



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:35 PM UTC

PDB ID : 7QF6 / pdb_00007qf6
Title : N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase
sidF
Authors : Poonsiri, T.; Demitri, N.; Stefano, B.
Deposited on : 2021-12-03
Resolution : 1.87 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:

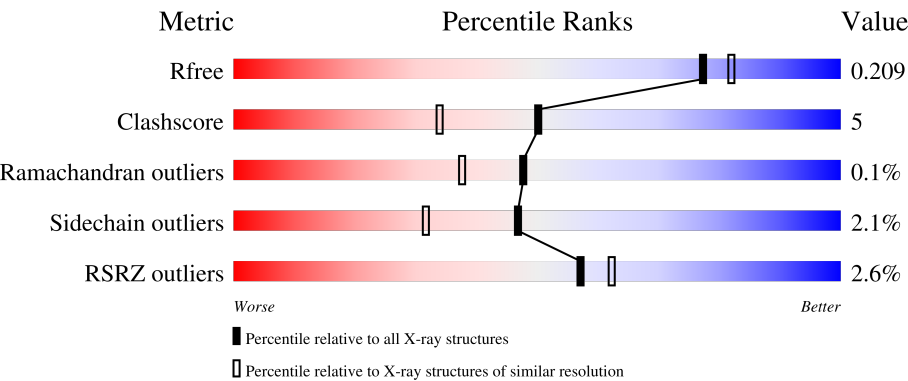
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	462	% 84%10%• 5%
1	B	462	2% 83%11%• 5%
1	C	462	2% 79%13%• 5%
1	D	462	% 83%11%• 5%
1	E	462	3% 82%11%• 5%

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Mol	Chain	Length	Quality of chain
1	F	462	 3% 82% 10% • 6%
1	G	462	 2% 83% 11% • 5%
1	H	462	 5% 78% 16% • 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30901 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 N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	3	0
			3610	2307	646	648	9			
1	B	440	Total	C	N	O	S	0	1	0
			3621	2313	650	649	9			
1	C	438	Total	C	N	O	S	0	3	0
			3607	2306	644	648	9			
1	D	438	Total	C	N	O	S	0	1	0
			3598	2300	643	646	9			
1	E	439	Total	C	N	O	S	0	1	0
			3605	2303	646	647	9			
1	F	433	Total	C	N	O	S	0	1	0
			3553	2270	634	640	9			
1	G	439	Total	C	N	O	S	0	1	0
			3618	2312	651	646	9			
1	H	438	Total	C	N	O	S	0	1	0
			3600	2301	646	644	9			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



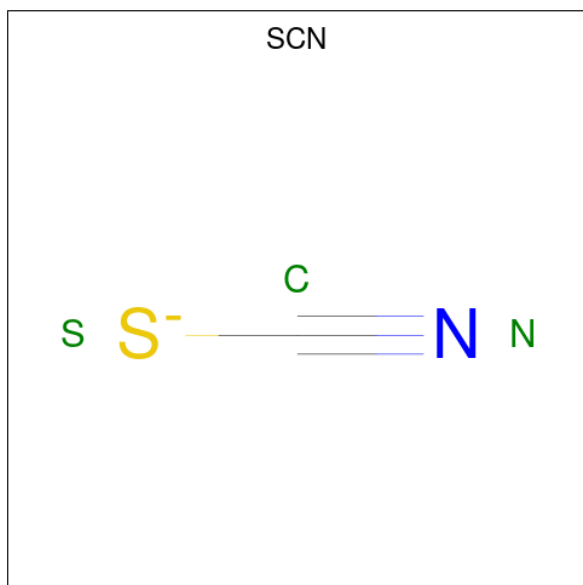
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	S	0	0
			3	1	1	1		
3	D	1	Total	C	N	S	0	0
			3	1	1	1		
3	G	1	Total	C	N	S	0	0
			3	1	1	1		
3	G	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		

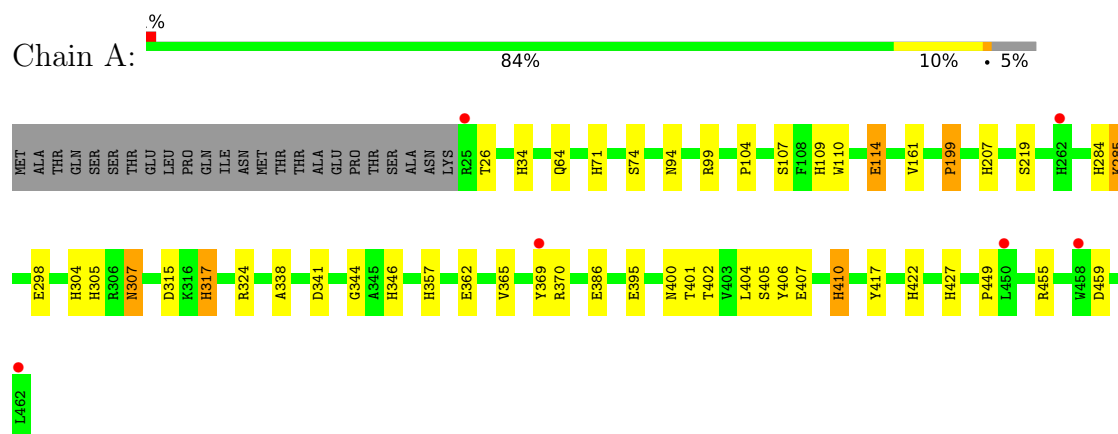
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	293	Total 293	O 293	0	0
5	B	300	Total 300	O 300	0	0
5	C	239	Total 239	O 239	0	0
5	D	223	Total 223	O 223	0	0
5	E	267	Total 267	O 267	0	0
5	F	224	Total 224	O 224	0	0
5	G	228	Total 228	O 228	0	0
5	H	199	Total 199	O 199	0	0

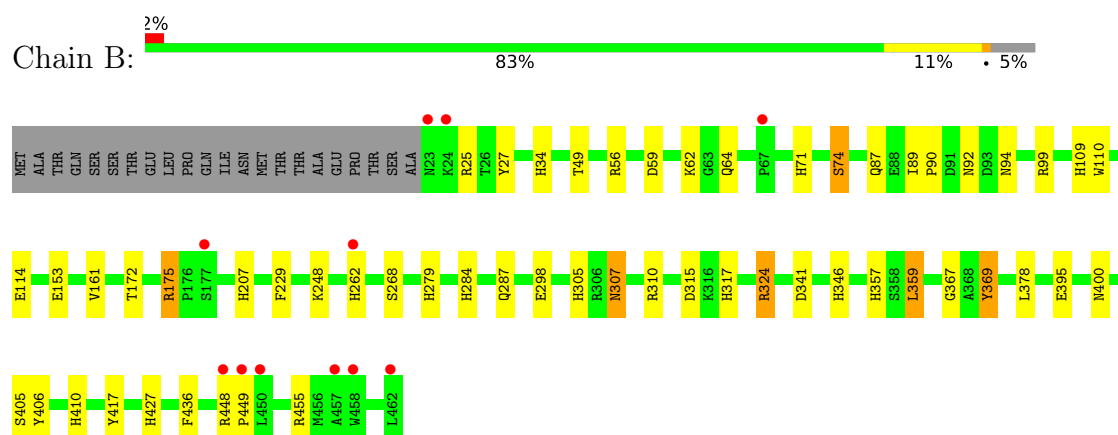
3 Residue-property plots [i](#)

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

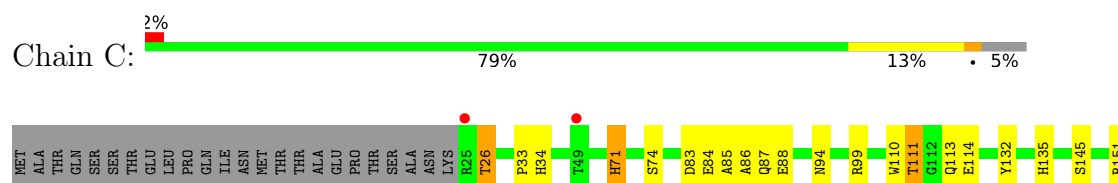
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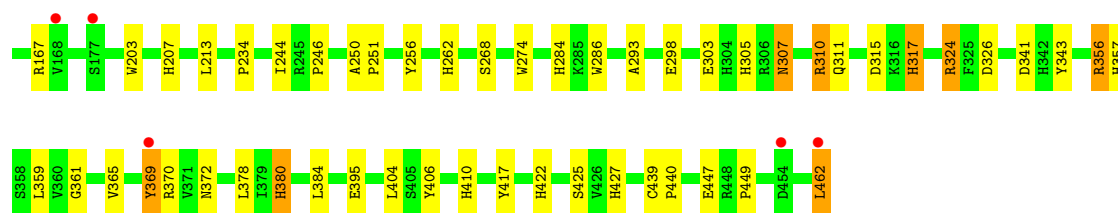


- Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF

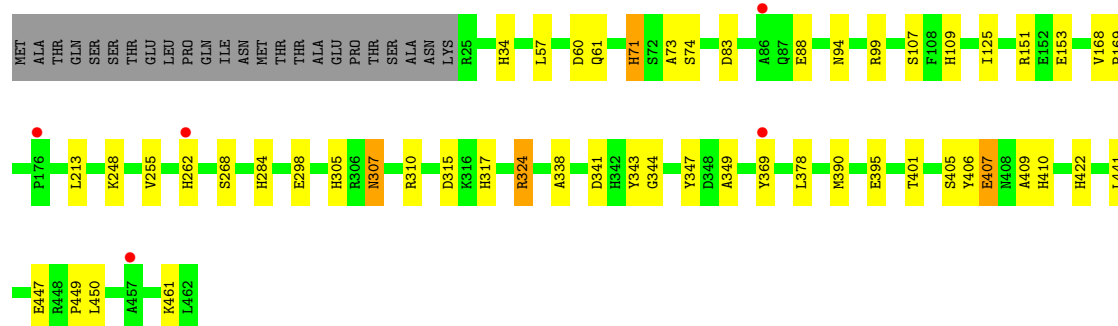
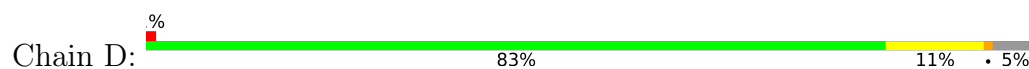


- Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF

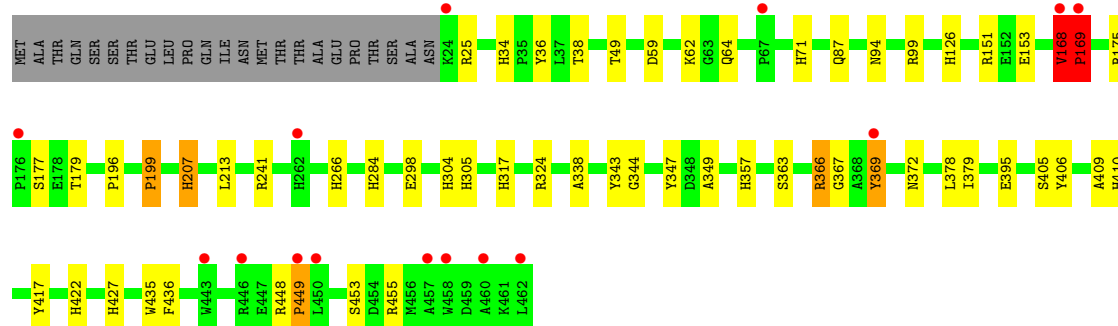
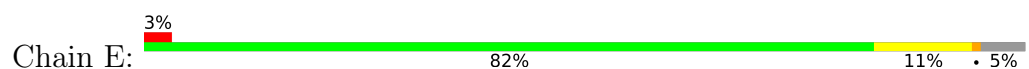




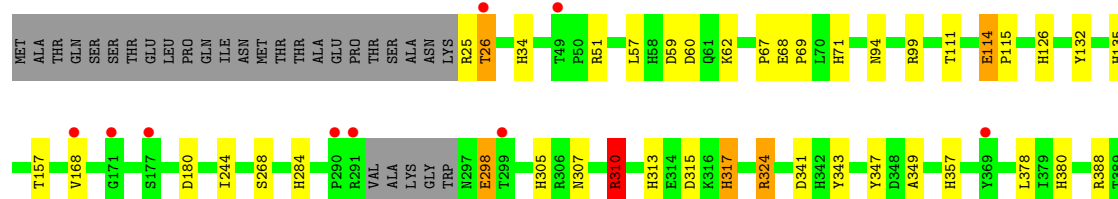
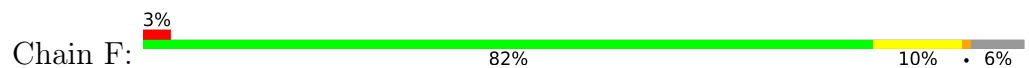
• Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF

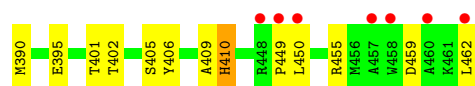


• Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF

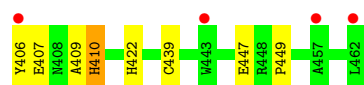
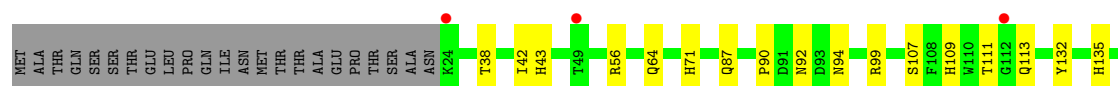
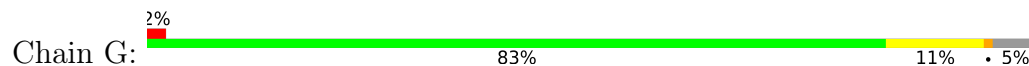


• Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF

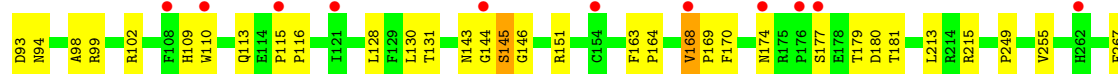
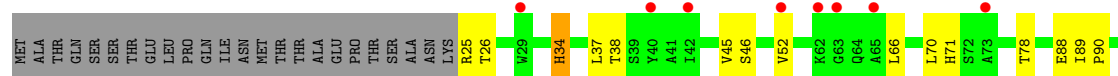
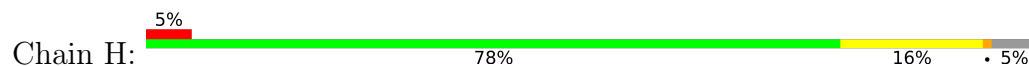




- Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF



- Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.27Å 80.84Å 179.84Å 101.17° 91.67° 117.25°	Depositor
Resolution (Å)	174.82 – 1.87 174.81 – 1.87	Depositor EDS
% Data completeness (in resolution range)	97.1 (174.82-1.87) 97.1 (174.81-1.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.172 , 0.209 0.172 , 0.209	Depositor DCC
R_{free} test set	15716 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	30901	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: K, GOL, SCN

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	1.02	3/3746 (0.1%)	1.28	14/5109 (0.3%)
1	B	1.03	4/3751 (0.1%)	1.28	18/5115 (0.4%)
1	C	0.98	7/3744 (0.2%)	1.31	18/5110 (0.4%)
1	D	0.94	4/3728 (0.1%)	1.25	12/5086 (0.2%)
1	E	0.98	9/3735 (0.2%)	1.31	13/5096 (0.3%)
1	F	0.98	5/3681 (0.1%)	1.31	11/5023 (0.2%)
1	G	0.97	1/3748 (0.0%)	1.31	18/5110 (0.4%)
1	H	1.01	4/3730 (0.1%)	1.39	17/5088 (0.3%)
All	All	0.99	37/29863 (0.1%)	1.30	121/40737 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	G	0	1
All	All	0	2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	427	HIS	CE1-NE2	10.72	1.43	1.32
1	E	427	HIS	CE1-NE2	8.51	1.41	1.32
1	H	279	HIS	CE1-NE2	8.20	1.40	1.32
1	B	34	HIS	CE1-NE2	8.08	1.40	1.32
1	E	34	HIS	CE1-NE2	8.01	1.40	1.32
1	C	34	HIS	CE1-NE2	7.69	1.40	1.32
1	H	380	HIS	CE1-NE2	7.17	1.39	1.32
1	C	425	SER	CA-CB	-7.16	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	210	HIS	CE1-NE2	7.15	1.39	1.32
1	D	422	HIS	CE1-NE2	7.06	1.39	1.32
1	A	427	HIS	CE1-NE2	6.98	1.39	1.32
1	C	207	HIS	CE1-NE2	6.94	1.39	1.32
1	C	380	HIS	CE1-NE2	6.71	1.39	1.32
1	C	427	HIS	CE1-NE2	6.54	1.39	1.32
1	E	422	HIS	CE1-NE2	6.43	1.39	1.32
1	D	422	HIS	CG-ND1	6.33	1.45	1.38
1	E	266	HIS	CE1-NE2	6.21	1.38	1.32
1	C	422	HIS	CE1-NE2	5.92	1.38	1.32
1	H	317	HIS	CE1-NE2	5.90	1.38	1.32
1	H	34	HIS	CE1-NE2	5.80	1.38	1.32
1	E	317	HIS	CE1-NE2	5.76	1.38	1.32
1	E	207	HIS	CE1-NE2	5.72	1.38	1.32
1	F	380	HIS	CE1-NE2	5.60	1.38	1.32
1	D	71	HIS	CG-ND1	5.58	1.44	1.38
1	E	304	HIS	CE1-NE2	5.54	1.38	1.32
1	B	109	HIS	CE1-NE2	5.51	1.38	1.32
1	F	313	HIS	CE1-NE2	5.50	1.38	1.32
1	A	34	HIS	CE1-NE2	5.49	1.38	1.32
1	B	279	HIS	CE1-NE2	5.44	1.38	1.32
1	C	71	HIS	CE1-NE2	5.43	1.38	1.32
1	F	34	HIS	CE1-NE2	5.41	1.38	1.32
1	F	126	HIS	CE1-NE2	5.36	1.38	1.32
1	F	410	HIS	CE1-NE2	5.23	1.37	1.32
1	A	304	HIS	CE1-NE2	5.23	1.37	1.32
1	D	34	HIS	CE1-NE2	5.23	1.37	1.32
1	E	422	HIS	CG-ND1	5.21	1.44	1.38
1	E	126	HIS	CE1-NE2	5.03	1.37	1.32

