



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:06 AM UTC

PDB ID : 5TUO / pdb_00005tuo
Title : Crystal structure of the complex of Helicobacter pylori alpha-carbonic anhydrase with 5-amino-1,3,4-thiadiazole-2-sulfonamide inhibitor.
Authors : Modak, J.K.; Roujeinikova, A.
Deposited on : 2016-11-06
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

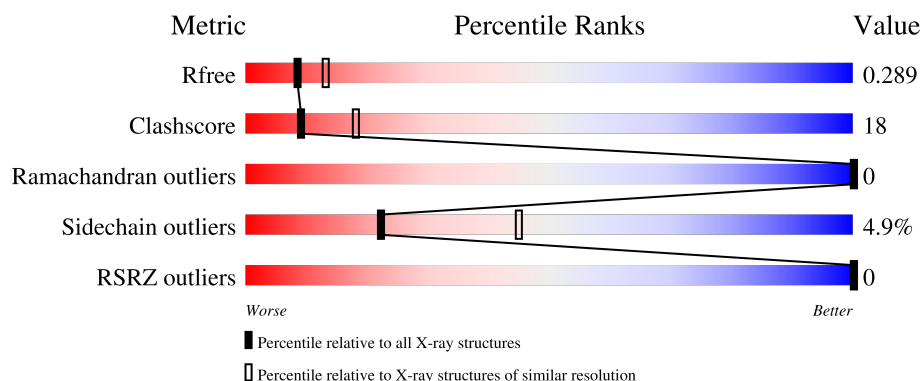
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

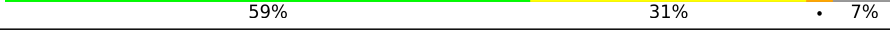
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	234	
1	B	234	
1	C	234	
1	D	234	
1	E	234	

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Mol	Chain	Length	Quality of chain
1	F	234	
1	G	234	
1	H	234	

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
4	1SA	A	303	-	X	-	-
4	1SA	B	303	-	X	-	-
4	1SA	C	303	-	X	-	-
4	1SA	D	303	-	X	-	-
4	1SA	E	303	-	X	-	-
4	1SA	F	302	-	X	-	-
4	1SA	G	303	-	X	-	-
4	1SA	H	303	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14560 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 Alpha-carbonic anhydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	1	0
			1838	1179	322	333	4			
1	B	217	Total	C	N	O	S	0	1	0
			1776	1138	310	324	4			
1	C	226	Total	C	N	O	S	0	1	0
			1853	1188	325	336	4			
1	D	218	Total	C	N	O	S	0	0	0
			1781	1144	311	323	3			
1	E	228	Total	C	N	O	S	0	1	0
			1868	1196	328	340	4			
1	F	199	Total	C	N	O	S	0	0	0
			1619	1046	280	289	4			
1	G	225	Total	C	N	O	S	0	1	0
			1846	1183	323	336	4			
1	H	218	Total	C	N	O	S	0	0	0
			1781	1142	312	323	4			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

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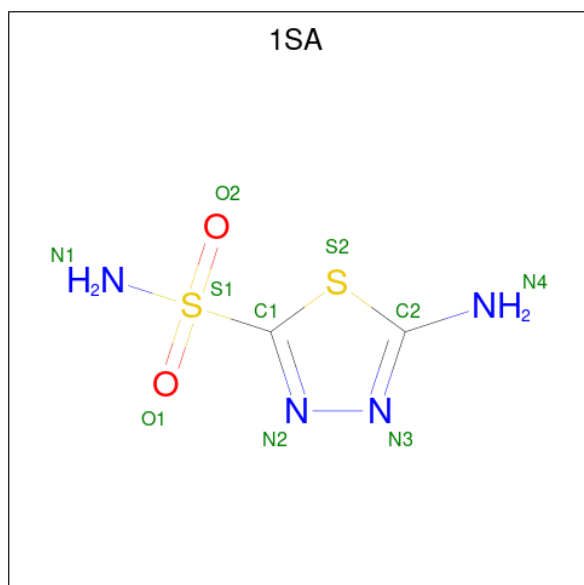
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 5-AMINO-1,3,4-THIADIAZOLE-2-SULFONAMIDE (CCD ID: 1SA) (formula: C₂H₄N₄O₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			10	2	4	2	2		
4	B	1	Total	C	N	O	S	0	0
			10	2	4	2	2		
4	C	1	Total	C	N	O	S	0	0
			10	2	4	2	2		
4	D	1	Total	C	N	O	S	0	0
			10	2	4	2	2		
4	E	1	Total	C	N	O	S	0	0
			10	2	4	2	2		
4	F	1	Total	C	N	O	S	0	0
			10	2	4	2	2		
4	G	1	Total	C	N	O	S	0	0
			10	2	4	2	2		
4	H	1	Total	C	N	O	S	0	0
			10	2	4	2	2		

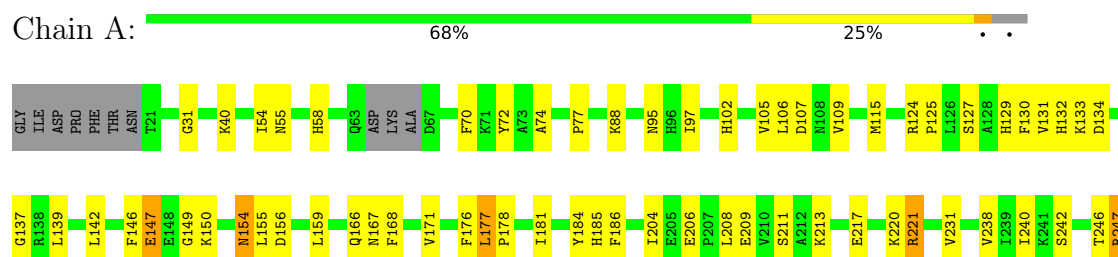
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	14	Total	O	0	0
			14	14		
5	C	17	Total	O	0	0
			17	17		
5	D	11	Total	O	0	0
			11	11		
5	E	5	Total	O	0	0
			5	5		
5	F	8	Total	O	0	0
			8	8		
5	G	21	Total	O	0	0
			21	21		
5	H	14	Total	O	0	0
			14	14		

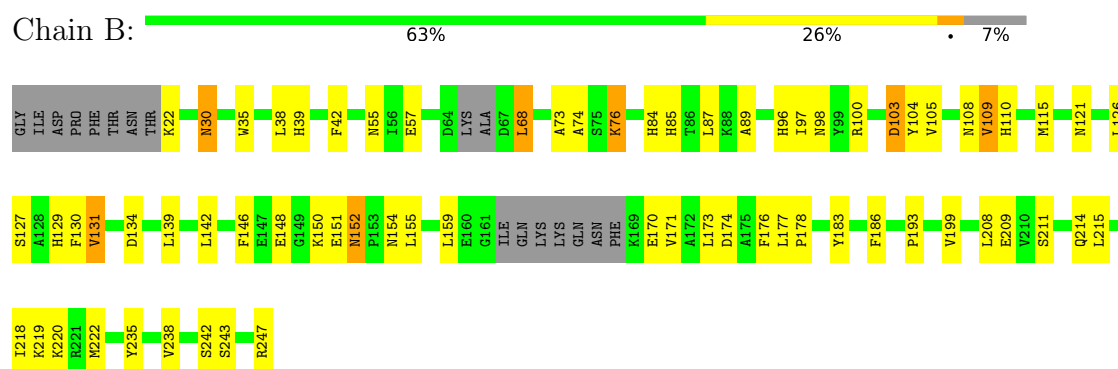
3 Residue-property plots

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

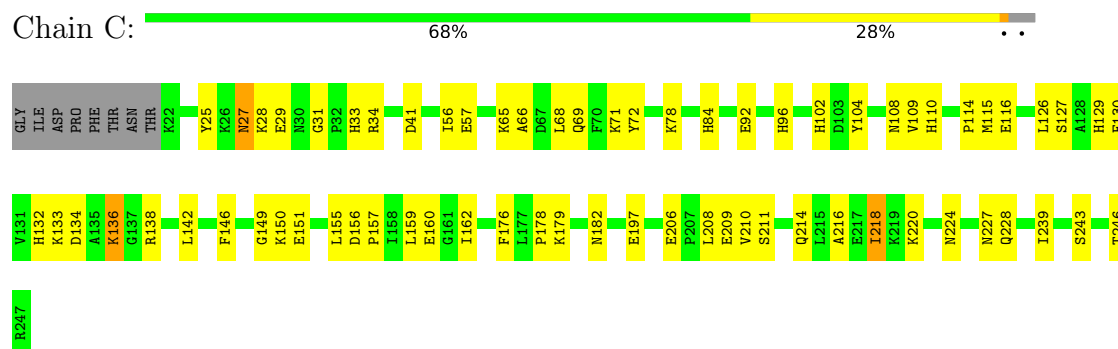
- Molecule 1: Alpha-carbonic anhydrase



- Molecule 1: Alpha-carbonic anhydrase



- Molecule 1: Alpha-carbonic anhydrase



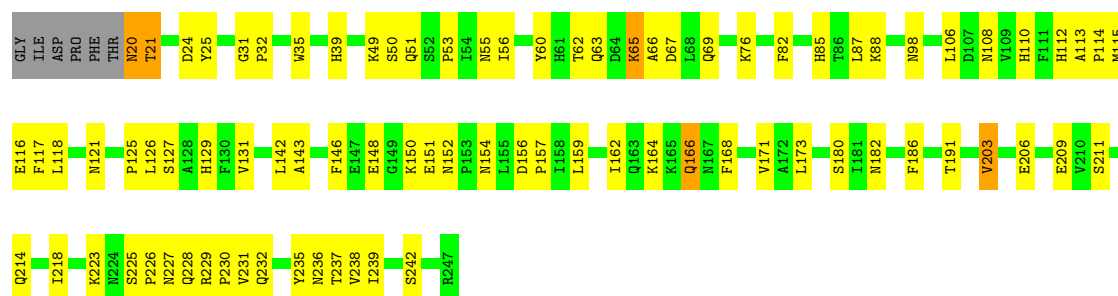
- Molecule 1: Alpha-carbonic anhydrase

Chain D: 

