



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:27 PM UTC

PDB ID : 4RDT / pdb_00004rdt
Title : Structure of the bacterial Zn-transporter ZnuD from *Neisseria meningitidis*
(flexible conformation bound to a zinc ion)
Authors : Calmettes, C.; El Bakkouri, M.; Moraes, T.F.
Deposited on : 2014-09-19
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (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

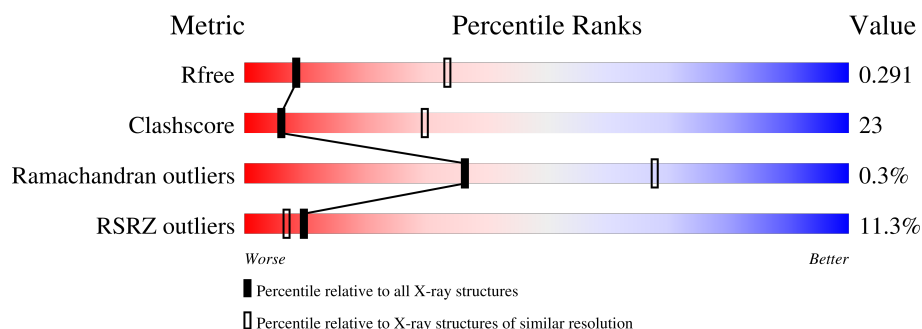
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	748	5% 54% 30% • 15%
1	B	748	14% 55% 29% • 15%

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	C8E	A	806	-	-	X	-
5	SO4	A	807	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	B	802	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10159 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 ZnuD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	635	Total	C	N	O	S	0	1	0
			5044	3158	932	945	9			
1	B	635	Total	C	N	O	S	0	0	0
			5032	3150	927	946	9			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q9JZN9
A	-12	ALA	-	expression tag	UNP Q9JZN9
A	-11	HIS	-	expression tag	UNP Q9JZN9
A	-10	HIS	-	expression tag	UNP Q9JZN9
A	-9	HIS	-	expression tag	UNP Q9JZN9
A	-8	HIS	-	expression tag	UNP Q9JZN9
A	-7	HIS	-	expression tag	UNP Q9JZN9
A	-6	HIS	-	expression tag	UNP Q9JZN9
A	-5	LEU	-	expression tag	UNP Q9JZN9
A	-4	VAL	-	expression tag	UNP Q9JZN9
A	-3	PRO	-	expression tag	UNP Q9JZN9
A	-2	ARG	-	expression tag	UNP Q9JZN9
A	-1	GLY	-	expression tag	UNP Q9JZN9
A	0	SER	-	expression tag	UNP Q9JZN9
B	-13	MET	-	expression tag	UNP Q9JZN9
B	-12	ALA	-	expression tag	UNP Q9JZN9
B	-11	HIS	-	expression tag	UNP Q9JZN9
B	-10	HIS	-	expression tag	UNP Q9JZN9
B	-9	HIS	-	expression tag	UNP Q9JZN9
B	-8	HIS	-	expression tag	UNP Q9JZN9
B	-7	HIS	-	expression tag	UNP Q9JZN9
B	-6	HIS	-	expression tag	UNP Q9JZN9
B	-5	LEU	-	expression tag	UNP Q9JZN9
B	-4	VAL	-	expression tag	UNP Q9JZN9
B	-3	PRO	-	expression tag	UNP Q9JZN9

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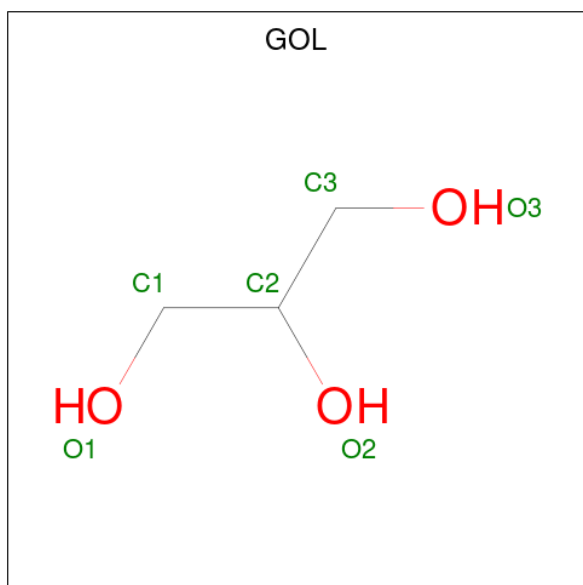
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ARG	-	expression tag	UNP Q9JZN9
B	-1	GLY	-	expression tag	UNP Q9JZN9
B	0	SER	-	expression tag	UNP Q9JZN9

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

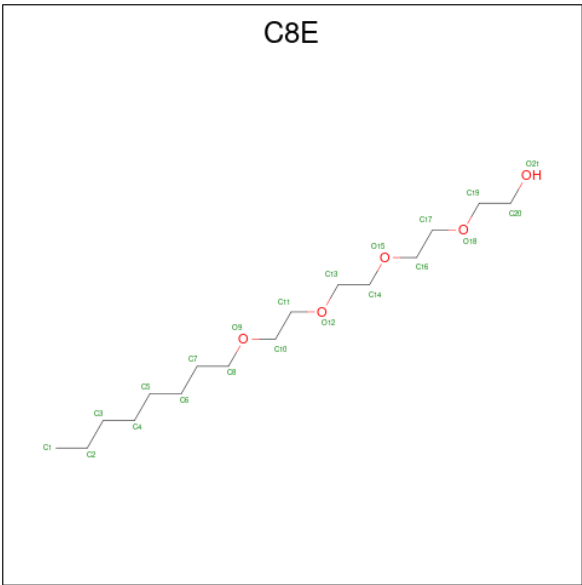
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



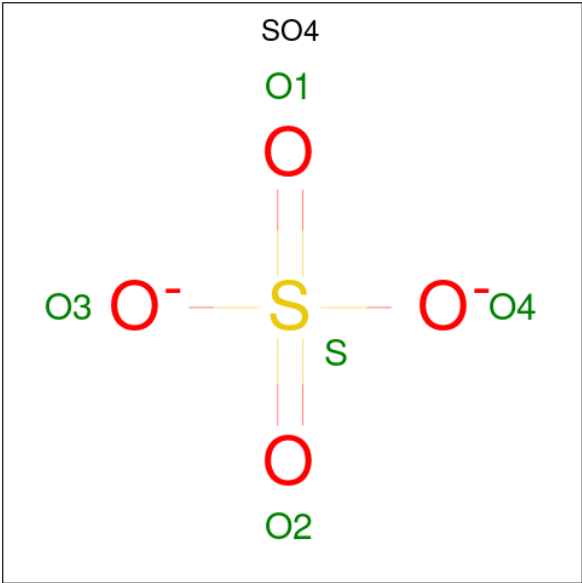
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	16	5		
4	A	1	Total	C	O	0	0
			21	16	5		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

