



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 03:43 PM EDT

PDB ID : 1GGJ / pdb_00001ggj
Title : CRYSTAL STRUCTURE OF CATALASE HP11 FROM ESCHERICHIA COLI, ASN201ALA VARIANT.
Authors : Melik-Adamyan, W.R.; Bravo, J.; Carpena, X.; Switala, J.; Mate, M.J.; Fita, I.; Loewen, P.C.
Deposited on : 2000-08-21
Resolution : 1.92 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

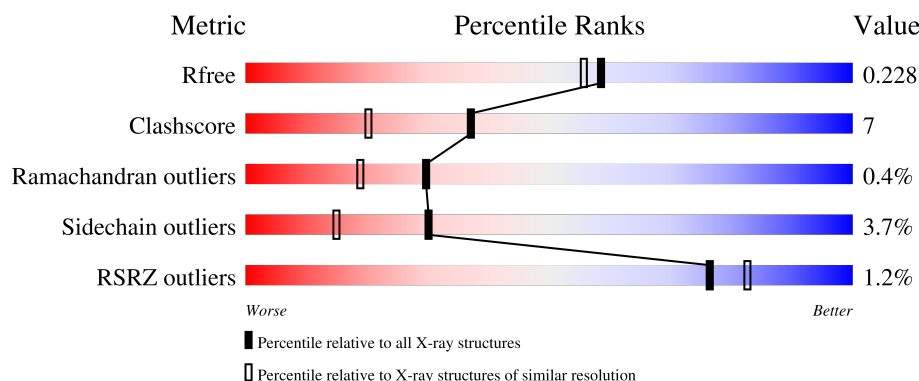
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	753	% 78% 17% ..
1	B	753	% 73% 20% ..
1	C	753	% 74% 19% ..
1	D	753	% 75% 18% ...

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HDD	C	760	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25962 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.

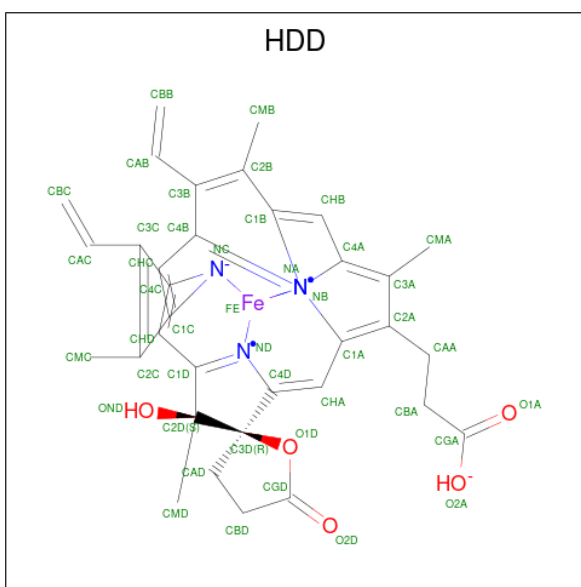
- Molecule 1 is a protein called CATALASE HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5743	3646	1004	1081	12			
1	B	727	Total	C	N	O	S	0	0	0
			5743	3646	1004	1081	12			
1	C	727	Total	C	N	O	S	0	0	0
			5743	3646	1004	1081	12			
1	D	727	Total	C	N	O	S	0	0	0
			5743	3646	1004	1081	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	ALA	ASN	engineered mutation	UNP P21179
B	201	ALA	ASN	engineered mutation	UNP P21179
C	201	ALA	ASN	engineered mutation	UNP P21179
D	201	ALA	ASN	engineered mutation	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: C₃₄H₃₂FeN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 34	Fe 1	N 4	O 5	0	0
2	B	1	Total 44	C 34	Fe 1	N 4	O 5	0	0
2	C	1	Total 44	C 34	Fe 1	N 4	O 5	0	0
2	D	1	Total 44	C 34	Fe 1	N 4	O 5	0	0

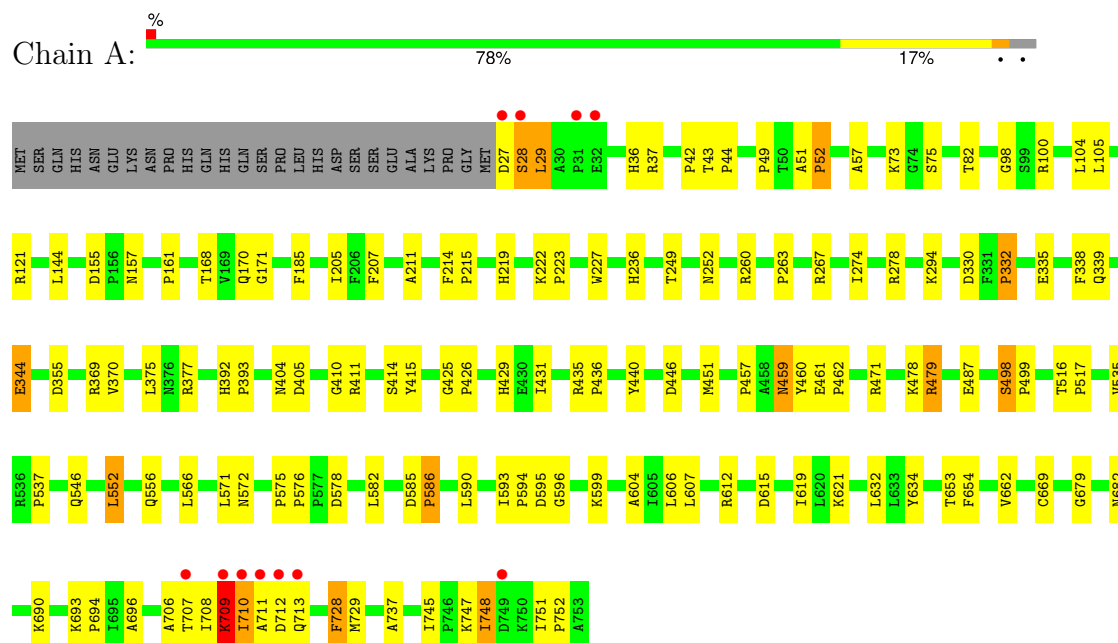
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	731	Total O 731 731	0	0
3	B	655	Total O 655 655	0	0
3	C	704	Total O 704 704	0	0
3	D	724	Total O 724 724	0	0

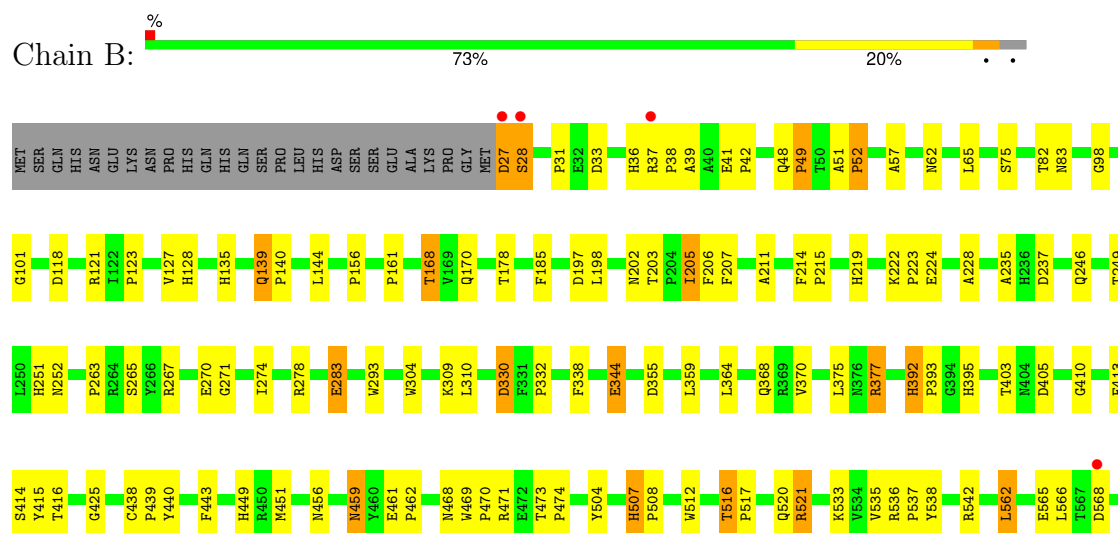
3 Residue-property plots [i](#)

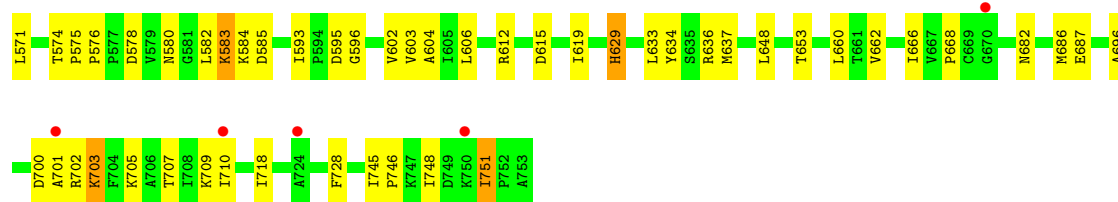
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CATALASE HPII

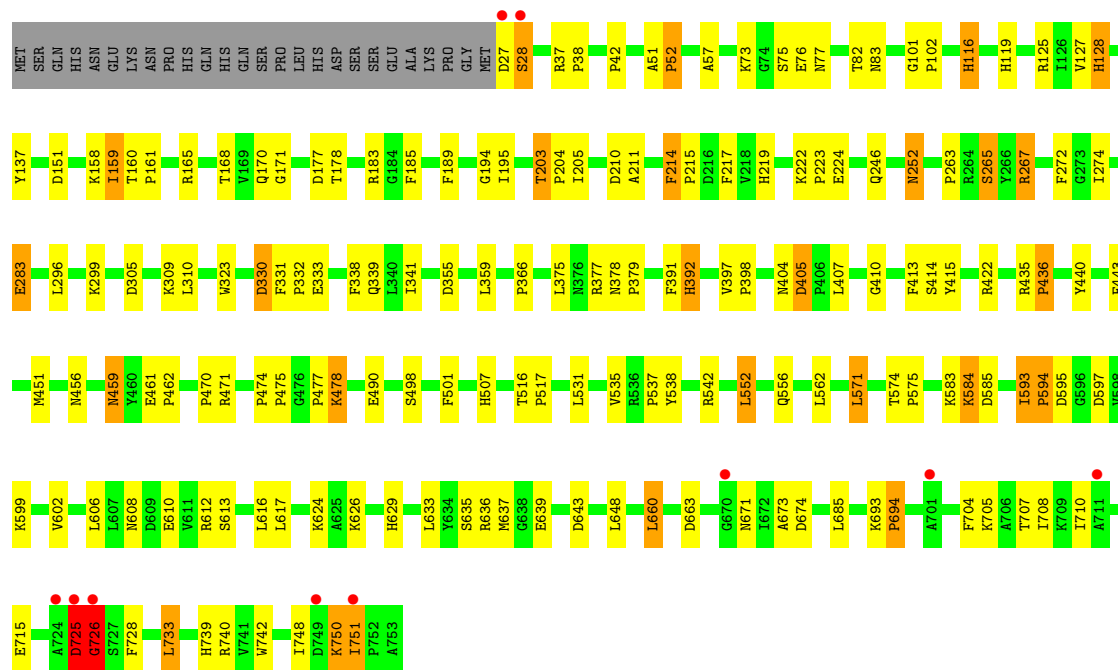
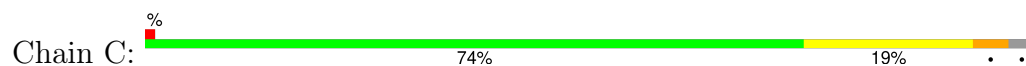


• Molecule 1: CATALASE HPII

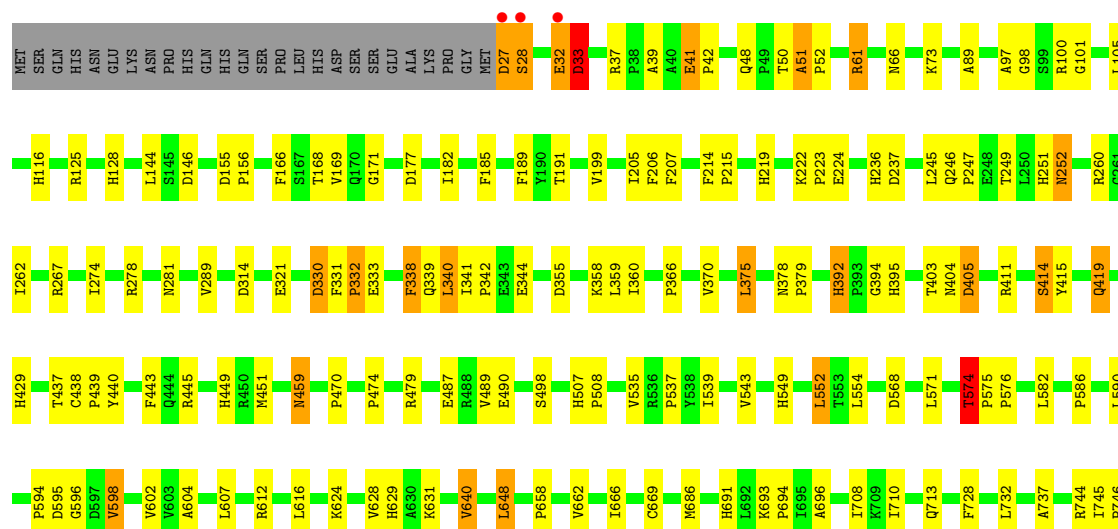
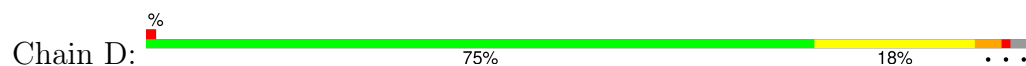


