



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:49 AM UTC

PDB ID : 1PJQ / pdb_00001pjq
Title : Structure and function of CysG, the multifunctional methyltransferase/dehydrogenase/ferrochelatase for siroheme synthesis
Authors : Stroupe, M.E.; Leech, H.K.; Daniels, D.S.; Warren, M.J.; Getzoff, E.D.
Deposited on : 2003-06-03
Resolution : 2.21 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

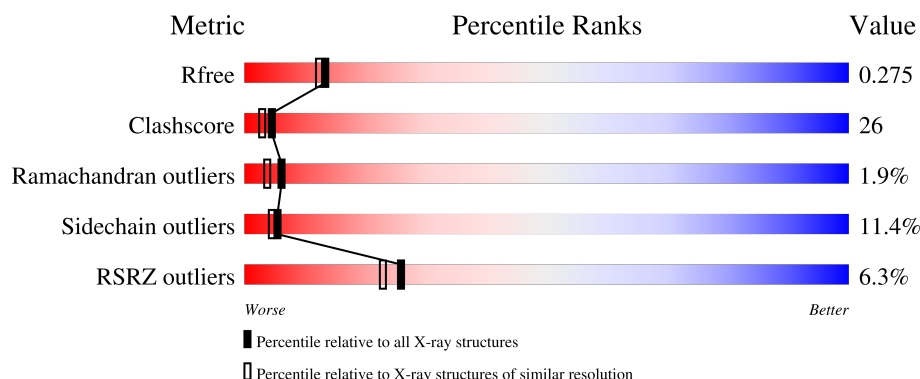
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	457	
1	B	457	

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
1	SEP	B	128	-	-	X	-
2	ACT	A	504	-	-	X	-
2	ACT	A	505	-	-	X	-
3	PGE	A	502	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7503 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.

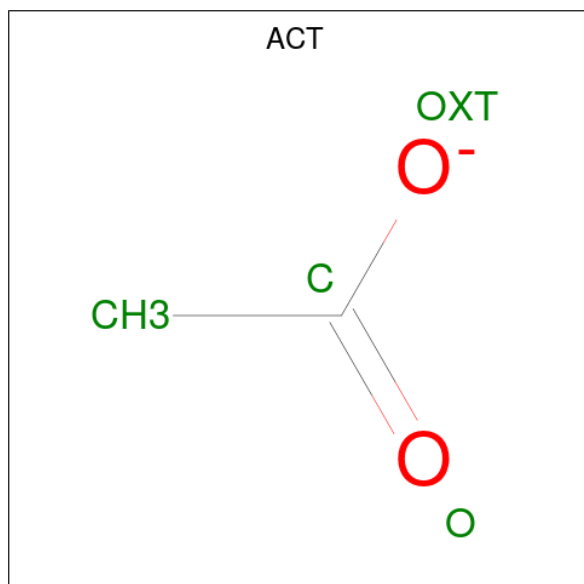
- Molecule 1 is a protein called Siroheme synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	P	S	0	13	0
			3581	2249	650	663	1	18			
1	B	455	Total	C	N	O	P	S	0	4	0
			3548	2228	643	659	1	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	SEP	SER	modified residue	UNP P25924
B	128	SEP	SER	modified residue	UNP P25924

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



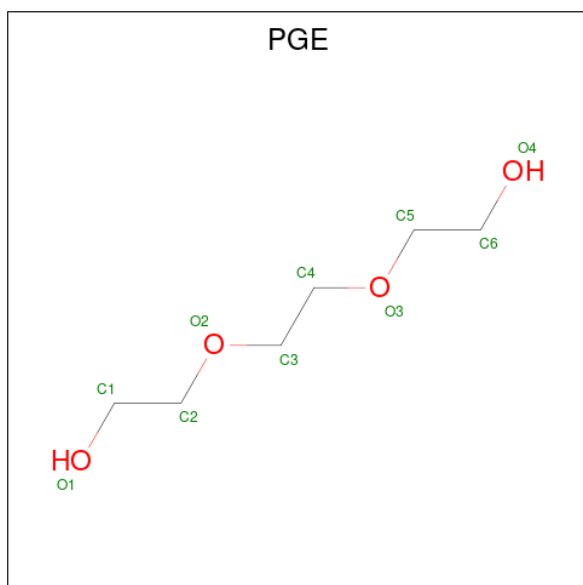
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

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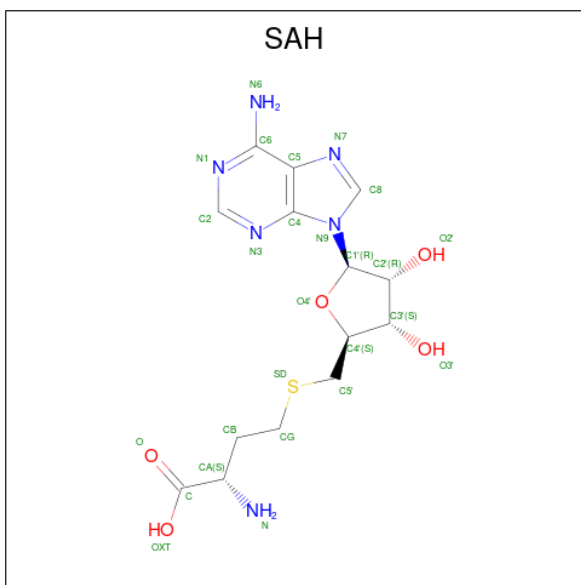
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

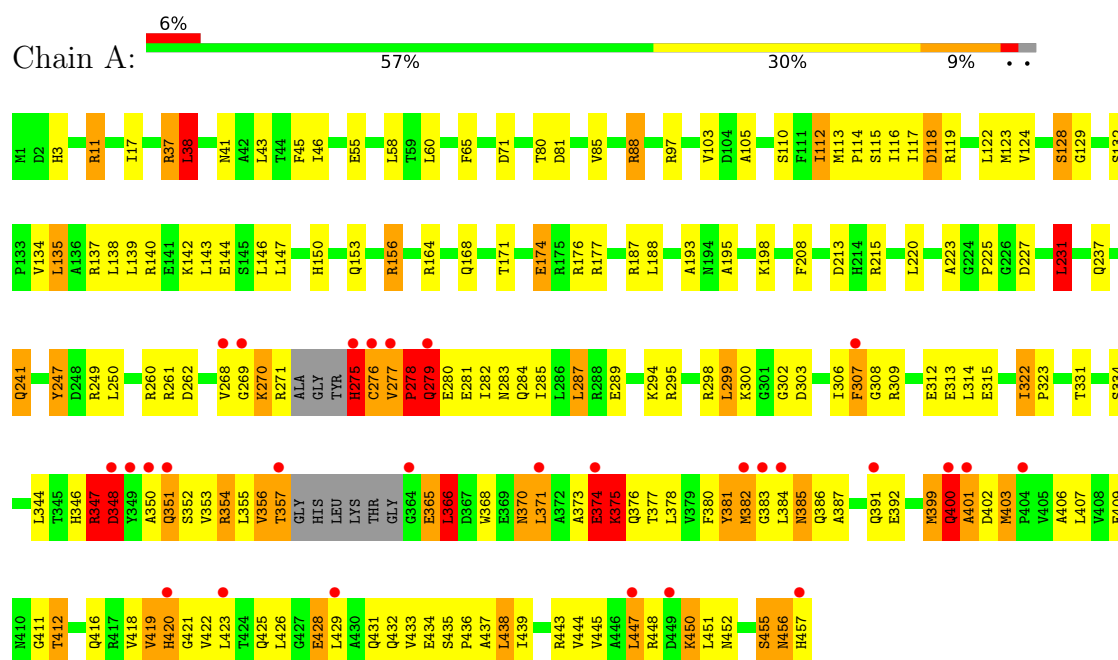
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	147	Total O 147 147	0	0
5	B	179	Total O 179 179	0	0