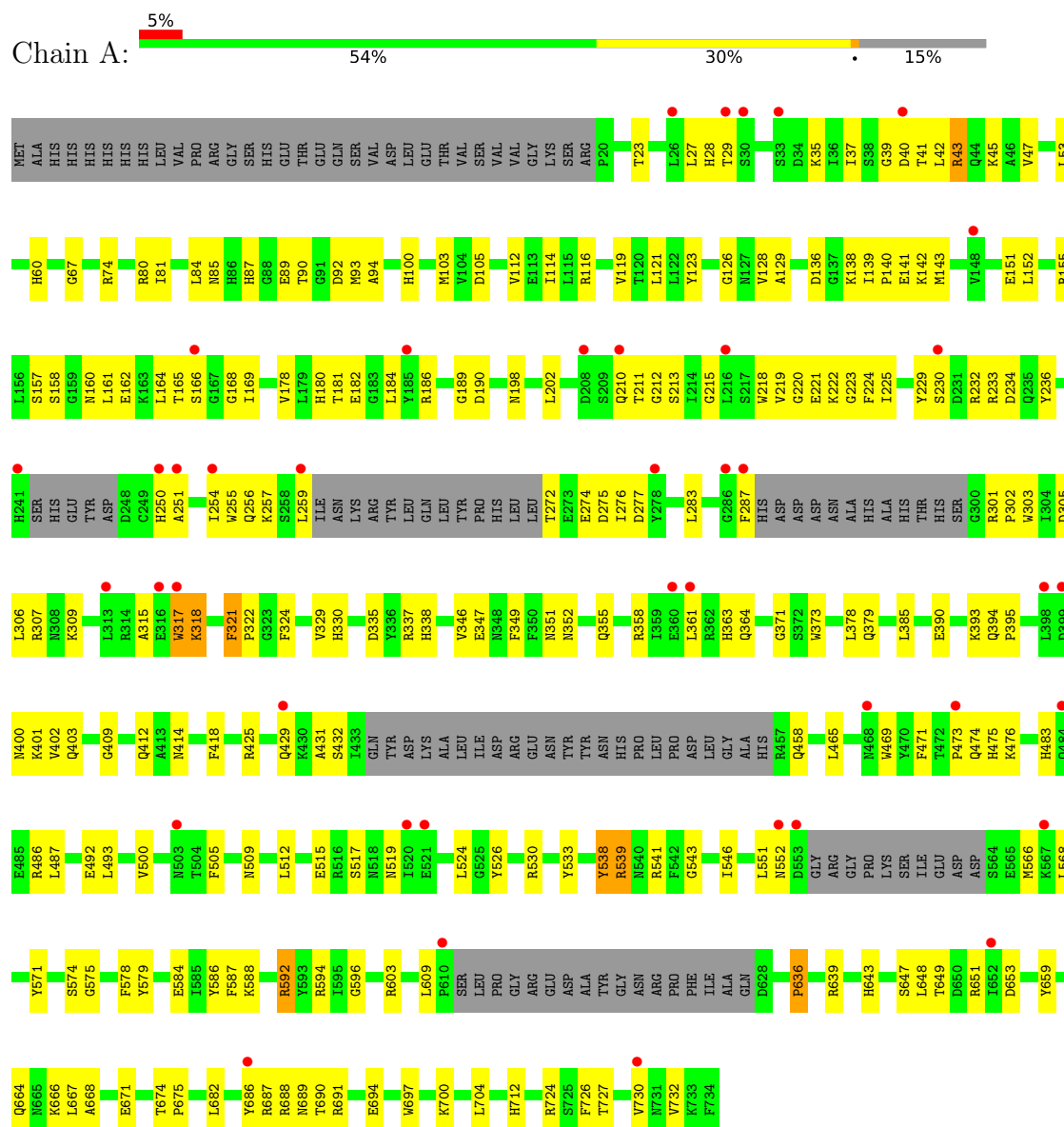
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total 9	O 9	0	0
6	B	2	Total 2	O 2	0	0

3 Residue-property plots

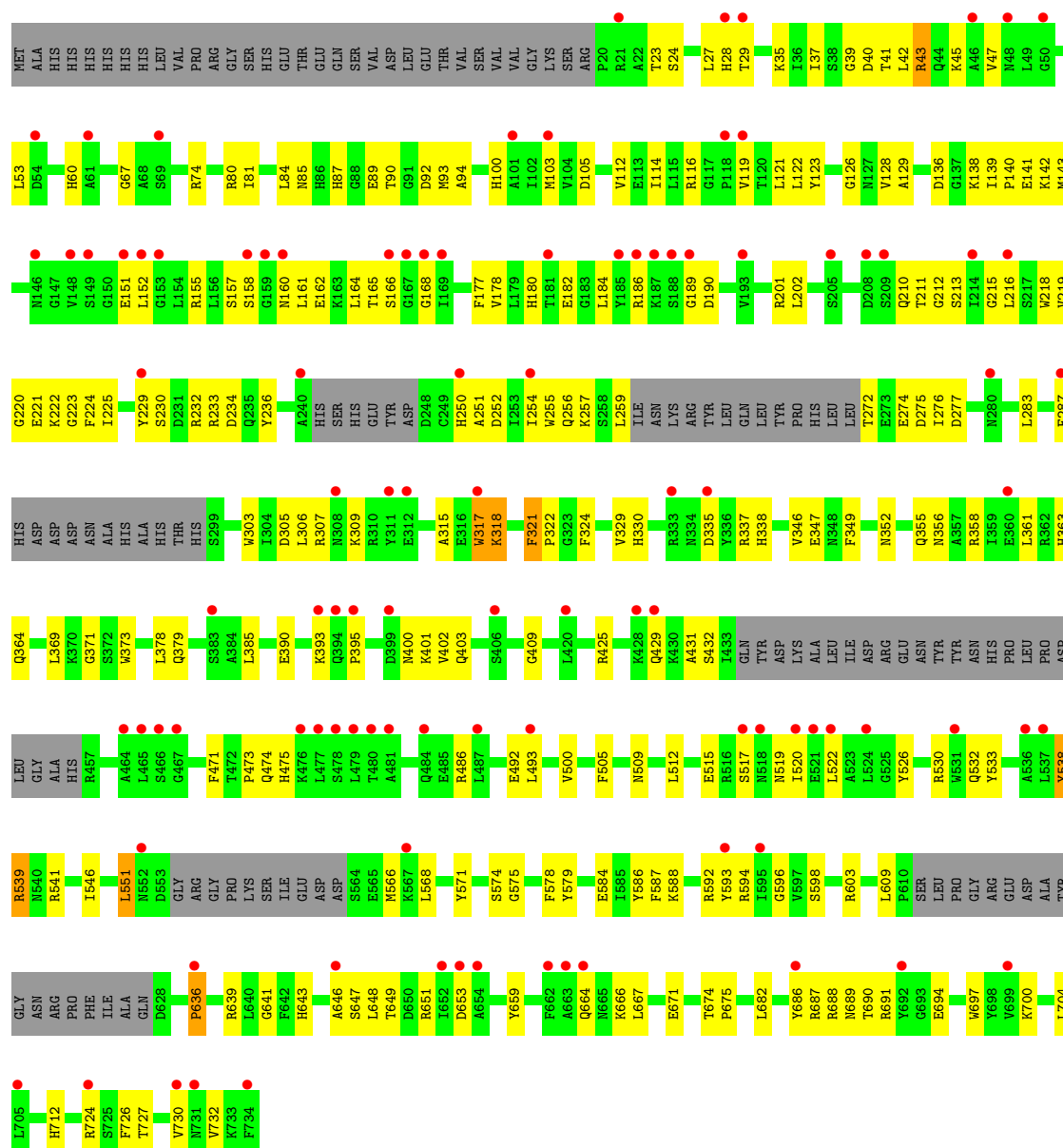
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ZnuD



• Molecule 1: ZnuD





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.34Å 156.23Å 158.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 3.20 49.93 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.93-3.20) 93.4 (49.93-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.270 , 0.305 (Not available) , 0.291	Depositor DCC
R_{free} test set	1664 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.882	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 85.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.040 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10159	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4419e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, C8E, ZN, GOL

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	0.53	0/5160	1.04	19/6969 (0.3%)
1	B	0.47	0/5144	1.02	16/6948 (0.2%)
All	All	0.50	0/10304	1.03	35/13917 (0.3%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	ARG	N-CA-C	7.85	119.91	111.36
1	A	539	ARG	CB-CG-CD	7.77	129.16	111.30
1	B	539	ARG	CB-CG-CD	7.56	128.69	111.30
1	A	43	ARG	CA-CB-CG	7.32	128.73	114.10
1	B	39	GLY	N-CA-C	7.31	121.50	112.73
1	B	43	ARG	CA-CB-CG	7.20	128.49	114.10
1	A	139	ILE	CA-C-N	7.14	128.77	119.84
1	A	139	ILE	C-N-CA	7.14	128.77	119.84
1	A	39	GLY	N-CA-C	7.04	121.17	112.73
1	B	592	ARG	N-CA-C	6.98	118.97	111.36
1	B	139	ILE	CA-C-N	6.97	128.56	119.84
1	B	139	ILE	C-N-CA	6.97	128.56	119.84
1	A	317	TRP	CA-CB-CG	6.48	125.92	113.60
1	A	275	ASP	N-CA-C	-6.47	105.35	113.18
1	B	317	TRP	CA-CB-CG	6.43	125.81	113.60
1	B	475	HIS	N-CA-C	-6.29	96.67	107.61
1	A	475	HIS	N-CA-C	-6.27	96.76	107.23
1	B	318	LYS	N-CA-C	6.26	120.62	112.92
1	A	318	LYS	N-CA-C	6.24	120.59	112.92
1	B	471	PHE	N-CA-C	-6.16	104.65	111.36
1	B	275	ASP	N-CA-C	-6.11	105.31	112.89
1	B	551	LEU	N-CA-C	6.05	117.77	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	PHE	N-CA-C	-6.04	104.78	111.36
1	A	551	LEU	N-CA-C	5.91	117.58	109.18
1	B	321	PHE	CA-C-N	-5.57	113.84	120.13
1	B	321	PHE	C-N-CA	-5.57	113.84	120.13
1	B	538	TYR	N-CA-C	5.43	117.64	109.23
1	A	321	PHE	CA-C-N	-5.35	114.08	120.13
1	A	321	PHE	C-N-CA	-5.35	114.08	120.13
1	A	28	HIS	N-CA-C	5.33	117.15	108.63
1	B	28	HIS	N-CA-C	5.27	117.06	108.63
1	A	543	GLY	N-CA-C	-5.06	106.27	113.86
1	A	483	HIS	CA-C-N	-5.05	115.36	122.94
1	A	483	HIS	C-N-CA	-5.05	115.36	122.94
1	A	538	TYR	N-CA-C	5.01	117.00	109.23

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	5044	0	4883	229	0
1	B	5032	0	4868	215	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	18	0	24	2	0
4	A	42	0	68	26	0
5	A	5	0	0	3	0
5	B	5	0	0	2	0
6	A	9	0	0	0	0
6	B	2	0	0	1	0
All	All	10159	0	9843	451	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 23.