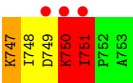


● Molecule 1: CATALASE HP11



● Molecule 1: CATALASE HP11





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.04Å 132.34Å 121.20Å 90.00° 109.63° 90.00°	Depositor
Resolution (Å)	87.71 – 1.92 87.71 – 1.92	Depositor EDS
% Data completeness (in resolution range)	91.7 (87.71-1.92) 92.0 (87.71-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.182 , 0.235 0.181 , 0.228	Depositor DCC
R_{free} test set	9705 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	7.3	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25962	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: HDD

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	0.52	0/5899	1.45	49/8020 (0.6%)
1	B	0.53	0/5899	1.50	84/8020 (1.0%)
1	C	0.53	0/5899	1.46	79/8020 (1.0%)
1	D	0.52	0/5899	1.47	67/8020 (0.8%)
All	All	0.52	0/23596	1.47	279/32080 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (279) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	521	ARG	CD-NE-CZ	12.76	142.27	124.40
1	C	725	ASP	CA-C-N	11.56	144.07	121.41
1	C	725	ASP	C-N-CA	11.56	144.07	121.41
1	C	725	ASP	CA-C-O	10.59	135.65	120.51
1	D	33	ASP	CA-CB-CG	9.95	122.55	112.60
1	C	330	ASP	CA-CB-CG	9.59	122.19	112.60
1	D	449	HIS	CA-CB-CG	9.31	123.11	113.80
1	C	414	SER	N-CA-C	9.16	120.87	111.07
1	D	330	ASP	CA-CB-CG	9.13	121.73	112.60
1	A	414	SER	N-CA-C	9.07	121.25	111.36
1	A	575	PRO	N-CA-CB	9.03	108.25	103.19
1	B	575	PRO	N-CA-CB	9.02	108.24	103.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	PHE	CA-CB-CG	8.96	122.76	113.80
1	B	474	PRO	N-CA-CB	8.62	108.02	103.19
1	D	575	PRO	N-CA-CB	8.24	107.81	103.19
1	A	728	PHE	CA-CB-CG	8.21	122.01	113.80
1	D	27	ASP	CA-CB-CG	7.98	120.58	112.60
1	A	44	PRO	N-CA-CB	7.92	107.34	103.22
1	B	414	SER	N-CA-C	7.89	119.57	110.97
1	D	474	PRO	N-CA-CB	7.87	107.60	103.19
1	D	445	ARG	NE-CZ-NH1	7.87	129.37	121.50
1	B	283	GLU	CA-CB-CG	7.80	129.71	114.10
1	A	576	PRO	N-CA-CB	7.62	107.46	103.19
1	A	170	GLN	N-CA-C	7.55	119.29	111.14
1	D	414	SER	N-CA-C	7.54	119.13	111.07
1	D	61	ARG	NE-CZ-NH2	7.52	125.97	119.20
1	C	585	ASP	CA-C-N	7.49	127.16	119.82
1	C	585	ASP	C-N-CA	7.49	127.16	119.82
1	B	392	HIS	CA-C-N	7.46	127.09	119.56
1	B	392	HIS	C-N-CA	7.46	127.09	119.56
1	C	217	PHE	CA-CB-CG	-7.43	106.37	113.80
1	C	338	PHE	CA-CB-CG	7.23	121.03	113.80
1	B	405	ASP	CA-C-N	7.23	126.86	119.19
1	B	405	ASP	C-N-CA	7.23	126.86	119.19
1	D	100	ARG	CD-NE-CZ	7.04	134.25	124.40
1	D	61	ARG	CD-NE-CZ	7.02	134.23	124.40
1	A	572	ASN	CA-CB-CG	-7.02	105.58	112.60
1	C	128	HIS	CB-CG-CD2	-7.00	122.10	131.20
1	A	43	THR	CA-C-N	6.89	124.62	119.66
1	A	43	THR	C-N-CA	6.89	124.62	119.66
1	C	726	GLY	N-CA-C	-6.88	96.87	113.18
1	C	28	SER	N-CA-C	-6.86	102.19	112.54
1	B	728	PHE	CA-CB-CG	6.78	120.58	113.80
1	C	185	PHE	CA-CB-CG	6.78	120.58	113.80
1	D	338	PHE	CA-CB-CG	6.76	120.56	113.80
1	C	575	PRO	N-CA-CB	6.64	106.91	103.19
1	B	224	GLU	CA-C-N	6.61	126.39	119.05
1	B	224	GLU	C-N-CA	6.61	126.39	119.05
1	D	185	PHE	CA-CB-CG	6.56	120.36	113.80
1	A	168	THR	N-CA-C	-6.52	99.65	109.96
1	A	585	ASP	CA-C-N	6.50	126.19	119.56
1	A	585	ASP	C-N-CA	6.50	126.19	119.56
1	D	182	ILE	N-CA-C	-6.49	102.98	110.05
1	B	98	GLY	N-CA-C	-6.49	104.63	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ARG	CD-NE-CZ	6.48	133.48	124.40
1	D	281	ASN	CA-CB-CG	6.47	119.07	112.60
1	A	100	ARG	CD-NE-CZ	6.47	133.46	124.40
1	B	449	HIS	CA-CB-CG	6.46	120.26	113.80
1	C	341	ILE	CB-CA-C	-6.39	103.70	110.16
1	D	392	HIS	CA-C-N	6.34	125.96	119.56
1	D	392	HIS	C-N-CA	6.34	125.96	119.56
1	C	170	GLN	N-CA-C	6.32	117.96	111.14
1	C	501	PHE	CA-CB-CG	6.30	120.10	113.80
1	B	330	ASP	CA-CB-CG	6.28	118.88	112.60
1	C	593	ILE	CA-C-N	6.23	126.59	119.93
1	C	593	ILE	C-N-CA	6.23	126.59	119.93
1	B	536	ARG	CA-C-O	6.17	123.30	119.29
1	D	479	ARG	CD-NE-CZ	6.17	133.03	124.40
1	B	278	ARG	CD-NE-CZ	6.15	133.01	124.40
1	C	101	GLY	CA-C-N	6.14	126.09	119.76
1	C	101	GLY	C-N-CA	6.14	126.09	119.76
1	A	171	GLY	N-CA-C	6.13	119.08	112.33
1	D	342	PRO	N-CA-CB	6.12	108.67	103.35
1	D	405	ASP	CA-C-N	6.11	125.73	119.56
1	D	405	ASP	C-N-CA	6.11	125.73	119.56
1	C	391	PHE	CA-CB-CG	6.10	119.90	113.80
1	B	139	GLN	CA-C-N	6.09	126.00	119.85
1	B	139	GLN	C-N-CA	6.09	126.00	119.85
1	C	158	LYS	CA-C-N	-6.08	115.26	123.10
1	C	158	LYS	C-N-CA	-6.08	115.26	123.10
1	C	102	PRO	N-CA-CB	6.05	108.70	103.31
1	C	116	HIS	CA-CB-CG	-6.05	107.75	113.80
1	D	171	GLY	N-CA-C	6.05	118.98	112.33
1	C	165	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	B	574	THR	CA-C-N	6.03	124.06	119.66
1	B	574	THR	C-N-CA	6.03	124.06	119.66
1	A	748	ILE	N-CA-C	6.03	119.52	111.44
1	C	392	HIS	CA-C-N	6.00	125.68	119.56
1	C	392	HIS	C-N-CA	6.00	125.68	119.56
1	C	339	GLN	N-CA-C	-5.99	98.96	108.73
1	D	574	THR	CA-C-N	5.99	124.03	119.66
1	D	574	THR	C-N-CA	5.99	124.03	119.66
1	A	185	PHE	CA-CB-CG	5.97	119.77	113.80
1	B	595	ASP	CA-CB-CG	5.95	118.55	112.60
1	C	474	PRO	N-CA-CB	5.93	106.51	103.19
1	A	338	PHE	CA-CB-CG	5.92	119.72	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	ILE	N-CA-C	-5.92	103.15	108.95
1	D	224	GLU	CA-C-N	5.89	125.43	119.19
1	D	224	GLU	C-N-CA	5.89	125.43	119.19
1	C	203	THR	CA-C-N	5.88	125.99	119.87
1	C	203	THR	C-N-CA	5.88	125.99	119.87
1	D	445	ARG	CD-NE-CZ	5.82	132.55	124.40
1	D	189	PHE	CA-CB-CG	5.82	119.62	113.80
1	A	355	ASP	CA-C-N	5.81	126.57	120.12
1	A	355	ASP	C-N-CA	5.81	126.57	120.12
1	D	246	GLN	CA-C-N	5.80	125.48	119.56
1	D	246	GLN	C-N-CA	5.80	125.48	119.56
1	C	574	THR	CA-C-N	5.80	123.89	119.66
1	C	574	THR	C-N-CA	5.80	123.89	119.66
1	D	366	PRO	N-CA-CB	5.79	108.39	103.35
1	B	701	ALA	N-CA-C	-5.79	105.71	112.89
1	B	42	PRO	N-CA-CB	5.79	108.48	103.27
1	D	612	ARG	CD-NE-CZ	5.79	132.50	124.40
1	B	648	LEU	CA-C-N	5.78	125.97	119.90
1	B	648	LEU	C-N-CA	5.78	125.97	119.90
1	C	52	PRO	N-CA-CB	5.76	108.38	103.19
1	C	475	PRO	N-CA-CB	5.76	108.36	103.35
1	B	521	ARG	CA-CB-CG	5.75	125.60	114.10
1	C	57	ALA	CA-C-N	5.75	125.61	119.28
1	C	57	ALA	C-N-CA	5.75	125.61	119.28
1	C	471	ARG	N-CA-C	5.75	119.42	110.17
1	B	246	GLN	CA-C-N	5.74	125.41	119.56
1	B	246	GLN	C-N-CA	5.74	125.41	119.56
1	C	128	HIS	CB-CG-ND1	5.74	131.30	122.70
1	B	516	THR	CA-C-N	5.73	125.41	119.05
1	B	516	THR	C-N-CA	5.73	125.41	119.05
1	A	595	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	355	ASP	CA-C-N	5.72	125.82	119.87
1	B	355	ASP	C-N-CA	5.72	125.82	119.87
1	D	51	ALA	N-CA-C	5.72	113.36	108.22
1	B	170	GLN	CA-C-O	-5.71	114.82	120.70
1	A	57	ALA	CA-C-N	5.71	125.24	119.19
1	A	57	ALA	C-N-CA	5.71	125.24	119.19
1	C	189	PHE	CA-CB-CG	5.68	119.48	113.80
1	B	338	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	498	SER	CA-C-N	5.67	125.51	119.28
1	A	498	SER	C-N-CA	5.67	125.51	119.28
1	C	751	ILE	CA-C-O	5.66	122.49	119.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	436	PRO	N-CA-CB	5.66	108.27	103.35
1	B	304	TRP	N-CA-C	5.65	117.89	111.11
1	C	663	ASP	CA-CB-CG	-5.63	106.97	112.60
1	B	228	ALA	CA-C-N	5.62	132.52	122.13
1	B	228	ALA	C-N-CA	5.62	132.52	122.13
1	B	395	HIS	CA-CB-CG	5.62	119.42	113.80
1	C	210	ASP	CA-CB-CG	5.61	118.21	112.60
1	D	419	GLN	CB-CG-CD	-5.60	103.08	112.60
1	C	246	GLN	CA-C-N	5.59	125.27	119.56
1	C	246	GLN	C-N-CA	5.59	125.27	119.56
1	D	498	SER	CA-C-N	5.59	125.43	119.28
1	D	498	SER	C-N-CA	5.59	125.43	119.28
1	B	118	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	203	THR	CA-C-N	5.58	126.06	120.04
1	B	203	THR	C-N-CA	5.58	126.06	120.04
1	D	236	HIS	CA-CB-CG	5.55	119.35	113.80
1	A	263	PRO	N-CA-CB	5.54	108.17	103.35
1	C	151	ASP	CA-CB-CG	-5.54	107.06	112.60
1	D	166	PHE	CA-C-O	-5.54	114.75	121.28
1	A	161	PRO	N-CA-CB	5.53	108.23	103.31
1	C	272	PHE	CA-CB-CG	5.53	119.33	113.80
1	B	206	PHE	CA-CB-CG	-5.53	108.27	113.80
1	C	177	ASP	N-CA-C	5.52	117.38	111.36
1	B	593	ILE	CA-C-N	5.51	125.83	119.93
1	B	593	ILE	C-N-CA	5.51	125.83	119.93
1	C	224	GLU	CA-C-N	5.51	125.35	119.28
1	C	224	GLU	C-N-CA	5.51	125.35	119.28
1	B	596	GLY	N-CA-C	5.51	117.81	111.36
1	A	471	ARG	N-CA-C	5.50	119.03	110.17
1	B	237	ASP	N-CA-C	5.50	117.70	111.11
1	C	339	GLN	N-CA-CB	5.47	119.34	110.42
1	B	224	GLU	CB-CA-C	5.46	118.14	109.52
1	D	237	ASP	N-CA-C	5.45	117.66	111.11
1	A	339	GLN	N-CA-C	-5.44	98.90	108.20
1	B	37	ARG	CA-C-N	5.44	125.34	119.85
1	B	37	ARG	C-N-CA	5.44	125.34	119.85
1	B	507	HIS	CA-C-N	5.42	124.88	119.24
1	B	507	HIS	C-N-CA	5.42	124.88	119.24
1	C	422	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	D	403	THR	N-CA-CB	5.40	119.75	111.22
1	B	629	HIS	CA-CB-CG	-5.39	108.41	113.80
1	D	595	ASP	CA-CB-CG	5.39	117.99	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	THR	CA-C-N	-5.38	117.46	123.16
1	B	168	THR	C-N-CA	-5.38	117.46	123.16
1	C	366	PRO	N-CA-CB	5.38	108.33	103.33
1	D	206	PHE	CA-CB-CG	-5.37	108.43	113.80
1	D	658	PRO	N-CA-CB	5.37	108.88	103.25
1	B	330	ASP	CB-CA-C	-5.36	104.58	111.50
1	B	585	ASP	CA-C-N	5.36	125.69	119.47
1	B	585	ASP	C-N-CA	5.36	125.69	119.47
1	D	32	GLU	N-CA-C	-5.36	101.92	109.96
1	D	314	ASP	CA-C-N	5.35	125.44	119.87
1	D	314	ASP	C-N-CA	5.35	125.44	119.87
1	C	407	LEU	N-CA-C	-5.35	104.87	111.40
1	C	168	THR	N-CA-C	-5.35	101.51	109.96
1	B	425	GLY	CA-C-N	5.34	125.81	120.04
1	B	425	GLY	C-N-CA	5.34	125.81	120.04
1	B	101	GLY	CA-C-N	5.34	125.10	119.76
1	B	101	GLY	C-N-CA	5.34	125.10	119.76
1	D	751	ILE	CA-C-O	5.33	127.09	119.95
1	A	332	PRO	N-CA-CB	5.33	107.91	103.17
1	D	332	PRO	N-CA-CB	5.31	107.89	103.17
1	A	121	ARG	CD-NE-CZ	5.31	131.83	124.40
1	C	263	PRO	N-CA-CB	5.30	108.03	103.31
1	A	344	GLU	CA-CB-CG	5.30	124.70	114.10
1	B	636	ARG	CA-C-O	-5.29	115.61	121.33
1	C	674	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	377	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	C	405	ASP	CA-C-N	5.28	124.89	119.56
1	C	405	ASP	C-N-CA	5.28	124.89	119.56
1	A	446	ASP	N-CA-C	5.28	115.81	108.00
1	B	504	TYR	N-CA-C	5.28	121.46	114.12
1	B	62	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	52	PRO	N-CA-CB	5.27	107.88	103.25
1	B	38	PRO	N-CA-CB	5.26	108.23	103.33
1	B	456	ASN	CA-C-O	5.26	124.70	119.75
1	D	177	ASP	N-CA-C	5.26	118.16	111.69
1	D	330	ASP	CB-CA-C	-5.23	104.50	111.88
1	C	82	THR	N-CA-C	-5.23	103.13	110.35
1	D	594	PRO	N-CA-CB	5.23	107.85	103.25
1	A	615	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	283	GLU	CB-CG-CD	5.20	121.44	112.60
1	C	194	GLY	N-CA-C	5.20	117.33	112.08
1	B	52	PRO	N-CA-CB	5.19	107.82	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	GLY	N-CA-C	-5.19	106.20	112.48
1	C	456	ASN	CA-C-O	5.18	124.06	119.71
1	C	171	GLY	N-CA-C	5.18	119.17	112.54
1	A	425	GLY	CA-C-N	5.18	125.64	120.04
1	A	425	GLY	C-N-CA	5.18	125.64	120.04
1	B	121	ARG	N-CA-C	5.18	118.38	110.20
1	B	576	PRO	CA-C-N	5.17	125.07	119.85
1	B	576	PRO	C-N-CA	5.17	125.07	119.85
1	A	42	PRO	N-CA-CB	5.17	107.92	103.27
1	A	479	ARG	CD-NE-CZ	5.17	131.63	124.40
1	D	355	ASP	CA-C-N	5.16	125.24	119.87
1	D	355	ASP	C-N-CA	5.16	125.24	119.87
1	B	49	PRO	N-CA-CB	5.16	108.14	103.34
1	C	597	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	750	LYS	CA-C-N	-5.15	118.88	122.59
1	C	750	LYS	C-N-CA	-5.15	118.88	122.59
1	D	691	HIS	CA-C-N	5.14	129.86	122.40
1	D	691	HIS	C-N-CA	5.14	129.86	122.40
1	B	403	THR	N-CA-CB	5.14	119.89	111.31
1	C	498	SER	CA-C-N	5.13	125.17	119.32
1	C	498	SER	C-N-CA	5.13	125.17	119.32
1	D	586	PRO	N-CA-CB	5.13	108.61	103.48
1	B	82	THR	N-CA-C	-5.13	103.72	110.33
1	D	169	VAL	CB-CA-C	-5.12	107.36	111.71
1	D	116	HIS	CA-CB-CG	-5.11	108.69	113.80
1	C	214	PHE	CA-C-N	5.11	124.72	119.05
1	C	214	PHE	C-N-CA	5.11	124.72	119.05
1	A	155	ASP	CA-CB-CG	5.10	117.70	112.60
1	C	355	ASP	CA-C-O	5.10	123.09	119.32
1	D	98	GLY	N-CA-C	-5.10	105.34	112.18
1	B	156	PRO	N-CA-CB	5.10	108.58	103.48
1	B	504	TYR	N-CA-CB	-5.09	103.85	110.88
1	C	608	ASN	CA-C-O	-5.08	115.59	121.49
1	D	199	VAL	N-CA-C	5.08	114.50	106.32
1	D	437	THR	N-CA-C	-5.07	106.94	113.23
1	A	236	HIS	CA-CB-CG	5.07	118.87	113.80
1	B	521	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	D	199	VAL	N-CA-CB	-5.06	106.62	111.89
1	D	247	PRO	N-CA-CB	5.05	108.53	103.48
1	C	42	PRO	N-CA-CB	5.05	107.66	103.17
1	C	594	PRO	N-CA-CB	5.04	107.73	103.19
1	A	586	PRO	N-CA-CB	5.04	108.52	103.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	394	GLY	O-C-N	-5.04	116.99	122.68
1	B	123	PRO	N-CA-CB	5.03	107.79	103.31
1	D	262	ILE	CA-C-N	5.03	124.96	119.78
1	D	262	ILE	C-N-CA	5.03	124.96	119.78
1	A	82	THR	N-CA-C	-5.03	103.41	110.35
1	D	33	ASP	N-CA-CB	5.03	118.98	110.49
1	A	157	ASN	CA-CB-CG	-5.03	107.57	112.60
1	A	37	ARG	CA-C-N	5.02	124.93	119.76
1	A	37	ARG	C-N-CA	5.02	124.93	119.76
1	A	49	PRO	N-CA-CB	5.02	107.72	103.35
1	C	694	PRO	N-CA-CB	5.02	107.71	103.19
1	B	57	ALA	CA-C-N	5.02	124.63	119.56
1	B	57	ALA	C-N-CA	5.02	124.63	119.56
1	B	161	PRO	N-CA-CB	5.01	107.71	103.35
1	B	263	PRO	N-CA-CB	5.00	107.76	103.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	726	GLY	Mainchain