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	169	PRO	N-CA-CB	-12.13	90.51	103.25
1	E	169	PRO	CB-CA-C	9.63	127.45	111.56
1	G	307	ASN	CA-CB-CG	-9.17	103.43	112.60
1	G	169	PRO	CB-CA-C	8.07	124.88	111.56
1	F	115	PRO	O-C-N	-7.92	117.43	121.15
1	H	249	PRO	CB-CA-C	7.89	121.33	111.23
1	H	444	ASP	CA-CB-CG	7.75	120.35	112.60
1	A	114	GLU	CB-CG-CD	7.41	125.20	112.60
1	C	111	THR	CA-C-N	-7.34	111.05	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	THR	C-N-CA	-7.34	111.05	121.54
1	H	38	THR	CA-CB-OG1	-7.10	98.95	109.60
1	F	180	ASP	CA-CB-CG	7.03	119.63	112.60
1	C	167	ARG	CG-CD-NE	-6.97	96.67	112.00
1	A	346	HIS	CA-CB-CG	-6.78	107.02	113.80
1	D	447	GLU	CB-CG-CD	6.76	124.09	112.60
1	A	104	PRO	CB-CA-C	-6.75	102.11	110.95
1	G	169	PRO	N-CA-CB	-6.75	96.16	103.25
1	E	417	TYR	CB-CA-C	-6.75	97.04	109.46
1	H	417	TYR	CB-CA-C	-6.71	98.04	109.51
1	E	49	THR	CA-CB-OG1	-6.67	99.59	109.60
1	H	130	LEU	N-CA-C	-6.64	104.11	111.82
1	B	417	TYR	CB-CA-C	-6.46	98.46	109.51
1	E	196	PRO	N-CA-C	6.46	122.61	114.92
1	C	151	ARG	NE-CZ-NH1	-6.46	115.04	121.50
1	B	114	GLU	CB-CG-CD	6.36	123.41	112.60
1	B	114	GLU	CB-CA-C	6.34	117.11	109.31
1	F	402	THR	CA-CB-OG1	-6.32	100.12	109.60
1	A	410	HIS	CA-CB-CG	-6.21	107.59	113.80
1	D	255	VAL	N-CA-C	-6.20	107.21	113.47
1	A	417	TYR	CB-CA-C	-6.12	98.19	109.46
1	G	353	ASP	CA-CB-CG	6.09	118.69	112.60
1	H	131	THR	CA-CB-OG1	-6.07	100.50	109.60
1	C	88	GLU	CA-C-N	-6.07	118.22	122.59
1	C	88	GLU	C-N-CA	-6.07	118.22	122.59
1	H	78	THR	CA-CB-OG1	-6.05	100.53	109.60
1	B	359	LEU	N-CA-CB	-6.03	100.70	110.71
1	G	111	THR	CA-C-N	-6.00	112.96	121.54
1	G	111	THR	C-N-CA	-6.00	112.96	121.54
1	C	439	CYS	CB-CA-C	-6.00	106.94	111.20
1	A	199	PRO	CB-CA-C	-5.93	102.48	111.44
1	B	307	ASN	CB-CA-C	-5.93	100.77	110.85
1	B	175	ARG	N-CA-CB	-5.92	102.29	110.29
1	H	255	VAL	N-CA-C	-5.92	107.73	113.53
1	D	307	ASN	CA-CB-CG	-5.90	106.70	112.60
1	C	440	PRO	CA-C-O	-5.84	116.99	121.31
1	E	436	PHE	CA-CB-CG	-5.83	107.97	113.80
1	F	410	HIS	CA-CB-CG	-5.83	107.97	113.80
1	C	33	PRO	CB-CA-C	-5.80	103.64	111.12
1	B	400	ASN	CA-C-N	5.78	128.03	120.28
1	B	400	ASN	C-N-CA	5.78	128.03	120.28
1	D	74	SER	N-CA-CB	-5.72	102.00	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	THR	CA-CB-OG1	-5.68	101.07	109.60
1	C	417	TYR	CB-CA-C	-5.68	99.00	109.46
1	H	145	SER	CB-CA-C	5.68	117.96	110.06
1	G	164	PRO	CB-CA-C	-5.65	104.00	111.23
1	G	315	ASP	CB-CA-C	5.64	119.54	110.29
1	H	292	VAL	CA-C-N	5.60	128.06	120.38
1	H	292	VAL	C-N-CA	5.60	128.06	120.38
1	G	64	GLN	CB-CG-CD	-5.60	103.08	112.60
1	B	307	ASN	CA-CB-CG	-5.59	107.01	112.60
1	E	448	ARG	CB-CA-C	-5.59	100.50	108.88
1	H	442	PHE	CA-CB-CG	5.58	119.38	113.80
1	A	114	GLU	CB-CA-C	5.58	116.43	108.68
1	C	151	ARG	CD-NE-CZ	-5.55	116.63	124.40
1	A	401	THR	CA-CB-OG1	-5.55	101.28	109.60
1	A	207	HIS	CA-CB-CG	-5.54	108.26	113.80
1	B	436	PHE	CA-CB-CG	-5.50	108.30	113.80
1	D	441	LEU	N-CA-C	-5.50	106.78	112.93
1	E	64	GLN	CB-CA-C	5.50	119.05	109.65
1	G	439	CYS	CB-CA-C	-5.49	107.30	111.20
1	C	326	ASP	CA-C-N	-5.47	113.89	122.65
1	C	326	ASP	C-N-CA	-5.47	113.89	122.65
1	G	407	GLU	N-CA-C	-5.47	105.23	111.14
1	D	73	ALA	CA-C-O	5.46	126.14	119.05
1	H	88	GLU	CA-C-N	-5.46	113.70	121.23
1	H	88	GLU	C-N-CA	-5.46	113.70	121.23
1	C	356	ARG	CB-CG-CD	5.42	123.77	111.30
1	B	346	HIS	CA-CB-CG	-5.41	108.39	113.80
1	C	26	THR	CA-CB-OG1	5.39	117.68	109.60
1	B	448	ARG	CB-CA-C	5.39	117.32	110.16
1	F	310	ARG	CB-CG-CD	5.39	123.69	111.30
1	E	151	ARG	CD-NE-CZ	-5.38	116.86	124.40
1	B	229	PHE	CA-CB-CG	-5.37	108.43	113.80
1	G	169	PRO	N-CD-CG	-5.33	95.20	103.20
1	B	87	GLN	CB-CG-CD	5.32	121.64	112.60
1	G	222	PRO	CB-CA-C	-5.32	104.43	111.23
1	A	459	ASP	CA-C-N	5.31	127.65	120.38
1	A	459	ASP	C-N-CA	5.31	127.65	120.38
1	B	310	ARG	CB-CG-CD	5.30	123.49	111.30
1	F	388	ARG	NE-CZ-NH1	-5.29	116.20	121.50
1	A	386	GLU	CB-CA-C	-5.27	104.76	110.98
1	E	169	PRO	N-CD-CG	-5.27	95.30	103.20
1	D	407	GLU	N-CA-C	-5.26	105.44	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	449	PRO	CB-CA-C	5.26	118.26	110.85
1	C	246	PRO	CB-CA-C	-5.25	104.10	110.98
1	G	410	HIS	CA-CB-CG	-5.24	108.56	113.80
1	E	199	PRO	CB-CA-C	-5.22	104.43	111.85
1	H	164	PRO	CB-CA-C	-5.22	104.11	110.95
1	G	265	GLN	CB-CG-CD	-5.21	103.75	112.60
1	F	157	THR	CA-CB-OG1	-5.19	101.81	109.60
1	H	359	LEU	N-CA-CB	-5.17	101.77	111.13
1	D	447	GLU	CB-CA-C	5.15	120.56	110.67
1	A	307	ASN	CA-CB-CG	-5.14	107.46	112.60
1	F	26	THR	N-CA-CB	5.14	118.11	110.29
1	B	49	THR	CA-CB-OG1	-5.14	101.89	109.60
1	G	197	VAL	CA-C-N	-5.13	113.82	121.87
1	G	197	VAL	C-N-CA	-5.13	113.82	121.87
1	B	287	GLN	N-CA-C	-5.12	106.54	112.89
1	C	86	ALA	CA-C-N	5.10	127.63	120.28
1	C	86	ALA	C-N-CA	5.10	127.63	120.28
1	H	267	PHE	CA-CB-CG	-5.10	108.70	113.80
1	D	125	ILE	CA-C-N	5.10	127.42	120.54
1	D	125	ILE	C-N-CA	5.10	127.42	120.54
1	B	74	SER	N-CA-CB	-5.08	101.87	110.41
1	G	402	THR	CA-CB-OG1	-5.08	101.98	109.60
1	D	151	ARG	CD-NE-CZ	-5.05	117.33	124.40
1	F	111	THR	CA-C-N	-5.05	112.49	121.48
1	F	111	THR	C-N-CA	-5.05	112.49	121.48
1	E	175	ARG	CB-CG-CD	5.04	122.90	111.30
1	F	126	HIS	CA-CB-CG	5.02	118.82	113.80
1	D	88	GLU	CB-CG-CD	5.01	121.12	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	168	VAL	Peptide
1	G	168	VAL	Peptide

