



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:56 AM UTC

PDB ID : 3HHD / pdb_00003hhd
Title : Structure of the Human Fatty Acid Synthase KS-MAT Didomain as a Framework for Inhibitor Design.
Authors : Pappenberger, G.M.; Benz, J.; Thoma, R.; Rudolph, M.G.
Deposited on : 2009-05-15
Resolution : 2.15 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

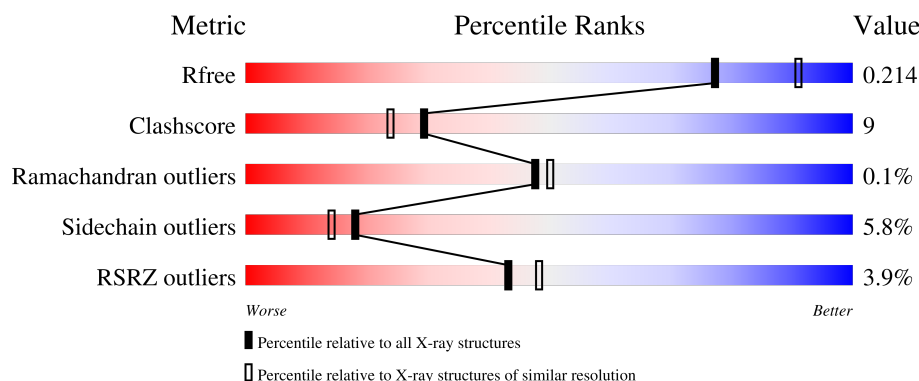
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	965	
1	B	965	
1	C	965	
1	D	965	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27836 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 Fatty acid synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	852	Total	C	N	O	S	0	2	0
			6497	4119	1144	1200	34			
1	B	852	Total	C	N	O	S	0	3	0
			6505	4125	1147	1199	34			
1	C	855	Total	C	N	O	S	0	1	0
			6512	4127	1147	1204	34			
1	D	854	Total	C	N	O	S	0	2	0
			6512	4129	1146	1203	34			

There are 12 discrepancies between the modelled and reference sequences:

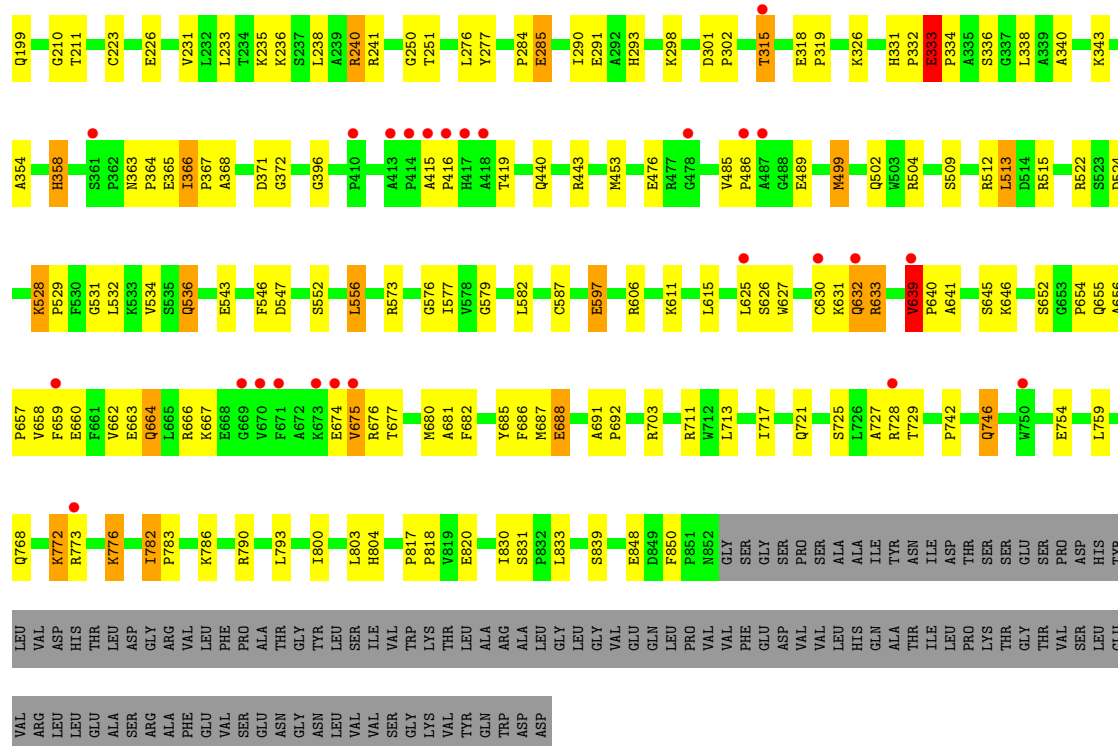
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P49327
A	0	THR	-	expression tag	UNP P49327
A	1	GLY	-	expression tag	UNP P49327
B	-1	SER	-	expression tag	UNP P49327
B	0	THR	-	expression tag	UNP P49327
B	1	GLY	-	expression tag	UNP P49327
C	-1	SER	-	expression tag	UNP P49327
C	0	THR	-	expression tag	UNP P49327
C	1	GLY	-	expression tag	UNP P49327
D	-1	SER	-	expression tag	UNP P49327
D	0	THR	-	expression tag	UNP P49327
D	1	GLY	-	expression tag	UNP P49327

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

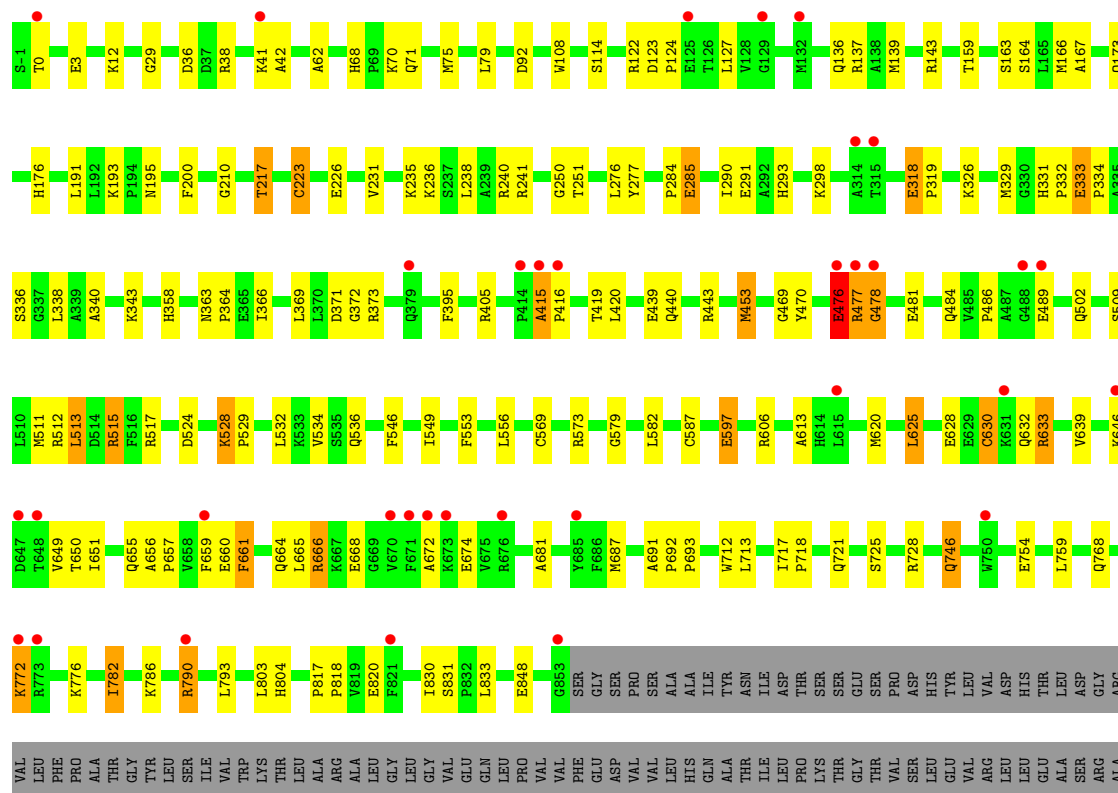
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	561	Total 561	O 561	0	0
3	B	371	Total 371	O 371	0	0
3	C	437	Total 437	O 437	0	0
3	D	439	Total 439	O 439	0	0