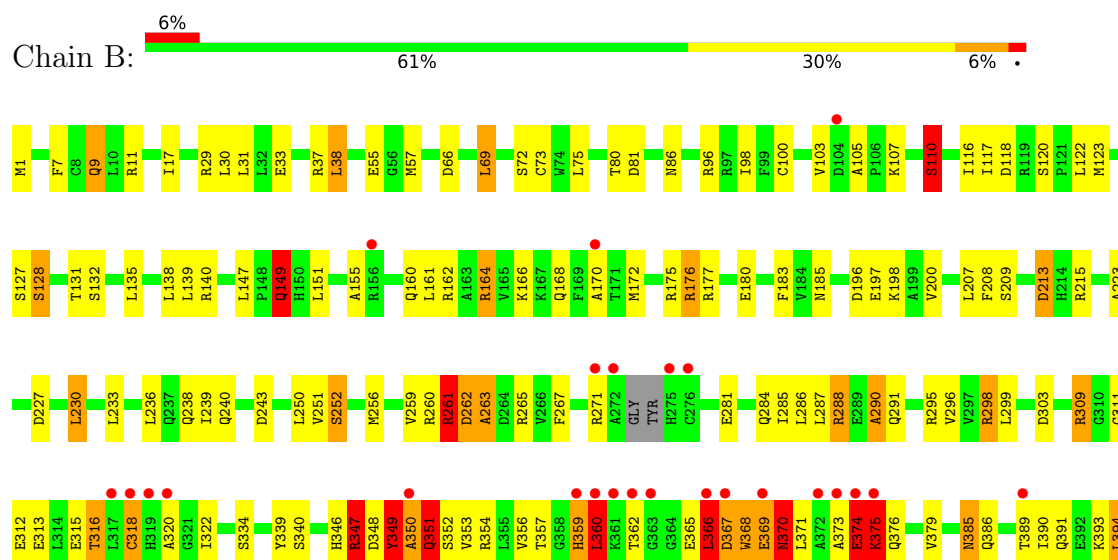
3 Residue-property plots [i](#)

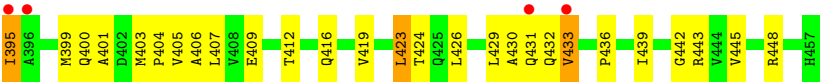
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Siroheme synthase



• Molecule 1: Siroheme synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.73Å 121.49Å 130.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.21 19.97 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.97-2.21) 99.1 (19.97-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.21Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.273 0.239 , 0.275	Depositor DCC
R_{free} test set	4899 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7503	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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: PGE, ACT, SAH, SEP

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	0.76	15/3627 (0.4%)	1.24	54/4903 (1.1%)
1	B	0.58	4/3594 (0.1%)	1.23	49/4861 (1.0%)
All	All	0.68	19/7221 (0.3%)	1.24	103/9764 (1.1%)

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	A	0	3
1	B	0	1
All	All	0	4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	LYS	CA-C	12.88	1.70	1.52
1	A	276	CYS	N-CA	-10.99	1.33	1.46
1	A	375	LYS	N-CA	10.79	1.60	1.46
1	A	276	CYS	CA-C	-9.41	1.42	1.53
1	A	375	LYS	CA-CB	-8.94	1.38	1.53
1	A	374[A]	GLU	CA-C	8.67	1.63	1.52
1	A	374[B]	GLU	CA-C	8.67	1.63	1.52
1	A	374[A]	GLU	C-O	-8.35	1.15	1.23
1	A	374[B]	GLU	C-O	-8.35	1.15	1.23
1	A	400	GLN	N-CA	7.52	1.55	1.46
1	A	275	HIS	C-N	-7.48	1.23	1.33
1	B	369	GLU	CA-C	-7.04	1.44	1.53
1	B	370	ASN	C-O	-6.60	1.15	1.24
1	A	374[A]	GLU	C-N	6.43	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374[B]	GLU	C-N	6.43	1.42	1.33
1	B	370	ASN	N-CA	-6.41	1.38	1.46
1	B	374	GLU	CA-C	6.27	1.61	1.52
1	A	276	CYS	CA-CB	-5.52	1.45	1.52
1	A	279	GLN	CA-C	-5.03	1.46	1.52

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	CYS	N-CA-CB	-18.43	87.23	110.45
1	B	350	ALA	N-CA-C	16.58	135.66	109.79
1	B	351	GLN	N-CA-C	15.27	131.89	111.28
1	A	276	CYS	N-CA-C	13.72	129.75	110.68
1	A	374[A]	GLU	N-CA-C	11.85	123.39	108.45
1	A	374[B]	GLU	N-CA-C	11.85	123.39	108.45
1	A	450	LYS	N-CA-C	-11.49	98.15	114.12
1	B	375	LYS	N-CA-C	11.03	134.30	110.80
1	B	370	ASN	N-CA-C	-10.72	87.97	110.80
1	A	375	LYS	CB-CA-C	10.49	131.30	110.42
1	A	347	ARG	N-CA-C	9.74	131.54	110.80
1	B	263	ALA	N-CA-C	-9.70	94.56	110.17
1	B	110	SER	N-CA-C	9.60	122.95	111.33
1	A	400	GLN	CB-CA-C	-9.18	92.14	110.42
1	B	366	LEU	N-CA-C	9.18	123.87	110.28
1	A	348	ASP	N-CA-C	-9.13	103.25	114.75
1	A	356	VAL	N-CA-C	8.89	123.36	108.86
1	B	320	ALA	N-CA-C	-8.80	102.95	114.31
1	B	262	ASP	N-CA-C	8.67	120.77	108.54
1	B	359	HIS	N-CA-C	8.66	123.44	108.02
1	B	369	GLU	N-CA-CB	7.97	123.76	110.53
1	A	351	GLN	N-CA-C	-7.93	101.80	114.09
1	B	352	SER	N-CA-C	-7.79	94.20	110.80
1	B	360	LEU	N-CA-C	-7.77	94.25	110.80
1	B	318	CYS	N-CA-C	7.72	120.78	111.82
1	A	365	GLU	N-CA-C	7.60	119.58	108.86
1	B	38	LEU	N-CA-C	7.49	122.05	109.76
1	A	276	CYS	O-C-N	7.47	132.99	122.68
1	B	116	ILE	N-CA-C	7.40	119.13	108.48
1	B	368	TRP	CA-C-N	-7.35	111.89	122.77
1	B	368	TRP	C-N-CA	-7.35	111.89	122.77
1	A	71	ASP	N-CA-C	7.25	121.77	112.34
1	A	88	ARG	N-CA-C	-7.22	103.44	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	ARG	CA-C-N	-7.22	113.24	123.20
1	B	261	ARG	C-N-CA	-7.22	113.24	123.20
1	A	386	GLN	N-CA-C	-7.03	104.81	113.53
1	A	374[A]	GLU	CA-C-N	-6.93	108.31	121.54
1	A	374[A]	GLU	C-N-CA	-6.93	108.31	121.54
1	A	374[B]	GLU	CA-C-N	-6.93	108.31	121.54
1	A	374[B]	GLU	C-N-CA	-6.93	108.31	121.54
1	B	243	ASP	N-CA-C	-6.83	103.96	112.90
1	B	369	GLU	CA-C-O	6.78	128.98	121.39
1	A	46	ILE	CA-C-N	6.77	128.30	119.84
1	A	46	ILE	C-N-CA	6.77	128.30	119.84
1	A	456	ASN	N-CA-C	-6.76	104.24	113.30
1	B	374	GLU	N-CA-C	6.73	125.13	110.80
1	B	349	TYR	CA-C-N	6.72	132.95	121.86
1	B	349	TYR	C-N-CA	6.72	132.95	121.86
1	A	38	LEU	N-CA-C	6.62	120.61	109.76
1	A	307	PHE	N-CA-C	6.59	119.74	111.24
1	B	350	ALA	N-CA-CB	-6.52	101.06	110.45
1	B	362	THR	N-CA-C	6.41	124.44	110.80
1	B	347	ARG	N-CA-C	6.34	124.31	110.80
1	B	103	VAL	N-CA-C	6.31	122.47	109.34
1	A	322	ILE	N-CA-C	6.29	114.90	107.73
1	A	279	GLN	CA-C-N	-6.10	111.63	120.29
1	A	279	GLN	C-N-CA	-6.10	111.63	120.29
1	A	118	ASP	N-CA-C	6.08	118.64	108.73
1	A	110	SER	N-CA-C	6.05	122.69	113.61
1	A	276	CYS	CA-C-O	-5.90	113.58	122.38
1	A	368	TRP	N-CA-C	5.85	118.61	111.82
1	A	308	GLY	N-CA-C	5.83	122.80	112.55
1	A	365	GLU	CA-C-N	5.82	132.65	121.54
1	A	365	GLU	C-N-CA	5.82	132.65	121.54
1	A	231	LEU	N-CA-C	-5.78	102.35	110.50
1	B	375	LYS	O-C-N	5.75	130.23	122.59
1	B	353	VAL	N-CA-C	-5.74	100.08	108.11
1	A	375	LYS	N-CA-CB	5.72	120.15	110.49
1	A	455	SER	N-CA-C	5.62	117.33	108.96
1	B	197	GLU	N-CA-C	5.56	118.06	111.33
1	B	155	ALA	N-CA-C	-5.55	105.14	111.07
1	A	279	GLN	N-CA-C	5.54	122.60	110.80
1	A	225	PRO	N-CA-C	5.51	120.82	114.20
1	A	400	GLN	N-CA-C	5.50	122.52	110.80
1	A	381[A]	TYR	N-CA-C	-5.50	101.51	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381[B]	TYR	N-CA-C	-5.50	101.51	109.59
1	B	303	ASP	CA-C-N	5.49	125.31	119.28
1	B	303	ASP	C-N-CA	5.49	125.31	119.28
1	A	399	MET	CA-C-N	5.48	132.01	121.54
1	A	399	MET	C-N-CA	5.48	132.01	121.54
1	A	105	ALA	CA-C-N	5.47	125.30	119.28
1	A	105	ALA	C-N-CA	5.47	125.30	119.28
1	B	105	ALA	CA-C-N	5.41	126.60	119.84
1	B	105	ALA	C-N-CA	5.41	126.60	119.84
1	B	359	HIS	CA-C-N	5.37	131.80	121.54
1	B	359	HIS	C-N-CA	5.37	131.80	121.54
1	A	55	GLU	N-CA-C	-5.34	105.99	112.88
1	B	376	GLN	N-CA-C	-5.31	101.10	109.50
1	B	290	ALA	N-CA-C	-5.31	105.16	111.69
1	B	251	VAL	N-CA-C	-5.26	100.83	108.36
1	B	296	VAL	N-CA-C	5.25	115.87	108.36
1	B	37	ARG	N-CA-C	-5.24	98.13	107.98
1	B	252	SER	N-CA-C	5.23	117.44	110.53
1	A	431	GLN	N-CA-C	-5.23	106.58	113.17
1	A	387	ALA	N-CA-C	5.23	117.66	111.33
1	A	399	MET	N-CA-C	5.18	117.68	109.24
1	B	356	VAL	N-CA-C	5.18	116.83	108.85
1	B	149	GLN	N-CA-C	5.16	117.57	111.33
1	B	170	ALA	N-CA-C	5.05	119.42	113.16
1	A	103	VAL	N-CA-C	5.03	119.80	109.34
1	B	118	ASP	N-CA-C	5.03	116.80	108.20
1	A	348	ASP	CA-C-N	5.00	127.29	120.54
1	A	348	ASP	C-N-CA	5.00	127.29	120.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	HIS	Mainchain
1	A	374[A]	GLU	Mainchain
1	A	374[B]	GLU	Mainchain
1	B	374	GLU	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3581	0	3611	239	0
1	B	3548	0	3584	163	0
2	A	8	0	6	14	0
2	B	4	0	3	1	0
3	A	10	0	13	8	0
4	B	26	0	19	0	0
5	A	147	0	0	9	0
5	B	179	0	0	4	0
All	All	7503	0	7236	378	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 26.

