



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:48 PM UTC

PDB ID : 1PJT / pdb_00001pjt
Title : The structure of the Ser128Ala point-mutant variant 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 : 2.80 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

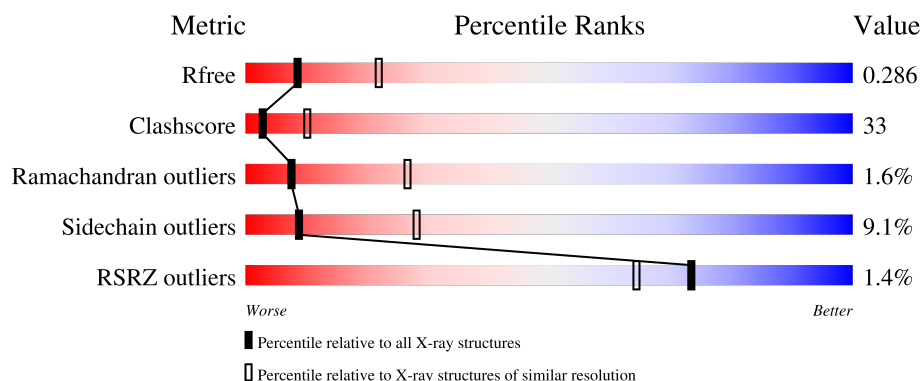
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	% 49% 40% 8% ..
1	B	457	2% 50% 42% 6% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7158 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.

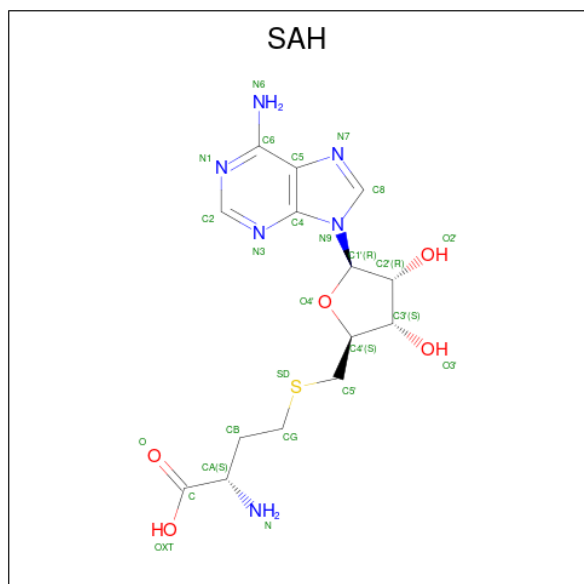
- Molecule 1 is a protein called Siroheme synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3462	2181	625	640	16			
1	B	455	Total	C	N	O	S	0	0	0
			3509	2210	635	648	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	ALA	SER	engineered mutation	UNP P25924
B	128	ALA	SER	engineered mutation	UNP P25924

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



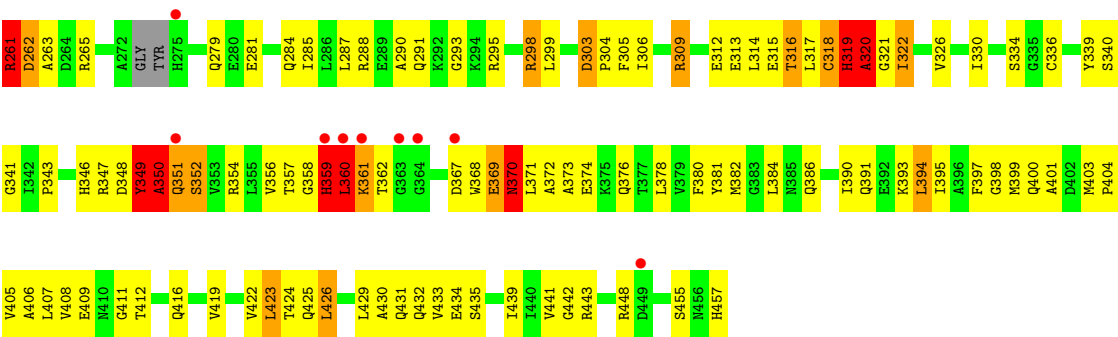
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	80	Total	O	0	0
			80	80		
4	B	50	Total	O	0	0
			50	50		

