257 (14%) 2 3	11, 25, 41, 60	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	477[A]	TYR	7.2
1	D	470[A]	ASP	7.0
1	A	476	CYS	6.8
1	D	464[A]	VAL	6.1
1	D	184[A]	ILE	5.8
1	D	204[A]	ILE	5.6
1	C	476	CYS	5.2
1	D	188[A]	ILE	5.1
1	D	401[A]	LEU	5.1
1	D	482[A]	HIS	5.1
1	D	343[A]	ALA	5.1
1	D	420[A]	GLY	5.1
1	D	441[A]	PHE	5.0
1	D	200[A]	LEU	5.0
1	D	265[A]	TRP	4.9
1	D	150[A]	GLY	4.9
1	D	46[A]	TYR	4.8
1	D	442[A]	ASP	4.8
1	D	421[A]	ALA	4.8
1	D	313[A]	TRP	4.8
1	D	399[A]	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	271[A]	SER	4.8
1	D	422[A]	LYS	4.7
1	D	474[A]	LYS	4.7
1	D	382[A]	ALA	4.6
1	B	476	CYS	4.6
1	D	41[A]	SER	4.6
1	D	258[A]	GLU	4.6
1	D	443[A]	ASN	4.5
1	D	471[A]	TYR	4.5
1	D	36[A]	GLY	4.5
1	D	400[A]	TYR	4.5
1	D	207[A]	ILE	4.4
1	D	483[A]	GLU	4.4
1	D	478[A]	GLN	4.4
1	D	112[A]	TYR	4.4
1	D	375[A]	VAL	4.4
1	D	37[A]	LYS	4.3
1	B	477[A]	TYR	4.3
1	D	192[A]	VAL	4.3
1	D	226[A]	TRP	4.3
1	B	482[A]	HIS	4.2
1	D	189[A]	ARG	4.1
1	D	480[A]	ASP	4.1
1	D	270[A]	ARG	4.1
1	D	201[A]	ALA	4.1
1	D	248[A]	ARG	4.1
1	D	315[A]	VAL	4.0
1	A	27	GLN	4.0
1	D	250[A]	GLY	3.9
1	D	473[A]	LYS	3.9
1	A	251	ASP	3.9
1	D	416[A]	SER	3.9
1	D	165[A]	ALA	3.9
1	C	477[A]	TYR	3.9
1	B	475[A]	ASP	3.8
1	D	233[A]	LEU	3.8
1	D	109[A]	THR	3.8
1	D	381[A]	ILE	3.8
1	D	415[A]	PHE	3.8
1	D	209[A]	LYS	3.8
1	D	169[A]	PHE	3.7
1	D	469[A]	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	251[A]	ASP	3.7
1	D	34[A]	SER	3.7
1	D	202[A]	THR	3.6
1	D	372[A]	PHE	3.6
1	D	151[A]	SER	3.6
1	D	249[A]	PHE	3.6
1	D	52[A]	GLY	3.6
1	D	316[A]	PHE	3.6
1	D	448[A]	PHE	3.6
1	D	230[A]	ALA	3.5
1	D	301[A]	LEU	3.5
1	D	156[A]	GLY	3.4
1	C	442	ASP	3.4
1	D	371[A]	PHE	3.4
1	D	370[A]	PRO	3.4
1	D	29[A]	THR	3.4
1	D	28[A]	LYS	3.4
1	D	50[A]	GLU	3.4
1	D	468[A]	SER	3.4
1	D	311[A]	ALA	3.4
1	D	268[A]	VAL	3.4
1	D	424[A]	ASN	3.3
1	D	312[A]	TYR	3.3
1	D	412[A]	GLU	3.3
1	D	479[A]	ILE	3.3
1	D	48[A]	LYS	3.3
1	B	416	SER	3.3
1	D	465[A]	VAL	3.3
1	D	27[A]	GLN	3.3
1	D	76[A]	TYR	3.3
1	D	222[A]	THR	3.3
1	D	361[A]	TYR	3.3
1	D	253[A]	ASP	3.2
1	D	289[A]	GLU	3.2
1	D	383[A]	GLY	3.2
1	D	379[A]	SER	3.2
1	D	320[A]	PHE	3.2
1	D	171[A]	ALA	3.2
1	D	354[A]	PRO	3.1
1	D	380[A]	VAL	3.1
1	D	49[A]	HIS	3.1