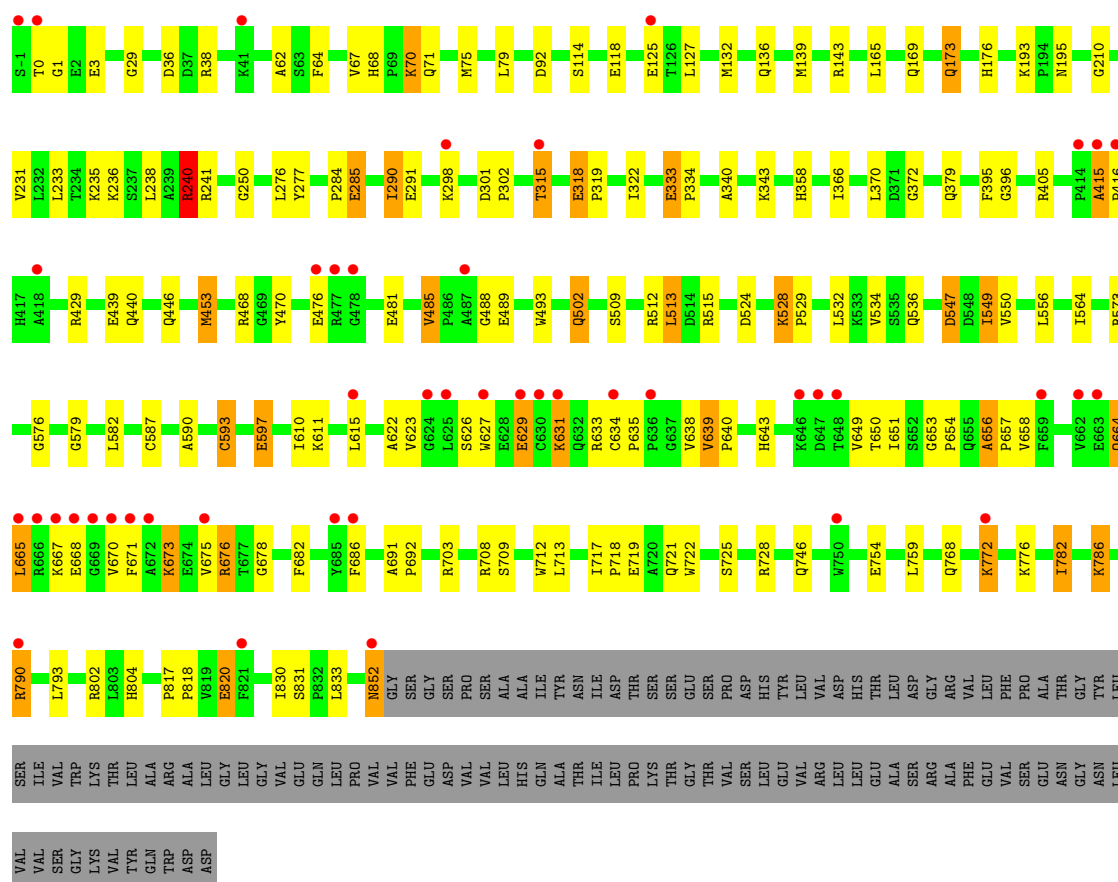
• Molecule 1: Fatty acid synthase



PHE
GLU
VAL
SER
GLU
ASN
GLY
ASN
VAL
VAL
SER
GLY
LYS
VAL
TYR
GLN
TRP
ASP
ASP

● Molecule 1: Fatty acid synthase

Chain D: 5% 71% 14% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.62Å 91.16Å 132.11Å 73.84° 86.83° 62.54°	Depositor
Resolution (Å)	45.64 – 2.15 45.64 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.3 (45.64-2.15) 97.7 (45.64-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.14Å)	Xtriage
Refinement program	BUSTER-TNT 2.5.1	Depositor
R, R_{free}	0.169 , 0.211 0.171 , 0.214	Depositor DCC
R_{free} test set	9152 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.9	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	0.96	EDS
Total number of atoms	27836	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.83% 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: CL

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	0.88	1/6662 (0.0%)	0.99	20/9058 (0.2%)
1	B	0.79	0/6673	0.99	21/9074 (0.2%)
1	C	0.81	3/6674 (0.0%)	0.98	23/9075 (0.3%)
1	D	0.81	1/6678 (0.0%)	0.98	24/9083 (0.3%)
All	All	0.82	5/26687 (0.0%)	0.99	88/36290 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	453	MET	SD-CE	-7.30	1.61	1.79
1	A	687	MET	SD-CE	-7.15	1.61	1.79
1	C	453	MET	SD-CE	-6.83	1.62	1.79
1	C	75	MET	SD-CE	5.84	1.94	1.79
1	C	511	MET	SD-CE	5.67	1.93	1.79

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	ILE	CA-C-N	11.60	132.55	119.32
1	B	366	ILE	C-N-CA	11.60	132.55	119.32
1	B	333	GLU	CA-C-N	-10.02	109.44	119.56
1	B	333	GLU	C-N-CA	-10.02	109.44	119.56
1	A	354	ALA	CA-C-N	-9.95	107.40	119.84
1	A	354	ALA	C-N-CA	-9.95	107.40	119.84
1	D	656	ALA	CA-C-N	7.82	127.47	119.19
1	D	656	ALA	C-N-CA	7.82	127.47	119.19
1	C	478	GLY	N-CA-C	-7.45	103.46	112.48
1	C	363	ASN	CA-C-N	7.44	127.11	119.82
1	C	363	ASN	C-N-CA	7.44	127.11	119.82
1	C	613	ALA	N-CA-C	-7.21	97.85	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	615	LEU	CA-C-N	7.20	124.91	119.66
1	D	615	LEU	C-N-CA	7.20	124.91	119.66
1	D	415	ALA	CA-C-N	7.13	126.39	118.97
1	D	415	ALA	C-N-CA	7.13	126.39	118.97
1	C	476	GLU	N-CA-C	-7.07	103.51	111.07
1	B	415	ALA	CA-C-N	7.05	126.30	118.97
1	B	415	ALA	C-N-CA	7.05	126.30	118.97
1	C	415	ALA	CA-C-N	6.96	126.21	118.97
1	C	415	ALA	C-N-CA	6.96	126.21	118.97
1	B	782	ILE	CA-C-N	6.74	127.29	120.14
1	B	782	ILE	C-N-CA	6.74	127.29	120.14
1	A	415	ALA	CA-C-N	6.72	128.25	119.84
1	A	415	ALA	C-N-CA	6.72	128.25	119.84
1	D	358	HIS	N-CA-C	6.72	121.06	112.86
1	D	653	GLY	CA-C-N	6.66	126.70	119.90
1	D	653	GLY	C-N-CA	6.66	126.70	119.90
1	A	333	GLU	CA-C-N	-6.60	112.83	119.56
1	A	333	GLU	C-N-CA	-6.60	112.83	119.56
1	A	240	ARG	N-CA-C	-6.28	104.58	112.93
1	B	639	VAL	N-CA-C	6.27	114.33	109.19
1	B	358	HIS	N-CA-C	6.24	120.47	112.86
1	B	240	ARG	N-CA-C	-6.24	104.64	112.93
1	D	366	ILE	CA-C-N	6.12	126.30	119.32
1	D	366	ILE	C-N-CA	6.12	126.30	119.32
1	A	159	THR	N-CA-C	-6.04	103.22	111.56
1	B	354	ALA	CA-C-N	-6.03	114.09	120.66
1	B	354	ALA	C-N-CA	-6.03	114.09	120.66
1	C	159	THR	N-CA-C	-6.01	103.26	111.56
1	D	549	ILE	N-CA-C	5.99	118.54	111.05
1	C	358	HIS	N-CA-C	5.97	120.14	112.86
1	C	549	ILE	N-CA-C	5.95	118.49	111.05
1	C	782	ILE	CA-C-N	5.93	126.43	120.14
1	C	782	ILE	C-N-CA	5.93	126.43	120.14
1	C	163	SER	N-CA-C	5.79	118.06	111.11
1	A	547	ASP	N-CA-C	-5.68	105.85	112.89
1	B	163	SER	N-CA-C	5.67	117.91	111.11
1	D	593	CYS	N-CA-C	5.63	120.15	113.28
1	D	240	ARG	N-CA-C	-5.60	105.48	112.93
1	B	776	LYS	CA-C-N	5.59	125.26	119.56
1	B	776	LYS	C-N-CA	5.59	125.26	119.56
1	D	782	ILE	CA-C-N	5.56	126.03	120.14
1	D	782	ILE	C-N-CA	5.56	126.03	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	488	GLY	N-CA-C	5.52	117.67	112.04
1	C	803	LEU	N-CA-C	-5.51	105.17	111.07
1	C	573	ARG	CA-C-N	-5.51	114.28	119.85
1	C	573	ARG	C-N-CA	-5.51	114.28	119.85
1	A	293	HIS	N-CA-C	-5.50	105.29	111.28
1	B	167	ALA	N-CA-C	-5.45	105.25	111.14
1	A	639	VAL	N-CA-C	5.43	113.64	109.19
1	A	371	ASP	N-CA-C	5.40	119.86	113.16
1	C	661	PHE	N-CA-C	-5.38	105.58	111.82
1	B	547	ASP	N-CA-C	-5.38	106.22	112.89
1	D	573	ARG	CA-C-N	-5.33	114.46	119.85
1	D	573	ARG	C-N-CA	-5.33	114.46	119.85
1	C	240	ARG	N-CA-C	-5.33	105.84	112.93
1	A	163	SER	N-CA-C	5.29	117.45	111.11
1	A	381	LEU	CA-C-N	-5.27	114.35	119.78
1	A	381	LEU	C-N-CA	-5.27	114.35	119.78
1	D	639	VAL	CA-C-N	5.21	128.12	120.46
1	D	639	VAL	C-N-CA	5.21	128.12	120.46
1	A	358	HIS	N-CA-C	5.21	119.21	112.86
1	C	137	ARG	N-CA-C	5.21	117.63	111.33
1	A	595	SER	N-CA-C	-5.17	103.86	110.53
1	D	485	VAL	N-CA-C	5.17	112.98	107.76
1	A	488	GLY	N-CA-C	5.14	117.28	112.04
1	B	573	ARG	CA-C-N	-5.13	114.67	119.85
1	B	573	ARG	C-N-CA	-5.13	114.67	119.85
1	C	728	ARG	N-CA-C	5.11	116.93	111.36
1	B	800	ILE	N-CA-C	-5.08	104.74	111.09
1	D	62	ALA	N-CA-C	5.03	117.42	111.33
1	C	122	ARG	N-CA-C	5.03	117.65	111.82
1	A	573	ARG	CA-C-N	-5.02	114.78	119.85
1	A	573	ARG	C-N-CA	-5.02	114.78	119.85
1	D	547	ASP	N-CA-C	-5.01	106.67	112.89
1	C	62	ALA	N-CA-C	5.01	117.39	111.33
1	C	293	HIS	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6497	0	6477	114	0
1	B	6505	0	6491	128	0
1	C	6512	0	6491	102	0
1	D	6512	0	6487	118	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	561	0	0	8	0
3	B	371	0	0	11	0
3	C	437	0	0	13	0
3	D	439	0	0	15	0
All	All	27836	0	25946	448	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 9.