All (378) 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:127:SER:C	1:B:128:SEP:N	1.67	1.46
1:B:128:SEP:CB	1:B:128:SEP:OG	1.83	1.27
1:A:374[A]:GLU:HG2	1:A:375:LYS:N	1.36	1.14
1:A:302:GLY:HA3	2:A:505:ACT:H2	1.25	1.13
1:A:374[B]:GLU:HG2	1:A:375:LYS:N	1.68	1.07
1:B:346:HIS:CE1	1:B:347:ARG:HD3	1.89	1.06
1:B:256:MET:O	1:B:259:VAL:HG12	1.60	1.01
1:A:284:GLN:HA	1:A:287:LEU:HD21	1.42	1.00
1:A:137[A]:ARG:NH2	1:B:176:ARG:HH12	1.65	0.95
1:A:346:HIS:HE1	1:A:347:ARG:HH21	1.00	0.95
1:A:142:LYS:NZ	3:A:502:PGE:H2	1.82	0.95
1:A:346:HIS:CE1	1:A:347:ARG:HH21	1.84	0.94
1:B:349:TYR:HD1	1:B:349:TYR:H	1.15	0.93
1:B:236:LEU:HD21	1:B:240:GLN:HE21	1.34	0.93
1:B:365:GLU:HG3	1:B:366:LEU:N	1.80	0.93
1:B:403:MET:HE1	1:B:442:GLY:HA2	1.47	0.92
1:A:407:LEU:HD22	1:A:439:ILE:HG12	1.50	0.91
1:B:265:ARG:HG3	1:B:265:ARG:HH11	1.35	0.91
1:B:374:GLU:HG3	1:B:375:LYS:HE2	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ASP:HB3	1:B:230:LEU:HD22	1.53	0.89
1:A:352:SER:HB3	1:A:376:GLN:HG2	1.52	0.89
1:A:287:LEU:HD23	1:A:287:LEU:H	1.38	0.88
1:B:412:THR:H	1:B:416:GLN:HE21	1.22	0.86
1:B:284[A]:GLN:HG3	1:B:288:ARG:HH21	1.43	0.84
1:A:142:LYS:HZ3	3:A:502:PGE:H2	1.43	0.83
1:A:268:VAL:HG12	1:A:268:VAL:O	1.75	0.82
1:A:401:ALA:O	1:A:422:VAL:HG12	1.80	0.82
1:B:162:ARG:HG3	1:B:166:LYS:HE2	1.62	0.81
1:A:374[B]:GLU:CG	1:A:375:LYS:N	2.26	0.81
1:A:374[B]:GLU:HG3	1:A:376:GLN:H	1.45	0.81
1:B:290:ALA:HB3	1:B:322:ILE:HD13	1.63	0.81
1:B:403:MET:HE1	1:B:442:GLY:CA	2.10	0.81
1:A:331[B]:THR:HG23	1:A:334:SER:H	1.46	0.80
1:B:128:SEP:CB	1:B:132:SER:H	1.97	0.78
1:B:407:LEU:CD2	1:B:439:ILE:HG12	2.14	0.78
1:A:137[A]:ARG:HH22	1:B:176:ARG:HH12	1.32	0.78
1:A:303:ASP:H	2:A:505:ACT:CH3	1.96	0.77
1:B:365:GLU:HG3	1:B:366:LEU:H	1.46	0.77
1:A:302:GLY:CA	2:A:505:ACT:H2	2.09	0.77
1:A:128:SEP:HB3	1:A:132:SER:H	1.48	0.76
1:A:401:ALA:O	1:A:422:VAL:CG1	2.33	0.76
1:B:127:SER:C	1:B:128:SEP:H	1.89	0.76
1:B:409:GLU:HB2	1:B:433:VAL:CG1	2.15	0.76
1:A:412:THR:H	1:A:416:GLN:HE21	1.33	0.76
1:A:370:ASN:HD21	1:B:370:ASN:HA	1.49	0.76
1:B:284[A]:GLN:HG3	1:B:288:ARG:NH2	2.01	0.75
1:A:287:LEU:HD23	1:A:287:LEU:N	2.01	0.75
1:A:366:LEU:HD12	1:A:371:LEU:HD11	1.69	0.75
1:B:284[A]:GLN:CG	1:B:288:ARG:HH21	1.99	0.75
1:A:112:ILE:HD12	1:A:129:GLY:HA2	1.69	0.75
1:A:356:VAL:HG12	1:A:357:THR:CG2	2.17	0.74
1:A:142:LYS:HZ3	3:A:502:PGE:H42	1.52	0.74
1:A:213:ASP:OD1	1:A:215:ARG:HG2	1.86	0.74
1:B:395:ILE:HG23	1:B:423:LEU:HD13	1.69	0.74
1:A:382[B]:MET:HB2	1:A:437:ALA:O	1.88	0.74
1:A:356:VAL:O	1:A:381[B]:TYR:HB2	1.87	0.74
1:B:351:GLN:HA	1:B:351:GLN:OE1	1.88	0.74
1:B:365:GLU:CG	1:B:366:LEU:N	2.52	0.73
1:B:281:GLU:O	1:B:285:ILE:HG13	1.87	0.73
1:B:66:ASP:O	1:B:69:LEU:HB2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:HIS:HE1	1:B:347:ARG:HD3	1.48	0.72
1:A:227:ASP:H	1:A:412:THR:CG2	2.03	0.72
1:A:137[A]:ARG:NH2	1:B:176:ARG:NH1	2.37	0.71
1:B:309:ARG:HB3	1:B:309:ARG:HH11	1.56	0.71
1:A:112:ILE:CD1	1:A:129:GLY:HA2	2.21	0.70
1:A:366:LEU:HD12	1:A:371:LEU:CD1	2.21	0.70
1:B:443:ARG:HG2	1:B:443:ARG:HH21	1.55	0.70
1:B:346:HIS:ND1	1:B:347:ARG:HD3	2.06	0.70
1:A:287:LEU:H	1:A:287:LEU:CD2	2.03	0.70
1:A:142:LYS:HZ1	3:A:502:PGE:H2	1.58	0.69
1:B:412:THR:H	1:B:416:GLN:NE2	1.88	0.69
1:A:356:VAL:HG12	1:A:357:THR:HG22	1.73	0.69
1:A:412:THR:H	1:A:416:GLN:NE2	1.90	0.69
1:A:283:ASN:O	1:A:287:LEU:CD2	2.39	0.69
1:B:100:CYS:H	1:B:110:SER:HB2	1.57	0.69
1:B:419:VAL:CG1	1:B:429:LEU:HD22	2.23	0.69
1:A:420[A]:HIS:CD2	1:A:421:GLY:N	2.60	0.69
1:A:447:LEU:HD23	1:A:447:LEU:H	1.57	0.68
1:A:122:LEU:HD21	1:B:139:LEU:HD11	1.75	0.68
1:A:418:VAL:H	1:A:457:HIS:CE1	2.11	0.68
1:A:420[A]:HIS:HD2	1:A:421:GLY:N	1.92	0.67
1:B:128:SEP:HB2	1:B:132:SER:H	1.59	0.67
1:A:227:ASP:H	1:A:412:THR:HG23	1.59	0.67
1:A:249:ARG:HG3	1:A:249:ARG:HH11	1.58	0.67
1:A:348:ASP:OD1	1:A:348:ASP:N	2.27	0.67
1:B:375:LYS:HD3	5:B:552:HOH:O	1.94	0.67
1:B:223:ALA:HB2	1:B:299:LEU:HD22	1.78	0.65
1:B:419:VAL:HG12	1:B:429:LEU:HD22	1.76	0.65
1:B:374:GLU:HG2	1:B:375:LYS:HG2	1.78	0.65
1:B:407:LEU:HD21	1:B:439:ILE:HG12	1.79	0.65
1:B:128:SEP:HB3	1:B:132:SER:H	1.60	0.65
1:A:277:VAL:HG12	1:A:281:GLU:HG2	1.78	0.65
1:A:352:SER:OG	1:B:354:ARG:HD3	1.97	0.64
1:A:309:ARG:HG2	1:A:312:GLU:OE1	1.97	0.64
1:B:367:ASP:OD1	1:B:367:ASP:N	2.20	0.64
1:A:419:VAL:HG21	1:A:429:LEU:HB3	1.80	0.63
1:B:162:ARG:O	1:B:166:LYS:HD2	1.97	0.63
1:A:164:ARG:HD2	1:A:208:PHE:CE2	2.34	0.63
1:A:399:MET:SD	1:A:423:LEU:HD11	2.38	0.63
1:A:429:LEU:O	1:A:432:GLN:HB2	1.98	0.63
1:A:85:VAL:HG22	1:A:88:ARG:HH21	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:617:HOH:O	1:B:318:CYS:HB2	1.99	0.63
1:A:384[B]:LEU:HD22	1:A:435:SER:OG	1.99	0.63
1:A:400:GLN:O	1:A:402:ASP:N	2.32	0.63
1:B:409:GLU:HB2	1:B:433:VAL:HG12	1.79	0.63
1:A:278:PRO:O	1:A:280:GLU:N	2.32	0.63
1:A:354:ARG:NH2	1:B:354:ARG:NH2	2.46	0.62
1:B:100:CYS:H	1:B:110:SER:CB	2.13	0.62
1:A:371:LEU:O	1:A:378:LEU:HD11	1.99	0.62
1:B:368:TRP:HH2	1:B:390:ILE:HG12	1.65	0.62
1:A:275:HIS:CG	1:A:276:CYS:H	2.11	0.62
1:A:187:ARG:HG3	1:A:187:ARG:HH11	1.64	0.62
1:A:374[B]:GLU:CG	1:A:376:GLN:H	2.13	0.62
1:A:331[B]:THR:CG2	1:A:334:SER:H	2.12	0.62
1:B:256:MET:O	1:B:259:VAL:CG1	2.44	0.62
1:A:307:PHE:CB	2:A:505:ACT:H3	2.30	0.62
1:A:357:THR:C	1:B:351:GLN:HG3	2.25	0.61
1:A:231:LEU:O	1:B:233:LEU:HD13	1.99	0.61
1:A:346:HIS:CE1	1:A:347:ARG:HD2	2.35	0.61
1:A:176:ARG:NH1	1:A:295:ARG:HD2	2.16	0.61
1:B:265:ARG:HG3	1:B:265:ARG:NH1	2.11	0.60
1:A:137[A]:ARG:HG2	1:A:137[A]:ARG:HH21	1.66	0.60
1:A:268:VAL:HA	1:A:277:VAL:HG21	1.83	0.60
1:A:277:VAL:O	1:A:282:ILE:HG13	2.01	0.60