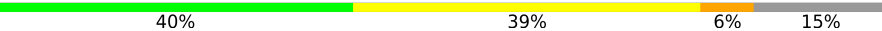


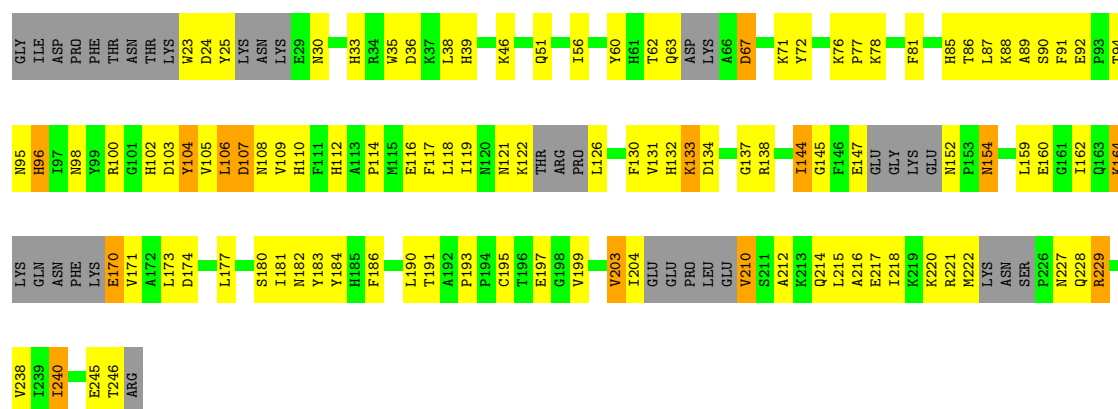
• Molecule 1: Alpha-carbonic anhydrase

Chain E: 



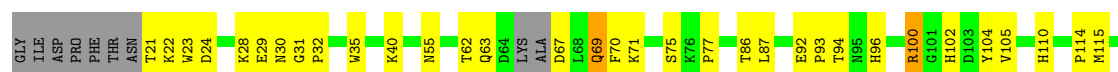
• Molecule 1: Alpha-carbonic anhydrase

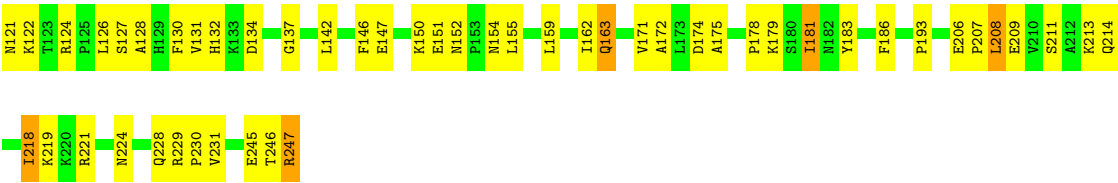
Chain F: 



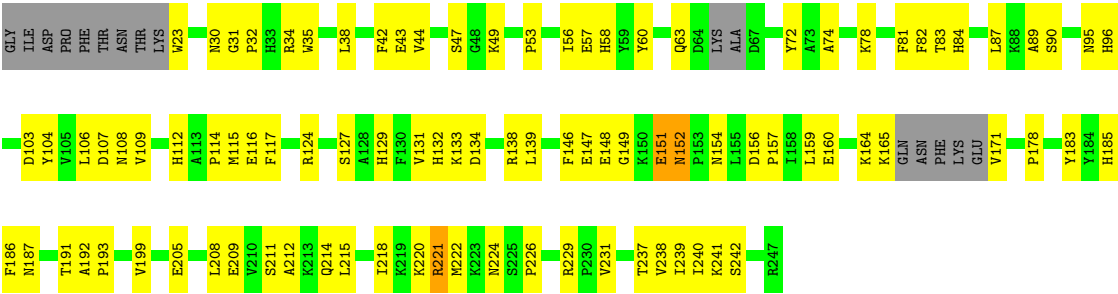
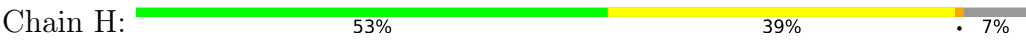
• Molecule 1: Alpha-carbonic anhydrase

Chain G: 





• Molecule 1: Alpha-carbonic anhydrase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.84Å 136.92Å 166.27Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	29.91 – 2.50 29.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.91-2.50) 99.6 (29.91-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.227 , 0.272 0.247 , 0.289	Depositor DCC
R_{free} test set	3273 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.120 for h,-k,-l	Xtriage
Reported twinning fraction	0.150 for h,-k,-l	Depositor
Outliers	1 of 64589 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14560	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ZN, 1SA

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	0.59	0/1895	0.96	6/2562 (0.2%)
1	B	0.65	0/1831	0.95	5/2476 (0.2%)
1	C	0.64	0/1911	0.92	2/2584 (0.1%)
1	D	0.54	0/1832	0.92	5/2476 (0.2%)
1	E	0.60	0/1926	0.93	4/2605 (0.2%)
1	F	0.58	0/1664	0.93	4/2248 (0.2%)
1	G	0.66	0/1903	0.95	5/2573 (0.2%)
1	H	0.66	0/1833	0.96	4/2479 (0.2%)
All	All	0.62	0/14795	0.94	35/20003 (0.2%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	100	ARG	N-CA-C	10.73	126.14	111.54
1	A	31	GLY	CA-C-N	9.20	129.80	119.32
1	A	31	GLY	C-N-CA	9.20	129.80	119.32
1	F	107	ASP	N-CA-C	8.61	120.28	111.07
1	A	156	ASP	CA-C-N	-8.00	111.55	119.87
1	A	156	ASP	C-N-CA	-8.00	111.55	119.87
1	E	31	GLY	CA-C-N	6.71	128.23	119.84
1	E	31	GLY	C-N-CA	6.71	128.23	119.84
1	B	76	LYS	CA-C-N	6.18	126.50	119.83
1	B	76	LYS	C-N-CA	6.18	126.50	119.83
1	G	31	GLY	CA-C-N	6.04	126.48	119.47
1	G	31	GLY	C-N-CA	6.04	126.48	119.47
1	D	31	GLY	CA-C-N	5.98	125.69	119.05
1	D	31	GLY	C-N-CA	5.98	125.69	119.05
1	H	31	GLY	CA-C-N	5.83	125.97	119.32
1	H	31	GLY	C-N-CA	5.83	125.97	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	206	GLU	CA-C-N	5.67	127.91	120.25
1	D	206	GLU	C-N-CA	5.67	127.91	120.25
1	B	152	ASN	CA-C-N	5.63	125.30	119.05
1	B	152	ASN	C-N-CA	5.63	125.30	119.05
1	G	181	ILE	N-CA-C	5.62	117.50	108.85
1	F	107	ASP	CB-CA-C	-5.60	102.09	110.88
1	F	154	ASN	N-CA-C	-5.46	105.48	111.82
1	E	76	LYS	CA-C-N	5.46	125.38	119.76
1	E	76	LYS	C-N-CA	5.46	125.38	119.76
1	A	70	PHE	N-CA-C	5.39	117.09	108.41
1	D	162	ILE	CB-CA-C	-5.38	105.08	111.97
1	C	31	GLY	CA-C-N	5.28	125.09	119.28
1	C	31	GLY	C-N-CA	5.28	125.09	119.28
1	G	183	TYR	N-CA-C	5.22	118.10	109.85
1	H	152	ASN	CA-C-N	5.10	124.89	119.28
1	H	152	ASN	C-N-CA	5.10	124.89	119.28
1	B	131	VAL	N-CA-C	5.08	115.89	108.58
1	F	199	VAL	CB-CA-C	-5.06	104.83	110.96
1	A	242	SER	N-CA-C	5.02	114.67	108.19

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	1838	0	1800	46	0
1	B	1776	0	1728	59	0
1	C	1853	0	1816	48	0
1	D	1781	0	1729	65	0
1	E	1868	0	1829	80	0
1	F	1619	0	1566	110	0
1	G	1846	0	1804	58	0
1	H	1781	0	1736	71	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	1	0
3	E	1	0	0	1	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	10	0	4	0	0
4	B	10	0	3	3	0
4	C	10	0	4	1	0
4	D	10	0	4	2	0
4	E	10	0	3	1	0
4	F	10	0	3	0	0
4	G	10	0	3	0	0
4	H	10	0	4	3	0
5	A	13	0	0	2	0
5	B	14	0	0	2	0
5	C	17	0	0	1	0
5	D	11	0	0	2	0
5	E	5	0	0	0	0
5	F	8	0	0	0	0
5	G	21	0	0	0	0
5	H	14	0	0	1	0
All	All	14560	0	14036	520	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 18.