All (448) 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:656:ALA:HB3	1:B:657:PRO:HD3	1.45	0.95
1:D:656:ALA:HB3	1:D:657:PRO:HD3	1.50	0.94
1:A:42:ALA:HB1	1:A:49:ARG:HD2	1.56	0.87
1:A:67:VAL:HG11	1:A:75:MET:HE1	1.55	0.86
1:A:499:MET:HE1	1:A:553:PHE:CE1	2.13	0.84
1:D:556:LEU:HD23	1:D:582:LEU:HD23	1.62	0.81
1:A:139:MET:HE3	1:D:395:PHE:CE1	2.18	0.78
1:A:656:ALA:HB3	1:A:657:PRO:HD3	1.68	0.75
1:C:333:GLU:HB2	1:C:334:PRO:HD2	1.68	0.75
1:A:200:PHE:CZ	1:D:132:MET:HE3	2.22	0.74
1:B:639:VAL:HG22	1:B:640:PRO:HD2	1.70	0.72
1:D:626:SER:OG	1:D:629:GLU:HB2	1.88	0.72
1:A:790:ARG:CD	1:A:790:ARG:H	2.01	0.72
1:A:680:MET:CE	1:A:687:MET:HE1	2.20	0.71
1:C:790:ARG:H	1:C:790:ARG:CD	2.03	0.69
1:B:728:ARG:HG2	1:B:729:THR:HG23	1.73	0.69
1:D:633:ARG:NH2	1:D:668:GLU:OE1	2.25	0.69
1:B:368:ALA:HA	1:B:371:ASP:OD1	1.92	0.69
1:D:790:ARG:CD	1:D:790:ARG:H	2.03	0.69
1:C:848:GLU:HG2	3:C:1008:HOH:O	1.93	0.69
1:B:440:GLN:OE1	1:B:443:ARG:NH1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:GLN:OE1	1:A:443:ARG:NH1	2.26	0.69
1:D:786:LYS:NZ	3:D:1096:HOH:O	2.24	0.68
1:A:477:ARG:NH1	1:A:789:HIS:HE2	1.91	0.68
1:C:440:GLN:HG3	1:C:833:LEU:HD22	1.76	0.68
1:D:440:GLN:HG3	1:D:833:LEU:HD22	1.76	0.68
1:B:655:GLN:HG3	1:B:659:PHE:CE2	2.30	0.67
1:D:291:GLU:HG2	1:D:340:ALA:HB1	1.78	0.66
1:A:209:GLU:OE2	1:A:213:LYS:NZ	2.27	0.66
1:C:3:GLU:OE2	1:C:236:LYS:HD2	1.96	0.66
1:D:241:ARG:HB2	1:D:453:MET:HE1	1.78	0.65
1:D:515:ARG:HB2	3:D:1250:HOH:O	1.95	0.65
1:B:680:MET:CE	1:B:687:MET:HE1	2.27	0.65
1:C:477:ARG:HG3	1:C:478:GLY:H	1.61	0.65
3:A:1712:HOH:O	1:C:41:LYS:HD3	1.96	0.65
1:C:193:LYS:HE3	1:C:195:ASN:HB2	1.79	0.65
1:D:656:ALA:CB	1:D:657:PRO:HD3	2.25	0.65
1:B:656:ALA:O	1:B:660:GLU:HG2	1.97	0.64
1:B:680:MET:HE3	1:B:687:MET:HE1	1.77	0.64
1:C:241:ARG:HB2	1:C:453:MET:HE1	1.80	0.64
1:D:68[A]:HIS:HB3	1:D:71:GLN:OE1	1.97	0.64
1:A:3:GLU:OE2	1:A:236:LYS:HD2	1.98	0.64
1:A:663:GLU:OE1	1:A:663:GLU:HA	1.96	0.64
1:A:200:PHE:CE1	1:D:132:MET:HE3	2.33	0.64
1:A:786:LYS:NZ	3:A:1091:HOH:O	2.29	0.64
1:D:768:GLN:O	1:D:772:LYS:HD2	1.98	0.63
1:A:768:GLN:O	1:A:772:LYS:HD2	1.98	0.63
1:B:68:HIS:CE1	1:B:70:LYS:HG3	2.33	0.63
1:A:68:HIS:CE1	1:A:70:LYS:HG3	2.33	0.63
1:B:396:GLY:HA3	1:C:139:MET:HE1	1.81	0.63
1:D:67:VAL:HG11	1:D:75:MET:HE1	1.80	0.63
1:B:615:LEU:HD12	1:B:680:MET:HE1	1.80	0.63
1:C:333:GLU:HB2	1:C:334:PRO:CD	2.29	0.63
1:D:290:ILE:HG23	1:D:322:ILE:HG22	1.80	0.63
1:A:363:ASN:HB3	1:A:366:ILE:HD12	1.80	0.63
1:A:515:ARG:HB2	3:A:1251:HOH:O	1.99	0.62
1:A:680:MET:HE3	1:A:687:MET:HE1	1.79	0.62
1:B:768:GLN:O	1:B:772:LYS:HD2	1.99	0.62
1:C:217:THR:HG23	1:C:364:PRO:CD	2.28	0.62
1:C:666:ARG:NH1	1:C:672:ALA:O	2.32	0.62
1:C:318:GLU:HG2	3:C:1794:HOH:O	1.98	0.62
1:D:71:GLN:HB3	3:D:1519:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:GLN:O	1:A:667:LYS:HB2	1.99	0.62
1:C:768:GLN:O	1:C:772:LYS:HD2	1.99	0.62
1:D:691:ALA:HB3	1:D:692:PRO:HD3	1.82	0.62
1:B:645:SER:HA	1:B:746:GLN:CG	2.29	0.61
1:B:703:ARG:NH2	3:B:1065:HOH:O	2.29	0.61
1:C:285:GLU:HB3	3:C:1536:HOH:O	1.99	0.61
1:D:547:ASP:OD1	1:D:676:ARG:HD2	2.00	0.61
1:D:333:GLU:HB2	1:D:334:PRO:HD2	1.82	0.61
1:D:804:HIS:HB2	3:D:1053:HOH:O	2.00	0.61
1:A:68:HIS:HE1	1:A:70:LYS:HG3	1.65	0.61
1:B:645:SER:HA	1:B:746:GLN:HG2	1.81	0.61
1:C:556:LEU:HD23	1:C:582:LEU:HD23	1.82	0.61
1:B:333:GLU:HB2	1:B:334:PRO:HD2	1.83	0.61
1:B:3:GLU:OE2	1:B:236:LYS:HD2	2.01	0.61
1:A:790:ARG:H	1:A:790:ARG:NE	1.98	0.61
1:B:68:HIS:HE1	1:B:70:LYS:HG3	1.64	0.61
1:B:499:MET:HE3	1:B:682:PHE:CD2	2.36	0.61
1:C:691:ALA:HB3	1:C:692:PRO:HD3	1.83	0.60
1:B:691:ALA:HB3	1:B:692:PRO:HD3	1.82	0.60
1:D:3:GLU:OE2	1:D:236:LYS:HD2	2.01	0.60
1:A:333:GLU:HB2	1:A:334:PRO:HD2	1.82	0.60
1:D:193:LYS:HE3	1:D:195:ASN:HB2	1.82	0.60
1:C:661:PHE:O	1:C:665:LEU:HG	2.02	0.60
1:B:641:ALA:HB2	1:B:652:SER:HB2	1.84	0.60
1:B:746:GLN:HE21	1:B:746:GLN:CA	2.15	0.60
1:D:790:ARG:H	1:D:790:ARG:NE	1.99	0.60
1:A:193:LYS:HE3	1:A:195:ASN:HB2	1.84	0.60
1:A:417:HIS:ND1	1:A:422:ARG:NH2	2.49	0.60
1:B:285:GLU:O	1:B:285:GLU:HG3	1.99	0.60
1:D:754:GLU:HG2	1:D:776:LYS:HD3	1.84	0.60
1:B:531:GLY:HA2	3:B:1230:HOH:O	2.02	0.59
1:C:790:ARG:H	1:C:790:ARG:NE	2.00	0.59
1:B:476:GLU:HB2	3:B:1353:HOH:O	2.01	0.59
1:B:664:GLN:O	1:B:667:LYS:HB2	2.03	0.59
1:C:285:GLU:O	1:C:285:GLU:HG3	2.00	0.59
1:B:193:LYS:HE3	1:B:195:ASN:HB2	1.84	0.58
1:B:139:MET:HE3	1:C:395:PHE:CE1	2.39	0.58
1:B:627:TRP:CD1	1:B:631:LYS:HE2	2.37	0.58
1:B:632:GLN:HG3	1:B:633:ARG:HG2	1.84	0.58
1:C:754:GLU:HG2	1:C:776:LYS:HD3	1.84	0.58
1:B:746:GLN:HE21	1:B:746:GLN:C	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ARG:NH2	1:A:668:GLU:OE1	2.36	0.58
1:B:79:LEU:HD21	1:B:143[A]:ARG:HG3	1.86	0.58
1:C:42:ALA:HA	3:C:1704:HOH:O	2.04	0.58
1:D:290:ILE:CG2	1:D:322:ILE:HG22	2.34	0.58
1:D:470:TYR:CZ	1:D:481:GLU:HG3	2.39	0.58
1:A:691:ALA:HB3	1:A:692:PRO:HD3	1.85	0.58
1:A:241:ARG:HB2	1:A:453:MET:HE1	1.84	0.57
1:A:301:ASP:HB2	1:A:302:PRO:HD3	1.87	0.57
1:A:627:TRP:CD1	1:A:631:LYS:HE2	2.38	0.57
1:B:241:ARG:HB2	1:B:453:MET:HE1	1.86	0.57