All (451) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:MET:CG	1:B:219:VAL:HG21	1.65	1.26
1:B:283:LEU:HG	1:B:287:PHE:CE2	1.71	1.25
1:B:283:LEU:CG	1:B:287:PHE:HE2	1.54	1.20
1:A:465:LEU:HD12	4:A:806:C8E:C17	1.72	1.19
1:A:465:LEU:HD12	4:A:806:C8E:H171	1.26	1.12
1:A:143:MET:CG	1:A:219:VAL:HG21	1.80	1.11
1:B:143:MET:HG2	1:B:219:VAL:CG2	1.83	1.08
1:B:255:TRP:CE3	1:B:256:GLN:HG2	1.89	1.06
1:A:143:MET:HG2	1:A:219:VAL:HG21	1.08	1.05
1:B:283:LEU:HG	1:B:287:PHE:HE2	0.92	1.05
1:B:283:LEU:CG	1:B:287:PHE:CE2	2.35	1.03
1:B:283:LEU:O	1:B:287:PHE:HD2	1.42	1.01
1:B:283:LEU:CD1	1:B:287:PHE:CE2	2.44	1.01
1:B:143:MET:HG2	1:B:219:VAL:HG21	1.01	1.00
1:B:593:TYR:CD1	1:B:646:ALA:HB2	1.99	0.97
1:B:593:TYR:CE1	1:B:646:ALA:CB	2.47	0.97
1:A:283:LEU:O	1:A:287:PHE:HD2	1.48	0.96
1:A:256:GLN:HB3	1:A:257:LYS:HB3	1.50	0.94
1:A:493:LEU:HD12	1:A:512:LEU:HD12	1.51	0.92
1:B:593:TYR:CD1	1:B:646:ALA:CB	2.52	0.92
1:B:493:LEU:HD12	1:B:512:LEU:HD12	1.53	0.90
1:B:283:LEU:O	1:B:287:PHE:CD2	2.25	0.90
1:B:60:HIS:CE1	1:B:639:ARG:HH21	1.90	0.90
1:A:143:MET:HG2	1:A:219:VAL:CG2	2.01	0.90
1:B:283:LEU:HD11	1:B:287:PHE:CE2	2.09	0.88
1:A:465:LEU:HD12	4:A:806:C8E:H172	1.51	0.88
1:A:648:LEU:HA	1:A:649:THR:HG22	1.54	0.88
1:A:60:HIS:CE1	1:A:639:ARG:HH21	1.91	0.88
1:B:143:MET:SD	1:B:219:VAL:HG21	2.14	0.87
1:B:648:LEU:HA	1:B:649:THR:HG22	1.55	0.87
1:A:164:LEU:HD11	1:A:184:LEU:HD11	1.57	0.86
1:B:593:TYR:CE1	1:B:646:ALA:HB1	2.10	0.86
1:B:234:ASP:HB2	1:B:306:LEU:HG	1.60	0.83
1:B:47:VAL:HG21	1:B:186:ARG:HD2	1.60	0.83
1:A:530:ARG:HG3	1:A:587:PHE:HE1	1.43	0.82
1:B:283:LEU:HD11	1:B:287:PHE:CZ	2.14	0.82
1:B:493:LEU:CD1	1:B:512:LEU:HD12	2.10	0.82
1:A:648:LEU:HA	1:A:649:THR:CG2	2.09	0.82
1:A:493:LEU:CD1	1:A:512:LEU:HD12	2.09	0.82
1:A:493:LEU:HG	1:A:509:ASN:O	1.79	0.82
1:A:664:GLN:HG2	1:A:712:HIS:HD2	1.45	0.81
1:B:164:LEU:HD11	1:B:184:LEU:HD11	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:O	1:A:287:PHE:CD2	2.33	0.80
1:B:648:LEU:HA	1:B:649:THR:CG2	2.11	0.80
1:A:234:ASP:HB2	1:A:306:LEU:HG	1.61	0.80
1:B:493:LEU:HG	1:B:509:ASN:O	1.81	0.80
1:B:519:ASN:O	1:B:520:ILE:HG13	1.81	0.80
1:A:158:SER:HB3	1:A:726:PHE:H	1.47	0.79
1:A:47:VAL:HG21	1:A:186:ARG:HD2	1.65	0.77
1:A:168:GLY:O	1:A:169:ILE:HD13	1.85	0.77
1:A:539:ARG:HD3	5:A:807:SO4:O3	1.83	0.77
1:A:42:LEU:HD11	1:A:112:VAL:HG12	1.66	0.77
1:B:593:TYR:HD1	1:B:646:ALA:HB2	1.46	0.77
1:A:469:TRP:HE3	4:A:806:C8E:C4	1.99	0.76
1:A:160:ASN:HB3	1:A:162:GLU:H	1.51	0.76
1:B:42:LEU:HD11	1:B:112:VAL:HG12	1.66	0.76
1:A:469:TRP:CE3	4:A:806:C8E:H41	2.20	0.76
4:A:806:C8E:H13	4:A:806:C8E:C5	2.15	0.76
1:B:160:ASN:HB3	1:B:162:GLU:H	1.51	0.76
1:B:385:LEU:HD23	1:B:395:PRO:HB3	1.67	0.75
1:A:60:HIS:HD2	1:A:636:PRO:HB3	1.52	0.75
1:A:385:LEU:HD23	1:A:395:PRO:HB3	1.66	0.74
1:A:566:MET:O	1:A:566:MET:HG3	1.88	0.74
1:A:324:PHE:HD1	1:A:363:HIS:HA	1.53	0.74
1:B:324:PHE:HD1	1:B:363:HIS:HA	1.52	0.74
1:A:469:TRP:HE3	4:A:806:C8E:H42	1.54	0.73
1:B:60:HIS:HD2	1:B:636:PRO:HB3	1.54	0.72
1:A:250:HIS:HB2	1:A:254:ILE:HD11	1.71	0.72
1:A:592:ARG:HH21	1:A:649:THR:CG2	2.01	0.72
1:A:60:HIS:CD2	1:A:636:PRO:HB3	2.26	0.71
4:A:806:C8E:H13	4:A:806:C8E:H132	1.70	0.71
1:A:469:TRP:CE3	4:A:806:C8E:C4	2.74	0.71
1:B:158:SER:HB3	1:B:726:PHE:H	1.54	0.71
1:A:143:MET:SD	1:A:219:VAL:HG21	2.31	0.70
1:B:60:HIS:CD2	1:B:636:PRO:HB3	2.26	0.70
1:A:530:ARG:HG3	1:A:587:PHE:CE1	2.27	0.70
1:A:254:ILE:HG21	1:A:393:LYS:NZ	2.08	0.69
1:B:593:TYR:CD1	1:B:646:ALA:HB1	2.27	0.68
1:B:143:MET:SD	1:B:219:VAL:CG2	2.80	0.68
4:A:806:C8E:H13	4:A:806:C8E:H52	1.75	0.68
1:A:210:GLN:NE2	4:A:805:C8E:O12	2.27	0.68
1:B:40:ASP:OD1	1:B:41:THR:N	2.27	0.68
1:A:92:ASP:HB3	1:A:103:MET:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:MET:SD	1:A:178:VAL:CG2	2.82	0.67
1:A:40:ASP:OD1	1:A:41:THR:N	2.27	0.67
1:B:92:ASP:HB3	1:B:103:MET:HG2	1.77	0.67
1:A:250:HIS:HB2	1:A:254:ILE:CD1	2.26	0.66
1:B:222:LYS:HB2	1:B:317:TRP:HB2	1.76	0.66
1:B:221:GLU:HB3	1:B:222:LYS:HA	1.77	0.66
1:A:324:PHE:CD1	1:A:361:LEU:HD13	2.30	0.66
1:A:255:TRP:CE3	1:A:256:GLN:HG2	2.31	0.66
1:B:143:MET:SD	1:B:178:VAL:CG2	2.84	0.66
1:A:222:LYS:HB2	1:A:317:TRP:HB2	1.76	0.65
1:A:221:GLU:HB3	1:A:222:LYS:HA	1.79	0.65
1:A:105:ASP:OD2	1:A:211:THR:HG21	1.97	0.65
1:A:254:ILE:HG22	1:A:393:LYS:HE3	1.79	0.65
1:B:257:LYS:HE3	1:B:259:LEU:HD11	1.79	0.65
1:B:255:TRP:HE3	1:B:256:GLN:HG2	1.59	0.64
1:B:45:LYS:O	1:B:155:ARG:NH2	2.30	0.64
1:A:257:LYS:HE3	1:A:259:LEU:HD11	1.80	0.64
1:B:324:PHE:CD1	1:B:361:LEU:HD13	2.32	0.64
1:B:505:PHE:HB2	1:B:566:MET:CE	2.28	0.63
1:A:686:TYR:HB3	1:A:697:TRP:HB2	1.80	0.63
1:B:84:LEU:HD13	1:B:87:HIS:HA	1.81	0.63
1:A:256:GLN:CB	1:A:257:LYS:HB3	2.28	0.62
1:A:255:TRP:HB3	1:A:256:GLN:HG3	1.81	0.62
1:A:418:PHE:HE1	4:A:806:C8E:H31	1.65	0.61
1:A:586:TYR:CD1	1:A:596:GLY:HA3	2.35	0.61
1:A:164:LEU:CD1	1:A:184:LEU:HD11	2.29	0.61
1:A:219:VAL:HG12	1:A:220:GLY:N	2.15	0.61
1:B:105:ASP:OD2	1:B:211:THR:HG21	2.01	0.61
1:A:255:TRP:HB2	1:A:393:LYS:HG3	1.82	0.61
1:A:465:LEU:CD1	4:A:806:C8E:H172	2.29	0.61
1:B:80:ARG:NH2	1:B:546:ILE:O	2.34	0.61
1:A:84:LEU:HD13	1:A:87:HIS:HA	1.81	0.61
1:A:160:ASN:HB3	1:A:162:GLU:N	2.16	0.61
1:B:686:TYR:HB3	1:B:697:TRP:HB2	1.81	0.61
1:A:315:ALA:HB3	1:A:329:VAL:HG22	1.83	0.60
1:B:160:ASN:HB3	1:B:162:GLU:N	2.15	0.60
1:B:255:TRP:CE3	1:B:256:GLN:CG	2.77	0.60
1:A:80:ARG:NH2	1:A:546:ILE:O	2.35	0.60
1:A:180:HIS:O	1:A:215:GLY:N	2.32	0.60
1:B:143:MET:CG	1:B:219:VAL:CG2	2.57	0.60
1:B:315:ALA:HB3	1:B:329:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:TYR:CD1	1:B:596:GLY:HA3	2.36	0.60
1:B:250:HIS:HB2	1:B:254:ILE:HD11	1.84	0.59
1:B:255:TRP:HB2	1:B:393:LYS:HG3	1.82	0.59
1:A:45:LYS:O	1:A:155:ARG:NH2	2.34	0.59
1:A:254:ILE:CG2	1:A:393:LYS:HE3	2.33	0.59
1:B:143:MET:HG2	1:B:219:VAL:CB	2.32	0.59
1:B:647:SER:HB3	1:B:653:ASP:OD1	2.02	0.59
1:A:233:ARG:HD2	1:A:307:ARG:HG2	1.85	0.58
1:B:157:SER:HB2	1:B:162:GLU:HB3	1.83	0.58
1:B:180:HIS:O	1:B:215:GLY:N	2.32	0.58
1:A:157:SER:HB2	1:A:162:GLU:HB3	1.85	0.58
1:B:225:ILE:HD11	1:B:317:TRP:HZ3	1.69	0.58
1:A:469:TRP:HB2	4:A:806:C8E:C3	2.34	0.58
1:A:141:GLU:HG2	1:A:224:PHE:CZ	2.38	0.58
1:B:505:PHE:HB2	1:B:566:MET:HE3	1.86	0.58
1:A:355:GLN:HE21	1:A:379:GLN:HE21	1.52	0.57
1:A:647:SER:HB3	1:A:653:ASP:OD1	2.04	0.57
1:B:219:VAL:HG12	1:B:220:GLY:N	2.18	0.57
4:A:806:C8E:H13	4:A:806:C8E:H51	1.85	0.57
1:B:164:LEU:CD1	1:B:184:LEU:HD11	2.33	0.56
1:A:222:LYS:CB	1:A:317:TRP:HB2	2.36	0.56
1:B:539:ARG:NH1	5:B:802:SO4:O1	2.39	0.56
1:A:539:ARG:HD3	5:A:807:SO4:S	2.46	0.56
1:B:23:THR:HG23	1:B:87:HIS:HE1	1.70	0.56
1:B:168:GLY:HA2	1:B:182:GLU:HA	1.88	0.56
1:A:225:ILE:HD11	1:A:317:TRP:HZ3	1.70	0.55
1:B:222:LYS:CB	1:B:317:TRP:HB2	2.35	0.55
1:B:255:TRP:CD2	1:B:256:GLN:HG2	2.39	0.55
1:A:23:THR:HG23	1:A:87:HIS:HE1	1.71	0.55
1:A:168:GLY:HA2	1:A:182:GLU:HA	1.88	0.55
1:A:552:ASN:N	1:A:552:ASN:HD22	2.03	0.55
1:B:141:GLU:HG2	1:B:224:PHE:CZ	2.42	0.55
1:B:355:GLN:HE21	1:B:379:GLN:HE21	1.53	0.55
1:B:664:GLN:HG2	1:B:712:HIS:ND1	2.22	0.55
1:B:539:ARG:HG3	1:B:579:TYR:HB3	1.88	0.55
1:B:283:LEU:CD2	1:B:287:PHE:HE2	2.17	0.54
1:A:165:THR:O	1:A:184:LEU:HD12	2.08	0.54
1:A:469:TRP:HB2	4:A:806:C8E:H32	1.90	0.54
1:A:255:TRP:HE3	1:A:256:GLN:HG2	1.71	0.54
1:A:539:ARG:HG3	1:A:579:TYR:HB3	1.89	0.54
1:A:539:ARG:NH1	5:A:807:SO4:O3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ARG:HH12	1:A:689:ASN:H	1.56	0.53
1:B:651:ARG:HH12	1:B:689:ASN:H	1.57	0.53
1:B:321:PHE:HB2	1:B:322:PRO:CD	2.38	0.53
1:A:143:MET:SD	1:A:219:VAL:CG2	2.96	0.53
1:A:321:PHE:HB2	1:A:322:PRO:CD	2.39	0.53
1:A:37:ILE:HB	1:A:112:VAL:HG13	1.90	0.53
1:B:155:ARG:HE	1:B:164:LEU:HD23	1.73	0.53
1:B:218:TRP:HB2	1:B:225:ILE:H	1.74	0.52
1:A:155:ARG:HE	1:A:164:LEU:HD23	1.74	0.52
1:A:337[B]:ARG:HG3	1:A:351:ASN:OD1	2.10	0.52
1:B:161:LEU:H	1:B:189:GLY:H	1.57	0.52
1:B:255:TRP:CE3	1:B:256:GLN:NE2	2.78	0.52
1:B:324:PHE:CD1	1:B:363:HIS:HA	2.38	0.52
1:A:335:ASP:OD2	1:A:337[B]:ARG:NH2	2.43	0.52
1:A:363:HIS:ND1	1:A:364:GLN:O	2.40	0.52
1:B:530:ARG:O	1:B:587:PHE:HD1	1.93	0.52
1:A:225:ILE:HG23	1:A:315:ALA:HB2	1.91	0.52
1:B:505:PHE:HB2	1:B:566:MET:HE1	1.92	0.52
1:A:161:LEU:H	1:A:189:GLY:H	1.58	0.51
1:B:165:THR:O	1:B:184:LEU:HD12	2.10	0.51
1:B:539:ARG:HA	1:B:578:PHE:O	2.10	0.51
1:A:89:GLU:HG3	1:A:378:LEU:HD12	1.91	0.51
1:B:89:GLU:HG3	1:B:378:LEU:HD12	1.92	0.51
1:B:219:VAL:CG1	1:B:220:GLY:N	2.74	0.51
1:A:465:LEU:CD1	4:A:806:C8E:H171	2.19	0.51
1:B:309:LYS:HB2	1:B:335:ASP:HB3	1.93	0.51
1:A:67:GLY:HA3	1:A:236:TYR:CD1	2.45	0.51
1:A:74:ARG:HD3	1:A:538:TYR:CE1	2.46	0.51
1:A:198:ASN:OD1	3:A:803:GOL:O2	2.27	0.51
1:A:219:VAL:CG1	1:A:220:GLY:N	2.74	0.51
1:A:592:ARG:HH21	1:A:649:THR:HG22	1.76	0.51
1:B:60:HIS:CE1	1:B:639:ARG:NH2	2.71	0.51
1:A:539:ARG:HA	1:A:578:PHE:O	2.11	0.51
1:B:37:ILE:HB	1:B:112:VAL:HG13	1.91	0.51
1:B:588:LYS:HG2	1:B:594:ARG:HB2	1.93	0.51
1:A:373:TRP:CE3	1:A:409:GLY:HA3	2.46	0.50
1:B:363:HIS:ND1	1:B:364:GLN:O	2.38	0.50
1:A:255:TRP:CH2	1:A:394:GLN:NE2	2.80	0.50
1:A:324:PHE:CD1	1:A:363:HIS:HA	2.38	0.50
1:A:259:LEU:HD23	1:A:272:THR:HA	1.93	0.50
1:A:664:GLN:HG2	1:A:712:HIS:CD2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:LEU:HG	1:B:287:PHE:CD2	2.37	0.50
1:A:166:SER:HB3	1:A:184:LEU:HD13	1.93	0.50
1:A:222:LYS:HD2	1:A:317:TRP:CD1	2.47	0.50
1:A:254:ILE:O	1:A:255:TRP:HD1	1.95	0.50
1:A:648:LEU:O	1:A:648:LEU:HD12	2.12	0.50
1:B:143:MET:HG2	1:B:219:VAL:HG11	1.93	0.50
1:B:355:GLN:NE2	1:B:379:GLN:HE21	2.09	0.50
1:A:588:LYS:HG2	1:A:594:ARG:HB2	1.94	0.50
1:B:574:SER:CB	1:B:609:LEU:HD23	2.42	0.50
1:A:355:GLN:NE2	1:A:379:GLN:HE21	2.08	0.50
1:B:255:TRP:HE3	1:B:256:GLN:HE21	1.55	0.50
1:B:697:TRP:CD1	1:B:730:VAL:HG13	2.47	0.50
1:A:84:LEU:HD11	1:A:123:TYR:CD1	2.46	0.49
1:A:303:TRP:CZ3	1:A:305:ASP:HB2	2.47	0.49
1:B:85:ASN:HB2	1:B:90:THR:HG22	1.94	0.49
1:B:225:ILE:HG23	1:B:315:ALA:HB2	1.93	0.49
4:A:806:C8E:C5	4:A:806:C8E:C1	2.85	0.49
4:A:806:C8E:H132	4:A:806:C8E:C1	2.40	0.49
1:B:143:MET:SD	1:B:178:VAL:HG22	2.53	0.49
1:B:505:PHE:HB3	1:B:568:LEU:HD13	1.93	0.49
1:B:522:LEU:HD12	1:B:522:LEU:O	2.12	0.49
1:B:121:LEU:O	1:B:425:ARG:HD2	2.13	0.49
1:B:166:SER:HB3	1:B:184:LEU:HD13	1.93	0.49
1:A:221:GLU:CB	1:A:222:LYS:HA	2.42	0.49
1:B:539:ARG:CG	1:B:579:TYR:HB3	2.42	0.49
1:A:143:MET:SD	1:A:178:VAL:HG22	2.52	0.49
1:B:84:LEU:HD11	1:B:123:TYR:CD1	2.48	0.49
1:A:539:ARG:CG	1:A:579:TYR:HB3	2.43	0.49
1:A:574:SER:CB	1:A:609:LEU:HD23	2.43	0.49