All (520) 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:G:67:ASP:HB3	1:G:100:ARG:CG	1.71	1.19
1:B:159:LEU:HD21	1:B:218:ILE:CG1	1.73	1.17
1:A:181:ILE:HD12	1:A:246:THR:HG21	1.25	1.12
1:F:100:ARG:NH2	1:F:138:ARG:HH12	1.50	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:HIS:HA	1:E:223:LYS:HE2	1.33	1.06
1:E:236:ASN:ND2	1:F:100:ARG:HE	1.53	1.06
1:B:159:LEU:HD21	1:B:218:ILE:HG12	1.04	1.03
1:G:67:ASP:HB3	1:G:100:ARG:HG2	1.36	1.03
1:E:82:PHE:HZ	1:E:223:LYS:CE	1.72	1.00
1:F:100:ARG:HH21	1:F:138:ARG:NH1	1.62	0.98
1:C:108:ASN:HD21	1:C:110:HIS:HD1	1.14	0.96
1:E:82:PHE:CZ	1:E:223:LYS:HE2	2.02	0.94
1:B:159:LEU:CD2	1:B:218:ILE:HG12	1.98	0.94
1:A:181:ILE:HD12	1:A:246:THR:CG2	1.98	0.93
1:D:87:LEU:HD13	1:D:223:LYS:CE	1.98	0.93
1:E:127:SER:OG	3:E:302:CL:CL	2.23	0.92
1:F:91:PHE:CE2	1:F:109:VAL:HG12	2.05	0.91
1:G:67:ASP:HB3	1:G:100:ARG:HG3	1.50	0.90
1:F:116:GLU:OE1	1:F:191:THR:HG21	1.72	0.90
1:E:65:LYS:HB3	1:E:242:SER:OG	1.73	0.89
1:F:91:PHE:HE2	1:F:109:VAL:HG12	1.35	0.88
1:C:66:ALA:CB	1:C:243:SER:O	2.22	0.88
1:B:110:HIS:CE1	4:B:303:1SA:S2	2.68	0.87
1:E:85:HIS:ND1	1:E:223:LYS:HE3	1.89	0.87
1:E:82:PHE:HZ	1:E:223:LYS:HE2	1.33	0.86
1:C:216:ALA:O	1:C:220:LYS:HG3	1.76	0.86
1:E:82:PHE:HZ	1:E:223:LYS:NZ	1.72	0.85
1:A:124:ARG:NH1	1:A:147:GLU:OE1	2.09	0.85
1:H:220:LYS:HG2	1:H:224:ASN:HD21	1.41	0.85
1:D:178:PRO:HD3	1:D:208:LEU:HD21	1.58	0.84
1:G:67:ASP:CB	1:G:100:ARG:HG2	2.08	0.84
1:E:55:ASN:HD21	1:E:121:ASN:HA	1.43	0.83
1:C:66:ALA:HB2	1:C:243:SER:O	1.78	0.82
1:E:85:HIS:HA	1:E:223:LYS:CE	2.12	0.80
1:F:76:LYS:HG2	1:F:170:GLU:HG3	1.64	0.79
1:E:69:GLN:HG3	1:E:98:ASN:HB3	1.63	0.79
1:E:82:PHE:HZ	1:E:223:LYS:HZ3	1.26	0.78
1:B:183:TYR:OH	5:B:401:HOH:O	2.00	0.78
1:D:82:PHE:CE2	1:D:223:LYS:HA	2.19	0.78
1:E:82:PHE:CZ	1:E:223:LYS:CE	2.60	0.77
1:F:100:ARG:HH21	1:F:138:ARG:HH12	0.80	0.76
1:A:181:ILE:CD1	1:A:246:THR:HG21	2.13	0.75
1:H:107:ASP:OD2	1:H:108:ASN:ND2	2.18	0.75
1:F:104:TYR:OH	1:F:138:ARG:NH2	2.20	0.75
1:B:110:HIS:HE1	4:B:303:1SA:S2	2.09	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:ASP:OD1	1:E:214:GLN:NE2	2.21	0.74
1:B:98:ASN:ND2	1:B:103:ASP:OD1	2.21	0.73
1:D:87:LEU:HD13	1:D:223:LYS:HE2	1.70	0.73
1:F:114:PRO:HD2	1:F:228:GLN:CD	2.13	0.73
1:D:177:LEU:O	1:D:247:ARG:NH2	2.21	0.73
1:F:147:GLU:O	1:F:210:VAL:N	2.22	0.73
1:E:115:MET:HA	1:E:127:SER:HB2	1.71	0.73
1:F:71:LYS:HE3	1:F:96:HIS:HD2	1.52	0.73
1:G:28:LYS:HG2	1:G:29:GLU:H	1.54	0.73
1:C:115:MET:HG3	1:C:127:SER:HB3	1.72	0.72
1:G:71:LYS:HE2	1:G:96:HIS:HB2	1.70	0.72
1:B:152:ASN:O	1:B:214:GLN:NE2	2.24	0.71
1:E:159:LEU:HD21	1:E:218:ILE:HG12	1.71	0.71
1:F:118:LEU:HD22	1:F:122:LYS:HA	1.72	0.71
1:E:110:HIS:HE1	1:E:131:VAL:CG2	2.03	0.71
1:F:106:LEU:HB2	1:F:132:HIS:CE1	2.26	0.70
1:E:236:ASN:HD22	1:F:100:ARG:HE	1.38	0.70
1:B:68:LEU:HD11	1:B:97:ILE:HG23	1.73	0.69
1:F:112:HIS:O	1:F:126:LEU:HD12	1.92	0.69
1:D:58:HIS:O	5:D:401:HOH:O	2.11	0.69
1:F:105:VAL:O	1:F:132:HIS:HA	1.92	0.69
1:C:178:PRO:O	1:C:246:THR:OG1	2.10	0.69
1:G:67:ASP:CB	1:G:100:ARG:HE	2.06	0.69
1:G:92:GLU:HB3	1:G:93:PRO:HD2	1.75	0.69
1:F:117:PHE:O	1:F:118:LEU:HD23	1.92	0.69
1:G:63:GLN:HE22	1:H:63:GLN:HE22	1.41	0.69
1:F:102:HIS:HB2	1:F:104:TYR:HE1	1.58	0.69
1:C:130:PHE:HB2	1:C:142:LEU:HB2	1.73	0.68
1:D:112:HIS:CE1	1:D:116:GLU:OE2	2.46	0.68
1:D:112:HIS:ND1	1:D:116:GLU:OE2	2.26	0.68
1:F:217:GLU:O	1:F:221:ARG:N	2.26	0.68
1:C:176:PHE:O	5:C:402:HOH:O	2.12	0.68
1:H:82:PHE:HB2	1:H:221:ARG:NH1	2.08	0.68
1:F:112:HIS:CE1	1:F:116:GLU:OE2	2.47	0.68
1:H:187:ASN:ND2	5:H:401:HOH:O	2.08	0.68
1:C:159:LEU:HD21	1:C:218:ILE:HD12	1.75	0.68
1:A:177:LEU:O	1:A:247:ARG:NH2	2.26	0.68
1:C:108:ASN:ND2	1:C:110:HIS:HD1	1.90	0.67
1:G:152:ASN:HB3	1:G:155:LEU:HB2	1.74	0.67
1:A:178:PRO:O	1:A:246:THR:OG1	2.11	0.67
1:D:49:LYS:O	5:D:402:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:TYR:OH	1:A:132:HIS:NE2	2.28	0.67
1:D:33:HIS:O	1:D:33:HIS:ND1	2.27	0.67
1:A:124:ARG:HH11	1:A:147:GLU:CD	2.03	0.67
1:D:87:LEU:HD13	1:D:223:LYS:HE3	1.74	0.66
1:D:161:GLY:O	1:D:168:PHE:HE1	1.77	0.66
1:E:191:THR:N	4:E:303:1SA:O2	2.27	0.66
1:A:102:HIS:HE1	1:A:134:ASP:OD2	1.79	0.65
1:D:162:ILE:HG21	1:D:223:LYS:HZ3	1.62	0.65
1:B:178:PRO:HD3	1:B:208:LEU:HD21	1.79	0.65
1:C:220:LYS:HA	1:C:224:ASN:ND2	2.11	0.64
1:G:211:SER:HB2	1:G:214:GLN:HG3	1.79	0.63
1:H:109:VAL:HA	1:H:129:HIS:O	1.98	0.63
1:D:63:GLN:N	1:D:63:GLN:OE1	2.32	0.63
1:E:110:HIS:CE1	1:E:131:VAL:CG2	2.80	0.63
1:H:87:LEU:H	1:H:222:MET:HE2	1.63	0.62
1:H:124:ARG:HB3	1:H:146:PHE:O	2.00	0.62
1:G:126:LEU:HB3	1:G:146:PHE:HB2	1.81	0.62
1:D:219:LYS:O	1:D:224:ASN:HA	2.00	0.62
1:G:181:ILE:HA	1:G:206:GLU:OE2	1.99	0.62
1:A:134:ASP:OD1	1:A:137:GLY:N	2.32	0.62
1:D:86:THR:OG1	1:D:111:PHE:O	2.18	0.62
1:D:82:PHE:HD2	1:D:223:LYS:HG2	1.65	0.62
1:C:33:HIS:CD2	1:C:34:ARG:HG3	2.35	0.61
1:B:76:LYS:HA	1:B:170:GLU:HA	1.81	0.61
1:E:20:ASN:O	1:E:21:THR:HG22	2.01	0.61
1:F:62:THR:OG1	1:F:63:GLN:N	2.31	0.61
1:D:76:LYS:HD3	1:D:168:PHE:O	2.01	0.61
1:D:54:ILE:HA	1:D:231:VAL:HG13	1.83	0.60
1:F:126:LEU:HD13	1:F:218:ILE:HD13	1.82	0.60
1:E:110:HIS:CE1	1:E:131:VAL:HG21	2.36	0.60
1:F:100:ARG:NH2	1:F:138:ARG:NH1	2.35	0.60
1:F:88:LYS:HG3	1:F:108:ASN:OD1	2.02	0.60
1:H:178:PRO:HD3	1:H:208:LEU:HD21	1.82	0.60
1:H:183:TYR:CZ	1:H:242:SER:HB3	2.37	0.60
1:A:54:ILE:HA	1:A:231:VAL:HG13	1.83	0.60
1:F:23:TRP:HZ3	1:F:25:TYR:HE1	1.48	0.60
1:G:186:PHE:HA	1:H:238:VAL:HG21	1.84	0.59
1:A:217:GLU:HA	1:A:220:LYS:HB3	1.84	0.59
1:F:100:ARG:O	1:F:100:ARG:HG2	2.02	0.59
1:C:78:LYS:NZ	1:C:92:GLU:HG3	2.16	0.59
1:D:129:HIS:NE2	3:D:302:CL:CL	2.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:THR:OG1	1:E:63:GLN:N	2.34	0.59
1:E:69:GLN:HE21	1:E:98:ASN:CG	2.10	0.59
1:G:67:ASP:HB2	1:G:100:ARG:HE	1.65	0.59
1:A:88:LYS:NZ	5:A:401:HOH:O	2.35	0.59
1:F:116:GLU:OE1	1:F:191:THR:CG2	2.50	0.59
1:H:47:SER:O	1:H:49:LYS:NZ	2.36	0.59