1:C:405:ARG:NH1	3:C:1194:HOH:O	2.34	0.57
1:B:685:TYR:O	1:B:688:GLU:HB2	2.03	0.57
1:C:0:THR:HG23	1:C:176:HIS:HE1	1.69	0.57
1:C:477:ARG:CG	1:C:478:GLY:H	2.15	0.57
1:B:504[B]:ARG:NH2	1:B:543:GLU:OE1	2.38	0.57
1:D:703:ARG:NH1	3:D:1142:HOH:O	2.38	0.57
1:A:625:LEU:HD12	1:A:629:GLU:HB3	1.87	0.56
1:C:291:GLU:HG2	1:C:340:ALA:HB1	1.86	0.56
1:B:293:HIS:O	1:B:326:LYS:HE2	2.04	0.56
1:B:132:MET:HE3	1:C:200:PHE:CZ	2.40	0.56
1:B:363:ASN:HB3	1:B:366:ILE:HD12	1.88	0.56
1:B:654:PRO:HB2	1:B:657:PRO:HD2	1.86	0.56
1:B:75:MET:HE3	1:B:79:LEU:HD23	1.87	0.55
1:B:658:VAL:O	1:B:662:VAL:HG23	2.06	0.55
1:C:502:GLN:HG3	1:C:546:PHE:HB3	1.88	0.55
1:A:680:MET:HE1	1:A:687:MET:HE1	1.86	0.55
1:D:639:VAL:HG22	1:D:640:PRO:N	2.21	0.55
1:D:440:GLN:HG3	1:D:833:LEU:CD2	2.36	0.55
1:D:852:ASN:HD22	1:D:852:ASN:C	2.15	0.55
1:A:754:GLU:HG2	1:A:776:LYS:HD3	1.89	0.54
1:D:509:SER:O	1:D:512:ARG:HD3	2.06	0.54
1:B:440:GLN:HG2	1:B:833:LEU:HD11	1.89	0.54
1:C:217:THR:HG23	1:C:364:PRO:HD2	1.88	0.54
1:B:235:LYS:HE2	1:B:238:LEU:HD13	1.89	0.54
1:C:440:GLN:HG3	1:C:833:LEU:CD2	2.37	0.54
1:D:627:TRP:HA	1:D:649:VAL:HG21	1.89	0.54
1:A:291:GLU:HG2	1:A:340:ALA:HB1	1.89	0.54
1:B:597:GLU:CD	1:B:597:GLU:H	2.16	0.54
1:D:319:PRO:HB3	1:D:372:GLY:O	2.08	0.54
1:A:654:PRO:HB2	1:A:657:PRO:HD2	1.89	0.54
1:D:333:GLU:CB	1:D:334:PRO:CD	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:GLN:HG3	1:B:546:PHE:HB3	1.90	0.54
1:B:556:LEU:HD22	1:B:582:LEU:HD23	1.90	0.54
1:A:685:TYR:O	1:A:688:GLU:HB2	2.08	0.53
1:C:332:PRO:HG2	1:C:336:SER:HA	1.89	0.53
1:A:285:GLU:HB3	3:A:1073:HOH:O	2.07	0.53
1:B:509:SER:O	1:B:512:ARG:HD3	2.09	0.53
1:C:333:GLU:CB	1:C:334:PRO:CD	2.87	0.53
1:C:366:ILE:HB	1:C:369:LEU:HD12	1.90	0.53
1:A:440:GLN:HG2	1:A:833:LEU:HD11	1.91	0.53
1:D:285:GLU:O	1:D:285:GLU:HG3	2.00	0.53
1:D:597:GLU:H	1:D:597:GLU:CD	2.17	0.53
1:A:502:GLN:HG3	1:A:546:PHE:HB3	1.91	0.52
1:A:509:SER:O	1:A:512:ARG:HD3	2.09	0.52
1:A:556:LEU:HD22	1:A:582:LEU:HD23	1.89	0.52
1:B:333:GLU:HB2	1:B:334:PRO:CD	2.38	0.52
1:A:597:GLU:H	1:A:597:GLU:CD	2.17	0.52
1:D:550:VAL:HG23	1:D:611:LYS:HD2	1.92	0.52
1:A:240:ARG:NH1	1:A:821:PHE:CE2	2.78	0.52
1:A:319:PRO:HB3	1:A:372:GLY:O	2.09	0.52
1:C:656:ALA:HB3	1:C:657:PRO:CD	2.40	0.52
1:A:79:LEU:HD21	1:A:143[A]:ARG:HG3	1.92	0.52
1:B:365:GLU:O	1:B:367:PRO:HD3	2.09	0.52
1:B:663:GLU:HA	1:B:663:GLU:OE1	2.09	0.52
1:D:649:VAL:CG1	1:D:650:THR:N	2.73	0.52
1:A:396:GLY:HA3	1:D:139:MET:HE1	1.92	0.52
1:B:68:HIS:HE1	1:B:70:LYS:CG	2.22	0.52
1:D:622:ALA:HB3	1:D:673:LYS:HG2	1.92	0.52
1:C:579:GLY:HA3	1:C:587:CYS:SG	2.50	0.52
1:A:250:GLY:HA3	1:A:276:LEU:HD21	1.92	0.51
1:B:717:ILE:HD13	1:B:727:ALA:HB2	1.90	0.51
1:C:92:ASP:HB2	1:C:831:SER:HB3	1.91	0.51
1:B:75:MET:HE1	1:B:79:LEU:HG	1.92	0.51
1:B:291:GLU:HG2	1:B:340:ALA:HB1	1.92	0.51
1:B:522:ARG:HD2	3:B:1105:HOH:O	2.10	0.51
1:C:509:SER:O	1:C:512:ARG:HD3	2.10	0.51
1:C:524:ASP:OD1	1:C:534:VAL:N	2.43	0.51
1:A:549:ILE:HD11	1:A:553:PHE:CZ	2.45	0.51
1:B:639:VAL:CG2	1:B:640:PRO:HD2	2.41	0.51
1:C:486:PRO:HD2	3:C:1576:HOH:O	2.11	0.51
1:A:235:LYS:HE2	1:A:238:LEU:HD13	1.92	0.51
1:B:656:ALA:CB	1:B:657:PRO:HD3	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:LYS:HE2	1:C:238:LEU:HD13	1.92	0.51
1:B:210:GLY:C	1:B:223:CYS:HB2	2.36	0.51
1:C:329:MET:HE2	1:C:332:PRO:HD3	1.92	0.51
1:D:333:GLU:CB	1:D:334:PRO:HD2	2.41	0.51
1:A:68:HIS:HE1	1:A:70:LYS:CG	2.24	0.50
1:C:597:GLU:CD	1:C:597:GLU:H	2.18	0.50
1:D:671:PHE:CZ	1:D:673:LYS:HB3	2.45	0.50
1:B:92:ASP:HB2	1:B:831:SER:HB3	1.93	0.50
1:B:331:HIS:CD2	1:B:333:GLU:H	2.29	0.50
1:A:524:ASP:OD1	1:A:534:VAL:N	2.44	0.50
1:B:319:PRO:HB3	1:B:372:GLY:O	2.11	0.50
1:D:405:ARG:NH1	3:D:1100:HOH:O	2.35	0.50
1:D:627:TRP:CD1	1:D:627:TRP:C	2.90	0.50
1:C:173:GLN:HG3	3:C:992:HOH:O	2.11	0.50
1:D:92:ASP:HB2	1:D:831:SER:HB3	1.92	0.50
1:D:493:TRP:CD2	1:D:576:GLY:HA3	2.46	0.50
1:C:0:THR:HG23	1:C:176:HIS:CE1	2.46	0.49
1:C:166:MET:HE1	1:C:251:THR:OG1	2.12	0.49
1:D:639:VAL:CG2	1:D:640:PRO:N	2.75	0.49
1:A:633:ARG:NH1	1:A:668:GLU:OE1	2.45	0.49
1:D:127:LEU:HD12	1:D:127:LEU:C	2.37	0.49
1:D:675:VAL:HG12	1:D:676:ARG:N	2.28	0.49
1:C:484:GLN:OE1	3:C:1480:HOH:O	2.19	0.49
1:C:681:ALA:O	1:C:687:MET:HE3	2.11	0.49
1:D:524:ASP:OD1	1:D:534:VAL:N	2.46	0.49
1:A:499:MET:HE1	1:A:553:PHE:HE1	1.72	0.49
1:B:343:LYS:HD3	1:B:343:LYS:C	2.38	0.49
1:A:92:ASP:HB2	1:A:831:SER:HB3	1.93	0.49
1:A:759:LEU:HD23	1:A:782:ILE:HB	1.95	0.49
1:A:333:GLU:CB	1:A:334:PRO:CD	2.90	0.49
1:D:627:TRP:CA	1:D:649:VAL:HG21	2.43	0.48
1:A:71:GLN:HB2	3:A:1037:HOH:O	2.12	0.48
1:A:210:GLY:C	1:A:223:CYS:HB2	2.38	0.48
1:A:285:GLU:O	1:A:285:GLU:HG3	2.06	0.48
1:D:719:GLU:HG3	1:D:722:TRP:CE3	2.48	0.48
1:B:139:MET:CE	1:C:395:PHE:CE1	2.96	0.48
1:A:416:PRO:O	1:A:419:THR:OG1	2.31	0.48
1:D:235:LYS:HE2	1:D:238:LEU:HD13	1.94	0.48
1:B:524:ASP:OD1	1:B:534:VAL:N	2.46	0.48
1:B:656:ALA:HB3	1:B:657:PRO:CD	2.29	0.48
1:B:754:GLU:HG2	1:B:776:LYS:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLY:C	1:C:223:CYS:HB2	2.37	0.48