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	5743	0	5577	77	0
1	B	5743	0	5577	84	0
1	C	5743	0	5577	84	0
1	D	5743	0	5577	92	0
2	A	44	0	31	7	0
2	B	44	0	31	5	0
2	C	44	0	31	5	0
2	D	44	0	31	4	0
3	A	731	0	0	6	0
3	B	655	0	0	4	0
3	C	704	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	724	0	0	10	0
All	All	25962	0	22432	324	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 7.

All (324) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:HIS:ND1	1:B:415:TYR:HB2	1.13	1.42
1:D:392:HIS:ND1	1:D:415:TYR:HB2	1.12	1.38
1:C:392:HIS:ND1	1:C:415:TYR:HB2	1.09	1.38
1:A:392:HIS:ND1	1:A:415:TYR:HB2	1.09	1.37
1:B:392:HIS:ND1	1:B:415:TYR:CB	2.05	1.19
1:A:392:HIS:ND1	1:A:415:TYR:CB	2.06	1.18
1:D:392:HIS:ND1	1:D:415:TYR:CB	2.06	1.17
1:C:392:HIS:ND1	1:C:415:TYR:CB	2.06	1.16
2:B:760:HDD:HBC1	2:B:760:HDD:HMC1	1.33	1.07
1:B:451:MET:HE2	1:D:451:MET:HE2	1.39	1.05
1:A:451:MET:HE2	1:C:451:MET:HE2	1.35	1.03
1:C:274:ILE:HD12	2:C:760:HDD:HMB1	1.56	0.87
1:D:392:HIS:CE1	1:D:415:TYR:HB2	2.11	0.85
1:B:392:HIS:CE1	1:B:415:TYR:HB2	2.11	0.85
2:A:760:HDD:HBC1	2:A:760:HDD:HMC1	1.56	0.85
1:D:750:LYS:HD3	1:D:751:ILE:H	1.50	0.76
2:C:760:HDD:HMC1	2:C:760:HDD:HBC1	1.68	0.74
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.52	0.73
1:A:392:HIS:CE1	1:A:415:TYR:HB2	2.16	0.73
2:B:760:HDD:HBC1	2:B:760:HDD:CMC	2.13	0.72
1:B:267:ARG:HG3	3:B:1240:HOH:O	1.88	0.72
1:C:392:HIS:CE1	1:C:415:TYR:HB2	2.14	0.71
1:A:392:HIS:CG	1:A:415:TYR:HB2	2.19	0.71
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.18	0.70
1:C:137:TYR:HB2	1:C:159:ILE:HD13	1.73	0.70
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.72	0.70
1:C:477:PRO:HB2	1:C:478:LYS:HD3	1.74	0.69
1:A:556:GLN:HG3	1:A:566:LEU:HD12	1.75	0.69
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.76	0.67
1:A:274:ILE:HD12	2:A:760:HDD:HMB1	1.77	0.67
1:B:309:LYS:HG2	1:B:660:LEU:HD11	1.76	0.66
1:B:51:ALA:HB1	1:B:52:PRO:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:ALA:HB2	1:A:662:VAL:HG11	1.77	0.66
1:B:583:LYS:O	1:B:584:LYS:HB3	1.93	0.65
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.78	0.65
2:A:760:HDD:HMB1	2:A:760:HDD:HBB1	1.78	0.64
1:C:725:ASP:HA	1:C:728:PHE:HB3	1.80	0.64
2:A:760:HDD:HMC1	2:A:760:HDD:CBC	2.26	0.64
1:B:468:ASN:HD22	1:D:27:ASP:N	1.96	0.64
1:D:629:HIS:HD2	3:D:1117:HOH:O	1.81	0.64
1:A:546:GLN:HG3	3:A:1455:HOH:O	1.98	0.64
1:A:29:LEU:HB2	3:C:1365:HOH:O	1.98	0.63
1:B:416:THR:HG21	3:D:1401:HOH:O	1.99	0.63
1:C:267:ARG:HD3	3:C:1249:HOH:O	1.99	0.62
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.81	0.62
1:D:274:ILE:HD12	2:D:760:HDD:HMB1	1.80	0.62
1:C:624:LYS:HD3	3:C:1400:HOH:O	2.00	0.61
1:C:748:ILE:O	1:C:751:ILE:HG22	2.01	0.61
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.83	0.61
1:B:686:MET:HB3	1:B:751:ILE:HD11	1.83	0.60
1:D:267:ARG:HG3	3:D:1241:HOH:O	2.01	0.60
1:B:451:MET:CE	1:D:451:MET:HE2	2.26	0.59
1:B:583:LYS:H	1:B:583:LYS:CE	2.16	0.59
1:A:745:ILE:O	1:A:748:ILE:HG12	2.03	0.59
1:D:222:LYS:HB3	1:D:223:PRO:HD2	1.85	0.59
1:D:27:ASP:O	1:D:28:SER:HB2	2.02	0.59
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.18	0.58
1:D:321:GLU:HG3	3:D:1307:HOH:O	2.03	0.58
1:D:750:LYS:CD	1:D:751:ILE:H	2.17	0.58
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.84	0.57
1:A:52:PRO:HG3	3:C:1012:HOH:O	2.04	0.57
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.86	0.57
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.85	0.57
1:B:521:ARG:HH21	1:B:745:ILE:CG2	2.15	0.57
2:A:760:HDD:HBC1	2:A:760:HDD:CMC	2.29	0.57
1:B:274:ILE:HD12	2:B:760:HDD:HMB1	1.86	0.57
1:B:666:ILE:HG12	1:B:696:ALA:HB3	1.86	0.57
1:A:621:LYS:HE3	3:A:1486:HOH:O	2.04	0.57
1:B:83:ASN:HB3	1:D:429:HIS:CD2	2.40	0.56
3:B:955:HOH:O	1:D:52:PRO:HG3	2.05	0.56
1:D:32:GLU:O	1:D:33:ASP:HB3	2.04	0.56
1:D:744:ARG:HA	1:D:747:LYS:HD3	1.86	0.56
1:A:751:ILE:HD12	1:A:751:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:ILE:O	1:A:710:ILE:HB	2.05	0.56
1:A:556:GLN:HG3	1:A:566:LEU:CD1	2.34	0.56
1:D:745:ILE:O	1:D:748:ILE:HG12	2.06	0.56
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.88	0.56
1:A:679:GLY:HA3	1:D:750:LYS:O	2.06	0.55
1:C:299:LYS:HE3	1:C:595:ASP:OD1	2.07	0.55
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.35	0.54
2:A:760:HDD:HBB1	2:A:760:HDD:CMB	2.37	0.54
1:B:606:LEU:O	1:B:668:PRO:HD2	2.08	0.54
1:B:438:CYS:HB2	1:B:439:PRO:HD2	1.89	0.54
1:B:745:ILE:HB	1:B:746:PRO:HD3	1.89	0.54
1:C:323:TRP:CZ3	1:C:379:PRO:HD2	2.43	0.53
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.44	0.53
1:A:708:ILE:O	1:A:709:LYS:C	2.52	0.53
1:B:507:HIS:N	1:B:508:PRO:HD2	2.23	0.53
1:B:359:LEU:H	1:B:507:HIS:HD2	1.57	0.53
1:A:748:ILE:O	1:A:751:ILE:HG13	2.08	0.53
1:B:178:THR:HG21	1:B:310:LEU:HD23	1.90	0.52
1:C:435:ARG:HD3	3:C:1118:HOH:O	2.09	0.52
1:A:478:LYS:HG2	3:A:1246:HOH:O	2.09	0.52
1:A:28:SER:CB	1:D:245:LEU:HD22	2.40	0.52
1:B:583:LYS:H	1:B:583:LYS:HE2	1.75	0.52
1:C:584:LYS:HZ3	1:C:584:LYS:HB2	1.74	0.52
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.91	0.52
1:C:629:HIS:HD2	3:C:1079:HOH:O	1.92	0.52
1:D:640:VAL:HG23	1:D:648:LEU:HB2	1.91	0.52
1:C:222:LYS:HB3	1:C:223:PRO:HD2	1.91	0.52
1:D:41:GLU:CD	1:D:42:PRO:HD2	2.35	0.52
1:B:604:ALA:HB2	1:B:662:VAL:HG11	1.90	0.52
1:D:602:VAL:HG13	1:D:662:VAL:HA	1.90	0.52
1:A:706:ALA:O	1:A:709:LYS:HD2	2.10	0.51
1:C:599:LYS:HE2	3:C:1054:HOH:O	2.10	0.51
1:C:613:SER:HB3	1:C:643:ASP:OD1	2.10	0.51
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.19	0.51
1:C:265:SER:OG	1:C:267:ARG:HB2	2.10	0.51
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.92	0.51
1:B:469:TRP:CE3	1:B:471:ARG:HG3	2.45	0.51
1:C:51:ALA:HB1	1:C:52:PRO:HD2	1.91	0.51
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.91	0.51
1:A:104:LEU:HB3	3:A:900:HOH:O	2.11	0.51
1:C:183:ARG:HG2	3:C:1294:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:GLU:O	1:D:33:ASP:CB	2.59	0.51
1:C:195:ILE:HD11	1:C:436:PRO:HA	1.92	0.50
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.46	0.50
1:A:709:LYS:HE3	1:A:709:LYS:HA	1.93	0.50
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.47	0.50
1:C:535:VAL:O	1:C:537:PRO:HD3	2.11	0.50
1:C:751:ILE:HB	3:C:1357:HOH:O	2.10	0.50
1:B:52:PRO:HG3	3:D:1050:HOH:O	2.11	0.50
1:C:556:GLN:NE2	3:C:1394:HOH:O	2.44	0.50
1:A:222:LYS:HB3	1:A:223:PRO:HD2	1.94	0.49
1:A:596:GLY:HA3	1:A:737:ALA:O	2.12	0.49
1:D:27:ASP:O	1:D:28:SER:CB	2.60	0.49
1:A:457:PRO:HG2	1:C:37:ARG:HH21	1.77	0.49
1:A:27:ASP:O	1:A:28:SER:C	2.55	0.49
1:A:267:ARG:HG2	1:A:332:PRO:HB3	1.94	0.49
1:A:586:PRO:HB2	1:A:593:ILE:HD11	1.95	0.49
1:B:36:HIS:HD1	1:B:36:HIS:H	1.59	0.49
1:B:128:HIS:HA	1:B:168:THR:O	2.13	0.49
1:D:666:ILE:HG12	1:D:696:ALA:HB3	1.94	0.49
1:A:710:ILE:HD11	1:A:747:LYS:HB3	1.94	0.49
1:B:700:ASP:O	1:B:703:LYS:HD3	2.12	0.49
1:D:359:LEU:H	1:D:507:HIS:HD2	1.61	0.49
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.95	0.49
1:B:535:VAL:O	1:B:537:PRO:HD3	2.13	0.49
1:B:271:GLY:HA3	1:B:293:TRP:HB2	1.95	0.49
1:B:748:ILE:O	1:B:751:ILE:HG22	2.12	0.49
1:A:619:ILE:HA	1:A:729:MET:HE2	1.95	0.48
1:C:404:ASN:O	1:C:405:ASP:C	2.54	0.48
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.95	0.48
1:A:28:SER:HB2	1:D:245:LEU:HD13	1.94	0.48
1:D:214:PHE:HB3	1:D:215:PRO:HD3	1.94	0.48
1:C:739:HIS:CD2	1:C:740:ARG:HG2	2.49	0.48
1:D:607:LEU:HD13	1:D:640:VAL:HG21	1.94	0.48
1:B:359:LEU:H	1:B:507:HIS:CD2	2.31	0.48
1:B:637:MET:HB2	1:C:562:LEU:HA	1.96	0.48
1:D:549:HIS:O	1:D:576:PRO:HD3	2.14	0.48
1:B:629:HIS:HD2	3:B:1022:HOH:O	1.95	0.48
1:C:490:GLU:HA	1:D:489:VAL:O	2.14	0.48
1:D:604:ALA:HB2	1:D:662:VAL:HG11	1.95	0.48
1:D:146:ASP:HB2	3:D:1382:HOH:O	2.14	0.47
1:C:305:ASP:O	1:C:309:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:HIS:N	1:B:508:PRO:CD	2.77	0.47
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.15	0.47
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.45	0.46