- 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	59.54Å 120.32Å 130.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.84 – 2.80 19.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.6 (19.84-2.80) 93.3 (19.84-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.06 (at 2.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.291 0.222 , 0.286	Depositor DCC
R_{free} test set	2194 reflections (9.75%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7158	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: PO4, SAH

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	0.69	6/3517 (0.2%)	1.21	45/4759 (0.9%)
1	B	0.72	10/3566 (0.3%)	1.25	42/4826 (0.9%)
All	All	0.71	16/7083 (0.2%)	1.23	87/9585 (0.9%)

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	4
1	B	0	2
All	All	0	6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	360	LEU	CA-C	17.17	1.76	1.52
1	A	364	GLY	N-CA	-12.72	1.25	1.45
1	A	279	GLN	CA-C	-9.20	1.40	1.52
1	B	359	HIS	CA-C	8.90	1.61	1.53
1	B	319	HIS	CA-C	-8.57	1.41	1.52
1	B	359	HIS	C-O	-8.29	1.10	1.23
1	B	360	LEU	C-O	-8.01	1.12	1.23
1	A	365	GLU	CA-C	7.59	1.62	1.52
1	B	320	ALA	CA-CB	-6.89	1.41	1.53
1	A	278	PRO	C-O	6.74	1.32	1.24
1	B	361	LYS	N-CA	6.38	1.55	1.46
1	A	365	GLU	C-O	5.89	1.31	1.24
1	A	366	LEU	N-CA	5.64	1.53	1.46
1	B	350	ALA	CA-CB	-5.49	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	359	HIS	C-N	5.12	1.40	1.33
1	B	360	LEU	N-CA	5.03	1.52	1.46