1:D:627:TRP:CE3	1:D:643:HIS:HB2	2.48	0.48
1:D:627:TRP:HE1	1:D:631:LYS:NZ	2.12	0.48
1:A:417:HIS:HE1	3:A:1365:HOH:O	1.97	0.48
1:C:29:GLY:HA2	3:C:1031:HOH:O	2.14	0.48
1:D:549:ILE:HG23	1:D:678:GLY:HA3	1.95	0.48
1:D:626:SER:HG	1:D:629:GLU:HB2	1.77	0.48
1:D:515:ARG:CB	3:D:1250:HOH:O	2.56	0.47
1:D:79:LEU:HD21	1:D:143:ARG:HG3	1.97	0.47
1:A:139:MET:CE	1:D:395:PHE:CE1	2.95	0.47
1:A:333:GLU:HB2	1:A:334:PRO:CD	2.43	0.47
1:A:170:ASN:HA	1:A:173:GLN:HG3	1.96	0.47
1:B:804:HIS:HB2	3:B:1104:HOH:O	2.14	0.47
1:C:127:LEU:C	1:C:127:LEU:HD12	2.39	0.47
1:C:319:PRO:HB3	1:C:372:GLY:O	2.13	0.47
1:A:493:TRP:CD2	1:A:576:GLY:HA3	2.50	0.47
1:A:499:MET:CE	1:A:553:PHE:HE1	2.28	0.47
1:A:675:VAL:HG12	1:A:676:ARG:N	2.29	0.47
1:B:675:VAL:HG12	1:B:677:THR:HG23	1.96	0.47
1:C:513:LEU:HD22	1:C:793:LEU:HD13	1.97	0.47
1:D:664:GLN:O	1:D:664:GLN:HG2	2.10	0.47
1:C:68:HIS:HB2	1:C:71:GLN:OE1	2.15	0.47
1:C:759:LEU:HD23	1:C:782:ILE:HB	1.97	0.47
1:D:318:GLU:HG2	3:D:984:HOH:O	2.15	0.47
1:A:633:ARG:HH12	1:A:668:GLU:CD	2.23	0.47
1:D:0:THR:HG23	1:D:176:HIS:HE1	1.80	0.47
1:D:634:CYS:SG	1:D:638:VAL:HG12	2.55	0.47
1:B:36:ASP:OD1	1:B:38:ARG:HB2	2.15	0.46
1:B:711:ARG:NE	3:B:1120:HOH:O	2.47	0.46
1:B:515:ARG:HB2	3:B:988:HOH:O	2.15	0.46
1:B:536:GLN:NE2	3:B:1011:HOH:O	2.47	0.46
1:B:654:PRO:HG3	1:B:686:PHE:CZ	2.50	0.46
1:D:0:THR:HG23	1:D:176:HIS:CE1	2.50	0.46
1:B:250:GLY:HA3	1:B:276:LEU:HD21	1.98	0.46
1:B:645:SER:HA	1:B:746:GLN:HG3	1.97	0.46
1:B:675:VAL:HG12	1:B:677:THR:CG2	2.45	0.46
1:D:240:ARG:NE	3:D:1005:HOH:O	2.47	0.46
1:A:67:VAL:HG11	1:A:75:MET:CE	2.38	0.46
1:B:759:LEU:HD23	1:B:782:ILE:HB	1.97	0.46
1:D:68[A]:HIS:CE1	1:D:70:LYS:HG3	2.51	0.46
1:A:68:HIS:CE1	1:A:70:LYS:CG	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ASP:OD1	1:D:38:ARG:HB2	2.16	0.46
1:A:528:LYS:N	1:A:529:PRO:CD	2.79	0.46
1:C:470:TYR:CZ	1:C:481:GLU:HG3	2.50	0.46
1:C:477:ARG:HA	1:C:477:ARG:HD3	1.48	0.46
1:A:72:ALA:HA	1:A:75:MET:HE3	1.98	0.46
1:A:513:LEU:HD22	1:A:793:LEU:HD13	1.97	0.46
1:B:68:HIS:CE1	1:B:70:LYS:CG	2.96	0.46
1:B:315:THR:O	1:B:315:THR:HG23	2.15	0.46
1:C:692:PRO:HB2	1:C:693:PRO:HD3	1.98	0.46
1:C:371:ASP:OD2	1:C:373:ARG:NH2	2.47	0.46
1:A:208:PRO:HD2	1:A:220:ASN:ND2	2.31	0.45
1:B:333:GLU:CB	1:B:334:PRO:CD	2.94	0.45
1:C:664:GLN:O	1:C:668:GLU:HG3	2.16	0.45
1:A:485:VAL:HA	1:A:486:PRO:HD3	1.83	0.45
1:C:439:GLU:HB2	3:C:1046:HOH:O	2.16	0.45
1:C:625:LEU:CD1	1:C:630:CYS:SG	3.04	0.45
1:C:649:VAL:CG1	1:C:650:THR:N	2.79	0.45
1:C:660:GLU:O	1:C:664:GLN:HG3	2.17	0.45
1:D:502[A]:GLN:CG	1:D:676:ARG:NH2	2.80	0.45
1:D:654:PRO:O	1:D:658:VAL:HG23	2.16	0.45
1:D:708:ARG:HG2	1:D:712:TRP:CZ3	2.52	0.45
1:A:712:TRP:CD1	1:A:712:TRP:C	2.94	0.45
1:C:36:ASP:OD1	1:C:38:ARG:HB2	2.17	0.45
1:D:513:LEU:HD22	1:D:793:LEU:HD13	1.99	0.45
1:D:717:ILE:HA	1:D:718:PRO:HD3	1.87	0.45
1:B:332:PRO:HG2	1:B:336:SER:HA	1.99	0.45
1:B:528:LYS:N	1:B:529:PRO:CD	2.79	0.45
1:C:528:LYS:HB3	1:C:529:PRO:HD3	1.99	0.45
1:C:655:GLN:HG3	1:C:659:PHE:CE2	2.52	0.45
1:A:499:MET:CE	1:A:553:PHE:CE1	2.91	0.45
1:C:79:LEU:HD21	1:C:143:ARG:HG3	1.99	0.45
1:D:528:LYS:N	1:D:529:PRO:CD	2.80	0.45
1:B:139:MET:HE3	1:C:395:PHE:HE1	1.81	0.45
1:C:633:ARG:HE	1:C:633:ARG:HB3	1.70	0.45
1:D:169:GLN:O	1:D:173:GLN:HG2	2.16	0.45
1:D:556:LEU:HD23	1:D:582:LEU:CD2	2.40	0.45
1:D:708:ARG:HD2	1:D:712:TRP:CZ3	2.52	0.45
1:B:817:PRO:HA	1:B:818:PRO:HD3	1.88	0.44
1:C:528:LYS:N	1:C:529:PRO:CD	2.80	0.44
1:C:553:PHE:CD1	1:C:582:LEU:HD22	2.52	0.44
1:D:759:LEU:HD23	1:D:782:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLU:HA	1:A:118:GLU:HG3	1.98	0.44
1:A:620:MET:HA	1:A:651:ILE:O	2.18	0.44
1:A:641:ALA:HB2	1:A:652:SER:HB2	1.99	0.44
1:B:92:ASP:HA	1:B:830:ILE:HB	1.99	0.44
1:C:476:GLU:O	1:C:477:ARG:HB2	2.17	0.44
1:C:579:GLY:CA	1:C:587:CYS:SG	3.05	0.44
1:D:564:ILE:HD13	1:D:590:ALA:HB2	1.99	0.44
1:A:168:LEU:HD12	1:A:185:VAL:HG21	1.99	0.44
1:A:582:LEU:HD13	1:A:606:ARG:HD3	1.99	0.44
1:A:127:LEU:C	1:A:127:LEU:HD12	2.42	0.44
1:B:641:ALA:O	1:B:742:PRO:HA	2.18	0.44
1:D:301:ASP:HB2	1:D:302:PRO:HD3	1.99	0.44
1:A:36:ASP:OD1	1:A:38:ARG:HB2	2.17	0.44
1:A:139:MET:HE3	1:D:395:PHE:HE1	1.79	0.44
1:B:79:LEU:HD21	1:B:143[B]:ARG:HG2	1.99	0.44
1:B:301:ASP:HB2	1:B:302:PRO:HD3	1.99	0.44
1:A:490:ARG:HA	1:A:491:PRO:HD2	1.90	0.44
1:A:499:MET:HB3	1:A:499:MET:HE2	1.69	0.44
1:B:127:LEU:C	1:B:127:LEU:HD12	2.43	0.43
1:C:620:MET:HA	1:C:651:ILE:O	2.17	0.43
1:D:468:ARG:HD2	1:D:485:VAL:HG21	2.00	0.43
1:D:654:PRO:HB2	1:D:657:PRO:HD2	2.00	0.43
1:A:301:ASP:CB	1:A:302:PRO:HD3	2.49	0.43
1:A:638:VAL:HG11	1:A:651:ILE:HD12	2.00	0.43
1:B:396:GLY:CA	1:C:139:MET:HE1	2.46	0.43
1:C:804:HIS:HB2	3:C:1176:HOH:O	2.18	0.43
1:A:635:PRO:HD3	1:A:661:PHE:CD1	2.53	0.43
1:B:343:LYS:HD3	1:B:343:LYS:O	2.18	0.43
1:C:582:LEU:HD13	1:C:606:ARG:HD3	2.00	0.43
1:D:649:VAL:HG12	1:D:650:THR:N	2.33	0.43
1:B:29:GLY:HA2	3:B:1085:HOH:O	2.18	0.43
1:C:250:GLY:HA3	1:C:276:LEU:HD21	2.01	0.43
1:C:515:ARG:HD3	1:C:569:CYS:SG	2.59	0.43
1:B:75:MET:CE	1:B:79:LEU:HG	2.48	0.43