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.50	0.46
1:D:411:ARG:HG2	2:D:760:HDD:C2C	2.45	0.46
1:C:309:LYS:HB3	1:C:660:LEU:HD21	1.98	0.46
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.97	0.46
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.51	0.46
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.43	0.46
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.31	0.46
1:C:583:LYS:O	1:C:584:LYS:HB3	2.15	0.46
1:C:671:ASN:HD21	1:C:673:ALA:HB3	1.80	0.46
1:D:535:VAL:O	1:D:537:PRO:HD3	2.14	0.46
1:B:602:VAL:HG22	1:B:629:HIS:HB2	1.98	0.46
1:B:461:GLU:HA	1:B:462:PRO:C	2.40	0.46
1:D:37:ARG:HB3	3:D:1462:HOH:O	2.15	0.46
1:B:634:TYR:O	1:B:653:THR:HA	2.15	0.46
1:D:338:PHE:HB3	1:D:340:LEU:HD13	1.97	0.46
1:A:426:PRO:HB2	1:C:116:HIS:CD2	2.51	0.46
1:B:473:THR:O	1:D:89:ALA:HA	2.16	0.46
1:A:330:ASP:OD2	1:A:599:LYS:NZ	2.48	0.46
1:D:507:HIS:N	1:D:508:PRO:HD2	2.31	0.46
1:D:624:LYS:HD3	1:D:624:LYS:C	2.41	0.46
1:B:139:GLN:HA	1:B:140:PRO:HD3	1.76	0.45
1:C:178:THR:HG21	1:C:310:LEU:HD23	1.97	0.45
1:C:359:LEU:H	1:C:507:HIS:CD2	2.34	0.45
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.98	0.45
1:D:574:THR:HG22	3:D:1165:HOH:O	2.15	0.45
1:A:457:PRO:HG2	1:C:37:ARG:NH2	2.30	0.45
1:B:344:GLU:CD	1:B:344:GLU:H	2.23	0.45
2:B:760:HDD:HMB1	2:B:760:HDD:HBB1	1.98	0.45
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.32	0.45
1:B:702:ARG:O	1:B:705:LYS:HD3	2.16	0.45
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.51	0.45
1:C:296:LEU:HD12	1:C:333:GLU:HB3	1.99	0.45
1:C:459:ASN:H	1:C:459:ASN:HD22	1.64	0.45
1:C:626:LYS:HG3	1:C:733:LEU:HG	1.98	0.45
1:C:159:ILE:HD12	1:C:159:ILE:C	2.42	0.45
1:A:713:GLN:NE2	3:A:1437:HOH:O	2.49	0.45
1:D:341:ILE:HD11	1:D:360:ILE:HD13	1.97	0.45
1:B:222:LYS:HB3	1:B:223:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.99	0.45
1:C:593:ILE:HA	1:C:594:PRO:HD2	1.73	0.45
1:C:704:PHE:O	1:C:707:THR:HG22	2.18	0.45
1:A:516:THR:HB	1:A:517:PRO:HD2	1.98	0.44
2:C:760:HDD:HBD2	3:C:959:HOH:O	2.16	0.44
1:A:227:TRP:CZ3	1:D:50:THR:HG21	2.52	0.44
1:A:708:ILE:O	1:A:710:ILE:N	2.51	0.44
1:C:516:THR:HB	1:C:517:PRO:HD2	1.99	0.44
1:C:636:ARG:NH2	1:C:639:GLU:O	2.50	0.44
1:D:39:ALA:H	1:D:48:GLN:NE2	2.16	0.44
1:D:693:LYS:HA	1:D:694:PRO:HD3	1.84	0.44
1:A:105:LEU:HD11	1:C:413:PHE:HB2	1.98	0.44
1:A:36:HIS:CD2	1:A:36:HIS:H	2.36	0.44
1:C:127:VAL:O	1:C:128:HIS:HB2	2.18	0.44
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.48	0.44
1:D:97:ALA:O	1:D:101:GLY:HA3	2.18	0.44
1:B:211:ALA:HB3	1:B:410:GLY:HA3	2.00	0.44
1:D:289:VAL:HA	1:D:339:GLN:O	2.18	0.44
1:B:368:GLN:O	1:B:370:VAL:HG23	2.18	0.44
1:C:28:SER:HA	3:C:1439:HOH:O	2.18	0.43
1:B:205:ILE:HD13	1:B:205:ILE:H	1.83	0.43
1:B:459:ASN:HD22	1:B:459:ASN:H	1.66	0.43
1:C:27:ASP:HB3	3:C:1391:HOH:O	2.17	0.43
1:C:705:LYS:HB3	1:C:710:ILE:HB	1.99	0.43
1:A:752:PRO:HB2	1:D:686:MET:SD	2.58	0.43
1:C:330:ASP:OD1	1:C:629:HIS:HE1	2.01	0.43
1:C:538:TYR:O	1:C:542:ARG:HG3	2.19	0.43
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.34	0.43
1:B:443:PHE:CE2	1:B:470:PRO:HD2	2.53	0.43
1:A:578:ASP:HB3	1:A:582:LEU:O	2.18	0.43
1:D:507:HIS:N	1:D:508:PRO:CD	2.81	0.43
1:D:748:ILE:O	1:D:751:ILE:HG22	2.17	0.43
1:A:211:ALA:HB3	1:A:410:GLY:HA3	2.00	0.43
1:C:331:PHE:HA	1:C:332:PRO:HD3	1.84	0.43
1:B:562:LEU:HA	1:C:637:MET:HB2	1.99	0.43
1:C:397:VAL:HB	1:C:398:PRO:HD2	2.00	0.43
1:A:429:HIS:CG	1:C:83:ASN:HB3	2.53	0.43
1:A:335:GLU:OE1	1:A:369:ARG:HG2	2.19	0.43
1:A:535:VAL:O	1:A:537:PRO:HD3	2.19	0.43
1:B:364:LEU:HD11	1:B:580:ASN:HB2	2.01	0.43
1:B:516:THR:HB	1:B:517:PRO:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:LEU:H	1:D:507:HIS:CD2	2.36	0.43
1:B:207:PHE:O	1:B:249:THR:HA	2.19	0.42
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.34	0.42
1:A:260:ARG:HD3	1:A:590:LEU:HD21	2.00	0.42
2:C:760:HDD:HMD3	2:C:760:HDD:HAD2	1.70	0.42
1:D:267:ARG:NH1	1:D:321:GLU:OE2	2.50	0.42
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.27	0.42
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.48	0.42
1:B:603:VAL:HG11	1:B:666:ILE:HD12	2.02	0.42
1:A:498:SER:HA	1:A:499:PRO:HD3	1.88	0.42
1:C:693:LYS:HA	1:C:694:PRO:HD3	1.95	0.42
1:D:392:HIS:HB3	1:D:395:HIS:CE1	2.55	0.42
1:A:207:PHE:O	1:A:249:THR:HA	2.19	0.42
1:A:461:GLU:HA	1:A:462:PRO:C	2.44	0.42
1:D:404:ASN:O	1:D:405:ASP:C	2.62	0.42
2:B:760:HDD:HBB1	2:B:760:HDD:CMB	2.49	0.42
1:C:125:ARG:HB3	2:C:760:HDD:HBD1	2.01	0.42
1:D:155:ASP:HA	1:D:156:PRO:HD2	1.90	0.42
1:B:309:LYS:NZ	1:B:687:GLU:OE2	2.50	0.42
1:C:461:GLU:HA	1:C:462:PRO:C	2.45	0.42
1:D:125:ARG:HB3	2:D:760:HDD:HBD1	2.02	0.42
1:D:332:PRO:HD2	1:D:375:LEU:O	2.20	0.42
1:A:606:LEU:HD22	1:A:654:PHE:CE2	2.55	0.42
1:A:693:LYS:HA	1:A:694:PRO:HD3	1.83	0.42
1:B:27:ASP:HB3	3:B:1386:HOH:O	2.19	0.42
1:C:610:GLU:HG3	1:C:610:GLU:O	2.20	0.42
1:C:740:ARG:HB2	1:C:742:TRP:CH2	2.54	0.42
1:D:438:CYS:HB2	1:D:439:PRO:HD2	2.00	0.42
1:D:669:CYS:SG	3:D:1450:HOH:O	2.45	0.42
1:A:144:LEU:HD11	1:A:370:VAL:HG13	2.01	0.42
1:A:479:ARG:NH2	3:A:1449:HOH:O	2.47	0.42
1:D:539:ILE:O	1:D:543:VAL:HG23	2.20	0.42
1:D:732:LEU:C	1:D:732:LEU:HD13	2.44	0.42
1:D:745:ILE:N	1:D:746:PRO:HD2	2.34	0.42
1:A:435:ARG:HA	1:A:436:PRO:HD3	1.88	0.41
1:A:612:ARG:HH11	1:A:669:CYS:CB	2.33	0.41
1:B:235:ALA:HB1	1:B:533:LYS:HD3	2.01	0.41
1:C:359:LEU:H	1:C:507:HIS:HD2	1.67	0.41
1:D:415:TYR:O	1:D:419:GLN:OE1	2.37	0.41
1:A:461:GLU:HB2	1:A:462:PRO:HA	2.01	0.41
1:A:634:TYR:O	1:A:653:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:PHE:HB3	1:B:215:PRO:HD3	2.03	0.41
1:D:27:ASP:N	3:D:861:HOH:O	2.53	0.41
1:A:459:ASN:HD22	1:A:460:TYR:HD2	1.68	0.41
1:C:214:PHE:HB3	1:C:215:PRO:HD3	2.01	0.41
1:C:214:PHE:N	1:C:215:PRO:CD	2.82	0.41
1:A:552:LEU:HD21	1:A:571:LEU:O	2.19	0.41
1:B:516:THR:HB	1:B:517:PRO:HD2	2.01	0.41
1:D:438:CYS:HB2	1:D:439:PRO:CD	2.51	0.41
1:A:593:ILE:HA	1:A:594:PRO:HD2	1.94	0.41
1:B:31:PRO:HB2	1:B:33:ASP:OD1	2.21	0.41
1:D:207:PHE:O	1:D:249:THR:HA	2.21	0.41
1:B:267:ARG:HD3	1:B:332:PRO:HG3	2.02	0.41
1:D:358:LYS:HD2	1:D:507:HIS:CE1	2.56	0.41
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.56	0.41
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.55	0.41
1:B:65:LEU:HD21	1:B:135:HIS:CG	2.56	0.41
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.50	0.41
1:C:76:GLU:O	1:C:77:ASN:HB2	2.21	0.41
1:C:203:THR:HB	1:C:204:PRO:HD2	2.02	0.41
1:A:404:ASN:O	1:A:405:ASP:C	2.64	0.41
1:B:39:ALA:HB1	1:B:41:GLU:HG2	2.03	0.41
1:B:413:PHE:HB2	1:D:105:LEU:HD11	2.02	0.41
1:C:584:LYS:HB2	1:C:584:LYS:NZ	2.34	0.41
1:D:568:ASP:HA	1:D:571:LEU:HD12	2.02	0.41
1:A:426:PRO:HG3	1:C:119:HIS:HB2	2.02	0.41
1:C:38:PRO:HG2	1:C:51:ALA:HB2	2.03	0.41
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.56	0.41
1:D:260:ARG:HD3	1:D:590:LEU:HD21	2.02	0.41
1:D:331:PHE:O	1:D:333:GLU:HG3	2.20	0.41
1:D:744:ARG:O	1:D:748:ILE:HG23	2.21	0.41
1:B:202:ASN:HA	1:B:270:GLU:O	2.21	0.41
1:D:252:ASN:HD22	1:D:252:ASN:HA	1.69	0.41
1:B:512:TRP:CH2	1:B:520:GLN:HB3	2.57	0.40
1:C:160:THR:HA	1:C:161:PRO:HD3	1.96	0.40
1:C:323:TRP:CH2	1:C:378:ASN:HB3	2.56	0.40
1:D:596:GLY:HA3	1:D:737:ALA:O	2.21	0.40
1:B:48:GLN:HB3	1:B:49:PRO:HD2	2.02	0.40
1:B:615:ASP:O	1:B:619:ILE:HG13	2.20	0.40
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.67	0.40
1:B:578:ASP:HB3	1:B:582:LEU:O	2.21	0.40
1:D:378:ASN:HB3	1:D:379:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:SER:OG	2:D:760:HDD:HHD	2.21	0.40
1:A:411:ARG:HG2	2:A:760:HDD:C2C	2.52	0.40
1:B:197:ASP:HB2	1:B:392:HIS:O	2.22	0.40
1:B:538:TYR:O	1:B:542:ARG:HG3	2.21	0.40
1:D:128:HIS:HA	1:D:168:THR:O	2.21	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	725/753 (96%)	697 (96%)	24 (3%)	4 (1%)	21	10
1	B	725/753 (96%)	697 (96%)	26 (4%)	2 (0%)	36	26
1	C	725/753 (96%)	699 (96%)	23 (3%)	3 (0%)	30	19
1	D	725/753 (96%)	700 (97%)	21 (3%)	4 (1%)	21	10
All	All	2900/3012 (96%)	2793 (96%)	94 (3%)	13 (0%)	30	19