1:B:373:TRP:CE3	1:B:409:GLY:HA3	2.48	0.49
1:A:505:PHE:HB3	1:A:568:LEU:HD13	1.95	0.49
1:A:667:LEU:HB2	1:A:671:GLU:HB2	1.94	0.49
1:B:103:MET:SD	1:B:232:ARG:HD3	2.53	0.49
1:A:160:ASN:OD1	3:A:804:GOL:H12	2.12	0.49
1:B:574:SER:HB2	1:B:609:LEU:HD23	1.94	0.49
1:A:469:TRP:CE3	4:A:806:C8E:H42	2.41	0.48
1:A:697:TRP:CD1	1:A:730:VAL:HG13	2.47	0.48
1:B:259:LEU:HD23	1:B:272:THR:HA	1.95	0.48
1:B:574:SER:OG	1:B:575:GLY:N	2.45	0.48
1:A:103:MET:SD	1:A:232:ARG:HD3	2.53	0.48
1:A:330:HIS:HB3	1:A:358:ARG:HG3	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:SER:OG	1:A:575:GLY:N	2.45	0.48
1:B:222:LYS:HD2	1:B:317:TRP:CD1	2.47	0.48
1:A:85:ASN:HB2	1:A:90:THR:HG22	1.95	0.48
1:A:486:ARG:HB3	1:A:515:GLU:HB2	1.95	0.48
1:A:574:SER:HB2	1:A:609:LEU:HD23	1.96	0.48
1:A:274:GLU:HA	1:A:276:ILE:HG22	1.95	0.48
1:B:177:PHE:CE1	1:B:216:LEU:HD21	2.49	0.48
1:B:254:ILE:O	1:B:255:TRP:HD1	1.96	0.48
1:A:309:LYS:HB2	1:A:335:ASP:HB3	1.95	0.48
1:B:274:GLU:HA	1:B:276:ILE:HG22	1.95	0.48
1:A:143:MET:SD	1:A:178:VAL:HG23	2.53	0.47
1:A:465:LEU:CD1	4:A:806:C8E:C17	2.66	0.47
1:B:74:ARG:HD3	1:B:538:TYR:CE1	2.48	0.47
1:B:303:TRP:CZ3	1:B:305:ASP:HB2	2.49	0.47
1:B:330:HIS:HB3	1:B:358:ARG:HG3	1.95	0.47
1:A:121:LEU:O	1:A:425:ARG:HD2	2.14	0.47
1:B:639:ARG:HD2	1:B:659:TYR:CD1	2.50	0.47
1:A:697:TRP:HD1	1:A:730:VAL:HG13	1.80	0.47
1:B:67:GLY:HA3	1:B:236:TYR:CD1	2.49	0.47
1:B:403:GLN:O	1:B:429:GLN:HA	2.14	0.47
1:B:60:HIS:HE1	1:B:639:ARG:HH21	1.52	0.47
1:A:81:ILE:HG22	1:A:129:ALA:HB3	1.97	0.47
1:A:140:PRO:C	1:A:142:LYS:H	2.23	0.47
1:A:220:GLY:HA2	1:A:221:GLU:C	2.40	0.47
1:A:403:GLN:O	1:A:429:GLN:HA	2.14	0.46
1:A:53:LEU:HD22	1:A:114:ILE:HD11	1.97	0.46
1:A:255:TRP:HA	1:A:256:GLN:HA	1.52	0.46
1:A:390:GLU:HG2	1:A:395:PRO:HG3	1.96	0.46
1:B:29:THR:OG1	1:B:119:VAL:HG13	2.15	0.46
1:B:93:MET:SD	1:B:352:ASN:HB2	2.56	0.46
1:B:143:MET:SD	1:B:178:VAL:HG23	2.55	0.46
1:B:493:LEU:HD11	1:B:512:LEU:HD12	1.93	0.46
1:A:690:THR:HG23	1:A:691:ARG:O	2.15	0.46
1:B:648:LEU:HD12	1:B:648:LEU:O	2.14	0.46
1:B:648:LEU:CA	1:B:649:THR:CG2	2.89	0.46
1:A:60:HIS:CE1	1:A:639:ARG:NH2	2.71	0.46
1:A:538:TYR:O	1:A:579:TYR:HA	2.16	0.46
1:B:651:ARG:HA	1:B:687:ARG:HB3	1.98	0.46
1:B:390:GLU:HG2	1:B:395:PRO:HG3	1.98	0.46
1:A:682:LEU:HD22	1:A:704:LEU:HD11	1.97	0.46
1:B:136:ASP:CG	1:B:138:LYS:HD3	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:TRP:CZ3	1:B:256:GLN:NE2	2.84	0.46
1:B:690:THR:HG23	1:B:691:ARG:O	2.16	0.46
1:A:190:ASP:HB3	1:A:202:LEU:O	2.16	0.46
1:A:301:ARG:HA	1:A:302:PRO:HD3	1.83	0.46
1:B:667:LEU:HB2	1:B:671:GLU:HB2	1.96	0.46
1:A:74:ARG:HB3	1:A:538:TYR:CE2	2.51	0.46
1:A:639:ARG:HD2	1:A:659:TYR:CD1	2.50	0.46
1:B:222:LYS:HB2	1:B:317:TRP:CB	2.45	0.46
1:B:473:PRO:HA	1:B:474:GLN:HA	1.51	0.46
1:B:538:TYR:O	1:B:579:TYR:HA	2.16	0.46
1:A:651:ARG:HA	1:A:687:ARG:HB3	1.97	0.46
1:A:29:THR:OG1	1:A:119:VAL:HG13	2.16	0.45
1:A:686:TYR:HD1	1:A:687:ARG:N	2.14	0.45
1:B:218:TRP:O	1:B:219:VAL:HG23	2.15	0.45
1:B:697:TRP:HD1	1:B:730:VAL:HG13	1.80	0.45
1:A:93:MET:SD	1:A:352:ASN:HB2	2.56	0.45
1:A:674:THR:HG22	1:A:675:PRO:O	2.16	0.45
1:B:486:ARG:HB3	1:B:515:GLU:HB2	1.97	0.45
1:A:473:PRO:HA	1:A:474:GLN:HA	1.52	0.45
1:B:53:LEU:HD22	1:B:114:ILE:HD11	1.99	0.45
1:B:143:MET:HG2	1:B:219:VAL:CG1	2.45	0.45
1:B:178:VAL:O	1:B:216:LEU:HA	2.15	0.45
1:B:486:ARG:HH21	1:B:515:GLU:CD	2.25	0.45
1:A:418:PHE:CE1	4:A:806:C8E:H31	2.47	0.45
1:B:140:PRO:C	1:B:142:LYS:H	2.25	0.45
1:B:221:GLU:CB	1:B:222:LYS:HA	2.40	0.45
1:B:566:MET:HG3	1:B:566:MET:O	2.16	0.45
1:A:152:LEU:O	1:A:732:VAL:N	2.46	0.45
1:B:682:LEU:HD22	1:B:704:LEU:HD11	1.97	0.45
1:A:60:HIS:HE1	1:A:639:ARG:HH21	1.53	0.45
1:A:218:TRP:CE3	1:A:219:VAL:O	2.70	0.45
1:A:526:TYR:HB3	1:A:533:TYR:CE2	2.52	0.45
1:B:219:VAL:CG1	1:B:220:GLY:H	2.29	0.45
1:B:674:THR:HG22	1:B:675:PRO:O	2.17	0.45
1:A:486:ARG:HH21	1:A:515:GLU:CD	2.25	0.44
1:A:221:GLU:OE1	1:A:318:LYS:HE2	2.17	0.44
1:B:35:LYS:HE3	1:B:584:GLU:OE2	2.18	0.44
1:B:347:GLU:HB3	1:B:500:VAL:HG11	1.99	0.44
1:B:74:ARG:HB3	1:B:538:TYR:CE2	2.52	0.44
1:A:74:ARG:HH11	1:A:116:ARG:HD3	1.82	0.44
1:B:74:ARG:HH11	1:B:116:ARG:CD	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:TYR:HD1	1:B:687:ARG:N	2.15	0.44
1:A:74:ARG:HH11	1:A:116:ARG:CD	2.31	0.44
1:A:210:GLN:CD	4:A:805:C8E:C13	2.91	0.44
1:A:694:GLU:O	1:A:732:VAL:HA	2.18	0.44
1:B:81:ILE:HG22	1:B:129:ALA:HB3	2.00	0.44
1:B:152:LEU:O	1:B:732:VAL:N	2.46	0.44
1:B:539:ARG:HD2	1:B:541:ARG:HH12	1.83	0.44
1:A:321:PHE:N	1:A:321:PHE:CD1	2.85	0.44
1:A:43:ARG:HD2	1:A:151:GLU:OE1	2.18	0.44
1:A:84:LEU:HD22	1:A:87:HIS:C	2.43	0.44
1:A:160:ASN:H	1:A:161:LEU:HA	1.83	0.44
1:A:84:LEU:HD11	1:A:123:TYR:CE1	2.53	0.44
1:A:254:ILE:HG21	1:A:393:LYS:HZ1	1.79	0.44
1:A:346:VAL:HG11	1:A:349:PHE:CE1	2.53	0.44
1:A:493:LEU:HD11	1:A:512:LEU:HD12	1.95	0.44
1:B:43:ARG:HD2	1:B:151:GLU:OE1	2.17	0.44
1:B:694:GLU:O	1:B:732:VAL:HA	2.18	0.44
1:B:122:LEU:O	1:B:358:ARG:NH2	2.32	0.43
1:B:335:ASP:OD2	1:B:337:ARG:NH2	2.50	0.43
1:A:324:PHE:CE1	1:A:361:LEU:CD1	3.02	0.43
1:A:324:PHE:CE1	1:A:361:LEU:HD13	2.52	0.43
1:B:233:ARG:HD2	1:B:307:ARG:HD3	2.00	0.43
1:A:222:LYS:HB2	1:A:317:TRP:CB	2.45	0.43
1:A:469:TRP:CB	4:A:806:C8E:H32	2.47	0.43
1:B:517:SER:OG	1:B:519:ASN:OD1	2.36	0.43
1:B:84:LEU:HD11	1:B:123:TYR:CE1	2.52	0.43
1:B:401:LYS:HB3	1:B:432:SER:HB2	2.00	0.43
1:B:221:GLU:OE1	1:B:318:LYS:HE2	2.19	0.43
1:B:324:PHE:CE1	1:B:361:LEU:HD13	2.54	0.43
1:B:690:THR:OG1	1:B:691:ARG:N	2.52	0.43
1:A:347:GLU:HB3	1:A:500:VAL:HG11	1.99	0.43
1:B:94:ALA:HA	1:B:100:HIS:HB2	2.00	0.43
1:B:539:ARG:HH11	1:B:539:ARG:HD3	1.63	0.43
1:A:35:LYS:HE3	1:A:584:GLU:OE2	2.19	0.43
1:A:136:ASP:CG	1:A:138:LYS:HD3	2.43	0.43
1:A:210:GLN:O	1:A:232:ARG:HA	2.19	0.43
1:A:648:LEU:CA	1:A:649:THR:CG2	2.89	0.43
1:B:210:GLN:O	1:B:232:ARG:HA	2.19	0.43
1:B:321:PHE:CD1	1:B:321:PHE:N	2.86	0.43
1:A:213:SER:HA	1:A:229:TYR:O	2.19	0.43
1:A:220:GLY:N	1:A:223:GLY:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:GLU:HA	1:A:571:TYR:CD2	2.54	0.43
1:A:552:ASN:ND2	1:A:552:ASN:O	2.52	0.43
1:A:592:ARG:NH2	1:A:649:THR:CG2	2.77	0.43
1:B:700:LYS:HB3	1:B:727:THR:HB	2.01	0.43
1:A:126:GLY:O	1:A:128:VAL:HG13	2.19	0.42
1:A:458:GLN:OE1	1:A:458:GLN:N	2.53	0.42
1:B:190:ASP:O	1:B:201:ARG:HD3	2.19	0.42
1:A:94:ALA:HA	1:A:100:HIS:HB2	2.02	0.42
1:A:210:GLN:CD	4:A:805:C8E:O12	2.62	0.42
1:A:700:LYS:HB3	1:A:727:THR:HB	2.02	0.42
1:B:37:ILE:HB	1:B:112:VAL:CG1	2.50	0.42
1:B:643:HIS:HE1	1:B:659:TYR:OH	2.02	0.42
1:A:512:LEU:HD13	1:A:546:ILE:HD13	2.02	0.42
1:B:160:ASN:H	1:B:161:LEU:HA	1.84	0.42
1:B:603:ARG:NH2	1:B:666:LYS:HE3	2.35	0.42
1:A:530:ARG:HD2	1:A:530:ARG:HA	1.95	0.42
1:B:24:SER:O	1:B:123:TYR:OH	2.22	0.42
1:B:84:LEU:HD22	1:B:87:HIS:C	2.45	0.42
1:B:346:VAL:HG11	1:B:349:PHE:CE1	2.55	0.42
1:B:526:TYR:HB3	1:B:533:TYR:CE2	2.54	0.42
1:A:212:GLY:O	1:A:230:SER:HA	2.20	0.42
1:B:212:GLY:O	1:B:230:SER:HA	2.20	0.42
1:A:218:TRP:HE3	1:A:219:VAL:O	2.02	0.42
1:A:476:LYS:O	1:A:524:LEU:HD12	2.20	0.42
1:B:274:GLU:HG2	1:B:277:ASP:HB3	2.02	0.42
1:B:306:LEU:HB2	1:B:338:HIS:HB3	2.01	0.42
1:B:519:ASN:C	1:B:520:ILE:HG13	2.43	0.42
1:B:593:TYR:HE1	1:B:646:ALA:CB	2.20	0.42
1:A:306:LEU:HB2	1:A:338:HIS:HB3	2.02	0.42
1:B:252:ASP:O	1:B:254:ILE:HG13	2.19	0.42
1:B:598:SER:O	1:B:641:GLY:N	2.36	0.42
1:A:60:HIS:HE1	1:A:639:ARG:NH2	2.16	0.42
1:A:138:LYS:HE2	1:A:213:SER:OG	2.19	0.42
1:A:274:GLU:HG2	1:A:277:ASP:HB3	2.02	0.41
1:A:27:LEU:HD22	1:A:371:GLY:HA2	2.02	0.41
1:A:37:ILE:HB	1:A:112:VAL:CG1	2.50	0.41
1:A:401:LYS:HB3	1:A:432:SER:HB2	2.01	0.41
1:A:539:ARG:HD2	1:A:541:ARG:HH12	1.84	0.41
1:A:42:LEU:HD11	1:A:112:VAL:CG1	2.45	0.41
1:A:169:ILE:N	1:A:181:THR:O	2.45	0.41
1:B:60:HIS:HE1	1:B:639:ARG:NH2	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:THR:OG1	1:A:691:ARG:N	2.53	0.41
1:B:492:GLU:HA	1:B:571:TYR:CD2	2.55	0.41
1:A:686:TYR:C	1:A:686:TYR:CD1	2.98	0.41
1:A:552:ASN:N	1:A:552:ASN:ND2	2.69	0.41
1:B:324:PHE:CE1	1:B:361:LEU:CD1	3.03	0.41
1:B:400:ASN:HD22	1:B:402:VAL:HG23	1.85	0.41
1:B:532:GLN:O	1:B:586:TYR:N	2.44	0.41
1:B:686:TYR:C	1:B:686:TYR:CD1	2.98	0.41
1:A:259:LEU:HB2	1:A:272:THR:HA	2.03	0.41
1:B:27:LEU:HD22	1:B:371:GLY:HA2	2.02	0.41
1:A:458:GLN:HB3	1:A:487:LEU:HD21	2.03	0.41
1:A:530:ARG:O	1:A:587:PHE:HD1	2.03	0.41
1:B:190:ASP:HB3	1:B:202:LEU:O	2.21	0.41
1:A:401:LYS:HD3	1:A:432:SER:HB2	2.03	0.41
1:A:649:THR:C	1:A:651:ARG:H	2.29	0.41
1:A:651:ARG:NH1	1:A:688:ARG:HA	2.36	0.41
1:A:686:TYR:HD1	1:A:686:TYR:C	2.29	0.41
1:B:651:ARG:NH1	1:B:688:ARG:HA	2.36	0.41
1:A:400:ASN:HD22	1:A:402:VAL:HG23	1.85	0.40
1:A:429:GLN:HE21	1:A:431:ALA:HB2	1.86	0.40
1:A:517:SER:OG	1:A:519:ASN:OD1	2.39	0.40
1:A:603:ARG:NH2	1:A:666:LYS:HE3	2.35	0.40
1:A:643:HIS:HE1	1:A:659:TYR:OH	2.03	0.40
1:A:667:LEU:HD12	1:A:668:ALA:O	2.22	0.40
1:A:724:ARG:HD3	1:A:726:PHE:CE1	2.56	0.40
1:B:356:ASN:ND2	6:B:901:HOH:O	2.47	0.40
1:B:369:LEU:HD12	1:B:369:LEU:O	2.21	0.40
1:B:686:TYR:HD1	1:B:686:TYR:C	2.29	0.40
1:A:412:GLN:NE2	1:A:414:ASN:HD21	2.19	0.40
1:B:126:GLY:O	1:B:128:VAL:HG13	2.21	0.40
1:B:223:GLY:HA3	1:B:317:TRP:HA	2.02	0.40
1:A:161:LEU:N	1:A:189:GLY:H	2.19	0.40
1:B:259:LEU:HB2	1:B:272:THR:HA	2.03	0.40
1:B:539:ARG:HD3	5:B:802:SO4:S	2.62	0.40
1:B:649:THR:C	1:B:651:ARG:H	2.29	0.40
1:B:724:ARG:HD3	1:B:726:PHE:CE1	2.57	0.40
4:A:806:C8E:H52	4:A:806:C8E:C1	2.48	0.40
1:B:429:GLN:HE21	1:B:431:ALA:HB2	1.86	0.40
1:B:551:LEU:HD23	1:B:551:LEU:HA	1.79	0.40
1:B:213:SER:HA	1:B:229:TYR:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	587/748 (78%)	536 (91%)	49 (8%)	2 (0%)	36	68
1	B	621/748 (83%)	569 (92%)	50 (8%)	2 (0%)	36	68
All	All	1208/1496 (81%)	1105 (92%)	99 (8%)	4 (0%)	36	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	ALA
1	B	251	ALA
1	A	636	PRO
1	B	636	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z > 2$
3	GOL	A	803	-	5,5,5	0.42	0	5,5,5	0.17	0
5	SO4	B	802	-	4,4,4	0.23	0	6,6,6	0.07	0
4	C8E	A	805	-	20,20,20	0.32	0	19,19,19	0.50	0
4	C8E	A	806	-	20,20,20	0.33	0	19,19,19	0.46	0
3	GOL	A	802	-	5,5,5	0.38	0	5,5,5	0.27	0
5	SO4	A	807	-	4,4,4	0.23	0	6,6,6	0.06	0
3	GOL	A	804	-	5,5,5	0.41	0	5,5,5	0.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	803	-	-	2/4/4/4	-
4	C8E	A	805	-	-	9/18/18/18	-
4	C8E	A	806	-	-	10/18/18/18	-
3	GOL	A	802	-	-	4/4/4/4	-
3	GOL	A	804	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	GOL	O1-C1-C2-C3
3	A	804	GOL	O1-C1-C2-C3
4	A	806	C8E	O15-C16-C17-O18