1:B:162:ARG:CG	1:B:166:LYS:HE2	2.29	0.60
1:A:261[B]:ARG:NH1	5:A:627:HOH:O	2.33	0.60
1:A:303:ASP:H	2:A:505:ACT:H1	1.66	0.60
1:B:29:ARG:O	1:B:33:GLU:HG3	2.01	0.60
1:A:140[A]:ARG:HG2	1:A:140[A]:ARG:HH11	1.67	0.60
1:A:346:HIS:ND1	1:A:347:ARG:HD2	2.17	0.60
1:B:196:ASP:O	1:B:200:VAL:HG23	2.01	0.60
1:B:238:GLN:HE22	1:B:295:ARG:HH21	1.48	0.60
1:A:112:ILE:HG13	1:B:7:PHE:HB2	1.84	0.59
1:B:160:GLN:O	1:B:161:LEU:HD23	2.02	0.59
1:B:166:LYS:HA	1:B:175:ARG:HD3	1.83	0.59
1:A:384[B]:LEU:CD2	1:A:435:SER:OG	2.50	0.59
1:A:268:VAL:O	1:A:268:VAL:CG1	2.48	0.59
1:A:357:THR:HG21	5:A:633:HOH:O	2.02	0.58
1:A:220:LEU:HD23	1:A:298:ARG:HB3	1.84	0.58
1:A:425:GLN:O	1:A:428:GLU:HG3	2.02	0.58
1:A:261[B]:ARG:HD2	5:A:506:HOH:O	2.02	0.58
1:A:450:LYS:O	1:A:451:LEU:HD23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ARG:HG2	1:B:443:ARG:NH2	2.15	0.58
1:A:146:LEU:C	1:A:146:LEU:HD23	2.28	0.58
1:A:356:VAL:HG12	1:A:357:THR:HG23	1.86	0.57
1:B:368:TRP:CD1	1:B:393:LYS:HD3	2.39	0.57
1:A:171:THR:OG1	1:A:174:GLU:HG2	2.04	0.57
1:A:277:VAL:O	1:A:278:PRO:C	2.47	0.57
1:A:400:GLN:O	1:A:401:ALA:C	2.44	0.57
1:A:307:PHE:HB2	2:A:505:ACT:CH3	2.35	0.57
1:B:368:TRP:NE1	1:B:393:LYS:HD3	2.20	0.57
1:B:267:PHE:HE2	1:B:271[A]:ARG:HG3	1.70	0.57
1:A:261[B]:ARG:NH2	1:B:30:LEU:HD13	2.21	0.56
1:A:380:PHE:O	1:A:438:LEU:HD23	2.05	0.56
1:A:223:ALA:HB2	1:A:299:LEU:HD22	1.86	0.56
1:B:290:ALA:CB	1:B:322:ILE:HD13	2.33	0.56
1:B:412:THR:N	1:B:416:GLN:HE21	2.00	0.56
1:A:261[B]:ARG:CZ	1:B:30:LEU:HD13	2.35	0.56
1:A:277:VAL:HB	1:A:282:ILE:HG13	1.87	0.56
1:B:122:LEU:HD13	1:B:123:MET:N	2.20	0.56
1:B:298:ARG:NH1	1:B:313:GLU:OE2	2.39	0.56
1:A:283:ASN:O	1:A:287:LEU:HD22	2.04	0.55
1:A:351:GLN:HB2	1:B:357:THR:HG22	1.88	0.55
1:B:401:ALA:HB1	1:B:424:THR:HG23	1.86	0.55
1:B:391:GLN:O	1:B:395:ILE:HG12	2.06	0.55
1:B:346:HIS:H	1:B:350:ALA:HB2	1.72	0.55
1:A:117:ILE:HD13	1:A:143:LEU:CB	2.37	0.55
1:A:374[A]:GLU:HG2	1:A:376:GLN:H	1.72	0.55
1:A:117:ILE:CD1	1:A:143:LEU:HB2	2.37	0.54
1:A:418:VAL:N	1:A:457:HIS:CE1	2.75	0.54
1:B:117:ILE:N	1:B:117:ILE:HD12	2.22	0.54
1:A:383[B]:GLY:HA3	5:A:633:HOH:O	2.08	0.54
1:A:391:GLN:NE2	1:A:423:LEU:O	2.40	0.54
1:A:400:GLN:HB3	1:A:402:ASP:OD2	2.08	0.54
1:A:354:ARG:NH2	1:A:370:ASN:OD1	2.40	0.54
1:A:374[B]:GLU:HG3	1:A:376:GLN:N	2.19	0.54
1:B:239:ILE:HD11	1:B:299:LEU:HD21	1.90	0.54
1:B:404:PRO:HB2	1:B:445:VAL:HB	1.90	0.54
1:A:41:ASN:OD1	1:A:65:PHE:HA	2.07	0.53
1:A:307:PHE:HB2	2:A:505:ACT:H3	1.89	0.53
1:B:66:ASP:HB3	1:B:69:LEU:HD22	1.89	0.53
1:B:400:GLN:HG3	5:B:682:HOH:O	2.08	0.53
1:B:311:GLY:O	1:B:315:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:GLN:OE1	1:B:351:GLN:CA	2.56	0.53
1:A:346:HIS:CE1	1:A:347:ARG:CD	2.91	0.53
1:A:227:ASP:N	1:A:412:THR:HG23	2.23	0.53
1:A:346:HIS:HE1	1:A:347:ARG:NH2	1.86	0.53
1:B:265:ARG:HH11	1:B:265:ARG:CG	2.13	0.53
1:A:456:ASN:O	1:A:457:HIS:HB2	2.09	0.53
1:A:118:ASP:OD2	1:A:123[B]:MET:HE1	2.09	0.53
1:A:115:SER:HB3	1:A:140[A]:ARG:HD3	1.91	0.52
1:A:140[B]:ARG:NH2	1:A:144:GLU:HG3	2.25	0.52
1:B:374:GLU:CG	1:B:375:LYS:HE2	2.32	0.52
1:B:346:HIS:O	1:B:350:ALA:HB3	2.10	0.52
1:A:17:ILE:HG13	1:A:38:LEU:HD21	1.92	0.52
1:A:81:ASP:H	2:A:504:ACT:H3	1.74	0.52
1:B:128:SEP:O1P	2:B:503:ACT:H1	2.09	0.52
1:B:164:ARG:HD2	1:B:208:PHE:CE2	2.45	0.52
1:A:117:ILE:HD13	1:A:143:LEU:HB3	1.92	0.51
1:A:270:LYS:O	1:A:271:ARG:C	2.53	0.51
1:B:288:ARG:HG2	1:B:288:ARG:HH11	1.74	0.51
1:A:135:LEU:HG	1:B:183:PHE:CD2	2.45	0.51
1:A:198:LYS:HG2	5:A:603:HOH:O	2.11	0.51
1:A:58:LEU:C	1:A:58:LEU:HD12	2.35	0.51
1:A:123[B]:MET:HE2	1:B:1:MET:HG3	1.91	0.51
1:B:430:ALA:C	1:B:432:GLN:H	2.18	0.51
1:A:168:GLN:HE21	1:A:168:GLN:HA	1.75	0.51
1:A:45:PHE:CE1	1:A:60:LEU:HD22	2.45	0.51
1:A:374[B]:GLU:O	1:A:375:LYS:HB2	2.10	0.51
1:B:236:LEU:HD23	1:B:236:LEU:C	2.35	0.51
1:A:403:MET:O	1:A:422:VAL:HG13	2.11	0.50
5:A:526:HOH:O	1:B:9:GLN:HG3	2.10	0.50
1:A:277:VAL:HG12	1:A:281:GLU:CG	2.39	0.50
1:A:347:ARG:HG2	1:A:348:ASP:OD1	2.11	0.50
1:A:350:ALA:HA	1:A:375:LYS:O	2.11	0.50
1:A:352:SER:HG	1:B:354:ARG:HD3	1.76	0.50
1:A:356:VAL:C	1:A:357:THR:HG23	2.35	0.50
1:B:309:ARG:HH11	1:B:309:ARG:CB	2.22	0.50
1:A:374[A]:GLU:O	1:A:375:LYS:HB2	2.10	0.50
1:A:150:HIS:CD2	1:A:153:GLN:HE22	2.29	0.50
1:A:307:PHE:CB	2:A:505:ACT:CH3	2.90	0.50
1:A:303:ASP:N	2:A:505:ACT:CH3	2.72	0.50
1:A:373:ALA:O	1:A:374[B]:GLU:HB2	2.11	0.50
1:A:445:VAL:HG12	1:A:445:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123[B]:MET:CE	1:B:1:MET:HG3	2.42	0.49
1:B:166:LYS:HA	1:B:175:ARG:HH11	1.78	0.49
1:B:349:TYR:CD1	1:B:349:TYR:N	2.66	0.49
1:A:134:VAL:O	1:A:138:LEU:HG	2.12	0.49
1:A:354:ARG:HH22	1:B:354:ARG:NH2	2.08	0.49
1:A:377[A]:THR:HG23	1:A:377[A]:THR:O	2.13	0.49
1:A:150:HIS:HB3	1:A:153:GLN:NE2	2.27	0.49
1:A:344:LEU:O	1:A:377[A]:THR:HG21	2.13	0.49
1:B:265:ARG:NH1	1:B:265:ARG:CG	2.74	0.49
1:A:241:GLN:HE21	1:A:295:ARG:HH12	1.60	0.49
1:A:241:GLN:HE21	1:A:295:ARG:NH1	2.10	0.49
1:B:17:ILE:HD11	1:B:31:LEU:HD22	1.95	0.48
1:A:289:GLU:OE2	1:A:294:LYS:HD2	2.13	0.48
1:A:284:GLN:CA	1:A:287:LEU:HD21	2.28	0.48
1:A:309:ARG:O	1:A:313:GLU:HG3	2.13	0.48
1:A:268:VAL:HG13	1:A:282:ILE:HG12	1.96	0.48
1:A:371:LEU:HD23	1:A:378:LEU:HD22	1.96	0.48
1:B:291:GLN:HG3	1:B:322:ILE:HD11	1.95	0.48
1:A:365:GLU:O	1:A:366:LEU:HD23	2.14	0.48
1:B:73[B]:CYS:SG	1:B:75:LEU:O	2.72	0.48
1:A:97:ARG:NE	1:B:72:SER:HA	2.28	0.47
1:B:309:ARG:NH1	1:B:312:GLU:OE1	2.47	0.47
1:A:277:VAL:HB	1:A:282:ILE:CG1	2.44	0.47
1:B:349:TYR:HD1	1:B:349:TYR:N	1.97	0.47
1:B:359:HIS:CG	1:B:386:GLN:NE2	2.82	0.47
1:A:303:ASP:H	2:A:505:ACT:H2	1.75	0.47
1:A:374[A]:GLU:CG	1:A:375:LYS:N	2.19	0.47