1:C:416:PRO:O	1:C:419:THR:OG1	2.36	0.43
1:B:416:PRO:O	1:B:419:THR:OG1	2.35	0.43
1:B:513:LEU:HD22	1:B:793:LEU:HD13	2.00	0.43
1:B:582:LEU:HD13	1:B:606:ARG:HD3	1.99	0.43
1:B:633:ARG:HE	1:B:633:ARG:HB3	1.49	0.43
1:B:49:ARG:H	1:B:49:ARG:HG2	1.68	0.43
1:D:502[A]:GLN:HG2	1:D:676:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:ASN:C	1:A:852:ASN:HD22	2.26	0.43
1:B:499:MET:CE	1:B:682:PHE:CD2	3.01	0.43
1:C:517:ARG:HD2	3:C:1631:HOH:O	2.17	0.43
1:C:712:TRP:CD1	1:C:712:TRP:C	2.96	0.43
1:B:191:LEU:HG	1:B:226:GLU:HG2	2.01	0.43
1:C:326:LYS:HE3	1:C:331:HIS:CD2	2.54	0.43
1:C:477:ARG:CG	1:C:478:GLY:N	2.80	0.43
1:D:29:GLY:HA2	3:D:1089:HOH:O	2.18	0.43
1:A:343:LYS:HD3	1:A:343:LYS:C	2.44	0.42
1:C:108:TRP:HB3	1:C:167:ALA:HB1	2.01	0.42
1:C:692:PRO:HB2	1:C:693:PRO:CD	2.48	0.42
1:D:439:GLU:HB2	3:D:1126:HOH:O	2.19	0.42
1:A:804:HIS:HB2	3:A:1291:HOH:O	2.19	0.42
1:B:196:THR:HA	1:B:199:GLN:HE21	1.84	0.42
1:C:123:ASP:HA	1:C:124:PRO:HD2	1.94	0.42
1:C:164:SER:HB2	1:C:338:LEU:HG	2.01	0.42
1:D:92:ASP:HA	1:D:830:ILE:HB	2.01	0.42
1:D:315:THR:O	1:D:315:THR:HG23	2.18	0.42
1:B:211:THR:CG2	1:B:358:HIS:CD2	3.02	0.42
1:C:469:GLY:HA2	1:C:481:GLU:O	2.19	0.42
1:D:633:ARG:O	1:D:635:PRO:HD3	2.20	0.42
1:B:803:LEU:HD12	1:B:803:LEU:HA	1.82	0.42
1:C:277:TYR:CZ	1:C:284:PRO:HG3	2.55	0.42
1:C:420:LEU:HD21	1:C:512:ARG:HB3	2.00	0.42
1:C:746:GLN:HE21	1:C:746:GLN:HB3	1.61	0.42
1:A:528:LYS:HB3	1:A:529:PRO:HD3	2.01	0.42
1:D:0:THR:HG23	1:D:1:GLY:N	2.35	0.42
1:A:431:PRO:HG2	1:B:839:SER:HB2	2.01	0.42
1:B:240:ARG:HA	1:B:240:ARG:HD2	1.86	0.42
1:D:528:LYS:HB3	1:D:529:PRO:HD3	2.02	0.42
1:A:165:LEU:HD22	1:A:392:SER:HB2	2.02	0.42
1:D:550:VAL:HG23	1:D:611:LYS:CD	2.49	0.42
1:D:665:LEU:HD23	1:D:665:LEU:HA	1.82	0.42
1:B:185:VAL:HG12	1:B:338:LEU:HD11	2.01	0.41
1:B:579:GLY:HA3	1:B:587:CYS:SG	2.60	0.41
1:B:782:ILE:HA	1:B:783:PRO:HD2	1.93	0.41
1:C:191:LEU:HG	1:C:226:GLU:HG2	2.02	0.41
1:C:817:PRO:HA	1:C:818:PRO:HD3	1.91	0.41
1:D:277:TYR:CZ	1:D:284:PRO:HG3	2.55	0.41
1:A:92:ASP:HA	1:A:830:ILE:HB	2.02	0.41
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:PRO:HB2	1:A:693:PRO:HD3	2.02	0.41
1:D:165:LEU:HD12	1:D:165:LEU:HA	1.90	0.41
1:C:12:LYS:HE3	3:C:1180:HOH:O	2.19	0.41
1:A:196:THR:HA	1:A:199:GLN:HE21	1.85	0.41
1:B:71:GLN:O	1:B:75:MET:HG3	2.21	0.41
1:B:681:ALA:C	1:B:687:MET:HE3	2.45	0.41
1:A:719:GLU:HA	1:A:722:TRP:CE2	2.55	0.41
3:A:1238:HOH:O	1:B:839:SER:HA	2.18	0.41
1:B:654:PRO:HG3	1:B:686:PHE:HZ	1.86	0.41
1:D:379:GLN:HG3	3:D:1343:HOH:O	2.19	0.41
1:D:493:TRP:CE2	1:D:576:GLY:HA3	2.56	0.41
1:D:746:GLN:HE21	1:D:746:GLN:HB3	1.64	0.41
1:D:817:PRO:HA	1:D:818:PRO:HD3	1.91	0.41
1:A:597:GLU:CD	1:A:597:GLU:N	2.79	0.41
1:B:277:TYR:CZ	1:B:284:PRO:HG3	2.56	0.41
1:B:656:ALA:CB	1:B:657:PRO:CD	2.96	0.41
1:B:848:GLU:OE2	3:B:1055:HOH:O	2.22	0.41
1:D:415:ALA:HB1	1:D:416:PRO:HD2	2.03	0.41
1:B:682:PHE:HB3	3:B:1187:HOH:O	2.20	0.41
1:D:64:PHE:CD1	1:D:429:ARG:HD3	2.56	0.41
1:A:277:TYR:CZ	1:A:284:PRO:HG3	2.55	0.41
1:A:717:ILE:HD13	1:A:727:ALA:HB2	2.02	0.41
1:B:118:GLU:HG2	1:B:850:PHE:CE1	2.56	0.41
1:B:576:GLY:C	1:B:577:ILE:HG13	2.45	0.41
1:D:210:GLY:HA2	3:D:1012:HOH:O	2.20	0.41
1:D:671:PHE:HZ	1:D:673:LYS:HD2	1.86	0.41
1:A:169:GLN:O	1:A:173:GLN:HG2	2.20	0.41
1:B:485:VAL:HA	1:B:486:PRO:HD3	1.84	0.41
1:D:67:VAL:HG11	1:D:75:MET:CE	2.49	0.41
1:D:250:GLY:HA3	1:D:276:LEU:HD21	2.02	0.41
1:D:579:GLY:HA3	1:D:587:CYS:SG	2.61	0.41
1:A:552:SER:O	1:A:556:LEU:HB2	2.21	0.40
1:B:123:ASP:HA	1:B:124:PRO:HD2	1.93	0.40
1:B:166:MET:HE1	1:B:251:THR:OG1	2.21	0.40
1:B:552:SER:O	1:B:556:LEU:HB2	2.20	0.40
1:B:746:GLN:HE21	1:B:746:GLN:HA	1.84	0.40
1:D:513:LEU:HD12	1:D:513:LEU:HA	1.98	0.40
1:A:417:HIS:CD2	1:A:417:HIS:H	2.39	0.40
1:B:363:ASN:OD1	1:B:364:PRO:HD2	2.22	0.40
1:C:92:ASP:HA	1:C:830:ILE:HB	2.02	0.40
1:C:415:ALA:HB1	1:C:416:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:717:ILE:HA	1:C:718:PRO:HD3	1.92	0.40
1:D:240:ARG:CD	3:D:1005:HOH:O	2.69	0.40
1:D:597:GLU:CD	1:D:597:GLU:N	2.79	0.40
1:D:654:PRO:HG3	1:D:686:PHE:CZ	2.56	0.40
1:A:142:ASN:HD22	1:D:396:GLY:HA3	1.85	0.40
1:A:164:SER:HB2	1:A:338:LEU:HG	2.03	0.40
1:A:185:VAL:HG12	1:A:338:LEU:HD11	2.03	0.40
1:B:579:GLY:CA	1:B:587:CYS:SG	3.09	0.40
1:C:754:GLU:HG2	1:C:776:LYS:CD	2.50	0.40
1:D:820:GLU:HB2	3:D:1042:HOH:O	2.20	0.40
1:A:817:PRO:HA	1:A:818:PRO:HD3	1.91	0.40
1:B:597:GLU:CD	1:B:597:GLU:N	2.78	0.40
1:A:87:TYR:CE2	1:A:97:PRO:HG2	2.57	0.40
1:A:687:MET:HB2	1:A:740:VAL:HG12	2.04	0.40
1:B:499:MET:H	1:B:499:MET:HG2	1.70	0.40
1:D:610:ILE:HD13	1:D:682:PHE:HE1	1.87	0.40
1:D:670:VAL:HG12	1:D:671:PHE:N	2.36	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	852/965 (88%)	837 (98%)	14 (2%)	1 (0%)	48	50
1	B	853/965 (88%)	836 (98%)	16 (2%)	1 (0%)	48	50
1	C	854/965 (88%)	840 (98%)	13 (2%)	1 (0%)	48	50
1	D	854/965 (88%)	837 (98%)	16 (2%)	1 (0%)	48	50
All	All	3413/3860 (88%)	3350 (98%)	59 (2%)	4 (0%)	48	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	GLU
1	B	333	GLU
1	C	333	GLU
1	D	333	GLU