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	709	LYS
1	A	711	ALA
1	D	28	SER
1	D	751	ILE
1	A	28	SER
1	C	75	SER
1	C	725	ASP
1	D	33	ASP
1	D	750	LYS
1	A	75	SER

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Mol	Chain	Res	Type
1	B	28	SER
1	B	75	SER
1	C	726	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	611/635 (96%)	598 (98%)	13 (2%)	47	33
1	B	611/635 (96%)	587 (96%)	24 (4%)	28	13
1	C	611/635 (96%)	582 (95%)	29 (5%)	23	9
1	D	611/635 (96%)	586 (96%)	25 (4%)	27	12
All	All	2444/2540 (96%)	2353 (96%)	91 (4%)	30	15

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	73	LYS
1	A	205	ILE
1	A	252	ASN
1	A	294	LYS
1	A	344	GLU
1	A	375	LEU
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	709	LYS
1	A	710	ILE
1	A	712	ASP
1	B	27	ASP
1	B	28	SER
1	B	127	VAL
1	B	198	LEU
1	B	205	ILE

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Mol	Chain	Res	Type
1	B	252	ASN
1	B	265	SER
1	B	283	GLU
1	B	344	GLU
1	B	375	LEU
1	B	377	ARG
1	B	440	TYR
1	B	459	ASN
1	B	562	LEU
1	B	565	GLU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	612	ARG
1	B	633	LEU
1	B	703	LYS
1	B	709	LYS
1	B	751	ILE
1	C	73	LYS
1	C	159	ILE
1	C	205	ILE
1	C	252	ASN
1	C	265	SER
1	C	267	ARG
1	C	283	GLU
1	C	375	LEU
1	C	377	ARG
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	531	LEU
1	C	552	LEU
1	C	571	LEU
1	C	584	LYS
1	C	602	VAL
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	617	LEU
1	C	633	LEU
1	C	635	SER

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Mol	Chain	Res	Type
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	715	GLU
1	C	733	LEU
1	C	750	LYS
1	D	41	GLU
1	D	73	LYS
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	340	LEU
1	D	344	GLU
1	D	375	LEU
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	598	VAL
1	D	616	LEU
1	D	631	LYS
1	D	640	VAL
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS
1	D	749	ASP
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	66	ASN
1	A	77	ASN
1	A	252	ASN
1	A	368	GLN
1	A	459	ASN
1	A	486	GLN

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Mol	Chain	Res	Type
1	A	515	GLN
1	A	556	GLN
1	A	671	ASN
1	A	713	GLN
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	368	GLN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	77	ASN
1	D	252	ASN
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN
1	D	556	GLN
1	D	629	HIS
1	D	682	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	HDD	C	760	1,3	49,52,52	2.88	18 (36%)	62,89,89	4.25	36 (58%)
2	HDD	B	760	1,3	49,52,52	2.90	21 (42%)	62,89,89	4.10	35 (56%)
2	HDD	D	760	1	49,52,52	3.03	19 (38%)	62,89,89	3.92	34 (54%)
2	HDD	A	760	1,3	49,52,52	3.00	20 (40%)	62,89,89	4.05	37 (59%)

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
2	HDD	B	760	1,3	-	2/9/89/89	0/1/9/9
2	HDD	A	760	1,3	-	2/9/89/89	0/1/9/9
2	HDD	D	760	1	-	4/9/89/89	0/1/9/9
2	HDD	C	760	1,3	1/1/8/14	4/9/89/89	0/1/9/9

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760	HDD	C3D-C2D	-11.76	1.27	1.55
2	C	760	HDD	C3D-C2D	-11.71	1.27	1.55
2	B	760	HDD	C3D-C2D	-11.69	1.27	1.55
2	A	760	HDD	C3D-C2D	-11.50	1.27	1.55
2	C	760	HDD	FE-NB	7.14	2.16	1.94
2	A	760	HDD	C1D-ND	7.12	1.40	1.35
2	D	760	HDD	CAD-C3D	6.33	1.64	1.53
2	A	760	HDD	O1D-C3D	6.27	1.56	1.46
2	D	760	HDD	C1D-ND	6.26	1.39	1.35
2	B	760	HDD	O1D-C3D	6.09	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HDD	FE-ND	6.08	2.13	1.94
2	D	760	HDD	O1D-C3D	5.91	1.56	1.46
2	C	760	HDD	O1D-C3D	5.48	1.55	1.46
2	B	760	HDD	FE-ND	5.45	2.11	1.94
2	A	760	HDD	OND-C2D	5.34	1.52	1.42
2	D	760	HDD	OND-C2D	5.24	1.52	1.42
2	C	760	HDD	C1D-ND	5.20	1.38	1.35
2	C	760	HDD	OND-C2D	5.19	1.52	1.42
2	B	760	HDD	OND-C2D	5.15	1.52	1.42
2	B	760	HDD	C1D-ND	4.99	1.38	1.35
2	A	760	HDD	FE-NB	4.92	2.10	1.94
2	D	760	HDD	FE-NA	4.34	2.09	1.95
2	C	760	HDD	FE-ND	4.33	2.08	1.94
2	D	760	HDD	FE-ND	4.28	2.08	1.94
2	D	760	HDD	FE-NC	4.27	2.09	1.95
2	B	760	HDD	FE-NC	4.23	2.09	1.95
2	B	760	HDD	FE-NA	3.90	2.08	1.95
2	A	760	HDD	C1B-NB	-3.66	1.33	1.40
2	D	760	HDD	C1B-NB	-3.59	1.34	1.40
2	B	760	HDD	C1B-NB	-3.47	1.34	1.40
2	D	760	HDD	O1D-CGD	-3.42	1.30	1.35
2	C	760	HDD	O1D-CGD	-3.38	1.30	1.35
2	B	760	HDD	O1D-CGD	-3.26	1.30	1.35
2	C	760	HDD	C1B-NB	-3.16	1.34	1.40
2	A	760	HDD	O1D-CGD	-3.06	1.30	1.35
2	D	760	HDD	CAB-C3B	2.99	1.55	1.47
2	B	760	HDD	CAB-C3B	2.87	1.55	1.47
2	A	760	HDD	CMB-C2B	2.85	1.56	1.50
2	C	760	HDD	FE-NA	2.75	2.04	1.95
2	A	760	HDD	FE-NA	2.73	2.04	1.95
2	C	760	HDD	CAB-C3B	2.72	1.54	1.47
2	D	760	HDD	C1A-C2A	2.71	1.50	1.44
2	A	760	HDD	FE-NC	2.66	2.03	1.95
2	B	760	HDD	CMB-C2B	2.63	1.56	1.50
2	A	760	HDD	C1A-C2A	2.62	1.49	1.44
2	C	760	HDD	CBA-CGA	2.55	1.56	1.50
2	B	760	HDD	CBA-CGA	2.51	1.56	1.50
2	A	760	HDD	CAB-C3B	2.50	1.54	1.47
2	A	760	HDD	CAC-C3C	2.48	1.54	1.47
2	B	760	HDD	CMC-C2C	2.48	1.55	1.50
2	D	760	HDD	C4A-C3A	2.45	1.48	1.43
2	C	760	HDD	CAC-C3C	2.43	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	760	HDD	C4A-C3A	2.38	1.48	1.43
2	C	760	HDD	CHA-C4D	2.38	1.44	1.37
2	A	760	HDD	CMC-C2C	2.37	1.55	1.50
2	B	760	HDD	CBA-CAA	2.37	1.60	1.51
2	C	760	HDD	C1A-C2A	2.37	1.49	1.44
2	D	760	HDD	CAC-C3C	2.35	1.53	1.47
2	B	760	HDD	C4A-C3A	2.34	1.48	1.43
2	B	760	HDD	C1A-C2A	2.33	1.49	1.44
2	B	760	HDD	CAD-C3D	2.33	1.57	1.53
2	B	760	HDD	CHA-C4D	2.32	1.43	1.37
2	A	760	HDD	C4A-C3A	2.29	1.48	1.43
2	C	760	HDD	CMB-C2B	2.29	1.55	1.50
2	B	760	HDD	CAC-C3C	2.29	1.53	1.47
2	A	760	HDD	CBA-CGA	2.25	1.55	1.50
2	D	760	HDD	CBA-CGA	2.20	1.55	1.50
2	D	760	HDD	CMC-C2C	2.19	1.55	1.50
2	A	760	HDD	CBA-CAA	2.19	1.59	1.51
2	A	760	HDD	C1B-C2B	2.17	1.48	1.44
2	C	760	HDD	C1B-C2B	2.17	1.48	1.44
2	A	760	HDD	CHA-C4D	2.15	1.43	1.37
2	C	760	HDD	CMC-C2C	2.13	1.55	1.50
2	D	760	HDD	CMA-C3A	2.12	1.55	1.50
2	B	760	HDD	C1B-C2B	2.11	1.48	1.44
2	B	760	HDD	C2A-C3A	-2.07	1.33	1.38
2	D	760	HDD	CHA-C4D	2.03	1.43	1.37
2	D	760	HDD	CBA-CAA	2.03	1.59	1.51