1:F:106:LEU:HB2	1:F:132:HIS:ND1	2.17	0.58
1:G:122:LYS:HE3	1:G:124:ARG:HH11	1.68	0.58
1:H:109:VAL:HG13	1:H:109:VAL:O	2.02	0.58
1:A:130:PHE:HB2	1:A:142:LEU:HB3	1.85	0.58
1:E:69:GLN:HE21	1:E:98:ASN:HB3	1.67	0.58
1:E:112:HIS:CE1	1:E:116:GLU:OE2	2.56	0.58
1:G:147:GLU:HG2	1:G:207:PRO:HB2	1.85	0.58
1:E:25:TYR:CE2	1:E:227:ASN:HB2	2.38	0.58
1:G:55:ASN:ND2	1:G:121:ASN:OD1	2.35	0.58
1:F:71:LYS:HE3	1:F:96:HIS:CD2	2.38	0.58
1:F:91:PHE:HE2	1:F:109:VAL:CG1	2.11	0.58
1:C:65:LYS:HB2	1:H:63:GLN:HB2	1.86	0.58
1:C:33:HIS:HD2	1:C:34:ARG:HG3	1.69	0.57
1:E:21:THR:HG23	1:E:21:THR:O	2.04	0.57
1:G:163:GLN:HA	1:G:221:ARG:HH12	1.69	0.57
1:H:104:TYR:HB3	1:H:132:HIS:HB3	1.85	0.57
1:B:151:GLU:HA	1:B:211:SER:HB3	1.85	0.57
1:B:174:ASP:OD1	1:B:174:ASP:N	2.36	0.57
1:D:104:TYR:HB3	1:D:132:HIS:HB3	1.87	0.57
1:F:78:LYS:HG3	1:F:92:GLU:HG2	1.86	0.57
1:C:78:LYS:HZ1	1:C:92:GLU:HG3	1.70	0.57
1:C:126:LEU:HB3	1:C:146:PHE:HB2	1.87	0.57
1:G:67:ASP:CB	1:G:100:ARG:CG	2.64	0.57
1:F:72:TYR:OH	1:F:132:HIS:HE1	1.89	0.56
1:H:82:PHE:HB2	1:H:221:ARG:HH12	1.69	0.56
1:F:86:THR:OG1	1:F:110:HIS:HB2	2.05	0.56
1:A:149:GLY:HA3	1:A:209:GLU:CD	2.30	0.56
1:B:219:LYS:HA	1:B:222:MET:HE3	1.86	0.56
1:C:102:HIS:CD2	1:C:136:LYS:HE3	2.40	0.56
1:F:119:ILE:HD13	1:F:184:TYR:HE2	1.71	0.56
1:F:152:ASN:O	1:F:214:GLN:NE2	2.38	0.56
1:B:159:LEU:CD2	1:B:218:ILE:CG1	2.65	0.56
1:E:69:GLN:HE21	1:E:98:ASN:CB	2.18	0.56
1:F:105:VAL:O	1:F:132:HIS:CA	2.54	0.56
1:H:35:TRP:HA	1:H:38:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ILE:HG21	1:A:204:ILE:HG12	1.88	0.56
1:C:211:SER:HB3	1:C:214:GLN:HG3	1.87	0.56
1:C:27:ASN:HD22	1:C:27:ASN:H	1.53	0.56
1:A:155:LEU:O	1:A:159:LEU:HD12	2.06	0.55
1:H:32:PRO:HA	1:H:35:TRP:CE2	2.41	0.55
1:H:53:PRO:HG3	1:H:116:GLU:HB3	1.88	0.55
1:C:56:ILE:HG23	1:C:239:ILE:HD13	1.87	0.55
1:F:104:TYR:CD1	1:F:104:TYR:N	2.73	0.55
1:G:130:PHE:HB2	1:G:142:LEU:HB3	1.88	0.55
1:B:55:ASN:HD21	1:B:121:ASN:ND2	2.05	0.55
1:E:65:LYS:O	1:E:66:ALA:HB3	2.05	0.55
1:F:95:ASN:ND2	1:F:173:LEU:HD13	2.22	0.55
1:F:98:ASN:ND2	1:F:103:ASP:OD1	2.34	0.55
1:G:63:GLN:HE22	1:H:63:GLN:NE2	2.02	0.55
1:D:62:THR:OG1	1:D:63:GLN:N	2.34	0.55
1:E:110:HIS:HE1	1:E:131:VAL:HG21	1.71	0.55
1:G:179:LYS:O	1:G:245:GLU:HA	2.07	0.55
1:B:84:HIS:O	1:B:85:HIS:HB2	2.07	0.55
1:B:177:LEU:O	1:B:247:ARG:NH1	2.31	0.55
1:E:55:ASN:HD21	1:E:121:ASN:CA	2.17	0.55
1:F:144:ILE:HA	1:F:204:ILE:HG12	1.88	0.55
1:F:107:ASP:OD1	1:F:108:ASN:ND2	2.35	0.54
1:C:66:ALA:O	1:C:68:LEU:N	2.39	0.54
1:H:221:ARG:HD2	1:H:221:ARG:O	2.08	0.54
1:F:78:LYS:HD3	1:F:92:GLU:OE2	2.07	0.54
1:C:220:LYS:HG2	1:C:224:ASN:HD21	1.72	0.54
1:C:84:HIS:HB2	4:C:303:1SA:HN41	1.73	0.53
1:D:120:ASN:O	1:D:121:ASN:HB2	2.08	0.53
1:D:172:ALA:HB1	1:D:175:ALA:HB3	1.89	0.53
1:E:53:PRO:HG3	1:E:116:GLU:HB3	1.90	0.53
1:F:104:TYR:N	1:F:104:TYR:HD1	2.07	0.53
1:H:124:ARG:NH1	1:H:147:GLU:OE1	2.41	0.53
1:A:150:LYS:NZ	5:A:403:HOH:O	2.40	0.53
1:E:67:ASP:OD2	1:F:60:TYR:CZ	2.62	0.53
1:F:67:ASP:OD1	1:F:183:TYR:OH	2.26	0.53
1:H:89:ALA:O	1:H:108:ASN:HB2	2.09	0.53
1:F:56:ILE:HD11	1:F:203:VAL:HG11	1.91	0.53
1:D:107:ASP:OD2	1:D:108:ASN:ND2	2.41	0.53
1:F:105:VAL:O	1:F:132:HIS:HB3	2.09	0.53
1:B:38:LEU:O	1:B:39:HIS:ND1	2.42	0.52
1:D:191:THR:O	1:D:229:ARG:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:ILE:HG23	1:E:239:ILE:HD13	1.91	0.52
1:E:164:LYS:HD2	1:E:168:PHE:HA	1.90	0.52
1:H:35:TRP:CE3	1:H:193:PRO:HD3	2.43	0.52
1:H:164:LYS:HG2	1:H:165:LYS:H	1.74	0.52
1:D:82:PHE:CD2	1:D:223:LYS:HG2	2.44	0.52
1:E:151:GLU:HA	1:E:211:SER:HB3	1.92	0.52
1:B:74:ALA:HA	1:B:171:VAL:O	2.09	0.52
1:F:109:VAL:O	1:F:109:VAL:HG13	2.09	0.52
1:H:82:PHE:CE1	1:H:222:MET:HA	2.45	0.52
1:B:174:ASP:OD2	5:B:402:HOH:O	2.19	0.52
1:A:166:GLN:HG2	1:A:167:ASN:N	2.24	0.52
1:E:21:THR:OG1	1:E:39:HIS:CE1	2.63	0.52
1:F:190:LEU:HB2	1:F:195:CYS:HA	1.90	0.52
1:F:36:ASP:HB3	1:F:46:LYS:HD3	1.90	0.52
1:B:152:ASN:HB2	1:B:209:GLU:O	2.10	0.52
1:B:68:LEU:HD11	1:B:97:ILE:CG2	2.37	0.52
1:F:184:TYR:HA	1:F:240:ILE:O	2.09	0.52
1:F:23:TRP:CZ3	1:F:25:TYR:HE1	2.27	0.52
1:F:103:ASP:C	1:F:104:TYR:HD1	2.18	0.52
1:H:84:HIS:O	4:H:303:1SA:N4	2.42	0.51
1:F:91:PHE:CE2	1:F:109:VAL:CG1	2.86	0.51
1:E:60:TYR:CE2	1:F:240:ILE:HD12	2.46	0.51
1:F:25:TYR:CD2	1:F:227:ASN:HA	2.45	0.51
1:B:159:LEU:HD11	1:B:218:ILE:HD11	1.92	0.51
1:F:114:PRO:HD2	1:F:228:GLN:HG2	1.91	0.51
1:F:212:ALA:HA	1:F:215:LEU:HB3	1.92	0.51
1:H:148:GLU:OE2	1:H:212:ALA:HB2	2.10	0.51
1:H:164:LYS:HG2	1:H:165:LYS:N	2.26	0.51
1:H:215:LEU:O	1:H:218:ILE:HG22	2.10	0.51
1:C:159:LEU:O	1:C:162:ILE:HG22	2.10	0.51
1:G:24:ASP:OD2	1:G:30:ASN:HB2	2.11	0.51
1:G:75:SER:N	1:G:171:VAL:O	2.40	0.51
1:B:89:ALA:O	1:B:108:ASN:HB2	2.11	0.51
1:G:219:LYS:HG2	1:G:224:ASN:HA	1.93	0.51
1:E:223:LYS:HB3	1:E:225:SER:HB3	1.92	0.50
1:A:181:ILE:CG2	1:A:204:ILE:HG12	2.40	0.50
1:E:87:LEU:HD12	1:E:88:LYS:H	1.75	0.50
1:F:114:PRO:HD2	1:F:228:GLN:CG	2.41	0.50
1:G:114:PRO:HD2	1:G:228:GLN:HB2	1.93	0.50
1:G:178:PRO:HD3	1:G:208:LEU:HD11	1.93	0.50
1:B:159:LEU:HD21	1:B:218:ILE:HG13	1.82	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:134:ASP:OD2	1:H:138:ARG:HD3	2.12	0.50
1:F:102:HIS:HB2	1:F:104:TYR:CE1	2.44	0.50
1:F:174:ASP:OD1	1:F:174:ASP:N	2.43	0.50
1:D:32:PRO:HA	1:D:35:TRP:CD2	2.46	0.50
1:D:162:ILE:CG2	1:D:223:LYS:NZ	2.74	0.50
1:F:216:ALA:O	1:F:220:LYS:HG2	2.12	0.50
1:H:221:ARG:HG3	1:H:221:ARG:HH11	1.76	0.50
1:A:154:ASN:ND2	1:A:176:PHE:HA	2.26	0.49
1:F:24:ASP:HB3	1:F:30:ASN:HB2	1.92	0.49
1:G:70:PHE:CD1	1:G:246:THR:HG22	2.47	0.49
1:G:159:LEU:HD21	1:G:218:ILE:HG13	1.93	0.49
1:B:68:LEU:CD1	1:B:97:ILE:HG23	2.42	0.49
1:H:151:GLU:HG2	1:H:214:GLN:CD	2.37	0.49
1:B:104:TYR:CE2	1:B:134:ASP:HB3	2.48	0.49
1:G:110:HIS:HE1	1:G:131:VAL:HG21	1.77	0.49
1:F:89:ALA:O	1:F:108:ASN:HB2	2.12	0.49
1:B:104:TYR:CD2	1:B:134:ASP:HB3	2.47	0.49
1:C:133:LYS:HG2	1:C:134:ASP:O	2.12	0.49
1:F:72:TYR:OH	1:F:132:HIS:CE1	2.66	0.49