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Mol	Chain	Res	Type	Atoms
4	A	805	C8E	O15-C16-C17-O18
3	A	803	GOL	O1-C1-C2-O2
4	A	805	C8E	C6-C7-C8-O9
3	A	802	GOL	O1-C1-C2-C3
3	A	802	GOL	C1-C2-C3-O3
3	A	804	GOL	C1-C2-C3-O3
3	A	802	GOL	O1-C1-C2-O2
3	A	804	GOL	O1-C1-C2-O2
4	A	806	C8E	C4-C5-C6-C7
4	A	806	C8E	C6-C7-C8-O9
4	A	805	C8E	O18-C19-C20-O21
3	A	804	GOL	O2-C2-C3-O3
4	A	806	C8E	O9-C10-C11-O12
4	A	805	C8E	C4-C5-C6-C7
4	A	805	C8E	C5-C6-C7-C8
4	A	806	C8E	C11-C10-O9-C8
4	A	805	C8E	C20-C19-O18-C17
4	A	806	C8E	C10-C11-O12-C13
4	A	806	C8E	C13-C14-O15-C16
4	A	805	C8E	C14-C13-O12-C11
4	A	806	C8E	C7-C8-O9-C10
4	A	806	C8E	C1-C2-C3-C4
3	A	802	GOL	O2-C2-C3-O3
4	A	806	C8E	C2-C3-C4-C5
4	A	805	C8E	C1-C2-C3-C4
4	A	805	C8E	O12-C13-C14-O15