1:B:250:LEU:HD21	1:B:436:PRO:HG3	1.96	0.47
1:B:287:LEU:HD12	1:B:316:THR:O	2.14	0.47
1:A:356:VAL:CG1	1:A:357:THR:N	2.76	0.47
1:B:401:ALA:HB1	1:B:424:THR:CG2	2.44	0.47
1:A:187:ARG:HG3	1:A:187:ARG:NH1	2.28	0.47
1:B:31:LEU:HD23	1:B:38:LEU:HD13	1.96	0.47
1:A:11:ARG:HE	1:A:11:ARG:HB2	1.33	0.47
1:A:346:HIS:ND1	1:A:347:ARG:CD	2.77	0.47
1:A:400:GLN:HB3	1:A:400:GLN:HE21	1.45	0.47
1:A:425:GLN:C	1:A:428:GLU:HG3	2.39	0.47
1:B:128:SEP:O	1:B:131:THR:OG1	2.17	0.47
1:A:356:VAL:HG12	1:A:357:THR:N	2.29	0.47
1:B:9:GLN:HE21	1:B:9:GLN:C	2.22	0.47
1:A:435:SER:HB3	1:A:436:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:LYS:HD2	5:B:649:HOH:O	2.16	0.46
1:A:331[B]:THR:OG1	2:A:505:ACT:OXT	2.26	0.46
1:A:406:ALA:C	1:A:407:LEU:HD23	2.40	0.46
1:A:422:VAL:O	1:A:423:LEU:C	2.58	0.46
1:B:149:GLN:NE2	5:B:530:HOH:O	2.49	0.46
1:B:80:THR:H	1:B:86:ASN:HD21	1.64	0.46
1:B:286:LEU:HD21	1:B:298:ARG:HD2	1.98	0.46
1:A:306:ILE:HD12	1:A:331[A]:THR:HG21	1.98	0.46
1:A:447:LEU:HD12	1:A:451:LEU:HD11	1.98	0.46
1:B:263:ALA:O	1:B:265:ARG:NH1	2.49	0.46
1:B:400:GLN:O	1:B:403:MET:HB2	2.16	0.46
1:B:164:ARG:HD3	1:B:168:GLN:NE2	2.32	0.45
1:A:269:GLY:C	1:A:271:ARG:H	2.24	0.45
1:B:371:LEU:C	1:B:373:ALA:H	2.24	0.45
1:B:405:VAL:HG12	1:B:406:ALA:N	2.32	0.45
1:A:118:ASP:O	1:A:119:ARG:HD3	2.16	0.45
1:A:142:LYS:HZ3	3:A:502:PGE:C2	2.24	0.45
1:B:176:ARG:O	1:B:180:GLU:HG3	2.16	0.45
1:A:303:ASP:N	2:A:505:ACT:H2	2.31	0.45
1:B:403:MET:HE1	1:B:442:GLY:N	2.30	0.45
1:B:309:ARG:HH12	1:B:312:GLU:CD	2.23	0.45
1:A:113:MET:HE3	1:A:114:PRO:HD2	1.99	0.45
1:B:260:ARG:O	1:B:261:ARG:C	2.60	0.45
1:A:150:HIS:CD2	1:A:153:GLN:NE2	2.85	0.45
1:A:422:VAL:HG12	1:A:423:LEU:N	2.32	0.45
1:A:117:ILE:HD11	1:A:143:LEU:HB2	1.99	0.45
1:A:142:LYS:NZ	3:A:502:PGE:H42	2.26	0.45
1:A:124:VAL:HG21	1:A:147:LEU:HD11	1.98	0.44
1:A:384[A]:LEU:HD12	1:A:384[A]:LEU:HA	1.73	0.44
1:A:3:HIS:CE1	1:B:9:GLN:HG2	2.52	0.44
1:A:409:GLU:OE1	1:A:434:GLU:HG2	2.17	0.44
1:B:339:TYR:CD2	1:B:412:THR:HA	2.53	0.44
1:A:117:ILE:HD13	1:A:143:LEU:HB2	1.98	0.44
1:A:153:GLN:OE1	1:A:193:ALA:HA	2.18	0.44
1:B:177:ARG:NH2	1:B:213:ASP:OD2	2.48	0.44
1:A:381[B]:TYR:O	1:A:383[B]:GLY:N	2.50	0.44
1:A:452:ASN:ND2	5:A:519:HOH:O	2.45	0.44
1:B:9:GLN:HE22	1:B:11:ARG:HG3	1.83	0.44
1:B:185:ASN:HD22	1:B:207:LEU:HD21	1.82	0.44
1:B:339:TYR:HB3	1:B:416:GLN:HE22	1.83	0.44
1:A:137[A]:ARG:NH2	1:A:137[A]:ARG:HG2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:VAL:HG21	1:A:371:LEU:HD21	1.99	0.44
1:B:162:ARG:O	1:B:166:LYS:CD	2.63	0.44
1:A:117:ILE:CD1	1:A:143:LEU:CB	2.96	0.44
1:A:139:LEU:CD2	3:A:502:PGE:H5	2.48	0.44
1:A:400:GLN:O	1:A:402:ASP:OD2	2.36	0.44
1:A:237:GLN:O	1:A:241:GLN:HG2	2.18	0.43
1:A:261[A]:ARG:NH1	1:B:140:ARG:CZ	2.81	0.43
1:A:122:LEU:C	1:A:123[B]:MET:HG2	2.43	0.43
1:A:374[A]:GLU:CG	1:A:376:GLN:H	2.30	0.43
1:A:411:GLY:O	1:A:412:THR:HG22	2.17	0.43
1:A:80:THR:HA	2:A:504:ACT:H2	2.00	0.43
1:A:177:ARG:NH1	1:A:213:ASP:HB3	2.33	0.43
1:A:448:ARG:O	1:A:452:ASN:HB2	2.18	0.43
1:A:227:ASP:H	1:A:412:THR:HG21	1.82	0.43
1:B:287:LEU:C	1:B:287:LEU:HD23	2.44	0.43
1:B:340:SER:O	1:B:448:ARG:HG3	2.19	0.43
1:A:220:LEU:HD12	1:A:314:LEU:HD11	2.01	0.43
1:A:279:GLN:NE2	1:A:309:ARG:HD3	2.33	0.43
1:A:269:GLY:HA2	1:A:276:CYS:SG	2.58	0.42
1:A:425:GLN:HA	1:A:428:GLU:HG3	2.01	0.42
1:B:267:PHE:CE2	1:B:271[A]:ARG:HG3	2.53	0.42
1:A:122:LEU:HD12	1:B:127:SER:O	2.19	0.42
1:A:322:ILE:HA	1:A:323:PRO:HD3	1.90	0.42
1:A:420[B]:HIS:ND1	1:A:420[B]:HIS:N	2.68	0.42
1:B:166:LYS:HG3	1:B:175:ARG:NH1	2.34	0.42
1:B:395:ILE:HG22	1:B:399:MET:O	2.19	0.42
1:A:249:ARG:HG3	1:A:249:ARG:NH1	2.30	0.42
1:A:426:LEU:C	1:A:426:LEU:HD23	2.44	0.42
1:B:359:HIS:HB2	1:B:386:GLN:CD	2.44	0.42
1:A:275:HIS:CE1	1:A:278:PRO:HG3	2.55	0.42
1:B:96:ARG:HG3	1:B:98:ILE:HD12	2.00	0.42
1:A:281:GLU:O	1:A:285:ILE:HG13	2.20	0.42
1:A:132:SER:HB3	1:A:135:LEU:HB2	2.01	0.42
1:A:353:VAL:HG22	1:A:377[A]:THR:HG22	2.01	0.42
1:A:377[A]:THR:O	1:A:377[A]:THR:CG2	2.68	0.42
1:B:346:HIS:HE1	1:B:347:ARG:CD	2.25	0.42
1:B:309:ARG:HH11	1:B:309:ARG:CG	2.32	0.41
1:B:394:LEU:HD23	1:B:399:MET:SD	2.59	0.41
1:A:268:VAL:CG1	1:A:282:ILE:CD1	2.98	0.41
1:B:122:LEU:HD13	1:B:122:LEU:C	2.45	0.41
1:B:291:GLN:CG	1:B:322:ILE:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:HD3	5:A:595:HOH:O	2.20	0.41
1:A:247:TYR:CD2	1:A:247:TYR:N	2.87	0.41
1:B:359:HIS:HB2	1:B:386:GLN:HG3	2.02	0.41
1:B:385:ASN:HD22	1:B:385:ASN:HA	1.59	0.41
1:A:140[A]:ARG:HH11	1:A:140[A]:ARG:CG	2.32	0.41
1:A:247:TYR:H	1:A:247:TYR:HD2	1.68	0.41
1:B:375:LYS:HG2	1:B:375:LYS:H	1.63	0.41
1:B:409:GLU:HB2	1:B:433:VAL:HG11	2.00	0.41
1:A:300:LYS:NZ	1:A:300:LYS:HB3	2.35	0.41
1:A:357:THR:O	1:B:351:GLN:HG3	2.19	0.41
1:A:385[A]:ASN:OD1	1:A:385[A]:ASN:O	2.39	0.41
1:A:420[A]:HIS:CD2	1:A:420[A]:HIS:C	2.99	0.41
1:A:37:ARG:CG	1:A:37:ARG:HH21	2.34	0.41
1:A:139:LEU:HD21	3:A:502:PGE:H5	2.03	0.41
1:A:444:VAL:O	1:A:447:LEU:HD23	2.20	0.41
1:B:346:HIS:O	1:B:350:ALA:CB	2.69	0.41
1:A:116:ILE:HG22	1:A:117:ILE:N	2.36	0.41
1:A:391:GLN:HG3	1:A:392:GLU:N	2.36	0.41
1:A:260:ARG:NE	1:A:262:ASP:OD2	2.54	0.40
1:A:275:HIS:ND1	1:A:276:CYS:N	2.59	0.40
1:B:9:GLN:HE21	1:B:9:GLN:CA	2.33	0.40
1:B:55:GLU:HG3	1:B:57:MET:HG2	2.03	0.40
1:B:128:SEP:HB2	1:B:132:SER:N	2.32	0.40
1:B:350:ALA:HB1	1:B:351:GLN:H	1.64	0.40
1:A:268:VAL:CG1	1:A:282:ILE:HG12	2.51	0.40
1:A:261[A]:ARG:HH12	1:B:140:ARG:CZ	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	454/457 (99%)	419 (92%)	23 (5%)	12 (3%)	4	2
1	B	454/457 (99%)	428 (94%)	20 (4%)	6 (1%)	9	7
All	All	908/914 (99%)	847 (93%)	43 (5%)	18 (2%)	6	3