1:C:27:ASN:H	1:C:27:ASN:ND2	2.09	0.49
1:G:70:PHE:HB2	1:G:246:THR:O	2.12	0.49
1:H:96:HIS:HB3	1:H:103:ASP:OD1	2.13	0.49
1:H:151:GLU:HG2	1:H:214:GLN:OE1	2.13	0.49
1:H:154:ASN:O	1:H:157:PRO:HD2	2.12	0.49
1:B:30:ASN:ND2	1:B:38:LEU:HD21	2.27	0.49
1:G:175:ALA:HA	1:G:247:ARG:NH1	2.28	0.49
1:A:154:ASN:OD1	1:A:154:ASN:N	2.46	0.49
1:A:154:ASN:HD22	1:A:176:PHE:HA	1.75	0.48
1:C:116:GLU:HA	1:C:228:GLN:HG3	1.94	0.48
1:D:215:LEU:O	1:D:219:LYS:HG3	2.13	0.48
1:F:130:PHE:O	1:F:132:HIS:CD2	2.66	0.48
1:H:74:ALA:HA	1:H:171:VAL:O	2.13	0.48
1:C:149:GLY:HA3	1:C:209:GLU:HG2	1.95	0.48
1:A:238:VAL:HG21	1:B:186:PHE:HA	1.95	0.48
1:B:154:ASN:ND2	1:B:176:PHE:HA	2.28	0.48
1:A:95:ASN:O	1:A:105:VAL:HG23	2.14	0.48
1:D:192:ALA:CB	4:D:303:1SA:N2	2.76	0.48
1:E:117:PHE:O	1:E:118:LEU:HD23	2.14	0.48
1:F:184:TYR:HB2	1:F:203:VAL:HG13	1.95	0.48
1:G:154:ASN:ND2	1:G:172:ALA:HB3	2.29	0.48
1:H:23:TRP:CZ2	1:H:84:HIS:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LYS:HE3	1:A:139:LEU:HD21	1.95	0.48
1:F:191:THR:O	1:F:229:ARG:HD2	2.14	0.48
1:B:131:VAL:HG21	4:B:303:1SA:S2	2.54	0.47
1:G:70:PHE:CG	1:G:246:THR:HG22	2.49	0.47
1:H:205:GLU:OE2	1:H:241:LYS:NZ	2.47	0.47
1:H:23:TRP:HH2	4:H:303:1SA:N4	2.11	0.47
1:A:186:PHE:HA	1:B:238:VAL:HG21	1.95	0.47
1:D:80:VAL:HG11	1:D:162:ILE:HD13	1.96	0.47
1:G:115:MET:HA	1:G:127:SER:HB2	1.96	0.47
1:B:55:ASN:ND2	1:B:57:GLU:OE2	2.47	0.47
1:E:223:LYS:HB2	1:E:225:SER:H	1.79	0.47
1:F:104:TYR:CD1	1:F:134:ASP:HB3	2.48	0.47
1:H:57:GLU:HB2	1:H:58:HIS:CE1	2.49	0.47
1:D:146:PHE:CD1	1:D:208:LEU:HB2	2.49	0.47
1:E:32:PRO:HA	1:E:35:TRP:CE2	2.50	0.47
1:G:93:PRO:HA	1:G:105:VAL:HG11	1.96	0.47
1:A:178:PRO:O	1:A:181:ILE:HD11	2.14	0.47
1:C:114:PRO:HD2	1:C:228:GLN:HB3	1.97	0.47
1:E:25:TYR:CD2	1:E:227:ASN:HA	2.48	0.47
1:E:49:LYS:HA	1:E:49:LYS:HD3	1.73	0.47
1:H:220:LYS:HG2	1:H:224:ASN:ND2	2.21	0.47
1:B:126:LEU:HG	1:B:127:SER:N	2.29	0.47
1:G:152:ASN:HB2	1:G:209:GLU:O	2.15	0.47
1:F:121:ASN:O	1:F:122:LYS:HB2	2.14	0.47
1:G:86:THR:OG1	1:G:87:LEU:N	2.48	0.47
1:D:57:GLU:OE1	1:D:120:ASN:ND2	2.47	0.47
1:D:130:PHE:N	1:D:130:PHE:CD1	2.83	0.47
1:E:112:HIS:HB2	1:E:127:SER:HB3	1.96	0.47
1:E:152:ASN:HB2	1:E:209:GLU:O	2.15	0.47
1:C:71:LYS:HB2	1:C:96:HIS:HB2	1.96	0.47
1:F:24:ASP:CG	1:F:25:TYR:N	2.73	0.47
1:D:115:MET:HG3	1:D:127:SER:HB3	1.96	0.46
1:G:174:ASP:O	1:G:247:ARG:HD3	2.15	0.46
1:H:81:PHE:CE2	1:H:83:THR:HB	2.50	0.46
1:A:178:PRO:HD3	1:A:208:LEU:HD21	1.96	0.46
1:E:110:HIS:CE1	1:E:129:HIS:HB2	2.51	0.46
1:B:30:ASN:ND2	1:B:38:LEU:HD11	2.30	0.46
1:B:115:MET:HG3	1:B:127:SER:HB3	1.95	0.46
1:G:162:ILE:HG12	1:G:162:ILE:O	2.14	0.46
1:D:217:GLU:O	1:D:220:LYS:HG2	2.16	0.46
1:A:74:ALA:HA	1:A:171:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:LEU:O	1:D:218:ILE:HG22	2.15	0.46
1:H:149:GLY:O	1:H:211:SER:HA	2.14	0.46
1:H:112:HIS:CD2	1:H:129:HIS:CE1	3.04	0.46
1:C:25:TYR:CD2	1:C:227:ASN:HA	2.50	0.46
1:H:56:ILE:HG23	1:H:239:ILE:HD13	1.98	0.46
1:H:152:ASN:HB2	1:H:209:GLU:O	2.16	0.46
1:H:237:THR:O	1:H:239:ILE:HG13	2.16	0.46
1:E:143:ALA:HB3	1:E:203:VAL:HG13	1.98	0.46
1:E:106:LEU:HD23	1:E:173:LEU:HD13	1.98	0.45
1:A:40:LYS:HE2	1:A:40:LYS:HB3	1.65	0.45
1:D:55:ASN:ND2	1:D:57:GLU:HG2	2.32	0.45
1:G:104:TYR:HB3	1:G:132:HIS:HB3	1.98	0.45
1:F:88:LYS:HA	1:F:110:HIS:HA	1.99	0.45
1:D:118:LEU:HD23	1:D:122:LYS:O	2.16	0.45
1:E:82:PHE:CZ	1:E:223:LYS:NZ	2.58	0.45
1:E:116:GLU:HA	1:E:228:GLN:HG3	1.99	0.45
1:F:217:GLU:CD	1:F:217:GLU:H	2.24	0.45
1:B:109:VAL:HA	1:B:129:HIS:O	2.15	0.45
1:B:220:LYS:HA	1:B:220:LYS:HD3	1.61	0.45
1:D:116:GLU:HG3	1:D:129:HIS:HE1	1.81	0.45
1:E:20:ASN:HD22	1:E:20:ASN:HA	1.60	0.45
1:H:35:TRP:CZ3	1:H:193:PRO:HD3	2.52	0.45
1:E:154:ASN:O	1:E:157:PRO:HD2	2.17	0.45
1:E:182:ASN:ND2	1:E:206:GLU:OE2	2.44	0.45
1:H:90:SER:HA	1:H:108:ASN:HB3	1.99	0.45
1:A:55:ASN:OD1	1:A:231:VAL:HG21	2.17	0.45
1:B:183:TYR:CZ	1:B:242:SER:HB3	2.52	0.45
1:D:211:SER:HB3	1:D:214:GLN:HB2	1.99	0.45
1:E:157:PRO:HB2	1:E:171:VAL:HG22	1.97	0.45
1:B:155:LEU:HB2	1:B:214:GLN:HE21	1.80	0.45
1:C:197:GLU:O	1:D:49:LYS:HG3	2.16	0.45
1:D:146:PHE:CE1	1:D:208:LEU:HB2	2.52	0.45
1:E:114:PRO:HA	1:E:125:PRO:O	2.17	0.45
1:C:156:ASP:N	1:C:157:PRO:HD2	2.32	0.45
1:D:81:PHE:CE1	1:D:83:THR:HB	2.52	0.45
1:D:144:ILE:HD13	1:D:177:LEU:HD22	1.98	0.45
1:E:126:LEU:HB3	1:E:146:PHE:HB2	1.97	0.45
1:H:220:LYS:HB3	1:H:220:LYS:HE3	1.74	0.45
1:B:76:LYS:HB2	1:B:170:GLU:HG2	2.00	0.44
1:D:87:LEU:HB2	1:D:223:LYS:HE3	1.98	0.44
1:E:35:TRP:HZ3	1:E:229:ARG:HD2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:PRO:HA	1:G:35:TRP:CE2	2.52	0.44
1:H:78:LYS:HB3	1:H:90:SER:OG	2.16	0.44
1:C:150:LYS:N	1:C:209:GLU:OE1	2.47	0.44
1:F:94:THR:HG23	1:F:95:ASN:OD1	2.17	0.44
1:G:77:PRO:HD3	1:G:171:VAL:HG23	1.98	0.44
1:A:106:LEU:HD12	1:A:131:VAL:O	2.18	0.44
1:B:235:TYR:N	1:B:235:TYR:CD1	2.84	0.44
1:F:38:LEU:C	1:F:39:HIS:CD2	2.96	0.44
1:A:40:LYS:HG3	1:C:41:ASP:OD1	2.17	0.44
1:G:151:GLU:HG2	1:G:214:GLN:CD	2.42	0.44
1:A:77:PRO:HD2	1:A:168:PHE:HB3	1.98	0.44
1:F:177:LEU:HB3	1:F:246:THR:HG21	1.98	0.44
1:D:157:PRO:HB2	1:D:171:VAL:HG22	2.00	0.44
1:A:181:ILE:HG23	1:A:204:ILE:HG23	2.00	0.44
1:A:217:GLU:O	1:A:221:ARG:N	2.43	0.44
1:B:139:LEU:HB2	1:B:199:VAL:HG22	1.99	0.44
1:C:129:HIS:HA	1:C:142:LEU:O	2.18	0.44
1:E:24:ASP:O	1:E:32:PRO:HD3	2.18	0.44
1:F:180:SER:HA	1:F:245:GLU:HG2	2.00	0.44
1:H:156:ASP:O	1:H:160:GLU:HG2	2.18	0.44
1:B:38:LEU:C	1:B:39:HIS:ND1	2.75	0.44
1:C:72:TYR:OH	1:C:132:HIS:NE2	2.37	0.44
1:C:130:PHE:HB3	1:C:132:HIS:HE1	1.83	0.44
1:D:192:ALA:HB2	4:D:303:1SA:N2	2.33	0.44
1:F:78:LYS:CG	1:F:92:GLU:HG2	2.46	0.44
1:C:133:LYS:HA	1:C:138:ARG:O	2.18	0.43
1:D:57:GLU:CD	1:D:120:ASN:HA	2.43	0.43
1:C:130:PHE:HB3	1:C:132:HIS:CE1	2.52	0.43
1:H:34:ARG:O	1:H:34:ARG:HG3	2.19	0.43
1:D:35:TRP:CZ3	1:D:193:PRO:HD3	2.52	0.43
1:D:113:ALA:HA	1:D:114:PRO:HA	1.78	0.43
1:E:150:LYS:N	1:E:209:GLU:OE1	2.30	0.43
1:F:33:HIS:O	1:F:46:LYS:NZ	2.38	0.43