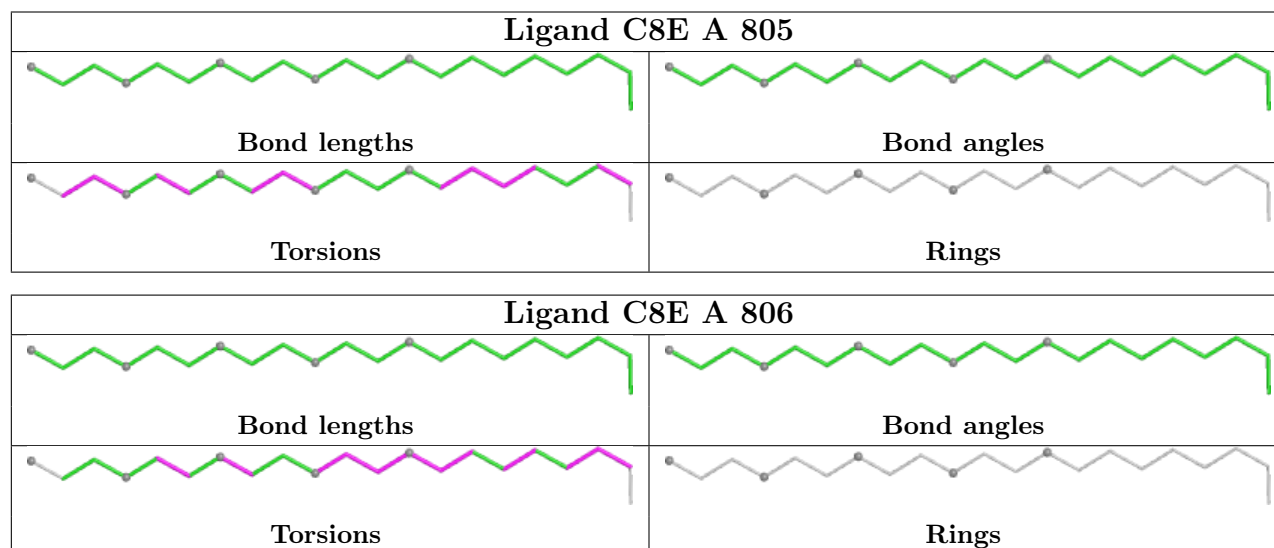
There are no ring outliers.