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HDD	C3B-C4B-NB	-13.91	99.48	109.47
2	A	760	HDD	C3B-C4B-NB	-13.63	99.68	109.47
2	C	760	HDD	C3B-C4B-NB	-13.44	99.81	109.47
2	D	760	HDD	C3B-C4B-NB	-12.82	100.26	109.47
2	C	760	HDD	OND-C2D-CMD	-10.33	89.48	109.45
2	A	760	HDD	C4B-C3B-C2B	9.97	116.45	107.28
2	C	760	HDD	C4B-C3B-C2B	9.95	116.42	107.28
2	B	760	HDD	C4B-C3B-C2B	9.61	116.11	107.28
2	C	760	HDD	C3D-O1D-CGD	8.89	119.43	111.14
2	D	760	HDD	CHC-C4B-NB	8.87	133.97	124.42
2	B	760	HDD	C3B-C2B-C1B	-8.86	99.76	106.41
2	A	760	HDD	C4C-CHD-C1D	-8.24	112.67	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	760	HDD	CHC-C4B-NB	8.18	133.22	124.42
2	A	760	HDD	C3B-C2B-C1B	-8.13	100.31	106.41
2	D	760	HDD	C4C-CHD-C1D	-8.11	112.89	125.99
2	C	760	HDD	CHD-C4C-NC	7.81	132.95	124.45
2	A	760	HDD	CHD-C4C-NC	7.77	132.92	124.45
2	C	760	HDD	C3B-C2B-C1B	-7.75	100.59	106.41
2	D	760	HDD	C3D-O1D-CGD	7.73	118.35	111.14
2	C	760	HDD	C4C-CHD-C1D	-7.66	113.62	125.99
2	B	760	HDD	CHC-C4B-NB	7.63	132.63	124.42
2	A	760	HDD	CHC-C4B-NB	7.62	132.62	124.42
2	B	760	HDD	C4C-CHD-C1D	-7.47	113.92	125.99
2	D	760	HDD	C3B-C2B-C1B	-7.47	100.80	106.41
2	D	760	HDD	C4B-C3B-C2B	6.82	113.55	107.28
2	A	760	HDD	C1B-NB-C4B	6.59	113.01	105.21
2	B	760	HDD	CHD-C4C-NC	6.27	131.28	124.45
2	A	760	HDD	O1D-CGD-CBD	-6.25	104.47	110.17
2	D	760	HDD	C1B-NB-C4B	6.23	112.59	105.21
2	B	760	HDD	C3D-O1D-CGD	6.16	116.88	111.14
2	C	760	HDD	C1B-NB-C4B	6.09	112.42	105.21
2	B	760	HDD	C1B-NB-C4B	6.06	112.38	105.21
2	A	760	HDD	OND-C2D-CMD	-6.00	97.86	109.45
2	D	760	HDD	CHD-C4C-NC	5.71	130.67	124.45
2	B	760	HDD	C2D-C1D-CHD	-5.70	114.30	123.28
2	B	760	HDD	CHD-C1D-ND	5.58	140.64	124.51
2	B	760	HDD	C2A-C1A-NA	-5.49	104.06	110.15
2	D	760	HDD	C4A-C3A-C2A	-5.42	100.61	106.82
2	D	760	HDD	C2A-C1A-NA	-5.36	104.21	110.15
2	B	760	HDD	CHC-C1C-NC	5.25	130.17	124.45
2	A	760	HDD	C4C-C3C-C2C	5.23	111.35	106.81
2	C	760	HDD	C2D-C1D-CHD	-5.23	115.05	123.28
2	D	760	HDD	OND-C2D-CMD	-5.15	99.49	109.45
2	B	760	HDD	OND-C2D-CMD	-5.11	99.57	109.45
2	C	760	HDD	C2A-C1A-NA	-5.09	104.51	110.15
2	D	760	HDD	O2A-CGA-O1A	5.05	136.32	123.33
2	B	760	HDD	C1A-C2A-C3A	4.85	114.37	106.87
2	B	760	HDD	O2A-CGA-O1A	4.84	135.78	123.33
2	B	760	HDD	C4C-C3C-C2C	4.77	110.95	106.81
2	A	760	HDD	CMD-C2D-C3D	4.66	127.37	115.11
2	B	760	HDD	CHB-C1B-NB	4.58	130.04	124.37
2	C	760	HDD	CHD-C1D-ND	4.56	137.68	124.51
2	D	760	HDD	O1A-CGA-CBA	-4.56	108.63	123.09
2	A	760	HDD	C2A-C1A-NA	-4.54	105.11	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	760	HDD	CHC-C1C-NC	4.51	129.37	124.45
2	D	760	HDD	C1A-CHA-C4D	4.51	134.18	125.87
2	B	760	HDD	CAA-CBA-CGA	-4.49	101.75	113.67
2	D	760	HDD	C4C-C3C-C2C	4.41	110.64	106.81
2	D	760	HDD	C2D-C1D-CHD	-4.40	116.36	123.28
2	B	760	HDD	C4A-C3A-C2A	-4.33	101.86	106.82
2	A	760	HDD	CHD-C1D-ND	4.31	136.95	124.51
2	C	760	HDD	CAC-C3C-C4C	-4.29	114.59	124.82
2	C	760	HDD	C1A-C2A-C3A	4.28	113.50	106.87
2	C	760	HDD	C4C-C3C-C2C	4.26	110.51	106.81
2	B	760	HDD	O1A-CGA-CBA	-4.25	109.61	123.09
2	C	760	HDD	CBD-CAD-C3D	4.24	110.03	103.98
2	B	760	HDD	O1D-C3D-CAD	-4.24	95.22	103.06
2	A	760	HDD	CHC-C1C-NC	4.21	129.03	124.45
2	D	760	HDD	O1D-C3D-CAD	-4.20	95.29	103.06
2	A	760	HDD	C1A-C2A-C3A	4.18	113.33	106.87
2	C	760	HDD	O1D-C3D-CAD	-4.08	95.52	103.06
2	C	760	HDD	C4D-ND-C1D	3.91	109.85	105.27
2	D	760	HDD	C1A-C2A-C3A	3.86	112.84	106.87
2	C	760	HDD	O1A-CGA-CBA	-3.83	110.95	123.09
2	A	760	HDD	C4A-CHB-C1B	-3.81	117.28	126.25
2	C	760	HDD	C1C-CHC-C4B	-3.81	117.93	126.02
2	A	760	HDD	C2D-C1D-CHD	-3.76	117.36	123.28
2	D	760	HDD	CAA-CBA-CGA	-3.75	103.71	113.67
2	D	760	HDD	CAC-C3C-C4C	-3.75	115.87	124.82
2	A	760	HDD	CAC-C3C-C4C	-3.70	115.99	124.82
2	A	760	HDD	C4A-C3A-C2A	-3.68	102.60	106.82
2	A	760	HDD	O1A-CGA-CBA	-3.67	111.47	123.09
2	C	760	HDD	C4A-C3A-C2A	-3.66	102.63	106.82
2	D	760	HDD	CHB-C1B-NB	3.58	128.79	124.37
2	A	760	HDD	CBD-CAD-C3D	-3.58	98.88	103.98
2	C	760	HDD	O1D-CGD-CBD	-3.53	106.95	110.17
2	B	760	HDD	C4D-ND-C1D	3.53	109.41	105.27
2	A	760	HDD	O2A-CGA-O1A	3.43	132.16	123.33
2	D	760	HDD	C4D-ND-C1D	3.39	109.25	105.27
2	A	760	HDD	CMC-C2C-C1C	3.35	130.62	124.73
2	C	760	HDD	CAA-CBA-CGA	-3.32	104.86	113.67
2	B	760	HDD	CAC-C3C-C4C	-3.30	116.93	124.82
2	C	760	HDD	CHB-C4A-NA	3.24	129.74	123.86
2	A	760	HDD	C3D-O1D-CGD	3.21	114.13	111.14
2	C	760	HDD	O2A-CGA-O1A	3.21	131.58	123.33
2	A	760	HDD	OND-C2D-C3D	-3.19	102.98	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HDD	CAA-CBA-CGA	-3.14	105.34	113.67
2	D	760	HDD	C4C-NC-C1C	3.12	110.91	105.82
2	A	760	HDD	C4C-NC-C1C	3.08	110.84	105.82
2	B	760	HDD	C1C-CHC-C4B	-3.06	119.51	126.02
2	C	760	HDD	C4C-NC-C1C	2.86	110.48	105.82
2	D	760	HDD	OND-C2D-C3D	-2.84	103.81	110.46
2	B	760	HDD	CMA-C3A-C2A	2.80	131.57	125.62
2	A	760	HDD	C1C-CHC-C4B	-2.80	120.07	126.02
2	C	760	HDD	CHB-C4A-C3A	-2.79	119.32	127.43
2	C	760	HDD	O1D-CGD-O2D	-2.79	118.46	120.81
2	D	760	HDD	CHD-C1D-ND	2.76	132.48	124.51
2	A	760	HDD	CBC-CAC-C3C	-2.73	113.88	127.53
2	D	760	HDD	CHA-C1A-C2A	2.73	131.26	125.30
2	D	760	HDD	C4A-CHB-C1B	-2.72	119.85	126.25
2	D	760	HDD	C1C-CHC-C4B	-2.71	120.26	126.02
2	B	760	HDD	CMD-C2D-C3D	2.63	122.02	115.11
2	C	760	HDD	CHA-C1A-NA	2.62	128.60	123.86
2	B	760	HDD	CBC-CAC-C3C	-2.60	114.51	127.53
2	B	760	HDD	C4A-CHB-C1B	-2.56	120.23	126.25
2	D	760	HDD	CMB-C2B-C1B	2.55	129.01	125.03
2	B	760	HDD	C4C-NC-C1C	2.48	109.87	105.82
2	D	760	HDD	CBC-CAC-C3C	-2.45	115.27	127.53
2	A	760	HDD	O1D-C3D-CAD	-2.45	98.52	103.06
2	B	760	HDD	CHB-C1B-C2B	-2.42	120.08	126.95
2	C	760	HDD	CHC-C1C-NC	2.41	127.07	124.45
2	C	760	HDD	CMA-C3A-C2A	2.40	130.70	125.62
2	C	760	HDD	CHB-C1B-NB	2.38	127.31	124.37
2	C	760	HDD	CBC-CAC-C3C	-2.36	115.74	127.53
2	C	760	HDD	C4A-CHB-C1B	-2.35	120.72	126.25
2	A	760	HDD	CAA-C2A-C1A	-2.35	120.36	124.94
2	C	760	HDD	CAB-C3B-C4B	-2.28	114.30	124.39
2	B	760	HDD	C3C-C2C-C1C	-2.27	104.89	107.05
2	A	760	HDD	C4D-ND-C1D	2.27	107.93	105.27
2	A	760	HDD	CHA-C1A-NA	2.25	127.93	123.86
2	D	760	HDD	CBD-CAD-C3D	2.24	107.18	103.98
2	B	760	HDD	O1D-CGD-CBD	-2.24	108.13	110.17
2	A	760	HDD	CHD-C4C-C3C	-2.22	121.47	125.21
2	B	760	HDD	CAA-C2A-C1A	-2.19	120.66	124.94
2	A	760	HDD	C3C-C2C-C1C	-2.18	104.98	107.05
2	D	760	HDD	CAB-C3B-C4B	-2.17	114.78	124.39
2	D	760	HDD	CHB-C1B-C2B	-2.16	120.81	126.95
2	C	760	HDD	CHD-C4C-C3C	-2.10	121.66	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HDD	CMA-C3A-C2A	2.10	130.07	125.62
2	B	760	HDD	CMC-C2C-C1C	2.08	128.39	124.73
2	A	760	HDD	CHB-C1B-C2B	-2.05	121.12	126.95
2	B	760	HDD	OND-C2D-C3D	-2.03	105.70	110.46