1:B:30:ASN:HD22	1:B:30:ASN:HA	1.57	0.43
1:C:178:PRO:HD3	1:C:208:LEU:HD21	1.99	0.43
1:E:230:PRO:O	1:E:232:GLN:NE2	2.41	0.43
1:C:104:TYR:HB3	1:C:132:HIS:HB3	2.00	0.43
1:A:213:LYS:O	1:A:217:GLU:HG2	2.19	0.43
1:E:108:ASN:OD1	1:E:110:HIS:ND1	2.51	0.43
1:F:133:LYS:HA	1:F:138:ARG:O	2.18	0.43
1:D:206:GLU:HA	1:D:207:PRO:HD3	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:LEU:HD12	1:F:131:VAL:O	2.19	0.43
1:G:134:ASP:OD1	1:G:137:GLY:N	2.46	0.43
1:H:43:GLU:HG3	1:H:44:VAL:N	2.33	0.43
1:B:130:PHE:HB2	1:B:142:LEU:HB3	2.00	0.43
1:B:150:LYS:HB2	1:B:209:GLU:OE1	2.19	0.43
1:F:145:GLY:H	1:F:204:ILE:HD11	1.82	0.43
1:F:152:ASN:OD1	1:F:154:ASN:N	2.51	0.43
1:H:117:PHE:CE1	1:H:186:PHE:CZ	3.07	0.43
1:F:212:ALA:O	1:F:216:ALA:N	2.51	0.43
1:A:58:HIS:HB3	1:B:100:ARG:CZ	2.49	0.43
1:D:35:TRP:HA	1:D:38:LEU:HD13	2.01	0.43
1:F:105:VAL:O	1:F:132:HIS:CB	2.67	0.43
1:F:160:GLU:OE2	1:F:164:LYS:NZ	2.41	0.43
1:B:155:LEU:HB2	1:B:214:GLN:NE2	2.34	0.42
1:E:159:LEU:HA	1:E:159:LEU:HD23	1.82	0.42
1:F:215:LEU:HA	1:F:218:ILE:HG12	2.01	0.42
1:E:164:LYS:HD3	1:E:166:GLN:O	2.19	0.42
1:G:96:HIS:CD2	1:G:105:VAL:HG22	2.55	0.42
1:C:155:LEU:HD12	1:C:210:VAL:HG23	2.01	0.42
1:E:51:GLN:HB3	1:E:232:GLN:HG3	2.00	0.42
1:E:82:PHE:CE2	1:E:223:LYS:HE2	2.50	0.42
1:H:139:LEU:HD12	1:H:199:VAL:HG22	2.01	0.42
1:B:215:LEU:HD12	1:B:215:LEU:HA	1.86	0.42
1:F:35:TRP:CZ3	1:F:193:PRO:HD3	2.55	0.42
1:A:185:HIS:HB3	1:A:240:ILE:HD11	2.02	0.42
1:D:63:GLN:O	1:D:64:ASP:HB2	2.20	0.42
1:E:113:ALA:O	1:E:226:PRO:HA	2.19	0.42
1:F:177:LEU:CB	1:F:246:THR:HG21	2.50	0.42
1:H:82:PHE:HE1	1:H:222:MET:HG2	1.83	0.42
1:H:156:ASP:HB2	1:H:157:PRO:HD3	2.01	0.42
1:C:109:VAL:HA	1:C:129:HIS:O	2.19	0.42
1:F:90:SER:HA	1:F:108:ASN:HB3	2.01	0.42
1:H:72:TYR:CD1	1:H:95:ASN:HB3	2.54	0.42
1:B:96:HIS:CD2	1:B:105:VAL:HG23	2.54	0.42
1:D:82:PHE:CZ	1:D:85:HIS:HA	2.54	0.42
1:F:23:TRP:HZ3	1:F:25:TYR:CE1	2.34	0.42
1:H:114:PRO:HD3	1:H:226:PRO:HB3	2.01	0.42
1:C:66:ALA:HB1	1:C:243:SER:O	2.17	0.42
1:A:124:ARG:HB3	1:A:146:PHE:O	2.19	0.42
1:A:125:PRO:HD2	1:A:146:PHE:O	2.20	0.42
1:B:42:PHE:N	1:B:42:PHE:CD1	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:PHE:N	1:D:130:PHE:HD1	2.17	0.42
1:B:73:ALA:O	1:B:173:LEU:HD12	2.20	0.41
1:B:146:PHE:CD1	1:B:208:LEU:HB2	2.54	0.41
1:D:174:ASP:OD1	1:D:174:ASP:N	2.53	0.41
1:D:179:LYS:O	1:D:245:GLU:HA	2.20	0.41
1:G:55:ASN:HD21	1:G:121:ASN:CG	2.27	0.41
1:H:106:LEU:HD12	1:H:131:VAL:O	2.20	0.41
1:D:162:ILE:HG21	1:D:223:LYS:NZ	2.32	0.41
1:F:76:LYS:HD3	1:F:170:GLU:N	2.35	0.41
1:F:77:PRO:HD3	1:F:171:VAL:HG23	2.02	0.41
1:D:124:ARG:HA	1:D:125:PRO:HD3	1.92	0.41
1:D:159:LEU:HD23	1:D:159:LEU:HA	1.78	0.41
1:E:85:HIS:O	1:E:227:ASN:ND2	2.52	0.41
1:E:236:ASN:ND2	1:F:100:ARG:NE	2.39	0.41
1:F:25:TYR:CE2	1:F:227:ASN:HA	2.56	0.41
1:F:88:LYS:CG	1:F:108:ASN:OD1	2.69	0.41
1:H:42:PHE:CD1	1:H:42:PHE:N	2.86	0.41
1:D:87:LEU:HD11	1:D:162:ILE:HD12	2.01	0.41
1:G:23:TRP:CE3	1:G:193:PRO:HD2	2.55	0.41
1:G:229:ARG:HG2	1:G:230:PRO:HD2	2.01	0.41
1:A:155:LEU:HB3	1:A:159:LEU:HD11	2.02	0.41
1:C:179:LYS:O	1:C:246:THR:OG1	2.39	0.41
1:E:85:HIS:ND1	1:E:223:LYS:CE	2.74	0.41
1:H:81:PHE:HE2	1:H:83:THR:HB	1.86	0.41
1:H:185:HIS:HB3	1:H:240:ILE:HG13	2.02	0.41
1:E:21:THR:HG23	1:E:39:HIS:NE2	2.35	0.41
1:F:130:PHE:N	1:F:130:PHE:CD1	2.89	0.41
1:G:62:THR:HG21	1:H:60:TYR:CD2	2.56	0.41
1:F:24:ASP:HB3	1:F:30:ASN:C	2.44	0.41
1:F:106:LEU:HD13	1:F:132:HIS:CE1	2.56	0.41
1:A:109:VAL:HA	1:A:129:HIS:O	2.21	0.41
1:B:22:LYS:HE3	1:B:22:LYS:HB3	1.87	0.41
1:C:182:ASN:ND2	1:C:206:GLU:OE2	2.53	0.41
1:E:223:LYS:CB	1:E:225:SER:H	2.33	0.41
1:H:191:THR:O	1:H:229:ARG:HD2	2.21	0.41
1:E:49:LYS:HD2	1:E:235:TYR:CE2	2.56	0.41
1:E:238:VAL:HG21	1:F:186:PHE:HA	2.03	0.41
1:F:35:TRP:HA	1:F:38:LEU:HD13	2.02	0.41
1:G:213:LYS:HA	1:G:213:LYS:HD3	1.82	0.41
1:H:104:TYR:HB3	1:H:132:HIS:CB	2.51	0.41
1:G:162:ILE:HG21	1:G:221:ARG:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:TYR:HA	1:A:240:ILE:O	2.20	0.40
1:B:35:TRP:CZ3	1:B:193:PRO:HD3	2.56	0.40
1:B:87:LEU:HD13	1:B:218:ILE:HG23	2.02	0.40
1:D:42:PHE:N	1:D:42:PHE:CD1	2.87	0.40
1:D:97:ILE:O	1:D:104:TYR:N	2.36	0.40
1:E:87:LEU:HD12	1:E:88:LYS:N	2.36	0.40
1:E:186:PHE:HA	1:F:238:VAL:HG21	2.03	0.40
1:G:67:ASP:CB	1:G:100:ARG:NE	2.80	0.40
1:A:115:MET:HG3	1:A:127:SER:HB3	2.04	0.40
1:E:110:HIS:CE1	1:E:131:VAL:HG23	2.54	0.40
1:F:51:GLN:NE2	1:F:197:GLU:OE2	2.50	0.40
1:F:85:HIS:HB3	1:F:227:ASN:OD1	2.21	0.40
1:F:159:LEU:HA	1:F:162:ILE:HG23	2.02	0.40
1:G:128:ALA:HB2	1:G:146:PHE:HE2	1.86	0.40
1:H:104:TYR:HA	1:H:133:LYS:O	2.21	0.40
1:F:122:LYS:HB2	1:F:122:LYS:HE2	1.79	0.40
1:F:134:ASP:OD1	1:F:137:GLY:N	2.52	0.40
1:F:182:ASN:OD1	1:F:182:ASN:O	2.39	0.40
1:G:69:GLN:NE2	1:G:69:GLN:HA	2.37	0.40
1:G:151:GLU:HG3	1:G:211:SER:HB2	2.03	0.40
1:G:208:LEU:HD12	1:G:208:LEU:HA	1.85	0.40
1:F:81:PHE:C	1:F:87:LEU:HD12	2.47	0.40
1:H:115:MET:HG3	1:H:127:SER:HB3	2.04	0.40
1:H:192:ALA:HB2	4:H:303:1SA:S2	2.61	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	221/234 (94%)	206 (93%)	15 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	212/234 (91%)	201 (95%)	11 (5%)	0	100	100
1	C	225/234 (96%)	208 (92%)	17 (8%)	0	100	100
1	D	208/234 (89%)	201 (97%)	7 (3%)	0	100	100
1	E	227/234 (97%)	208 (92%)	19 (8%)	0	100	100
1	F	183/234 (78%)	168 (92%)	15 (8%)	0	100	100
1	G	222/234 (95%)	210 (95%)	12 (5%)	0	100	100
1	H	212/234 (91%)	200 (94%)	12 (6%)	0	100	100
All	All	1710/1872 (91%)	1602 (94%)	108 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	201/208 (97%)	192 (96%)	9 (4%)	24	49
1	B	194/208 (93%)	188 (97%)	6 (3%)	35	62
1	C	202/208 (97%)	193 (96%)	9 (4%)	24	49
1	D	194/208 (93%)	185 (95%)	9 (5%)	24	48
1	E	204/208 (98%)	191 (94%)	13 (6%)	16	33
1	F	175/208 (84%)	161 (92%)	14 (8%)	11	24
1	G	202/208 (97%)	190 (94%)	12 (6%)	18	37
1	H	194/208 (93%)	189 (97%)	5 (3%)	40	68
All	All	1566/1664 (94%)	1489 (95%)	77 (5%)	22	45