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	3610	0	3441	31	0
1	B	3621	0	3450	37	0
1	C	3607	0	3422	43	0
1	D	3598	0	3420	38	0
1	E	3605	0	3422	37	0
1	F	3553	0	3359	43	0
1	G	3618	0	3452	36	0
1	H	3600	0	3427	52	0
2	A	24	0	32	6	0
2	B	18	0	24	2	0
2	C	6	0	8	1	0
2	D	12	0	16	2	0
2	E	12	0	16	2	0
2	F	12	0	16	0	0
2	G	18	0	24	3	0
3	B	3	0	0	0	0
3	D	3	0	0	0	0
3	G	6	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	A	293	0	0	2	0
5	B	300	0	0	3	0
5	C	239	0	0	3	0
5	D	223	0	0	3	0
5	E	267	0	0	2	0
5	F	224	0	0	5	0
5	G	228	0	0	1	0
5	H	199	0	0	6	0
All	All	30901	0	27529	299	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 5.

All (299) 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:F:307:ASN:ND2	1:F:310:ARG:HH22	1.16	1.40
1:F:307:ASN:ND2	1:F:310:ARG:NH2	1.76	1.33
1:F:307:ASN:HD22	1:F:310:ARG:NH2	1.30	1.26
1:H:215:ARG:NH1	5:H:501:HOH:O	1.87	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:HIS:CD2	1:E:305:HIS:HD2	1.79	0.99
1:D:284:HIS:CD2	1:D:305:HIS:HD2	1.82	0.98
1:D:284:HIS:HD2	1:D:305:HIS:HD2	0.98	0.97
1:E:284:HIS:HD2	1:E:305:HIS:CD2	1.81	0.97
1:D:401:THR:HG21	1:D:461:LYS:NZ	1.80	0.96
1:H:26:THR:HG22	5:H:656:HOH:O	1.68	0.94
1:A:284:HIS:HD2	1:A:305:HIS:HD2	1.14	0.94
1:G:94:ASN:HD21	1:G:99:ARG:HH11	1.16	0.94
1:H:113:GLN:O	1:H:145:SER:OG	1.84	0.93
1:D:284:HIS:HD2	1:D:305:HIS:CD2	1.85	0.93
1:F:307:ASN:HD21	1:F:310:ARG:HH22	1.03	0.93
1:H:94:ASN:HD21	1:H:99:ARG:HH11	1.16	0.93
1:E:284:HIS:HD2	1:E:305:HIS:HD2	0.95	0.91
1:H:168:VAL:HB	1:H:169:PRO:HD3	1.51	0.91
1:G:284:HIS:HD2	1:G:305:HIS:HD2	1.16	0.91
1:H:179:THR:HG22	1:H:181:THR:H	1.33	0.90
1:B:94:ASN:HD21	1:B:99:ARG:HH11	1.20	0.89
1:A:284:HIS:CD2	1:A:305:HIS:HD2	1.91	0.89
1:F:94:ASN:HD21	1:F:99:ARG:HH11	1.14	0.89
1:A:94:ASN:HD21	1:A:99:ARG:HH11	1.17	0.88
1:G:307:ASN:HD21	1:G:310:ARG:HH21	1.20	0.88
1:D:94:ASN:HD21	1:D:99:ARG:HH11	1.16	0.88
1:B:284:HIS:HD2	1:B:305:HIS:HD2	1.16	0.88
1:C:94:ASN:HD21	1:C:99:ARG:HH11	1.23	0.87
1:G:284:HIS:CD2	1:G:305:HIS:HD2	1.93	0.87
1:C:284:HIS:HD2	1:C:305:HIS:HD2	1.20	0.85
1:B:284:HIS:CD2	1:B:305:HIS:HD2	1.94	0.85
1:B:25:ARG:NH2	5:B:602:HOH:O	2.08	0.84
1:F:284:HIS:HD2	1:F:305:HIS:HD2	1.23	0.83
1:G:284:HIS:HD2	1:G:305:HIS:CD2	1.96	0.83
1:H:284:HIS:HD2	1:H:305:HIS:HD2	1.27	0.83
1:H:284:HIS:CD2	1:H:305:HIS:HD2	1.97	0.83
1:E:453:SER:HA	1:F:450:LEU:HD11	1.60	0.83
1:D:315:ASP:OD1	1:D:317:HIS:HD2	1.64	0.81
1:B:284:HIS:HD2	1:B:305:HIS:CD2	1.98	0.81
1:F:284:HIS:CD2	1:F:305:HIS:HD2	2.00	0.80
1:F:25:ARG:HB2	5:F:602:HOH:O	1.83	0.79
1:E:94:ASN:HD21	1:E:99:ARG:HH11	1.28	0.78
1:A:405:SER:OG	1:A:449:PRO:HB2	1.83	0.78
1:C:284:HIS:CD2	1:C:305:HIS:HD2	2.02	0.78
1:C:298:GLU:O	1:C:305:HIS:HE1	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:401:THR:HG21	1:D:461:LYS:HZ1	1.47	0.78
1:G:307:ASN:ND2	1:G:310:ARG:HH21	1.81	0.78
1:H:298:GLU:O	1:H:305:HIS:HE1	1.66	0.77
1:G:307:ASN:HD21	1:G:310:ARG:NH2	1.82	0.77
1:A:284:HIS:HD2	1:A:305:HIS:CD2	2.00	0.75
1:E:363:SER:O	1:E:366:ARG:HD3	1.87	0.75
1:D:248:LYS:HA	2:D:501:GOL:H31	1.68	0.75
1:D:298:GLU:O	1:D:305:HIS:HE1	1.69	0.75
1:G:315:ASP:OD1	1:G:317:HIS:HD2	1.70	0.74
1:A:298:GLU:O	1:A:305:HIS:HE1	1.70	0.74
1:C:284:HIS:HD2	1:C:305:HIS:CD2	2.04	0.74
1:H:115:PRO:HG3	1:H:146:GLY:HA3	1.70	0.74
1:G:298:GLU:O	1:G:305:HIS:HE1	1.70	0.74
1:G:71:HIS:HD2	5:G:750:HOH:O	1.72	0.72
1:H:284:HIS:HD2	1:H:305:HIS:CD2	2.08	0.72
1:F:284:HIS:HD2	1:F:305:HIS:CD2	2.07	0.71
1:D:405:SER:OG	1:D:450:LEU:O	2.09	0.70
1:B:25:ARG:NH1	1:B:27:TYR:CE1	2.60	0.70
1:E:406:TYR:CE1	1:E:449:PRO:HG3	2.26	0.70
1:F:307:ASN:HD22	1:F:310:ARG:HH21	1.36	0.69
1:D:401:THR:HG21	1:D:461:LYS:HZ3	1.55	0.69
1:G:94:ASN:ND2	1:G:99:ARG:HH11	1.90	0.69
1:A:199:PRO:CD	2:A:502:GOL:H11	2.21	0.69
1:D:94:ASN:ND2	1:D:99:ARG:HH11	1.91	0.69
1:H:168:VAL:CB	1:H:169:PRO:HD3	2.22	0.68
1:B:298:GLU:O	1:B:305:HIS:HE1	1.76	0.68
2:D:501:GOL:H12	5:D:684:HOH:O	1.92	0.67
1:E:298:GLU:O	1:E:305:HIS:HE1	1.75	0.67
1:A:219:SER:HA	2:A:502:GOL:H12	1.76	0.67
1:F:317:HIS:HE1	1:F:341:ASP:OD1	1.77	0.66
1:B:94:ASN:ND2	1:B:99:ARG:HH11	1.92	0.66
1:H:317:HIS:HE1	1:H:341:ASP:OD1	1.78	0.66
1:C:307:ASN:ND2	1:C:310:ARG:HH21	1.93	0.66
1:C:84:GLU:O	1:C:87:GLN:HG2	1.95	0.66
1:B:369:TYR:HD1	1:B:369:TYR:H	1.44	0.65
1:C:369:TYR:HD1	1:C:369:TYR:H	1.44	0.65
1:F:94:ASN:ND2	1:F:99:ARG:HH11	1.90	0.64
1:B:315:ASP:OD1	1:B:317:HIS:HD2	1.81	0.64
1:A:315:ASP:OD1	1:A:317:HIS:HD2	1.81	0.64
1:A:422:HIS:HB3	5:D:801:HOH:O	1.97	0.64
1:E:168:VAL:HG12	1:E:169:PRO:CD	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:450:LEU:C	1:F:450:LEU:HD12	2.22	0.64
1:D:262:HIS:CD2	1:D:369:TYR:HB2	2.33	0.64
1:F:459:ASP:O	1:F:462:LEU:HG	1.98	0.64
1:B:317:HIS:HE1	1:B:341:ASP:OD1	1.81	0.62
1:H:94:ASN:ND2	1:H:99:ARG:HH11	1.92	0.62