6 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	GOL	1	0
5	B	802	SO4	2	0
4	A	805	C8E	3	0
4	A	806	C8E	23	0
5	A	807	SO4	3	0
3	A	804	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	635/748 (84%)	0.50	41 (6%) 25 16	43, 87, 164, 259	1 (0%)
1	B	635/748 (84%)	1.11	102 (16%) 4 3	94, 137, 213, 273	0
All	All	1270/1496 (84%)	0.81	143 (11%) 10 7	43, 119, 195, 273	1 (0%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	THR	6.5
1	B	103	MET	5.7
1	B	520	ILE	5.6
1	B	208	ASP	5.5
1	B	29	THR	5.0
1	B	664	GLN	4.8
1	A	250	HIS	4.5
1	B	686	TYR	4.4
1	B	429	GLN	4.4
1	B	652	ILE	4.4
1	B	48	ASN	4.4
1	B	479	LEU	4.3
1	A	552	ASN	4.2
1	B	311	TYR	4.1
1	A	254	ILE	4.1
1	B	166	SER	4.1
1	B	522	LEU	4.0
1	A	287	PHE	4.0
1	B	287	PHE	3.9
1	B	467	GLY	3.8
1	B	481	ALA	3.8
1	B	692	TYR	3.7
1	B	118	PRO	3.7
1	A	686	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	646	ALA	3.6
1	A	429	GLN	3.6
1	B	216	LEU	3.6
1	A	241	HIS	3.6
1	B	186	ARG	3.5
1	B	521	GLU	3.5
1	B	552	ASN	3.5
1	B	663	ALA	3.5
1	B	240	ALA	3.5
1	B	167	GLY	3.4
1	B	699	VAL	3.4
1	B	653	ASP	3.3
1	B	151	GLU	3.2
1	B	487	LEU	3.2
1	B	731	ASN	3.2
1	B	148	VAL	3.2
1	B	158	SER	3.2
1	A	468	ASN	3.1
1	B	169	ILE	3.1
1	A	40	ASP	3.1
1	B	465	LEU	3.1
1	B	705	LEU	3.1
1	B	119	VAL	3.0
1	B	567	LYS	3.0
1	B	536	ALA	3.0
1	B	254	ILE	3.0
1	B	724	ARG	2.9
1	B	21	ARG	2.9
1	B	595	ILE	2.9
1	A	216	LEU	2.8
1	B	593	TYR	2.8
1	B	160	ASN	2.8
1	B	229	TYR	2.8
1	B	466	SER	2.7
1	B	518	ASN	2.7
1	A	610	PRO	2.7
1	B	168	GLY	2.7
1	B	464	ALA	2.7
1	B	189	GLY	2.7
1	B	493	LEU	2.7
1	A	33	SER	2.6
1	B	517	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	312	GLU	2.6
1	B	360	GLU	2.6
1	A	521	GLU	2.6
1	A	313	LEU	2.6
1	A	286	GLY	2.5
1	B	69	SER	2.5
1	B	209	SER	2.5
1	B	50	GLY	2.5
1	B	159	GLY	2.5
1	B	54	ASP	2.5
1	B	734	PHE	2.5
1	B	524	LEU	2.5
1	B	61	ALA	2.4
1	B	280	ASN	2.4
1	B	335	ASP	2.4
1	B	476	LYS	2.4
1	B	480	THR	2.4
1	A	567	LYS	2.4
1	B	187	LYS	2.4
1	B	185	TYR	2.4
1	B	28	HIS	2.4
1	A	251	ALA	2.4
1	B	46	ALA	2.4
1	B	333	ARG	2.4
1	A	317	TRP	2.4
1	B	654	ALA	2.4
1	A	360	GLU	2.4
1	B	250	HIS	2.3
1	B	308	ASN	2.3
1	A	166	SER	2.3
1	A	473	PRO	2.3
1	B	636	PRO	2.3
1	A	520	ILE	2.3
1	A	259	LEU	2.3
1	B	484	GLN	2.3
1	B	420	LEU	2.3
1	B	662	PHE	2.3
1	A	316	GLU	2.3
1	B	193	VAL	2.3
1	A	652	ILE	2.2
1	B	153	GLY	2.2
1	B	477	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	185	TYR	2.2
1	B	428	LYS	2.2
1	B	146	ASN	2.2
1	A	398	LEU	2.2
1	B	101	ALA	2.2
1	B	395	PRO	2.2
1	A	278	TYR	2.2
1	A	30	SER	2.2
1	B	383	SER	2.2
1	B	394	GLN	2.2
1	A	26	LEU	2.2
1	A	553	ASP	2.2
1	A	730	VAL	2.2
1	A	208	ASP	2.2
1	B	531	TRP	2.2
1	B	537	LEU	2.1
1	B	152	LEU	2.1
1	B	188	SER	2.1
1	A	148	VAL	2.1
1	A	399	ASP	2.1
1	A	484	GLN	2.1
1	B	406	SER	2.1
1	A	503	ASN	2.1
1	B	317	TRP	2.1
1	A	361	LEU	2.1
1	A	210	GLN	2.1
1	B	399	ASP	2.1
1	B	393	LYS	2.0
1	B	730	VAL	2.0
1	A	230	SER	2.0
1	B	478	SER	2.0
1	B	181	THR	2.0
1	B	149	SER	2.0
1	B	205	SER	2.0
1	B	214	ILE	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](#)