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ILE
1	A	107	ASP

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Mol	Chain	Res	Type
1	A	147	GLU
1	A	154	ASN
1	A	177	LEU
1	A	206	GLU
1	A	211	SER
1	A	221	ARG
1	A	247	ARG
1	B	30	ASN
1	B	68	LEU
1	B	103	ASP
1	B	109	VAL
1	B	148	GLU
1	B	243	SER
1	C	27	ASN
1	C	28	LYS
1	C	29	GLU
1	C	57	GLU
1	C	69	GLN
1	C	136	LYS
1	C	151	GLU
1	C	160	GLU
1	C	218	ILE
1	D	44	VAL
1	D	50	SER
1	D	83	THR
1	D	97	ILE
1	D	107	ASP
1	D	144	ILE
1	D	179	LYS
1	D	182	ASN
1	D	213	LYS
1	E	20	ASN
1	E	21	THR
1	E	50[A]	SER
1	E	50[B]	SER
1	E	65	LYS
1	E	142	LEU
1	E	148	GLU
1	E	162	ILE
1	E	166	GLN
1	E	180	SER
1	E	203	VAL

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Mol	Chain	Res	Type
1	E	231	VAL
1	E	237	THR
1	F	67	ASP
1	F	96	HIS
1	F	104	TYR
1	F	106	LEU
1	F	133	LYS
1	F	144	ILE
1	F	164	LYS
1	F	170	GLU
1	F	181	ILE
1	F	203	VAL
1	F	210	VAL
1	F	222	MET
1	F	229	ARG
1	F	240	ILE
1	G	21	THR
1	G	22	LYS
1	G	40	LYS
1	G	69	GLN
1	G	94	THR
1	G	102	HIS
1	G	150	LYS
1	G	163	GLN
1	G	208	LEU
1	G	218	ILE
1	G	231	VAL
1	G	247	ARG
1	H	30	ASN
1	H	151	GLU
1	H	159	LEU
1	H	221	ARG
1	H	231	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	96	HIS
1	A	102	HIS
1	A	236	ASN
1	B	30	ASN

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Mol	Chain	Res	Type
1	B	121	ASN
1	B	232	GLN
1	B	236	ASN
1	C	27	ASN
1	C	63	GLN
1	C	96	HIS
1	C	108	ASN
1	C	120	ASN
1	C	182	ASN
1	C	224	ASN
1	D	58	HIS
1	D	61	HIS
1	D	154	ASN
1	D	182	ASN
1	E	20	ASN
1	E	39	HIS
1	E	55	ASN
1	E	69	GLN
1	E	167	ASN
1	E	236	ASN
1	F	39	HIS
1	F	61	HIS
1	F	96	HIS
1	F	121	ASN
1	F	132	HIS
1	F	214	GLN
1	G	55	ASN
1	G	61	HIS
1	G	69	GLN
1	G	224	ASN
1	H	30	ASN
1	H	63	GLN
1	H	85	HIS
1	H	95	ASN
1	H	96	HIS
1	H	102	HIS
1	H	112	HIS
1	H	121	ASN
1	H	224	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 23 ligands modelled in this entry, 15 are monoatomic - leaving 8 for Mogul analysis.

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$
4	1SA	B	303	2	10,10,10	3.50	6 (60%)	15,15,15	12.19	10 (66%)
4	1SA	E	303	2	10,10,10	3.51	6 (60%)	15,15,15	12.15	10 (66%)
4	1SA	G	303	2	10,10,10	3.52	6 (60%)	15,15,15	12.16	10 (66%)
4	1SA	D	303	2	10,10,10	3.51	6 (60%)	15,15,15	12.16	10 (66%)
4	1SA	H	303	2	10,10,10	3.51	6 (60%)	15,15,15	12.14	10 (66%)
4	1SA	A	303	2	10,10,10	3.51	6 (60%)	15,15,15	12.16	10 (66%)
4	1SA	F	302	2	10,10,10	3.51	6 (60%)	15,15,15	12.16	10 (66%)
4	1SA	C	303	2	10,10,10	3.54	6 (60%)	15,15,15	12.21	10 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1SA	B	303	2	-	2/6/6/6	0/1/1/1
4	1SA	E	303	2	-	0/6/6/6	0/1/1/1
4	1SA	G	303	2	-	0/6/6/6	0/1/1/1
4	1SA	D	303	2	-	0/6/6/6	0/1/1/1
4	1SA	H	303	2	-	4/6/6/6	0/1/1/1
4	1SA	A	303	2	-	4/6/6/6	0/1/1/1
4	1SA	F	302	2	-	0/6/6/6	0/1/1/1
4	1SA	C	303	2	-	0/6/6/6	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	303	1SA	C1-S2	6.25	1.79	1.73
4	E	303	1SA	C1-S2	6.22	1.79	1.73
4	B	303	1SA	C1-S2	6.22	1.79	1.73
4	D	303	1SA	C1-S2	6.21	1.79	1.73
4	G	303	1SA	C1-S2	6.21	1.79	1.73
4	A	303	1SA	C1-S2	6.19	1.79	1.73
4	F	302	1SA	C1-S2	6.19	1.79	1.73
4	C	303	1SA	N3-N2	-6.17	1.26	1.39
4	D	303	1SA	N3-N2	-6.16	1.26	1.39
4	H	303	1SA	C1-S2	6.15	1.79	1.73
4	F	302	1SA	N3-N2	-6.15	1.26	1.39
4	A	303	1SA	N3-N2	-6.14	1.26	1.39
4	G	303	1SA	N3-N2	-6.14	1.26	1.39
4	E	303	1SA	N3-N2	-6.14	1.26	1.39
4	B	303	1SA	N3-N2	-6.13	1.26	1.39
4	H	303	1SA	N3-N2	-6.11	1.26	1.39
4	H	303	1SA	C2-S2	3.87	1.79	1.74
4	A	303	1SA	C2-S2	3.83	1.79	1.74
4	F	302	1SA	C2-S2	3.81	1.79	1.74
4	G	303	1SA	C2-S2	3.81	1.79	1.74
4	D	303	1SA	C2-S2	3.81	1.79	1.74
4	E	303	1SA	C2-S2	3.80	1.79	1.74
4	C	303	1SA	C2-S2	3.79	1.79	1.74
4	B	303	1SA	C2-S2	3.74	1.79	1.74
4	C	303	1SA	C1-N2	3.40	1.32	1.29
4	H	303	1SA	S1-N1	3.34	1.66	1.58
4	B	303	1SA	S1-N1	3.34	1.66	1.58
4	E	303	1SA	S1-N1	3.34	1.66	1.58
4	A	303	1SA	S1-N1	3.33	1.66	1.58
4	F	302	1SA	S1-N1	3.33	1.66	1.58
4	G	303	1SA	S1-N1	3.32	1.66	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	303	1SA	S1-N1	3.32	1.66	1.58
4	H	303	1SA	C1-N2	3.32	1.32	1.29
4	G	303	1SA	C1-N2	3.30	1.32	1.29
4	D	303	1SA	S1-N1	3.30	1.66	1.58
4	B	303	1SA	C1-N2	3.30	1.32	1.29
4	A	303	1SA	C1-N2	3.30	1.32	1.29
4	D	303	1SA	C1-N2	3.28	1.32	1.29
4	F	302	1SA	C1-N2	3.27	1.32	1.29
4	E	303	1SA	C1-N2	3.25	1.32	1.29
4	E	303	1SA	C2-N4	2.34	1.39	1.34
4	D	303	1SA	C2-N4	2.34	1.39	1.34
4	G	303	1SA	C2-N4	2.32	1.39	1.34
4	H	303	1SA	C2-N4	2.32	1.39	1.34
4	A	303	1SA	C2-N4	2.31	1.39	1.34
4	F	302	1SA	C2-N4	2.29	1.39	1.34
4	B	303	1SA	C2-N4	2.27	1.39	1.34
4	C	303	1SA	C2-N4	2.25	1.39	1.34