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	ALA	N-CA-C	14.55	141.80	110.80
1	B	360	LEU	N-CA-C	-13.73	95.87	113.17
1	B	359	HIS	N-CA-C	13.38	128.11	109.11
1	B	360	LEU	O-C-N	-12.29	106.98	122.34
1	A	374	GLU	O-C-N	10.95	135.14	123.42
1	A	374	GLU	CA-C-N	10.88	142.33	121.54
1	A	374	GLU	C-N-CA	10.88	142.33	121.54
1	A	276	CYS	N-CA-C	10.87	125.71	113.21
1	A	308	GLY	N-CA-C	-10.67	87.89	113.18
1	B	359	HIS	CA-C-O	-10.57	107.17	121.86
1	B	110	SER	N-CA-C	10.13	123.59	111.33
1	B	351	GLN	N-CA-C	10.11	125.55	112.41
1	A	366	LEU	N-CA-C	9.77	125.67	109.06
1	A	351	GLN	N-CA-C	-9.05	99.54	113.02
1	B	318	CYS	CA-C-N	-8.98	104.38	121.54
1	B	318	CYS	C-N-CA	-8.98	104.38	121.54
1	B	38	LEU	N-CA-C	8.69	123.88	109.46
1	B	370	ASN	N-CA-C	-8.04	93.67	110.80
1	B	350	ALA	CA-C-N	-8.04	109.87	122.49
1	B	350	ALA	C-N-CA	-8.04	109.87	122.49
1	A	105	ALA	CA-C-N	7.99	127.70	119.56
1	A	105	ALA	C-N-CA	7.99	127.70	119.56
1	B	116	ILE	N-CA-C	7.95	119.93	108.48
1	A	365	GLU	N-CA-C	7.83	127.48	110.80
1	B	360	LEU	N-CA-CB	7.77	121.99	110.49
1	B	431	GLN	N-CA-C	-7.39	104.71	113.21
1	B	263	ALA	N-CA-C	-7.13	97.60	109.07
1	A	456	ASN	N-CA-C	-7.06	103.84	113.30
1	A	280	GLU	N-CA-C	7.05	119.82	111.71
1	B	149	GLN	N-CA-C	6.93	119.71	111.33
1	A	364	GLY	CA-C-O	-6.93	106.25	120.80
1	B	261	ARG	CA-C-N	-6.91	113.67	123.20
1	B	261	ARG	C-N-CA	-6.91	113.67	123.20
1	B	115	SER	N-CA-C	-6.84	99.39	110.20
1	A	279	GLN	CA-C-N	-6.81	110.47	120.28
1	A	279	GLN	C-N-CA	-6.81	110.47	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	GLN	CB-CA-C	-6.54	97.41	110.42
1	A	38	LEU	N-CA-C	6.49	120.23	109.46
1	A	73	CYS	N-CA-C	6.48	120.46	110.42
1	A	356	VAL	N-CA-C	6.45	119.60	108.95
1	A	398	GLY	N-CA-C	6.31	125.43	115.08
1	A	374	GLU	N-CA-C	6.30	118.44	108.79
1	B	398	GLY	N-CA-C	6.20	122.46	115.08
1	B	303	ASP	CA-C-N	6.19	125.68	119.24
1	B	303	ASP	C-N-CA	6.19	125.68	119.24
1	B	243	ASP	N-CA-C	-6.17	103.88	112.45
1	A	277	VAL	CA-C-N	-6.16	112.14	119.84
1	A	277	VAL	C-N-CA	-6.16	112.14	119.84
1	A	374	GLU	CA-C-O	-6.12	114.68	121.23
1	A	116	ILE	N-CA-C	6.12	117.40	108.53
1	A	367	ASP	N-CA-C	6.11	123.81	110.80
1	A	450	LYS	N-CA-C	-6.11	97.79	110.80
1	B	216	GLY	N-CA-C	6.08	119.54	111.03
1	B	252	SER	N-CA-C	6.05	118.11	110.24
1	B	170	ALA	N-CA-C	5.97	118.75	111.82
1	A	319	HIS	N-CA-C	-5.94	105.30	112.54
1	A	71	ASP	N-CA-C	5.92	120.04	112.34
1	B	359	HIS	CA-C-N	-5.89	112.82	122.54
1	B	359	HIS	C-N-CA	-5.89	112.82	122.54
1	A	171	THR	N-CA-C	5.81	119.02	110.59
1	B	319	HIS	N-CA-CB	5.80	120.30	110.49
1	B	374	GLU	N-CA-C	5.74	121.18	113.72
1	A	454	PHE	N-CA-C	5.73	117.39	111.03
1	A	88	ARG	N-CA-C	-5.67	105.24	111.82
1	B	352	SER	N-CA-C	-5.64	98.78	110.80
1	A	322	ILE	N-CA-C	5.64	114.09	107.77
1	A	55	GLU	N-CA-C	-5.61	105.03	112.94
1	A	276	CYS	O-C-N	5.51	132.26	122.34
1	A	375	LYS	N-CA-C	-5.48	99.14	110.80
1	A	375	LYS	CA-C-N	5.47	131.07	122.21
1	A	375	LYS	C-N-CA	5.47	131.07	122.21
1	B	109	ALA	CA-C-N	5.46	127.85	120.38
1	B	109	ALA	C-N-CA	5.46	127.85	120.38
1	A	381	TYR	N-CA-C	5.41	118.00	111.40
1	B	119	ARG	N-CA-C	-5.35	103.92	110.61
1	A	103	VAL	N-CA-C	5.25	120.27	109.34
1	A	182	PHE	N-CA-C	5.25	116.81	111.14
1	B	262	ASP	N-CA-C	5.19	115.86	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	349	TYR	CA-C-N	5.18	131.43	121.54
1	B	349	TYR	C-N-CA	5.18	131.43	121.54
1	A	365	GLU	CA-C-N	5.17	131.26	122.37
1	A	365	GLU	C-N-CA	5.17	131.26	122.37
1	A	110	SER	N-CA-C	5.15	120.20	112.94
1	B	372	ALA	N-CA-C	5.11	119.14	113.01
1	A	34	ALA	N-CA-C	-5.11	106.46	113.30
1	B	37	ARG	N-CA-C	-5.08	98.42	107.98
1	B	322	ILE	N-CA-C	5.04	113.47	107.73

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	GLN	Mainchain
1	A	364	GLY	Peptide,Mainchain
1	A	374	GLU	Mainchain
1	B	319	HIS	Sidechain
1	B	359	HIS	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	3462	0	3509	272	0
1	B	3509	0	3559	234	0
2	A	26	0	19	4	0
2	B	26	0	19	1	0
3	B	5	0	0	1	0
4	A	80	0	0	4	0
4	B	50	0	0	5	0
All	All	7158	0	7106	463	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 33.