1	D	254[A]	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	475	ASP	3.1
1	D	328[A]	SER	3.1
1	D	472[A]	VAL	3.1
1	D	377[A]	ASP	3.1
1	D	103[A]	TYR	3.1
1	D	83[A]	ARG	3.0
1	D	476[A]	CYS	3.0
1	D	333[A]	ILE	3.0
1	D	51[A]	ASN	3.0
1	D	435[A]	LEU	3.0
1	D	256[A]	ILE	3.0
1	D	445[A]	VAL	3.0
1	D	232[A]	TRP	3.0
1	D	40[A]	VAL	3.0
1	D	174[A]	TYR	3.0
1	D	69[A]	LEU	3.0
1	A	477[A]	TYR	3.0
1	D	119[A]	GLN	3.0
1	D	307[A]	VAL	2.9
1	D	42[A]	GLU	2.9
1	D	39[A]	VAL	2.9
1	D	185[A]	GLY	2.9
1	D	197[A]	TRP	2.9
1	D	154[A]	SER	2.9
1	D	279[A]	PRO	2.9
1	D	293[A]	GLY	2.9
1	D	418[A]	ILE	2.9
1	D	125[A]	TYR	2.9
1	D	63[A]	TRP	2.9
1	D	144[A]	GLY	2.9
1	B	422	LYS	2.9
1	D	467[A]	SER	2.9
1	D	281[A]	ILE	2.9
1	D	134[A]	ARG	2.8
1	D	365[A]	LEU	2.8
1	D	369[A]	PHE	2.8
1	D	291[A]	PRO	2.8
1	D	295[A]	HIS	2.8
1	D	413[A]	VAL	2.8
1	D	302[A]	TRP	2.8
1	D	463[A]	ILE	2.8
1	D	398[A]	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	337[A]	VAL	2.8
1	D	340[A]	ALA	2.8
1	B	465	VAL	2.7
1	D	298[A]	ASN	2.7
1	D	65[A]	LEU	2.7
1	D	106[A]	TYR	2.7
1	D	397[A]	GLY	2.7
1	D	31[A]	ILE	2.7
1	D	163[A]	ALA	2.7
1	D	269[A]	GLU	2.7
1	D	137[A]	ALA	2.7
1	D	466[A]	ASP	2.7
1	D	116[A]	ASN	2.7
1	D	290[A]	ILE	2.6
1	D	44[A]	GLY	2.6
1	D	278[A]	LYS	2.6
1	D	227[A]	PHE	2.6
1	D	461[A]	VAL	2.6
1	D	305[A]	TYR	2.6
1	D	223[A]	SER	2.6
1	D	241[A]	GLY	2.6
1	D	426[A]	TRP	2.6
1	D	191[A]	ASP	2.5
1	D	457[A]	GLY	2.5
1	D	376[A]	PRO	2.5
1	D	176[A]	ASP	2.5
1	D	459[A]	ASP	2.5
1	D	267[A]	PHE	2.5
1	B	443	ASN	2.5
1	D	394[A]	ALA	2.5
1	D	433[A]	GLY	2.5
1	D	434[A]	LYS	2.5
1	D	212[A]	LEU	2.5
1	D	321[A]	GLY	2.5
1	D	438[A]	ILE	2.5
1	D	126[A]	TRP	2.4
1	D	348[A]	TYR	2.4
1	B	483	GLU	2.4
1	D	218[A]	ARG	2.4
1	C	443	ASN	2.4
1	D	124[A]	GLY	2.4
1	D	296[A]	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	97[A]	VAL	2.4
1	D	153[A]	VAL	2.4
1	D	160[A]	VAL	2.4
1	D	166[A]	TYR	2.4
1	D	216[A]	HIS	2.4
1	D	346[A]	PRO	2.4
1	D	147[A]	CYS	2.3
1	D	206[A]	ALA	2.3
1	D	423[A]	LYS	2.3
1	D	367[A]	LEU	2.3
1	D	446[A]	HIS	2.3
1	B	251	ASP	2.3
1	D	338[A]	GLY	2.3
1	D	374[A]	ARG	2.3
1	D	310[A]	TYR	2.3
1	D	53[A]	THR	2.3
1	D	236[A]	ASN	2.3
1	D	55[A]	PHE	2.3
1	D	244[A]	ARG	2.3
1	C	482[A]	HIS	2.3
1	D	447[A]	LYS	2.3