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	760	HDD	NC

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	760	HDD	C2B-C3B-CAB-CBB
2	D	760	HDD	C2C-C3C-CAC-CBC
2	C	760	HDD	C4B-C3B-CAB-CBB
2	D	760	HDD	C4B-C3B-CAB-CBB
2	C	760	HDD	CAA-CBA-CGA-O1A
2	B	760	HDD	CAA-CBA-CGA-O1A
2	A	760	HDD	CAA-CBA-CGA-O1A
2	D	760	HDD	CAA-CBA-CGA-O1A
2	D	760	HDD	CAA-CBA-CGA-O2A
2	A	760	HDD	CAA-CBA-CGA-O2A
2	B	760	HDD	CAA-CBA-CGA-O2A
2	C	760	HDD	CAA-CBA-CGA-O2A

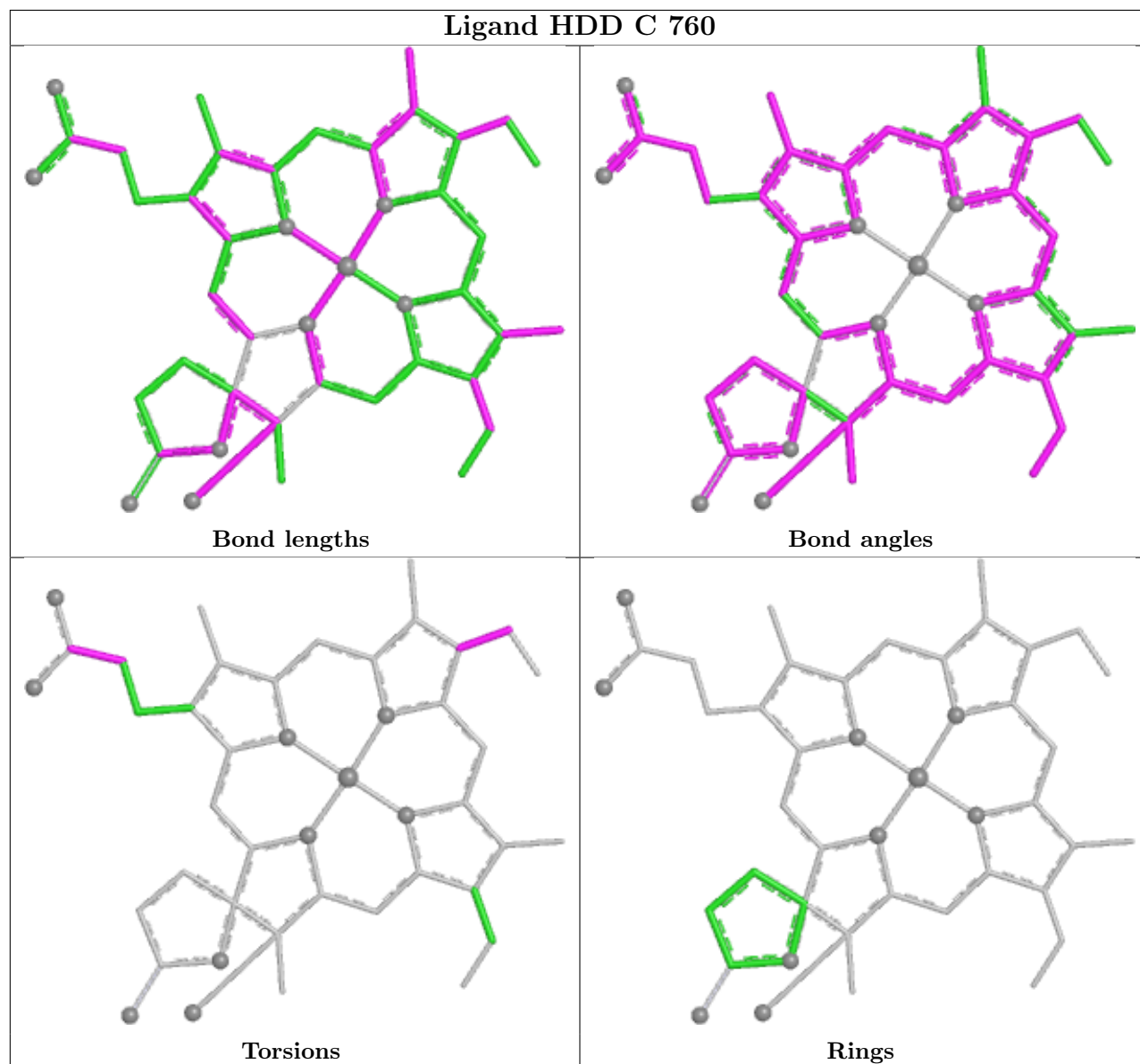
There are no ring outliers.

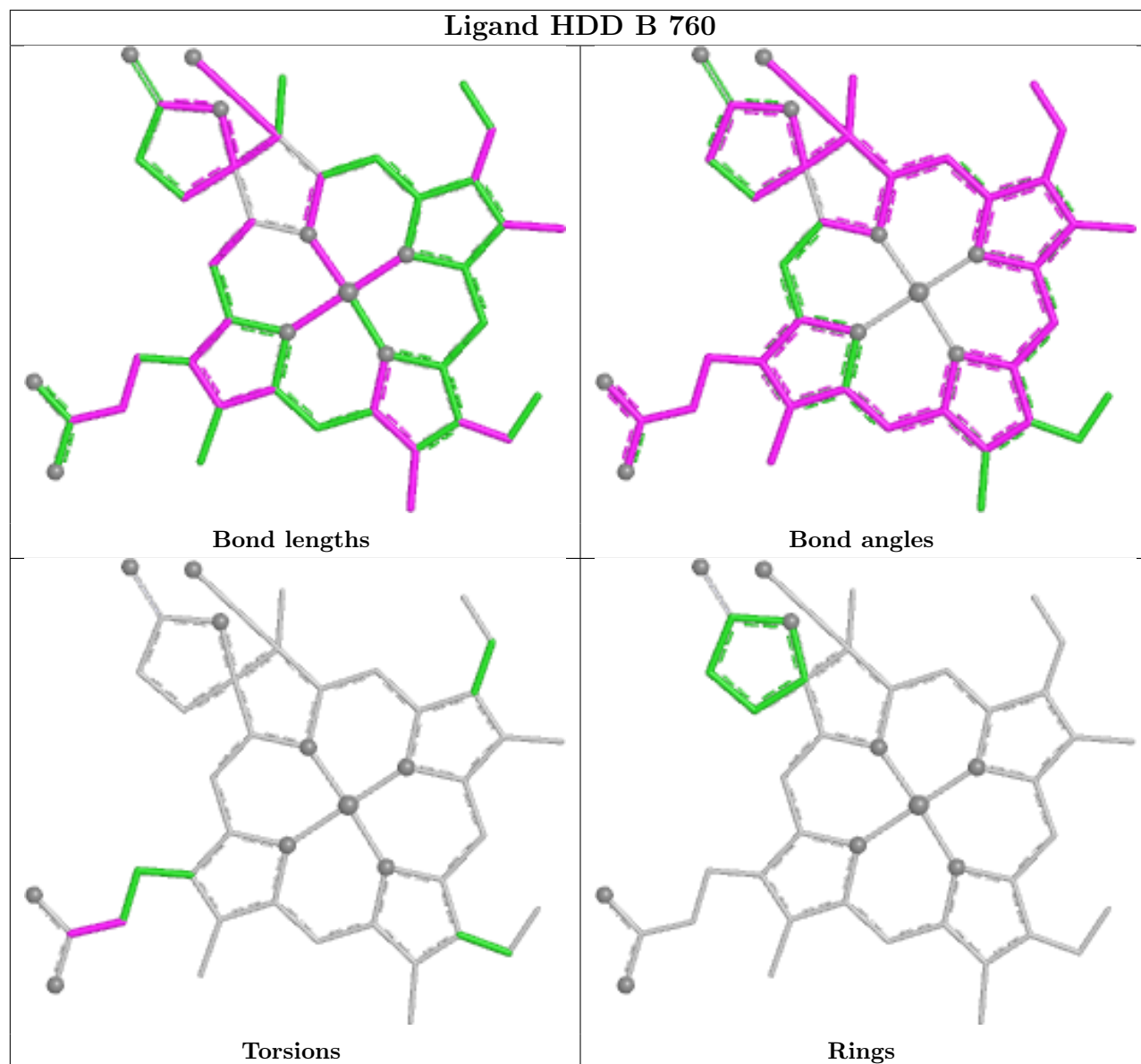
4 monomers are involved in 21 short contacts:

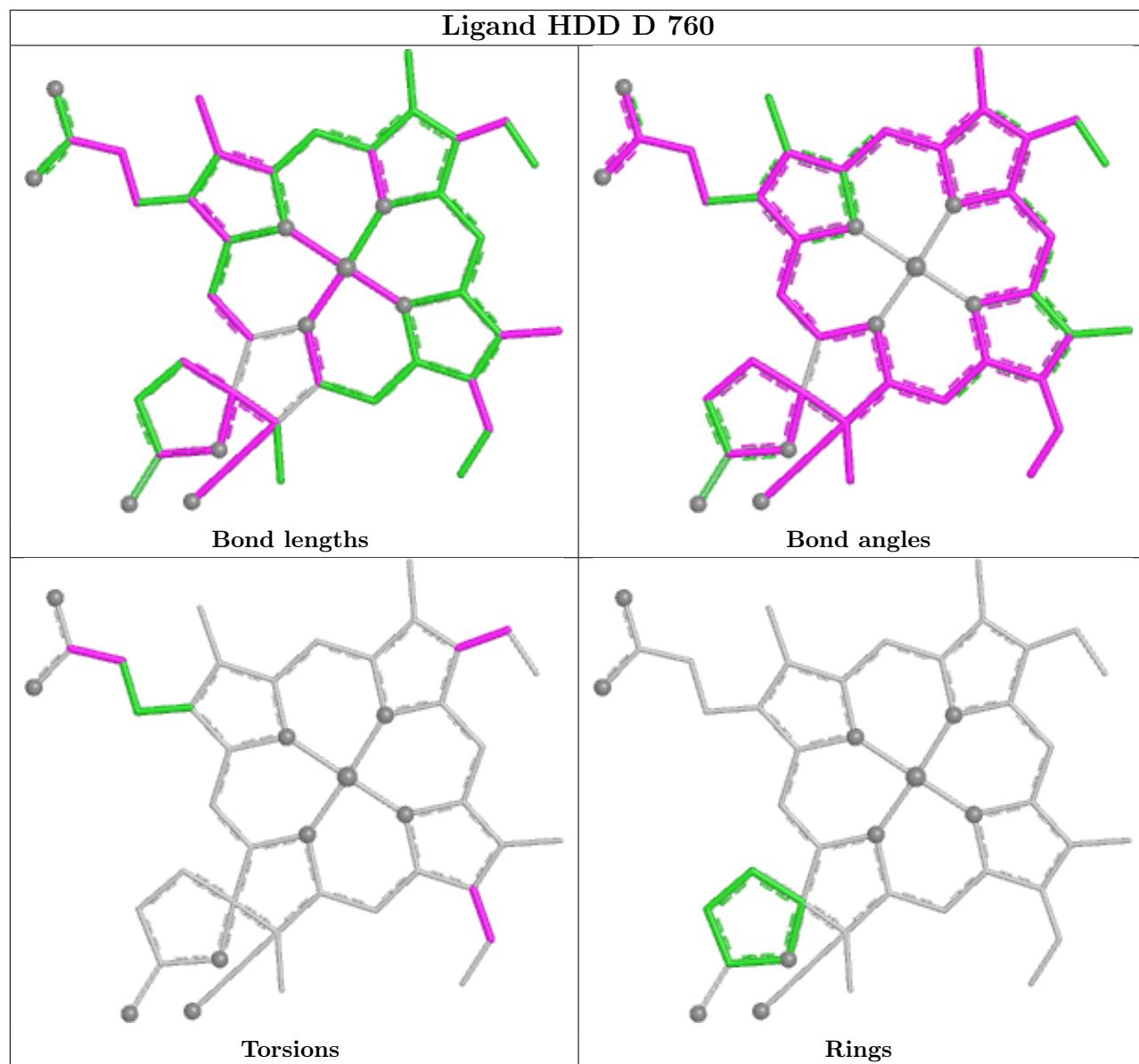
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	760	HDD	5	0
2	B	760	HDD	5	0
2	D	760	HDD	4	0
2	A	760	HDD	7	0