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	698/792 (88%)	664 (95%)	34 (5%)	22	19
1	B	698/792 (88%)	654 (94%)	44 (6%)	16	11
1	C	699/792 (88%)	661 (95%)	38 (5%)	20	16
1	D	699/792 (88%)	652 (93%)	47 (7%)	15	10
All	All	2794/3168 (88%)	2631 (94%)	163 (6%)	18	14

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LYS
1	A	114	SER
1	A	136	GLN
1	A	161	CYS
1	A	173	GLN
1	A	231	VAL
1	A	233	LEU
1	A	285	GLU
1	A	290	ILE
1	A	298	LYS
1	A	318	GLU
1	A	343	LYS
1	A	476	GLU
1	A	477	ARG
1	A	489	GLU
1	A	499	MET
1	A	513	LEU
1	A	515	ARG

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Mol	Chain	Res	Type
1	A	528	LYS
1	A	532	LEU
1	A	536	GLN
1	A	556	LEU
1	A	597	GLU
1	A	630	CYS
1	A	646	LYS
1	A	663	GLU
1	A	713	LEU
1	A	721	GLN
1	A	746	GLN
1	A	772	LYS
1	A	786	LYS
1	A	790	ARG
1	A	820	GLU
1	A	852	ASN
1	B	49	ARG
1	B	70	LYS
1	B	114	SER
1	B	118	GLU
1	B	136	GLN
1	B	195	ASN
1	B	231	VAL
1	B	233	LEU
1	B	285	GLU
1	B	290	ILE
1	B	298	LYS
1	B	315	THR
1	B	318	GLU
1	B	489	GLU
1	B	499	MET
1	B	513	LEU
1	B	528	LYS
1	B	532	LEU
1	B	536	GLN
1	B	556	LEU
1	B	597	GLU
1	B	611	LYS
1	B	625	LEU
1	B	626	SER
1	B	630	CYS
1	B	632	GLN