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	LYS
1	A	279	GLN
1	A	347	ARG
1	A	375	LYS
1	A	382[A]	MET
1	A	382[B]	MET
1	A	400	GLN
1	A	401	ALA
1	B	374	GLU
1	B	375	LYS
1	A	315	GLU
1	A	195	ALA
1	A	278	PRO
1	A	366	LEU
1	B	360	LEU
1	B	261	ARG
1	B	347	ARG
1	B	370	ASN

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	379/372 (102%)	338 (89%)	41 (11%)	6	5
1	B	375/372 (101%)	330 (88%)	45 (12%)	5	4
All	All	754/744 (101%)	668 (89%)	86 (11%)	5	4

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	37	ARG
1	A	38	LEU
1	A	43	LEU
1	A	112	ILE
1	A	135	LEU
1	A	156	ARG
1	A	174	GLU
1	A	188	LEU
1	A	231	LEU
1	A	241	GLN
1	A	247	TYR
1	A	250	LEU
1	A	277	VAL
1	A	278	PRO
1	A	279	GLN
1	A	287	LEU
1	A	299	LEU
1	A	347	ARG
1	A	348	ASP
1	A	354	ARG
1	A	355	LEU
1	A	357	THR
1	A	366	LEU
1	A	370	ASN
1	A	371	LEU
1	A	375	LYS
1	A	385[A]	ASN
1	A	385[B]	ASN
1	A	400	GLN
1	A	403	MET
1	A	412	THR
1	A	419	VAL
1	A	420[A]	HIS
1	A	420[B]	HIS
1	A	428	GLU
1	A	433	VAL
1	A	438	LEU
1	A	443	ARG
1	A	447	LEU
1	A	455	SER
1	B	9	GLN
1	B	69	LEU