1	D	385[A]	ASN	2.3
1	D	332[A]	PHE	2.3
1	D	430[A]	THR	2.3
1	D	57[A]	TRP	2.3
1	D	168[A]	LYS	2.2
1	D	356[A]	TYR	2.2
1	D	45[A]	ARG	2.2
1	D	32[A]	PRO	2.2
1	D	347[A]	TRP	2.2
1	D	306[A]	ASP	2.2
1	D	341[A]	TYR	2.2
1	D	440[A]	GLU	2.2
1	B	250	GLY	2.2
1	B	473	LYS	2.2
1	D	231[A]	PRO	2.2
1	D	339[A]	GLY	2.2
1	D	378[A]	GLN	2.2
1	D	35[A]	ASN	2.2
1	D	300[A]	LEU	2.2
1	A	253	ASP	2.2
1	D	352[A]	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	275[A]	LYS	2.2
1	D	224[A]	ALA	2.2
1	D	273[A]	ALA	2.2
1	D	133[A]	ILE	2.1
1	D	247[A]	GLN	2.1
1	D	33[A]	TRP	2.1
1	D	357[A]	ASN	2.1
1	D	453[A]	GLY	2.1
1	D	114[A]	PHE	2.1
1	D	81[A]	CYS	2.1
1	D	283[A]	GLY	2.1
1	D	431[A]	LYS	2.1
1	D	162[A]	GLN	2.1
1	A	420	GLY	2.1
1	D	182[A]	TRP	2.1
1	D	208[A]	ASP	2.1
1	A	482[A]	HIS	2.1
1	D	286[A]	ILE	2.1
1	B	424	ASN	2.0
1	D	101[A]	ASN	2.0
1	B	273	ALA	2.0
1	D	475[A]	ASP	2.0
1	D	280[A]	VAL	2.0
1	D	417[A]	LYS	2.0
1	D	456[A]	SER	2.0
1	D	104[A]	GLY	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 carbohydrates 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(\AA^2)	Q<0.9
3	MRD	C	484	8/8	0.62	0.35	74,76,77,78	0
2	SO4	A	15	5/5	0.63	0.22	22,22,26,36	0
2	SO4	B	13	5/5	0.77	0.27	83,83,84,84	0
2	SO4	A	6	5/5	0.78	0.20	74,74,75,76	0
4	MPD	C	485	8/8	0.80	0.34	38,44,46,46	0
3	MRD	B	485	8/8	0.84	0.30	51,53,55,57	0
4	MPD	C	17	8/8	0.86	0.21	47,47,48,49	0
2	SO4	A	12	5/5	0.87	0.18	67,67,69,69	0
2	SO4	B	7	5/5	0.88	0.15	74,74,75,76	0
3	MRD	B	18	8/8	0.89	0.22	48,49,51,53	0
3	MRD	A	485	8/8	0.90	0.18	45,46,48,48	0
3	MRD	C	20	8/8	0.90	0.14	29,34,37,39	0
3	MRD	A	19	8/8	0.91	0.19	37,41,44,46	0
3	MRD	B	484	8/8	0.92	0.11	34,36,38,41	0
3	MRD	A	484	8/8	0.93	0.15	32,35,40,42	0
2	SO4	A	3	5/5	0.94	0.15	54,55,56,57	0
2	SO4	C	8	5/5	0.94	0.14	63,64,65,65	0
2	SO4	A	5	5/5	0.96	0.13	50,51,53,55	0
2	SO4	B	16	5/5	0.96	0.13	56,57,58,59	0
2	SO4	C	14	5/5	0.97	0.15	57,58,59,60	0
2	SO4	A	9	5/5	0.97	0.10	43,44,44,45	0
2	SO4	C	11	5/5	0.98	0.11	36,37,38,38	0
2	SO4	C	1	5/5	0.98	0.13	44,45,47,47	0
2	SO4	B	10	5/5	0.98	0.14	38,39,40,41	0
2	SO4	B	2	5/5	0.98	0.12	46,47,49,49	0
2	SO4	C	4	5/5	0.99	0.15	41,42,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.