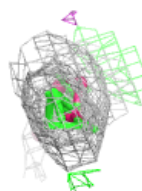
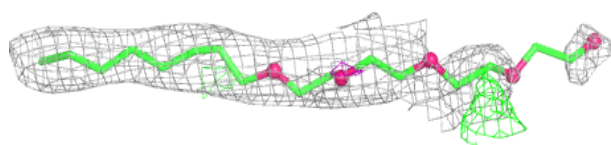
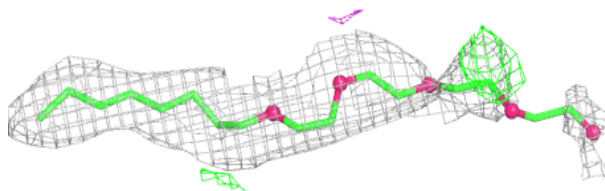
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	802	6/6	0.67	0.24	118,132,135,137	0
5	SO4	A	807	5/5	0.76	0.13	157,158,162,169	0
5	SO4	B	802	5/5	0.76	0.09	173,176,176,177	0
3	GOL	A	803	6/6	0.82	0.19	92,113,117,123	0
3	GOL	A	804	6/6	0.82	0.46	97,104,112,113	0
4	C8E	A	805	21/21	0.87	0.14	39,92,137,142	0
4	C8E	A	806	21/21	0.88	0.19	80,98,130,132	0
2	ZN	B	801	1/1	0.98	0.08	82,82,82,82	0
2	ZN	A	801	1/1	0.99	0.18	127,127,127,127	0

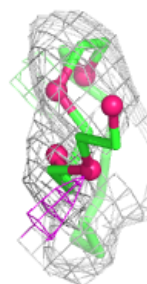
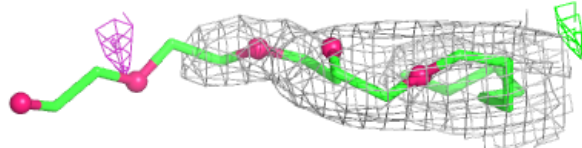
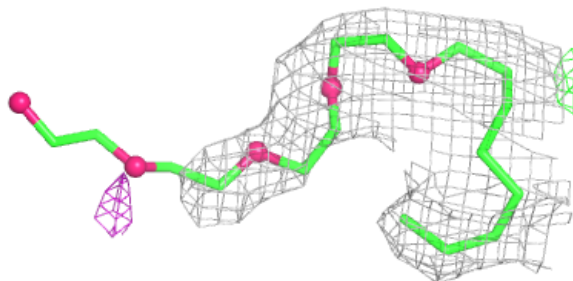
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E A 805:

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

**Electron density around C8E A 806:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.