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Mol	Chain	Res	Type
1	B	81	ASP
1	B	107	LYS
1	B	110	SER
1	B	120	SER
1	B	135	LEU
1	B	138	LEU
1	B	147	LEU
1	B	149	GLN
1	B	151	LEU
1	B	164	ARG
1	B	172	MET
1	B	176	ARG
1	B	209	SER
1	B	213	ASP
1	B	215	ARG
1	B	230	LEU
1	B	252	SER
1	B	261	ARG
1	B	262	ASP
1	B	288	ARG
1	B	298	ARG
1	B	309	ARG
1	B	316	THR
1	B	334	SER
1	B	347	ARG
1	B	348	ASP
1	B	349	TYR
1	B	351	GLN
1	B	360	LEU
1	B	366	LEU
1	B	367	ASP
1	B	369	GLU
1	B	374	GLU
1	B	375	LYS
1	B	379	VAL
1	B	385	ASN
1	B	389	THR
1	B	394	LEU
1	B	395	ILE
1	B	423	LEU
1	B	426	LEU
1	B	431	GLN

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Mol	Chain	Res	Type
1	B	433	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	150	HIS
1	A	153	GLN
1	A	168	GLN
1	A	190	GLN
1	A	194	ASN
1	A	238	GLN
1	A	241	GLN
1	A	279	GLN
1	A	284	GLN
1	A	346	HIS
1	A	391	GLN
1	A	400	GLN
1	A	416	GLN
1	A	452	ASN
1	A	457	HIS
1	B	9	GLN
1	B	48	GLN
1	B	54	ASN
1	B	86	ASN
1	B	101	ASN
1	B	149	GLN
1	B	150	HIS
1	B	238	GLN
1	B	240	GLN
1	B	291	GLN
1	B	359	HIS
1	B	385	ASN
1	B	386	GLN
1	B	416	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	B	128	1	8,9,10	5.11	6 (75%)	7,12,14	4.72	2 (28%)
1	SEP	A	128	1	8,9,10	3.55	3 (37%)	7,12,14	3.99	4 (57%)

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
1	SEP	B	128	1	-	3/6/8/10	-
1	SEP	A	128	1	-	1/6/8/10	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	SEP	OG-CB	10.20	1.83	1.44
1	A	128	SEP	P-OG	6.94	1.82	1.60
1	A	128	SEP	CB-CA	6.19	1.69	1.52
1	B	128	SEP	P-OG	5.42	1.77	1.60
1	B	128	SEP	CB-CA	5.23	1.66	1.52
1	B	128	SEP	O-C	4.52	1.37	1.20
1	B	128	SEP	CA-N	4.42	1.60	1.48
1	A	128	SEP	P-O1P	2.96	1.59	1.50
1	B	128	SEP	P-O1P	2.62	1.58	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	SEP	OG-CB-CA	11.97	119.79	108.14
1	A	128	SEP	OG-CB-CA	9.07	116.97	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	SEP	O3P-P-OG	-4.05	96.10	106.67
1	B	128	SEP	O3P-P-O2P	2.58	117.46	107.80
1	A	128	SEP	O3P-P-O2P	2.51	117.23	107.80
1	A	128	SEP	O2P-P-OG	2.18	112.36	106.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	128	SEP	CA-CB-OG-P
1	B	128	SEP	N-CA-CB-OG
1	B	128	SEP	C-CA-CB-OG
1	B	128	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	128	SEP	9	0
1	A	128	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SAH	B	501	-	27,28,28	1.84	3 (11%)	36,40,40	1.91	8 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PGE	A	502	-	9,9,9	2.09	2 (22%)	8,8,8	1.52	3 (37%)
2	ACT	A	504	-	3,3,3	0.97	0	3,3,3	0.85	0
2	ACT	A	505	-	3,3,3	0.94	0	3,3,3	0.88	0
2	ACT	B	503	-	3,3,3	1.03	0	3,3,3	0.84	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	PGE	A	502	-	-	2/7/7/7	-
4	SAH	B	501	-	-	0/15/31/31	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	SAH	C2-N1	7.43	1.47	1.33
3	A	502	PGE	O3-C4	-4.24	1.23	1.42
3	A	502	PGE	O4-C6	-3.63	1.23	1.42
4	B	501	SAH	O4'-C1'	3.01	1.48	1.42
4	B	501	SAH	C5-N7	-2.95	1.33	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	SAH	N3-C2-N1	-6.36	118.95	128.58
4	B	501	SAH	C5-C4-N3	-4.16	120.99	126.72
4	B	501	SAH	C2-N3-C4	3.84	121.21	111.83
4	B	501	SAH	N9-C8-N7	-3.36	109.17	113.94
4	B	501	SAH	C5-N7-C8	3.05	108.25	103.45
4	B	501	SAH	C4-C5-N7	-2.80	107.38	110.58
4	B	501	SAH	N3-C4-N9	2.74	131.83	127.17
3	A	502	PGE	O3-C5-C6	2.36	120.52	110.11
3	A	502	PGE	O2-C3-C4	2.19	120.34	110.35
4	B	501	SAH	C4-N9-C8	2.19	108.03	105.74
3	A	502	PGE	O3-C4-C3	2.18	120.29	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