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	303	1SA	S2-C1-N2	-30.50	100.04	116.10
4	B	303	1SA	S2-C1-N2	-30.45	100.07	116.10
4	D	303	1SA	S2-C1-N2	-30.40	100.10	116.10
4	A	303	1SA	S2-C1-N2	-30.38	100.11	116.10
4	G	303	1SA	S2-C1-N2	-30.37	100.11	116.10
4	E	303	1SA	S2-C1-N2	-30.35	100.12	116.10
4	F	302	1SA	S2-C1-N2	-30.34	100.13	116.10
4	H	303	1SA	S2-C1-N2	-30.30	100.14	116.10
4	C	303	1SA	S2-C2-N3	-19.47	99.83	113.79
4	B	303	1SA	S2-C2-N3	-19.41	99.88	113.79
4	F	302	1SA	S2-C2-N3	-19.39	99.89	113.79
4	A	303	1SA	S2-C2-N3	-19.37	99.90	113.79
4	G	303	1SA	S2-C2-N3	-19.37	99.90	113.79
4	H	303	1SA	S2-C2-N3	-19.35	99.92	113.79
4	E	303	1SA	S2-C2-N3	-19.34	99.93	113.79
4	D	303	1SA	S2-C2-N3	-19.33	99.93	113.79
4	C	303	1SA	C1-S2-C2	17.79	96.07	85.56
4	B	303	1SA	C1-S2-C2	17.77	96.06	85.56
4	F	302	1SA	C1-S2-C2	17.67	96.00	85.56
4	A	303	1SA	C1-S2-C2	17.67	96.00	85.56
4	G	303	1SA	C1-S2-C2	17.65	95.99	85.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	303	1SA	C1-S2-C2	17.65	95.99	85.56
4	E	303	1SA	C1-S2-C2	17.63	95.98	85.56
4	D	303	1SA	C1-S2-C2	17.63	95.97	85.56
4	D	303	1SA	C1-N2-N3	17.33	122.22	111.48
4	A	303	1SA	C1-N2-N3	17.31	122.20	111.48
4	E	303	1SA	C1-N2-N3	17.31	122.20	111.48
4	C	303	1SA	C1-N2-N3	17.30	122.20	111.48
4	F	302	1SA	C1-N2-N3	17.29	122.19	111.48
4	B	303	1SA	C1-N2-N3	17.29	122.19	111.48
4	H	303	1SA	C1-N2-N3	17.28	122.19	111.48
4	G	303	1SA	C1-N2-N3	17.25	122.16	111.48
4	C	303	1SA	C2-N3-N2	10.53	121.86	112.07
4	G	303	1SA	C2-N3-N2	10.51	121.83	112.07
4	B	303	1SA	C2-N3-N2	10.48	121.81	112.07
4	A	303	1SA	C2-N3-N2	10.46	121.79	112.07
4	F	302	1SA	C2-N3-N2	10.46	121.79	112.07
4	D	303	1SA	C2-N3-N2	10.45	121.78	112.07
4	E	303	1SA	C2-N3-N2	10.44	121.77	112.07
4	H	303	1SA	C2-N3-N2	10.43	121.76	112.07
4	C	303	1SA	N4-C2-N3	7.40	130.06	123.83
4	D	303	1SA	N4-C2-N3	7.39	130.06	123.83
4	G	303	1SA	N4-C2-N3	7.38	130.05	123.83
4	H	303	1SA	N4-C2-N3	7.37	130.04	123.83
4	A	303	1SA	N4-C2-N3	7.37	130.04	123.83
4	F	302	1SA	N4-C2-N3	7.35	130.02	123.83
4	B	303	1SA	N4-C2-N3	7.32	130.00	123.83
4	E	303	1SA	N4-C2-N3	7.31	129.99	123.83
4	G	303	1SA	S1-C1-N2	6.98	130.00	121.95
4	C	303	1SA	S1-C1-N2	6.97	130.00	121.95
4	E	303	1SA	S1-C1-N2	6.97	130.00	121.95
4	A	303	1SA	S1-C1-N2	6.96	129.99	121.95
4	B	303	1SA	S1-C1-N2	6.95	129.98	121.95
4	D	303	1SA	S1-C1-N2	6.95	129.98	121.95
4	F	302	1SA	S1-C1-N2	6.93	129.94	121.95
4	H	303	1SA	S1-C1-N2	6.93	129.94	121.95
4	C	303	1SA	S2-C1-S1	6.28	129.96	121.62
4	B	303	1SA	S2-C1-S1	6.28	129.95	121.62
4	B	303	1SA	S2-C2-N4	6.26	130.12	121.97
4	D	303	1SA	S2-C1-S1	6.26	129.93	121.62
4	F	302	1SA	S2-C1-S1	6.26	129.93	121.62
4	H	303	1SA	S2-C1-S1	6.25	129.91	121.62
4	C	303	1SA	S2-C2-N4	6.24	130.10	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	1SA	S2-C1-S1	6.24	129.91	121.62
4	F	302	1SA	S2-C2-N4	6.23	130.09	121.97
4	G	303	1SA	S2-C1-S1	6.23	129.89	121.62
4	E	303	1SA	S2-C2-N4	6.22	130.08	121.97
4	E	303	1SA	S2-C1-S1	6.22	129.88	121.62
4	A	303	1SA	S2-C2-N4	6.21	130.06	121.97
4	G	303	1SA	S2-C2-N4	6.20	130.05	121.97
4	H	303	1SA	S2-C2-N4	6.19	130.04	121.97
4	D	303	1SA	S2-C2-N4	6.17	130.01	121.97
4	H	303	1SA	O2-S1-O1	3.63	125.46	120.27
4	D	303	1SA	O2-S1-O1	3.60	125.43	120.27
4	A	303	1SA	O2-S1-O1	3.60	125.42	120.27
4	C	303	1SA	O2-S1-O1	3.59	125.41	120.27
4	B	303	1SA	O2-S1-O1	3.58	125.40	120.27
4	E	303	1SA	O2-S1-O1	3.58	125.40	120.27
4	G	303	1SA	O2-S1-O1	3.57	125.38	120.27
4	F	302	1SA	O2-S1-O1	3.57	125.37	120.27

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	1SA	N2-C1-S1-N1
4	A	303	1SA	S2-C1-S1-N1
4	H	303	1SA	N2-C1-S1-N1
4	H	303	1SA	S2-C1-S1-N1
4	B	303	1SA	N2-C1-S1-O2
4	A	303	1SA	S2-C1-S1-O2
4	B	303	1SA	S2-C1-S1-O2
4	H	303	1SA	S2-C1-S1-O2
4	A	303	1SA	N2-C1-S1-O2
4	H	303	1SA	N2-C1-S1-O2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	1SA	3	0
4	E	303	1SA	1	0
4	D	303	1SA	2	0
4	H	303	1SA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	303	1SA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	224/234 (95%)	-1.35	0 100 100	17, 48, 70, 86	1 (0%)
1	B	217/234 (92%)	-1.34	0 100 100	20, 49, 74, 88	1 (0%)
1	C	226/234 (96%)	-1.38	0 100 100	20, 41, 64, 78	1 (0%)
1	D	218/234 (93%)	-1.26	0 100 100	31, 56, 82, 95	0
1	E	228/234 (97%)	-1.34	0 100 100	26, 47, 70, 83	1 (0%)
1	F	199/234 (85%)	-1.10	0 100 100	46, 71, 87, 94	0
1	G	225/234 (96%)	-1.32	0 100 100	17, 52, 73, 90	1 (0%)
1	H	218/234 (93%)	-1.27	0 100 100	25, 51, 71, 82	0
All	All	1755/1872 (93%)	-1.30	0 100 100	17, 51, 79, 95	5 (0%)

There are no RSRZ outliers to report.

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
4	1SA	A	303	10/10	0.98	0.06	23,41,46,51	10
3	CL	E	302	1/1	0.99	0.03	40,40,40,40	0
3	CL	H	302	1/1	0.99	0.05	38,38,38,38	0
3	CL	D	302	1/1	0.99	0.07	53,53,53,53	0
4	1SA	B	303	10/10	0.99	0.04	37,43,55,58	10
4	1SA	C	303	10/10	0.99	0.04	28,46,57,59	0
4	1SA	D	303	10/10	0.99	0.05	43,55,64,70	0
4	1SA	E	303	10/10	0.99	0.04	36,45,54,64	10
4	1SA	F	302	10/10	0.99	0.03	54,55,59,61	10
4	1SA	G	303	10/10	0.99	0.05	32,38,49,53	0
4	1SA	H	303	10/10	0.99	0.06	40,54,60,70	10
2	ZN	A	301	1/1	1.00	0.01	32,32,32,32	0
2	ZN	B	301	1/1	1.00	0.01	32,32,32,32	0
3	CL	G	302	1/1	1.00	0.03	35,35,35,35	0
2	ZN	C	301	1/1	1.00	0.01	34,34,34,34	0
2	ZN	D	301	1/1	1.00	0.02	46,46,46,46	0
2	ZN	E	301	1/1	1.00	0.01	34,34,34,34	0
2	ZN	F	301	1/1	1.00	0.01	59,59,59,59	1
2	ZN	G	301	1/1	1.00	0.01	30,30,30,30	0
2	ZN	H	301	1/1	1.00	0.02	46,46,46,46	0
3	CL	A	302	1/1	1.00	0.02	34,34,34,34	0
3	CL	B	302	1/1	1.00	0.02	39,39,39,39	0
3	CL	C	302	1/1	1.00	0.02	34,34,34,34	0

6.5 Other polymers

There are no such residues in this entry.