1:C:307:ASN:ND2	1:C:310:ARG:NH2	2.46	0.62
1:F:406:TYR:O	1:F:410:HIS:HD2	1.82	0.62
1:H:310:ARG:HG2	1:H:310:ARG:HH11	1.64	0.62
1:B:406:TYR:O	1:B:410:HIS:HD2	1.83	0.62
1:F:67:PRO:O	1:F:68:GLU:HG3	2.00	0.62
1:A:199:PRO:HD2	2:A:502:GOL:H11	1.80	0.61
1:F:59:ASP:OD2	1:F:62:LYS:HE2	2.00	0.61
1:D:317:HIS:HE1	1:D:341:ASP:OD1	1.84	0.61
1:A:406:TYR:O	1:A:410:HIS:HD2	1.83	0.61
1:A:64:GLN:CD	1:B:64:GLN:HG2	2.25	0.61
1:A:94:ASN:ND2	1:A:99:ARG:HH11	1.95	0.61
1:D:284:HIS:CD2	1:D:305:HIS:CD2	2.72	0.61
1:H:179:THR:HG22	1:H:180:ASP:N	2.16	0.61
1:H:315:ASP:OD1	1:H:317:HIS:HD2	1.84	0.60
1:C:307:ASN:HD21	1:C:310:ARG:NH2	1.99	0.60
1:G:113:GLN:O	1:G:145:SER:OG	2.19	0.60
1:F:405:SER:OG	1:F:449:PRO:HB2	2.02	0.60
1:C:317:HIS:HE1	1:C:341:ASP:OD1	1.84	0.60
1:F:51:ARG:NH2	5:F:602:HOH:O	2.33	0.60
1:G:317:HIS:HE1	1:G:341:ASP:OD2	1.84	0.60
1:B:357:HIS:HE1	2:B:504:GOL:O3	1.84	0.59
1:D:213:LEU:HD23	1:E:153:GLU:HG2	1.83	0.59
1:E:284:HIS:CD2	1:E:305:HIS:CD2	2.69	0.59
1:D:390:MET:HE1	5:E:821:HOH:O	2.02	0.59
1:G:406:TYR:O	1:G:410:HIS:HD2	1.86	0.59
1:C:114:GLU:O	1:C:114:GLU:HG2	2.01	0.59
1:C:315:ASP:OD1	1:C:317:HIS:HD2	1.85	0.58
1:C:357:HIS:HE1	2:C:501:GOL:O1	1.86	0.58
1:F:315:ASP:OD1	1:F:317:HIS:HD2	1.86	0.58
1:E:369:TYR:HD1	1:E:369:TYR:H	1.51	0.58
1:D:406:TYR:O	1:D:410:HIS:HD2	1.85	0.58
1:E:71:HIS:HD2	5:E:674:HOH:O	1.84	0.58
1:F:298:GLU:O	1:F:305:HIS:HE1	1.86	0.57
1:H:307:ASN:HD21	1:H:310:ARG:HH21	1.50	0.57
1:G:307:ASN:ND2	1:G:310:ARG:NH2	2.47	0.57
1:F:268:SER:OG	1:F:324:ARG:HD3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:94:ASN:HD21	1:G:99:ARG:NH1	1.96	0.57
1:C:94:ASN:ND2	1:C:99:ARG:HH11	1.97	0.57
1:G:42:ILE:HB	2:G:503:GOL:H12	1.85	0.57
1:G:284:HIS:CD2	1:G:305:HIS:CD2	2.81	0.57
1:H:25:ARG:HG2	1:H:26:THR:O	2.05	0.57
1:F:114:GLU:O	1:F:114:GLU:HG2	2.05	0.56
1:C:262:HIS:CD2	1:C:369:TYR:HD2	2.23	0.56
1:D:71:HIS:HD2	5:D:641:HOH:O	1.88	0.56
1:H:406:TYR:O	1:H:410:HIS:HD2	1.88	0.56
1:H:94:ASN:ND2	1:H:99:ARG:HD2	2.20	0.55
1:A:365:VAL:HG13	1:A:370:ARG:HD3	1.89	0.55
1:F:284:HIS:CD2	1:F:305:HIS:CD2	2.89	0.55
1:C:71:HIS:HD2	5:C:673:HOH:O	1.89	0.54
1:B:367:GLY:HA3	1:B:369:TYR:CE1	2.43	0.54
1:D:60:ASP:OD1	1:D:61:GLN:NE2	2.33	0.54
1:B:359:LEU:C	1:B:359:LEU:HD23	2.33	0.54
1:A:219:SER:CA	2:A:502:GOL:H12	2.36	0.54
1:E:405:SER:OG	1:E:449:PRO:HB2	2.08	0.53
1:C:274:TRP:CZ2	1:C:310:ARG:HG3	2.44	0.53
1:H:168:VAL:HB	1:H:169:PRO:CD	2.32	0.53
1:B:284:HIS:CD2	1:B:305:HIS:CD2	2.82	0.53
1:G:151:ARG:NH1	1:G:180:ASP:O	2.36	0.53
1:B:367:GLY:HA3	1:B:369:TYR:HE1	1.74	0.53
1:E:347:TYR:CE2	1:E:349:ALA:HA	2.44	0.52
1:B:268:SER:OG	1:B:324:ARG:HD3	2.10	0.52
1:H:25:ARG:HG2	1:H:26:THR:N	2.24	0.52
1:F:401:THR:HG23	5:F:756:HOH:O	2.08	0.52
1:H:45:VAL:HB	1:H:52:VAL:HG12	1.91	0.52
1:E:94:ASN:ND2	1:E:99:ARG:HH11	2.03	0.52
1:E:406:TYR:O	1:E:410:HIS:HD2	1.92	0.52
1:C:293:ALA:HA	5:C:722:HOH:O	2.09	0.52
1:E:453:SER:CA	1:F:450:LEU:HD11	2.35	0.52
1:H:113:GLN:O	1:H:145:SER:CB	2.57	0.52
1:A:455:ARG:HB2	1:D:409:ALA:O	2.10	0.52
1:E:409:ALA:O	1:F:455:ARG:HB2	2.10	0.51
1:A:64:GLN:NE2	1:B:64:GLN:HG2	2.25	0.51
1:A:71:HIS:HD2	5:A:633:HOH:O	1.92	0.51
1:D:405:SER:OG	1:D:449:PRO:HB2	2.10	0.51
1:B:405:SER:OG	1:B:449:PRO:HB2	2.10	0.51
1:D:406:TYR:CE1	1:D:449:PRO:HG3	2.45	0.51
1:H:110:TRP:CE2	1:H:144:GLY:HA3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ARG:HH12	1:B:27:TYR:HE1	1.58	0.51
1:C:365:VAL:HG13	1:C:370:ARG:HD3	1.93	0.51
1:G:357:HIS:HE1	2:G:504:GOL:O1	1.93	0.51
1:A:317:HIS:HE1	1:A:341:ASP:OD1	1.93	0.51
1:C:359:LEU:HD23	1:C:359:LEU:C	2.36	0.50
1:E:36:TYR:OH	1:E:207:HIS:CE1	2.65	0.50
1:H:151:ARG:NH1	1:H:180:ASP:O	2.42	0.50
1:F:67:PRO:C	1:F:68:GLU:HG3	2.36	0.50
1:C:74:SER:O	1:C:110:TRP:HA	2.11	0.50
1:F:132:TYR:HB3	1:F:135:HIS:HD2	1.75	0.50
1:B:262:HIS:CD2	1:B:369:TYR:HB2	2.47	0.50
1:C:84:GLU:O	1:C:87:GLN:HB2	2.12	0.49
1:D:369:TYR:H	1:D:369:TYR:HD1	1.60	0.49
1:G:405:SER:HB3	1:G:449:PRO:HB2	1.93	0.49
1:G:87:GLN:OE1	1:G:87:GLN:HA	2.12	0.49
1:D:407:GLU:OE1	1:D:407:GLU:HA	2.12	0.49
1:H:109:HIS:CE1	5:H:521:HOH:O	2.65	0.49
1:D:57:LEU:HD11	1:D:60:ASP:HB3	1.95	0.48
1:E:453:SER:HB3	1:F:450:LEU:CD1	2.42	0.48
1:H:66:LEU:HD13	1:H:70:LEU:HG	1.95	0.48
1:E:357:HIS:HE1	2:E:501:GOL:O1	1.96	0.48
1:F:57:LEU:HD11	1:F:60:ASP:HB3	1.93	0.48
1:G:43:HIS:CD2	1:G:56:ARG:HD2	2.48	0.48
1:D:168:VAL:HG13	1:D:169:PRO:HA	1.94	0.48
1:D:315:ASP:OD1	1:D:317:HIS:CD2	2.55	0.48
1:D:338:ALA:O	1:D:344:GLY:HA3	2.14	0.48
1:C:406:TYR:CE1	1:C:449:PRO:HG3	2.49	0.47
1:H:338:ALA:O	1:H:344:GLY:HA3	2.14	0.47
1:B:94:ASN:HD21	1:B:99:ARG:NH1	2.01	0.47
1:B:455:ARG:HB2	1:G:409:ALA:O	2.14	0.47
1:H:276:ASN:OD1	1:H:276:ASN:C	2.57	0.47
1:G:132:TYR:HB3	1:G:135:HIS:HD2	1.79	0.47
1:B:64:GLN:HE22	1:B:207:HIS:CE1	2.33	0.47
1:H:347:TYR:CE2	1:H:349:ALA:HA	2.49	0.47