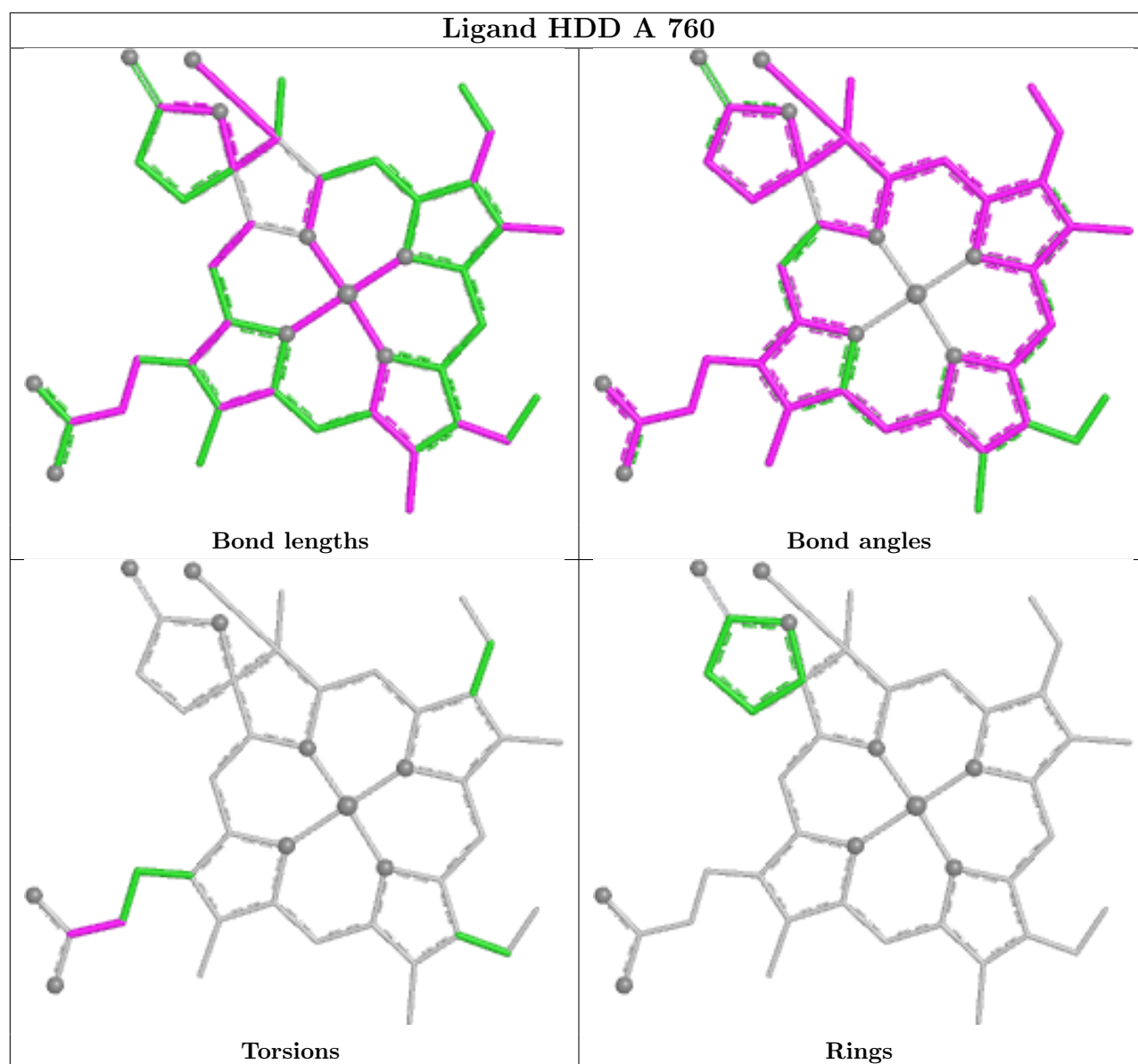
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	727/753 (96%)	-0.33	11 (1%) 72 79	2, 6, 21, 35	1 (0%)
1	B	727/753 (96%)	-0.29	9 (1%) 76 82	2, 7, 23, 33	1 (0%)
1	C	727/753 (96%)	-0.30	10 (1%) 73 80	2, 7, 23, 32	1 (0%)
1	D	727/753 (96%)	-0.36	6 (0%) 82 88	2, 7, 21, 33	1 (0%)
All	All	2908/3012 (96%)	-0.32	36 (1%) 76 82	2, 7, 22, 35	4 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ASP	6.8
1	A	711	ALA	5.5
1	A	712	ASP	5.1
1	A	28	SER	4.8
1	B	27	ASP	4.6
1	A	713	GLN	4.2
1	A	710	ILE	3.9
1	D	27	ASP	3.7
1	C	27	ASP	3.5
1	C	28	SER	3.5
1	D	28	SER	3.2
1	C	724	ALA	3.0
1	A	749	ASP	2.8
1	C	726	GLY	2.8
1	D	750	LYS	2.7
1	D	32	GLU	2.6
1	C	670	GLY	2.6
1	A	707	THR	2.5
1	B	750	LYS	2.5
1	B	28	SER	2.5
1	D	751	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	725	ASP	2.4
1	C	749	ASP	2.4
1	A	32	GLU	2.4
1	D	749	ASP	2.3
1	A	31	PRO	2.2
1	C	751	ILE	2.2
1	B	37	ARG	2.2
1	C	711	ALA	2.2
1	A	709	LYS	2.2
1	B	670	GLY	2.1
1	B	701	ALA	2.1
1	C	701	ALA	2.1
1	B	710	ILE	2.1
1	B	568	ASP	2.1
1	B	724	ALA	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](#)

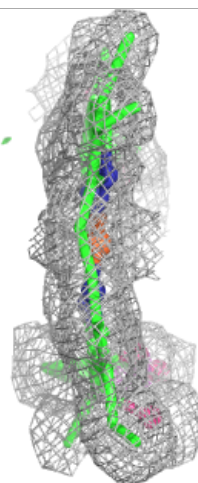
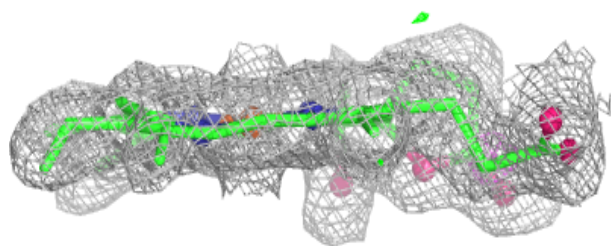
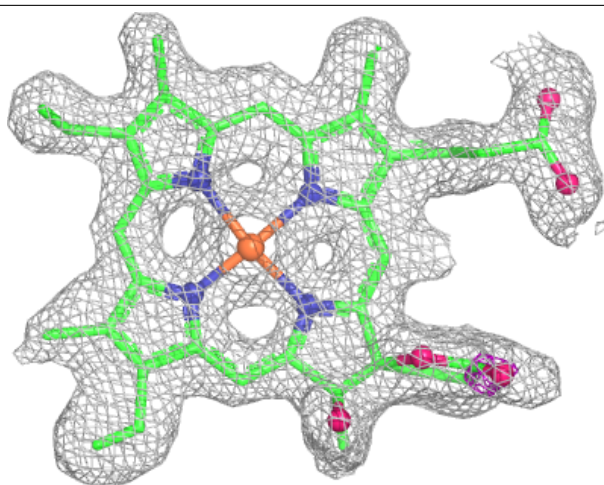
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	HDD	C	760	44/44	0.97	0.06	7,11,13,15	0
2	HDD	D	760	44/44	0.97	0.06	2,9,12,14	0
2	HDD	A	760	44/44	0.98	0.06	8,10,12,13	0
2	HDD	B	760	44/44	0.98	0.06	2,9,13,16	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

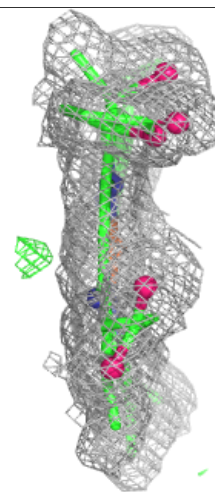
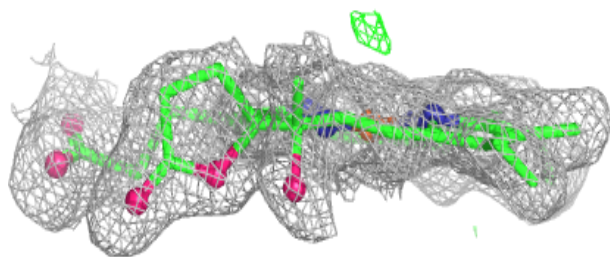
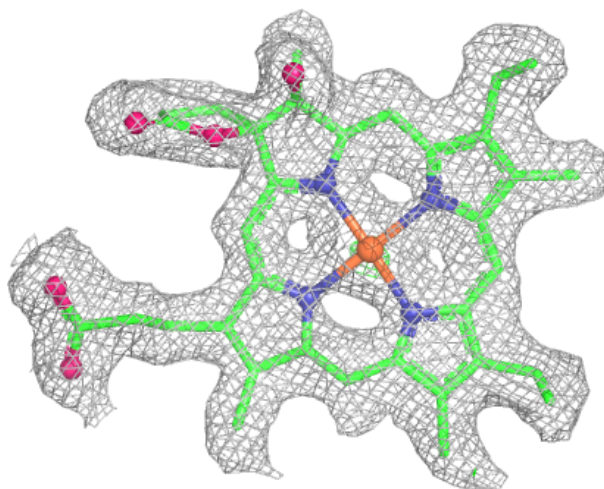
Electron density around HDD C 760:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



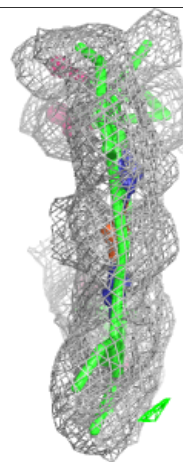
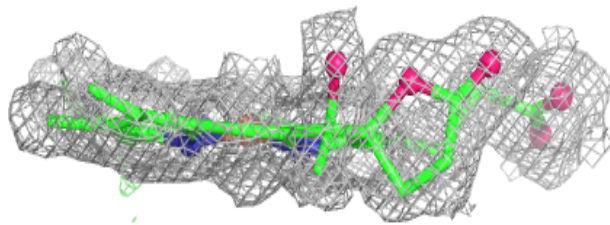
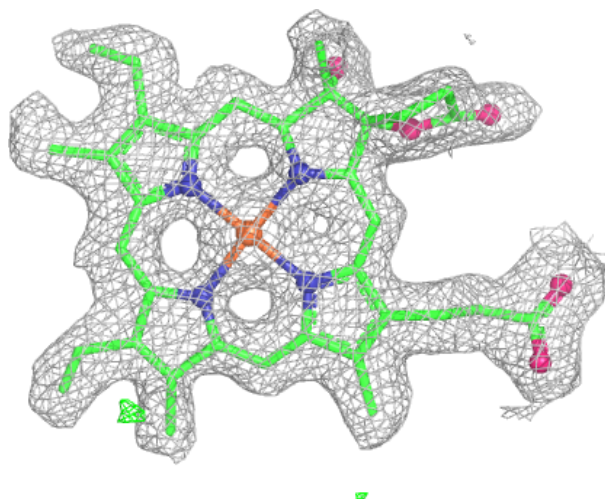
Electron density around HDD D 760:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



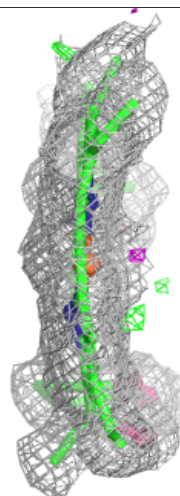
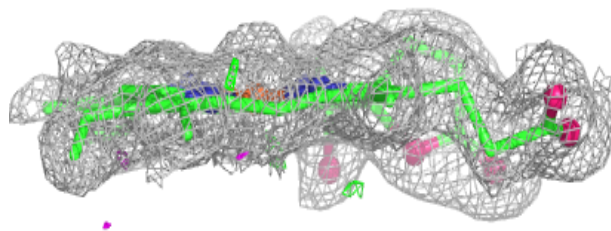
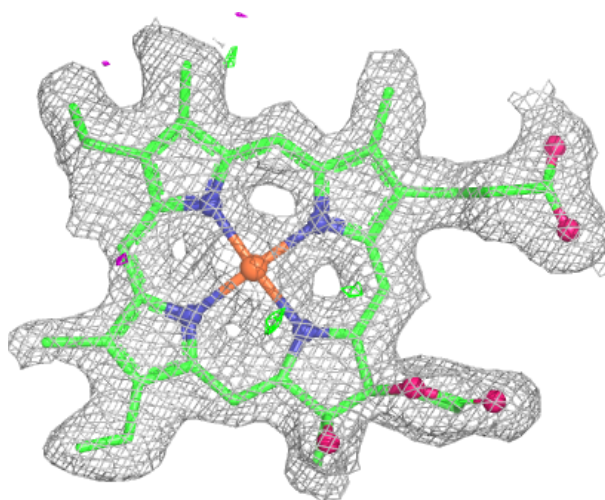
Electron density around HDD A 760:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HDD B 760:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.