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Mol	Chain	Res	Type
1	B	633	ARG
1	B	639	VAL
1	B	646	LYS
1	B	664	GLN
1	B	666	ARG
1	B	674	GLU
1	B	675	VAL
1	B	676	ARG
1	B	688	GLU
1	B	713	LEU
1	B	721	GLN
1	B	725	SER
1	B	746	GLN
1	B	772	LYS
1	B	773	ARG
1	B	786	LYS
1	B	790	ARG
1	B	820	GLU
1	C	70	LYS
1	C	114	SER
1	C	136	GLN
1	C	217	THR
1	C	223	CYS
1	C	231	VAL
1	C	285	GLU
1	C	290	ILE
1	C	298	LYS
1	C	318	GLU
1	C	343	LYS
1	C	443	ARG
1	C	476	GLU
1	C	477	ARG
1	C	489	GLU
1	C	513	LEU
1	C	515	ARG
1	C	528	LYS
1	C	532	LEU
1	C	536	GLN
1	C	597	GLU
1	C	625	LEU
1	C	628	GLU
1	C	630	CYS

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Mol	Chain	Res	Type
1	C	632	GLN
1	C	633	ARG
1	C	639	VAL
1	C	646	LYS
1	C	666	ARG
1	C	674	GLU
1	C	713	LEU
1	C	721	GLN
1	C	725	SER
1	C	746	GLN
1	C	772	LYS
1	C	786	LYS
1	C	790	ARG
1	C	820	GLU
1	D	70	LYS
1	D	114	SER
1	D	118	GLU
1	D	125	GLU
1	D	136	GLN
1	D	173	GLN
1	D	231	VAL
1	D	233	LEU
1	D	240	ARG
1	D	285	GLU
1	D	290	ILE
1	D	298	LYS
1	D	315	THR
1	D	318	GLU
1	D	343	LYS
1	D	370	LEU
1	D	446	GLN
1	D	476	GLU
1	D	489	GLU
1	D	502[A]	GLN
1	D	502[B]	GLN
1	D	513	LEU
1	D	528	LYS
1	D	532	LEU
1	D	536	GLN
1	D	593	CYS
1	D	597	GLU
1	D	623	VAL

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Mol	Chain	Res	Type
1	D	629	GLU
1	D	631	LYS
1	D	651	ILE
1	D	664	GLN
1	D	665	LEU
1	D	667	LYS
1	D	673	LYS
1	D	676	ARG
1	D	709	SER
1	D	713	LEU
1	D	721	GLN
1	D	725	SER
1	D	728	ARG
1	D	772	LYS
1	D	786	LYS
1	D	790	ARG
1	D	802	ARG
1	D	820	GLU
1	D	852	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	173	GLN
1	A	179	GLN
1	A	199	GLN
1	A	271	GLN
1	A	360	HIS
1	A	399	ASN
1	A	560	GLN
1	A	746	GLN
1	A	852	ASN
1	B	169	GLN
1	B	173	GLN
1	B	179	GLN
1	B	199	GLN
1	B	271	GLN
1	B	331	HIS
1	B	358	HIS
1	B	360	HIS
1	B	375	GLN

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Mol	Chain	Res	Type
1	B	399	ASN
1	B	483	GLN
1	B	536	GLN
1	B	632	GLN
1	B	723	HIS
1	B	746	GLN
1	B	751	HIS
1	C	68	HIS
1	C	169	GLN
1	C	170	ASN
1	C	173	GLN
1	C	179	GLN
1	C	199	GLN
1	C	271	GLN
1	C	331	HIS
1	C	360	HIS
1	C	399	ASN
1	C	483	GLN
1	C	560	GLN
1	C	632	GLN
1	C	746	GLN
1	D	169	GLN
1	D	170	ASN
1	D	173	GLN
1	D	199	GLN
1	D	271	GLN
1	D	331	HIS
1	D	399	ASN
1	D	560	GLN
1	D	596	GLN
1	D	746	GLN
1	D	852	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	852/965 (88%)	-0.14	23 (2%) 56 60	8, 22, 56, 78	2 (0%)
1	B	852/965 (88%)	0.29	30 (3%) 47 51	15, 31, 63, 91	3 (0%)
1	C	855/965 (88%)	0.15	34 (3%) 42 47	13, 28, 60, 78	1 (0%)
1	D	854/965 (88%)	0.11	45 (5%) 32 36	10, 27, 60, 85	2 (0%)
All	All	3413/3860 (88%)	0.11	132 (3%) 43 48	8, 27, 60, 91	8 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	415	ALA	5.1
1	D	627	TRP	5.0
1	C	750	TRP	4.8
1	B	416	PRO	4.8
1	C	671	PHE	4.8
1	C	821	PHE	4.7
1	D	-1	SER	4.4
1	A	415	ALA	4.4
1	D	750	TRP	4.3
1	A	413	ALA	4.2
1	D	315	THR	4.2
1	D	630	CYS	4.2
1	D	670	VAL	4.2
1	D	671	PHE	4.1
1	A	42	ALA	4.0
1	C	488	GLY	4.0
1	B	750	TRP	4.0
1	D	416	PRO	4.0
1	C	853	GLY	3.9
1	D	672	ALA	3.9
1	D	648	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	416	PRO	3.7
1	C	790	ARG	3.7
1	B	415	ALA	3.7
1	C	415	ALA	3.7
1	C	315	THR	3.7
1	C	772	LYS	3.6
1	A	414	PRO	3.6
1	D	647	ASP	3.5
1	C	0	THR	3.5
1	C	648	THR	3.5
1	B	413	ALA	3.5
1	B	478	GLY	3.4
1	B	418	ALA	3.4
1	B	670	VAL	3.3
1	D	634	CYS	3.2
1	D	631	LYS	3.2
1	D	669	GLY	3.2
1	B	675	VAL	3.2
1	C	41	LYS	3.2
1	C	647	ASP	3.1
1	D	662	VAL	3.1
1	B	417	HIS	3.1
1	D	0	THR	3.0
1	B	671	PHE	3.0
1	D	478	GLY	3.0
1	D	821	PHE	3.0
1	C	670	VAL	3.0
1	B	315	THR	3.0
1	A	410	PRO	3.0
1	B	410	PRO	3.0
1	B	414	PRO	3.0
1	D	685	TYR	3.0
1	A	477	ARG	3.0
1	A	417	HIS	3.0
1	D	476	GLU	2.9
1	C	685	TYR	2.9
1	C	476	GLU	2.8
1	C	646	LYS	2.8
1	A	750	TRP	2.8
1	B	1	GLY	2.7
1	D	418	ALA	2.7
1	D	666	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	686	PHE	2.7
1	C	672	ALA	2.6
1	A	671	PHE	2.6
1	B	486	PRO	2.6
1	C	416	PRO	2.6
1	D	636	PRO	2.6
1	D	667	LYS	2.5
1	C	659	PHE	2.5
1	D	772	LYS	2.5
1	D	487	ALA	2.5
1	A	686	PHE	2.5
1	B	673	LYS	2.5
1	A	665	LEU	2.5
1	D	665	LEU	2.5
1	C	132	MET	2.5
1	B	669	GLY	2.5
1	D	125	GLU	2.4
1	D	668	GLU	2.4
1	B	361	SER	2.4
1	A	418	ALA	2.4
1	B	487	ALA	2.4
1	D	625	LEU	2.4
1	A	125	GLU	2.4
1	C	129	GLY	2.3
1	D	646	LYS	2.3
1	A	670	VAL	2.3
1	D	615	LEU	2.3
1	B	773	ARG	2.3
1	B	659	PHE	2.3
1	C	414	PRO	2.3
1	B	2	GLU	2.3
1	D	659	PHE	2.3
1	B	42	ALA	2.3
1	D	624	GLY	2.2
1	C	489	GLU	2.2
1	B	632	GLN	2.2
1	D	414	PRO	2.2
1	D	852	ASN	2.2
1	C	314	ALA	2.2
1	A	370	LEU	2.2
1	A	412	PRO	2.2
1	B	728	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	130	TYR	2.2
1	C	631	LYS	2.2
1	A	675	VAL	2.1
1	B	625	LEU	2.1
1	C	673	LYS	2.1
1	A	130	TYR	2.1
1	A	852	ASN	2.1
1	A	647	ASP	2.1
1	A	674	GLU	2.1
1	C	676	ARG	2.1
1	D	477	ARG	2.1
1	C	615	LEU	2.1
1	C	478	GLY	2.1
1	C	379	GLN	2.1
1	D	790	ARG	2.1
1	D	41	LYS	2.1
1	B	639	VAL	2.1
1	D	675	VAL	2.1
1	B	674	GLU	2.0
1	C	773	ARG	2.0
1	D	298	LYS	2.0
1	C	125	GLU	2.0
1	D	629	GLU	2.0
1	D	663	GLU	2.0
1	C	477	ARG	2.0
1	B	630	CYS	2.0
1	A	419	THR	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	CL	C	964	1/1	0.89	0.27	76,76,76,76	0
2	CL	D	964	1/1	0.91	0.18	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.