1:A:284:HIS:CD2	1:A:305:HIS:CD2	2.83	0.47
1:H:71:HIS:HD2	5:H:586:HOH:O	1.97	0.47
1:H:284:HIS:CD2	1:H:305:HIS:CD2	2.87	0.46
1:H:404:LEU:HD11	1:H:426:VAL:CG2	2.46	0.46
1:A:161:VAL:HG11	1:F:244:ILE:HD13	1.96	0.46
1:H:98:ALA:O	1:H:102:ARG:HG3	2.16	0.46
1:A:199:PRO:HD3	2:A:502:GOL:H32	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:ASN:OD1	1:C:410:HIS:HE1	1.97	0.46
1:B:172:THR:HA	1:B:175:ARG:NH1	2.31	0.46
1:F:347:TYR:CE2	1:F:349:ALA:HA	2.50	0.46
1:D:83:ASP:C	1:D:83:ASP:OD1	2.57	0.46
1:D:307:ASN:OD1	1:D:310:ARG:NH2	2.35	0.46
1:D:94:ASN:HD21	1:D:99:ARG:NH1	1.98	0.46
1:H:357:HIS:HE1	5:H:541:HOH:O	1.98	0.45
1:C:274:TRP:CE2	1:C:310:ARG:HG3	2.52	0.45
1:G:42:ILE:H	2:G:503:GOL:C1	2.29	0.45
1:H:93:ASP:O	1:H:102:ARG:NH2	2.47	0.45
1:D:347:TYR:CE2	1:D:349:ALA:HA	2.51	0.45
1:E:409:ALA:O	1:F:455:ARG:HD3	2.16	0.45
1:A:338:ALA:O	1:A:344:GLY:HA3	2.17	0.45
1:B:161:VAL:HG11	1:C:244:ILE:HD13	1.97	0.45
5:A:745:HOH:O	1:F:390:MET:HE1	2.16	0.45
1:B:248:LYS:HG2	2:B:503:GOL:H11	1.99	0.45
1:H:461:LYS:HE3	1:H:461:LYS:HB2	1.65	0.45
1:A:94:ASN:ND2	1:A:99:ARG:HD2	2.32	0.45
1:H:89:ILE:HG23	1:H:90:PRO:HD2	1.97	0.45
1:A:107:SER:OG	1:A:109:HIS:HE1	2.00	0.44
1:C:234:PRO:HB3	1:H:170:PHE:CE2	2.53	0.44
1:E:455:ARG:HB2	1:F:409:ALA:O	2.18	0.44
1:H:163:PHE:O	1:H:177:SER:HB2	2.18	0.44
1:A:407:GLU:HA	1:A:407:GLU:OE1	2.18	0.44
1:B:89:ILE:O	1:B:90:PRO:C	2.61	0.44
1:C:268:SER:OG	1:C:324:ARG:HD3	2.17	0.44
1:C:286:TRP:CD2	1:C:361:GLY:HA3	2.53	0.43
1:C:307:ASN:O	1:C:311:GLN:HG3	2.19	0.43
1:H:110:TRP:CG	1:H:116:PRO:HD3	2.53	0.43
1:F:71:HIS:HD2	5:F:621:HOH:O	2.00	0.43
1:F:94:ASN:HD21	1:F:99:ARG:NH1	1.97	0.43
1:B:64:GLN:HG3	5:B:601:HOH:O	2.19	0.43
1:C:74:SER:HB2	1:C:111:THR:OG1	2.17	0.43
1:D:315:ASP:CG	1:D:317:HIS:HD2	2.27	0.43
1:E:241:ARG:HD3	2:E:502:GOL:O2	2.18	0.43
1:E:369:TYR:CD1	1:E:369:TYR:N	2.86	0.43
1:F:357:HIS:HE1	5:F:631:HOH:O	2.01	0.43
1:C:83:ASP:OD1	1:C:85:ALA:HB3	2.19	0.43
1:C:380:HIS:CE1	1:C:384:LEU:HD11	2.53	0.43
1:C:462:LEU:HA	5:C:616:HOH:O	2.19	0.43
1:H:168:VAL:CB	1:H:169:PRO:CD	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ASN:O	1:A:404:LEU:HD13	2.19	0.43
1:C:132:TYR:HB3	1:C:135:HIS:CD2	2.54	0.43
1:E:367:GLY:HA3	1:E:369:TYR:CE1	2.54	0.43
1:H:34:HIS:CE1	1:H:37:LEU:HD21	2.54	0.42
1:A:285:LYS:NZ	1:A:362:GLU:OE2	2.52	0.42
1:E:168:VAL:HG12	1:E:169:PRO:HD2	1.98	0.42
1:H:143:ASN:HA	5:H:566:HOH:O	2.19	0.42
1:A:74:SER:O	1:A:110:TRP:HA	2.19	0.42
1:E:379:ILE:HG21	1:E:435:TRP:CE2	2.54	0.42
1:H:310:ARG:HH11	1:H:310:ARG:CG	2.32	0.42
1:C:84:GLU:O	1:C:87:GLN:CB	2.68	0.42
1:D:268:SER:OG	1:D:324:ARG:HD3	2.20	0.42
1:B:153:GLU:HG2	1:C:213:LEU:HD23	2.01	0.42
1:C:84:GLU:O	1:C:87:GLN:CG	2.64	0.42
1:C:113:GLN:O	1:C:145:SER:OG	2.38	0.42
1:E:372:ASN:OD1	1:E:410:HIS:HE1	2.02	0.42
1:G:90:PRO:HB2	1:G:92:ASN:OD1	2.20	0.42
1:B:56:ARG:CZ	1:F:69:PRO:HG2	2.50	0.41
1:D:406:TYR:CZ	1:D:449:PRO:HG3	2.54	0.41
1:G:284:HIS:HA	1:G:305:HIS:CD2	2.54	0.41
1:A:357:HIS:HE1	2:A:501:GOL:O3	2.04	0.41
1:G:447:GLU:O	1:G:447:GLU:HG2	2.18	0.41
1:B:59:ASP:OD2	1:B:62:LYS:HE2	2.21	0.41
1:H:94:ASN:HD21	1:H:99:ARG:HD2	1.85	0.41
1:E:59:ASP:OD2	1:E:62:LYS:HD3	2.20	0.41
1:G:107:SER:OG	1:G:109:HIS:HE1	2.04	0.41
1:G:372:ASN:OD1	1:G:410:HIS:HE1	2.04	0.41
1:H:179:THR:CG2	1:H:180:ASP:N	2.81	0.41
1:H:315:ASP:CG	1:H:317:HIS:HD2	2.29	0.41
1:C:203:TRP:O	1:C:256:TYR:HA	2.21	0.41
1:E:338:ALA:O	1:E:344:GLY:HA3	2.21	0.41
1:E:409:ALA:C	1:F:455:ARG:HB2	2.46	0.41
1:H:284:HIS:HA	1:H:305:HIS:CD2	2.55	0.41
1:B:71:HIS:HD2	5:B:609:HOH:O	2.03	0.41
1:B:74:SER:O	1:B:110:TRP:HA	2.21	0.41
1:E:177:SER:OG	1:E:179:THR:HG22	2.21	0.41
1:F:298:GLU:O	1:F:305:HIS:CE1	2.70	0.41
1:G:338:ALA:O	1:G:344:GLY:HA3	2.20	0.41
1:G:359:LEU:C	1:G:359:LEU:HD23	2.46	0.41
1:H:365:VAL:O	1:H:365:VAL:HG12	2.21	0.41
1:B:92:ASN:O	1:G:422:HIS:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ALA:HA	1:C:251:PRO:HD3	1.96	0.40
1:C:307:ASN:HD21	1:C:310:ARG:HH21	1.59	0.40
1:D:153:GLU:HG2	1:E:213:LEU:HD23	2.03	0.40
1:E:36:TYR:OH	1:E:207:HIS:HE1	2.03	0.40
1:G:177:SER:OG	1:G:179:THR:HG22	2.22	0.40
1:G:315:ASP:OD1	1:G:317:HIS:CD2	2.62	0.40
1:D:107:SER:OG	1:D:109:HIS:HE1	2.04	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	439/462 (95%)	430 (98%)	9 (2%)	0	100	100
1	B	439/462 (95%)	431 (98%)	8 (2%)	0	100	100
1	C	439/462 (95%)	431 (98%)	8 (2%)	0	100	100
1	D	437/462 (95%)	429 (98%)	8 (2%)	0	100	100
1	E	438/462 (95%)	431 (98%)	6 (1%)	1 (0%)	43	34
1	F	430/462 (93%)	424 (99%)	6 (1%)	0	100	100
1	G	438/462 (95%)	431 (98%)	6 (1%)	1 (0%)	43	34
1	H	437/462 (95%)	427 (98%)	9 (2%)	1 (0%)	43	34
All	All	3497/3696 (95%)	3434 (98%)	60 (2%)	3 (0%)	48	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	169	PRO
1	G	169	PRO
1	H	168	VAL