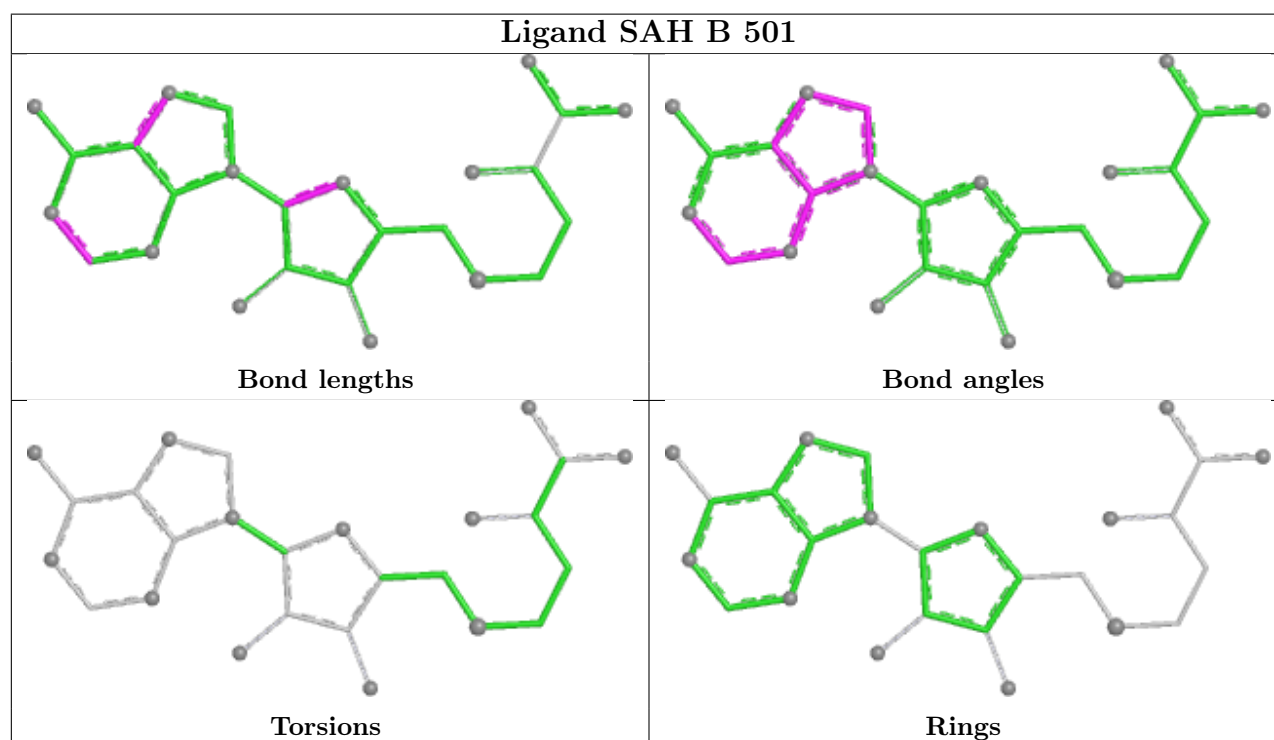
Mol	Chain	Res	Type	Atoms
3	A	502	PGE	O2-C3-C4-O3
3	A	502	PGE	C6-C5-O3-C4

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PGE	8	0
2	A	504	ACT	2	0
2	A	505	ACT	12	0
2	B	503	ACT	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	127:SER	C	128:SEP	N	1.67

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	447/457 (97%)	0.38	28 (6%) 26 23	13, 38, 67, 99	13 (2%)
1	B	454/457 (99%)	0.18	29 (6%) 25 22	14, 34, 64, 95	4 (0%)
All	All	901/914 (98%)	0.28	57 (6%) 26 23	13, 36, 65, 99	17 (1%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	384[A]	LEU	6.2
1	A	420[A]	HIS	4.0
1	A	277	VAL	3.9
1	B	360	LEU	3.9
1	A	276	CYS	3.9
1	B	374	GLU	3.8
1	B	362	THR	3.8
1	B	363	GLY	3.7
1	B	272	ALA	3.7
1	A	382[A]	MET	3.4
1	A	307	PHE	3.3
1	B	318	CYS	3.1
1	A	401	ALA	3.1
1	B	359	HIS	3.1
1	B	367	ASP	3.1
1	A	383[A]	GLY	3.0
1	B	372	ALA	3.0
1	B	396	ALA	3.0
1	B	395	ILE	3.0
1	A	349	TYR	3.0
1	B	320	ALA	2.9
1	B	275	HIS	2.9
1	B	319	HIS	2.9
1	B	366	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	357	THR	2.8
1	A	268	VAL	2.7
1	A	400	GLN	2.7
1	B	373	ALA	2.7
1	A	364	GLY	2.7
1	A	429	LEU	2.6
1	B	433	VAL	2.6
1	A	279	GLN	2.5
1	A	350	ALA	2.5
1	A	275	HIS	2.5
1	B	431	GLN	2.5
1	B	361	LYS	2.4
1	B	350	ALA	2.4
1	B	369	GLU	2.4
1	A	269	GLY	2.3
1	B	276	CYS	2.3
1	B	271[A]	ARG	2.3
1	A	371	LEU	2.3
1	B	156	ARG	2.3
1	A	447	LEU	2.2
1	A	404	PRO	2.2
1	B	389	THR	2.2
1	A	374[A]	GLU	2.2
1	A	457	HIS	2.2
1	B	170	ALA	2.2
1	A	348	ASP	2.1
1	A	391	GLN	2.1
1	A	423	LEU	2.0
1	A	449	ASP	2.0
1	B	104[A]	ASP	2.0
1	B	375	LYS	2.0
1	A	351	GLN	2.0
1	B	317	LEU	2.0

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

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
1	SEP	A	128	10/11	0.73	0.24	31,38,53,54	0
1	SEP	B	128	10/11	0.85	0.14	30,38,52,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

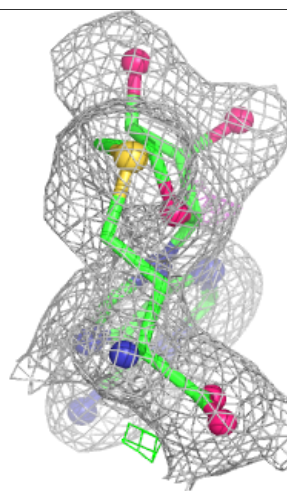
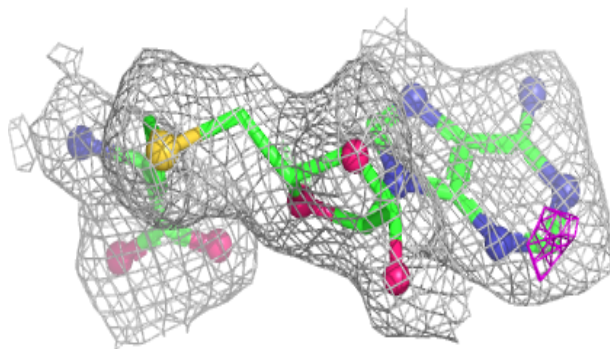
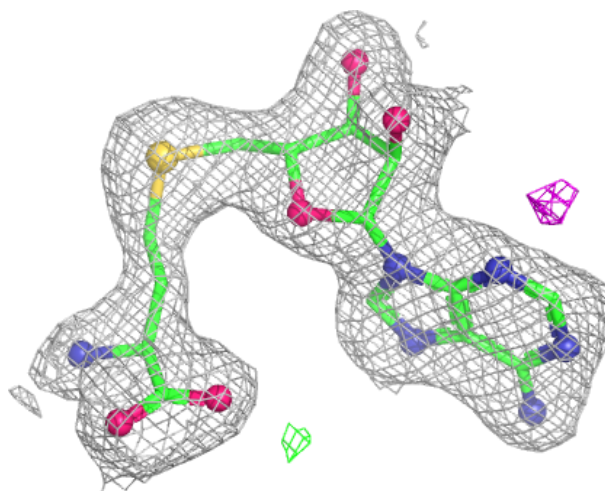
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	A	504	4/4	0.53	0.26	57,59,60,61	0
2	ACT	B	503	4/4	0.78	0.21	57,58,58,59	0
3	PGE	A	502	10/10	0.87	0.11	49,54,57,58	0
2	ACT	A	505	4/4	0.92	0.12	36,39,42,42	0
4	SAH	B	501	26/26	0.94	0.07	27,32,35,37	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 SAH B 501:

$2mF_o-DF_c$ (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.