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	389/407 (96%)	381 (98%)	8 (2%)	47	32
1	B	389/407 (96%)	384 (99%)	5 (1%)	61	50
1	C	387/407 (95%)	373 (96%)	14 (4%)	31	14
1	D	386/407 (95%)	382 (99%)	4 (1%)	68	60
1	E	386/407 (95%)	375 (97%)	11 (3%)	38	22
1	F	381/407 (94%)	371 (97%)	10 (3%)	40	24
1	G	388/407 (95%)	383 (99%)	5 (1%)	61	50
1	H	386/407 (95%)	377 (98%)	9 (2%)	44	29
All	All	3092/3256 (95%)	3026 (98%)	66 (2%)	47	32

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	114	GLU
1	A	285	LYS
1	A	307	ASN
1	A	317	HIS
1	A	324	ARG
1	A	369	TYR
1	A	395	GLU
1	B	307	ASN
1	B	324	ARG
1	B	369	TYR
1	B	378	LEU
1	B	395	GLU
1	C	26	THR
1	C	303	GLU
1	C	307	ASN
1	C	310	ARG
1	C	317	HIS
1	C	324	ARG

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Mol	Chain	Res	Type
1	C	343	TYR
1	C	356	ARG
1	C	369	TYR
1	C	378	LEU
1	C	395	GLU
1	C	404	LEU
1	C	447	GLU
1	C	462	LEU
1	D	324	ARG
1	D	343	TYR
1	D	378	LEU
1	D	395	GLU
1	E	25	ARG
1	E	38	THR
1	E	87	GLN
1	E	168	VAL
1	E	169	PRO
1	E	324	ARG
1	E	343	TYR
1	E	366	ARG
1	E	369	TYR
1	E	378	LEU
1	E	395	GLU
1	F	26	THR
1	F	114	GLU
1	F	168	VAL
1	F	298	GLU
1	F	310	ARG
1	F	317	HIS
1	F	324	ARG
1	F	343	TYR
1	F	378	LEU
1	F	395	GLU
1	G	38	THR
1	G	307	ASN
1	G	343	TYR
1	G	378	LEU
1	G	395	GLU
1	H	46	SER
1	H	128	LEU
1	H	174	ASN
1	H	213	LEU

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Mol	Chain	Res	Type
1	H	317	HIS
1	H	343	TYR
1	H	395	GLU
1	H	401	THR
1	H	404	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	94	ASN
1	A	109	HIS
1	A	113	GLN
1	A	207	HIS
1	A	226	ASN
1	A	284	HIS
1	A	305	HIS
1	A	317	HIS
1	A	357	HIS
1	A	408	ASN
1	A	410	HIS
1	A	415	GLN
1	B	71	HIS
1	B	94	ASN
1	B	109	HIS
1	B	207	HIS
1	B	226	ASN
1	B	284	HIS
1	B	305	HIS
1	B	317	HIS
1	B	342	HIS
1	B	357	HIS
1	B	410	HIS
1	C	71	HIS
1	C	94	ASN
1	C	109	HIS
1	C	135	HIS
1	C	174	ASN
1	C	226	ASN
1	C	284	HIS
1	C	305	HIS
1	C	307	ASN

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Mol	Chain	Res	Type
1	C	317	HIS
1	C	357	HIS
1	C	408	ASN
1	C	410	HIS
1	C	415	GLN
1	D	58	HIS
1	D	64	GLN
1	D	71	HIS
1	D	94	ASN
1	D	109	HIS
1	D	226	ASN
1	D	284	HIS
1	D	305	HIS
1	D	317	HIS
1	D	357	HIS
1	D	408	ASN
1	D	410	HIS
1	D	415	GLN
1	E	43	HIS
1	E	71	HIS
1	E	94	ASN
1	E	109	HIS
1	E	207	HIS
1	E	226	ASN
1	E	262	HIS
1	E	284	HIS
1	E	305	HIS
1	E	357	HIS
1	E	408	ASN
1	E	410	HIS
1	F	71	HIS
1	F	94	ASN
1	F	109	HIS
1	F	226	ASN
1	F	284	HIS
1	F	287	GLN
1	F	305	HIS
1	F	307	ASN
1	F	311	GLN
1	F	317	HIS
1	F	357	HIS
1	F	408	ASN

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Mol	Chain	Res	Type
1	F	410	HIS
1	G	43	HIS
1	G	71	HIS
1	G	94	ASN
1	G	109	HIS
1	G	135	HIS
1	G	226	ASN
1	G	284	HIS
1	G	305	HIS
1	G	307	ASN
1	G	317	HIS
1	G	357	HIS
1	G	410	HIS
1	H	71	HIS
1	H	94	ASN
1	H	207	HIS
1	H	226	ASN
1	H	284	HIS
1	H	305	HIS
1	H	307	ASN
1	H	317	HIS
1	H	357	HIS
1	H	410	HIS
1	H	415	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	$\# Z > 2$
2	GOL	B	502	-	5,5,5	0.17	0	5,5,5	0.69	0
2	GOL	A	501	-	5,5,5	0.19	0	5,5,5	0.74	0
3	SCN	G	501	-	1,2,2	0.39	0	0,1,1	-	-
2	GOL	F	501	-	5,5,5	0.31	0	5,5,5	0.84	0
2	GOL	D	502	-	5,5,5	0.31	0	5,5,5	1.16	0
2	GOL	E	501	-	5,5,5	0.25	0	5,5,5	0.42	0
2	GOL	A	502	-	5,5,5	0.15	0	5,5,5	0.83	0
2	GOL	G	505	-	5,5,5	0.11	0	5,5,5	0.39	0
2	GOL	F	502	-	5,5,5	0.22	0	5,5,5	0.51	0
2	GOL	G	503	-	5,5,5	0.38	0	5,5,5	0.62	0
2	GOL	G	504	-	5,5,5	0.23	0	5,5,5	0.47	0
2	GOL	B	504	-	5,5,5	0.37	0	5,5,5	0.77	0
2	GOL	C	501	-	5,5,5	0.24	0	5,5,5	0.36	0
2	GOL	D	501	-	5,5,5	0.40	0	5,5,5	1.20	0
2	GOL	A	503	-	5,5,5	0.23	0	5,5,5	1.12	0
2	GOL	A	504	-	5,5,5	0.16	0	5,5,5	0.56	0
3	SCN	G	502	-	1,2,2	0.51	0	0,1,1	-	-
2	GOL	B	503	-	5,5,5	0.54	0	5,5,5	0.47	0
2	GOL	E	502	-	5,5,5	0.31	0	5,5,5	0.37	0
3	SCN	D	503	-	1,2,2	1.20	0	0,1,1	-	-
3	SCN	B	501	-	1,2,2	2.58	1 (100%)	0,1,1	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	503	-	-	0/4/4/4	-
2	GOL	A	504	-	-	2/4/4/4	-
2	GOL	A	502	-	-	4/4/4/4	-
2	GOL	B	502	-	-	4/4/4/4	-
2	GOL	B	503	-	-	0/4/4/4	-
2	GOL	A	501	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	502	-	-	2/4/4/4	-
2	GOL	E	502	-	-	0/4/4/4	-
2	GOL	G	505	-	-	4/4/4/4	-
2	GOL	F	502	-	-	3/4/4/4	-
2	GOL	G	503	-	-	2/4/4/4	-
2	GOL	G	504	-	-	0/4/4/4	-
2	GOL	E	501	-	-	1/4/4/4	-
2	GOL	B	504	-	-	4/4/4/4	-
2	GOL	F	501	-	-	3/4/4/4	-
2	GOL	C	501	-	-	0/4/4/4	-
2	GOL	D	501	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	SCN	C-N	-2.58	1.06	1.15

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-C3
2	B	502	GOL	O1-C1-C2-C3
2	B	504	GOL	O1-C1-C2-C3
2	B	504	GOL	C1-C2-C3-O3
2	D	501	GOL	C1-C2-C3-O3
2	D	502	GOL	O1-C1-C2-C3
2	A	501	GOL	O1-C1-C2-O2
2	B	504	GOL	O1-C1-C2-O2
2	B	504	GOL	O2-C2-C3-O3
2	F	501	GOL	O1-C1-C2-O2
2	A	502	GOL	O1-C1-C2-C3
2	A	502	GOL	C1-C2-C3-O3
2	A	504	GOL	C1-C2-C3-O3
2	B	502	GOL	C1-C2-C3-O3
2	F	501	GOL	O1-C1-C2-C3
2	F	501	GOL	C1-C2-C3-O3
2	F	502	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	G	503	GOL	C1-C2-C3-O3
2	G	505	GOL	O1-C1-C2-C3
2	G	505	GOL	C1-C2-C3-O3
2	A	502	GOL	O1-C1-C2-O2
2	A	502	GOL	O2-C2-C3-O3
2	B	502	GOL	O1-C1-C2-O2
2	B	502	GOL	O2-C2-C3-O3
2	D	501	GOL	O2-C2-C3-O3
2	A	501	GOL	O2-C2-C3-O3
2	A	504	GOL	O2-C2-C3-O3
2	G	505	GOL	O2-C2-C3-O3
2	G	503	GOL	O2-C2-C3-O3
2	F	502	GOL	O1-C1-C2-C3
2	D	502	GOL	O1-C1-C2-O2
2	F	502	GOL	O1-C1-C2-O2
2	E	501	GOL	O2-C2-C3-O3
2	G	505	GOL	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GOL	1	0
2	E	501	GOL	1	0
2	A	502	GOL	5	0
2	G	503	GOL	2	0
2	G	504	GOL	1	0
2	B	504	GOL	1	0
2	C	501	GOL	1	0
2	D	501	GOL	2	0
2	B	503	GOL	1	0
2	E	502	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	438/462 (94%)	-0.34	6 (1%) 73 79	18, 27, 50, 79	3 (0%)
1	B	440/462 (95%)	-0.32	11 (2%) 58 64	17, 26, 54, 101	1 (0%)
1	C	438/462 (94%)	-0.11	7 (1%) 70 75	17, 29, 54, 93	3 (0%)
1	D	438/462 (94%)	-0.13	5 (1%) 78 82	19, 31, 56, 80	1 (0%)
1	E	439/462 (95%)	-0.16	15 (3%) 48 53	18, 29, 58, 82	1 (0%)
1	F	433/462 (93%)	-0.07	16 (3%) 45 49	19, 29, 62, 88	1 (0%)
1	G	439/462 (95%)	-0.01	10 (2%) 61 67	20, 31, 60, 87	1 (0%)
1	H	438/462 (94%)	0.45	22 (5%) 34 36	21, 35, 62, 92	1 (0%)
All	All	3503/3696 (94%)	-0.09	92 (2%) 57 62	17, 30, 57, 101	12 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	168	VAL	6.5
1	C	462	LEU	6.3
1	G	462	LEU	6.0
1	G	168	VAL	4.2
1	F	460	ALA	4.1
1	F	369	TYR	3.9
1	H	462	LEU	3.9
1	H	262	HIS	3.8
1	E	462	LEU	3.6
1	E	460	ALA	3.5
1	F	462	LEU	3.5
1	E	458	TRP	3.4
1	F	450	LEU	3.3
1	H	176	PRO	3.2
1	G	24	LYS	3.1
1	F	448	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	262	HIS	3.0
1	H	62	LYS	3.0
1	G	112	GLY	3.0
1	H	108	PHE	2.9
1	B	24	LYS	2.9
1	H	29	TRP	2.9
1	H	443	TRP	2.9
1	G	369	TYR	2.8
1	H	369	TYR	2.8
1	C	369	TYR	2.8
1	B	458	TRP	2.8
1	E	169	PRO	2.7
1	G	457	ALA	2.7
1	C	49	THR	2.7
1	G	169	PRO	2.7
1	C	25	ARG	2.6
1	H	174	ASN	2.6
1	E	262	HIS	2.6
1	C	177	SER	2.6
1	G	49	THR	2.6
1	E	443	TRP	2.6
1	H	73	ALA	2.5
1	E	67	PRO	2.5
1	E	446	ARG	2.5
1	H	144	GLY	2.5
1	B	449	PRO	2.5
1	E	176	PRO	2.5
1	B	448	ARG	2.4
1	B	23	ASN	2.4
1	G	406	TYR	2.4
1	E	450	LEU	2.4
1	F	177	SER	2.4
1	H	154	CYS	2.4
1	A	462	LEU	2.4
1	F	457	ALA	2.4
1	C	168	VAL	2.4
1	E	168	VAL	2.4
1	H	42	ILE	2.3
1	B	450	LEU	2.3
1	B	462	LEU	2.3
1	D	176	PRO	2.2
1	E	449	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	168	VAL	2.2
1	A	25	ARG	2.2
1	A	450	LEU	2.2
1	B	177	SER	2.2
1	H	177	SER	2.2
1	B	67	PRO	2.2
1	D	457	ALA	2.2
1	E	457	ALA	2.2
1	D	369	TYR	2.2
1	D	262	HIS	2.2
1	E	24	LYS	2.2
1	F	290	PRO	2.2
1	B	457	ALA	2.2
1	H	65	ALA	2.2
1	E	369	TYR	2.1
1	F	458	TRP	2.1
1	H	63	GLY	2.1
1	F	449	PRO	2.1
1	A	262	HIS	2.1
1	F	171	GLY	2.1
1	F	291	ARG	2.1
1	F	26	THR	2.1
1	A	458	TRP	2.1
1	D	86	ALA	2.1
1	G	443	TRP	2.0
1	H	110	TRP	2.0
1	C	454	ASP	2.0
1	H	121	ILE	2.0
1	F	49	THR	2.0
1	F	299	THR	2.0
1	A	369	TYR	2.0
1	H	40	TYR	2.0
1	H	115	PRO	2.0
1	H	52	VAL	2.0

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

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	GOL	A	504	6/6	0.87	0.12	40,57,65,77	0
2	GOL	G	503	6/6	0.87	0.13	34,49,54,54	0
2	GOL	F	501	6/6	0.89	0.12	41,49,57,60	0
2	GOL	A	502	6/6	0.89	0.13	38,45,52,65	0
2	GOL	B	504	6/6	0.90	0.11	31,43,45,49	0
2	GOL	A	503	6/6	0.91	0.11	34,41,50,56	0
2	GOL	F	502	6/6	0.91	0.12	37,45,46,55	0
2	GOL	D	502	6/6	0.91	0.12	35,45,50,52	0
3	SCN	G	501	3/3	0.91	0.15	20,20,26,62	0
4	K	B	505	1/1	0.91	0.14	75,75,75,75	0
2	GOL	A	501	6/6	0.92	0.10	32,42,46,47	0
2	GOL	E	501	6/6	0.94	0.08	30,37,39,41	0
2	GOL	G	504	6/6	0.94	0.09	36,44,45,49	0
2	GOL	C	501	6/6	0.94	0.09	37,41,42,54	0
2	GOL	B	502	6/6	0.94	0.09	31,40,48,50	0
4	K	E	503	1/1	0.94	0.10	45,45,45,45	0
2	GOL	G	505	6/6	0.95	0.09	36,46,49,50	0
2	GOL	E	502	6/6	0.95	0.07	35,37,39,40	0
2	GOL	D	501	6/6	0.96	0.08	26,36,38,45	0
3	SCN	B	501	3/3	0.96	0.09	17,17,24,55	0
3	SCN	D	503	3/3	0.96	0.12	41,41,48,49	0
2	GOL	B	503	6/6	0.97	0.07	23,27,36,37	0
3	SCN	G	502	3/3	0.97	0.09	38,38,39,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.