All (463) 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:360:LEU:C	1:B:360:LEU:CA	1.76	1.52
1:A:346:HIS:CE1	1:A:347:ARG:HD2	1.60	1.36
1:A:348:ASP:O	1:A:375:LYS:HE3	1.26	1.35
1:A:279:GLN:NE2	1:A:309:ARG:HD3	1.62	1.12
1:B:359:HIS:ND1	1:B:362:THR:HG22	1.73	1.04
1:A:347:ARG:NH2	1:B:315:GLU:OE2	1.91	1.02
1:A:366:LEU:CD1	1:A:371:LEU:HD11	1.92	0.99
1:B:256:MET:O	1:B:259:VAL:HG12	1.60	0.99
1:A:346:HIS:HE1	1:A:347:ARG:HD2	1.19	0.96
1:A:346:HIS:HE1	1:A:347:ARG:HH21	1.16	0.94
1:B:319:HIS:O	1:B:321:GLY:N	2.04	0.90
1:A:366:LEU:HD13	1:A:371:LEU:HD11	1.52	0.89
1:A:349:TYR:HD1	1:A:349:TYR:H	1.16	0.88
1:A:447:LEU:HD23	1:A:447:LEU:H	1.37	0.87
1:A:346:HIS:ND1	1:A:347:ARG:HD2	1.87	0.87
1:A:348:ASP:C	1:A:375:LYS:HE3	1.99	0.87
1:A:374:GLU:HG2	1:A:375:LYS:N	1.86	0.87
1:A:411:GLY:O	1:A:412:THR:HG22	1.77	0.84
1:A:148:PRO:HD2	1:A:151:LEU:HD22	1.58	0.84
1:A:279:GLN:HE21	1:A:309:ARG:HD3	1.42	0.84
1:B:359:HIS:CE1	1:B:362:THR:HG22	2.12	0.83
1:A:346:HIS:HE1	1:A:347:ARG:NH2	1.77	0.83
1:A:277:VAL:O	1:A:278:PRO:C	2.19	0.82
1:A:346:HIS:CE1	1:A:347:ARG:HH21	1.96	0.82
1:B:309:ARG:HB3	1:B:309:ARG:HH11	1.45	0.82
1:A:366:LEU:CD1	1:A:371:LEU:CD1	2.57	0.82
1:B:346:HIS:CD2	1:B:347:ARG:HG2	2.14	0.82
1:B:99:PHE:HD2	1:B:110:SER:HB3	1.46	0.81
1:A:346:HIS:CE1	1:A:347:ARG:CD	2.56	0.80
1:A:407:LEU:HD22	1:A:439:ILE:HG12	1.63	0.80
1:B:319:HIS:C	1:B:321:GLY:H	1.90	0.80
1:B:357:THR:HG23	1:B:382:MET:HE3	1.62	0.79
1:A:277:VAL:O	1:A:278:PRO:O	1.99	0.79
1:B:162:ARG:HG3	1:B:166:LYS:HE2	1.63	0.79
1:A:354:ARG:HH12	1:B:354:ARG:CZ	1.96	0.79
1:A:132:SER:HB3	1:A:135:LEU:HB2	1.66	0.78
1:A:331:THR:HG22	1:A:334:SER:HB2	1.64	0.77
1:B:359:HIS:ND1	1:B:362:THR:CG2	2.47	0.77
1:B:403:MET:HE1	1:B:442:GLY:CA	2.14	0.77
1:A:177:ARG:NH1	1:A:213:ASP:HB3	1.99	0.77
1:A:354:ARG:HH22	1:B:354:ARG:NH2	1.83	0.77
1:A:279:GLN:NE2	1:A:309:ARG:CD	2.45	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ARG:HH22	1:B:315:GLU:CD	1.92	0.76
1:A:386:GLN:O	1:A:390:ILE:HG13	1.85	0.76
1:B:360:LEU:C	1:B:360:LEU:N	2.44	0.76
1:A:233:LEU:HD23	1:B:233:LEU:HD12	1.66	0.75
1:A:268:VAL:HG12	1:A:268:VAL:O	1.86	0.75
1:A:223:ALA:HB2	1:A:299:LEU:HD22	1.69	0.75
1:A:279:GLN:HE21	1:A:309:ARG:CD	1.99	0.75
1:B:99:PHE:CD2	1:B:110:SER:HB3	2.22	0.74
1:A:51:VAL:O	1:A:55:GLU:HG3	1.87	0.74
1:B:318:CYS:O	1:B:319:HIS:CG	2.40	0.74
1:A:240:GLN:NE2	4:B:552:HOH:O	2.21	0.73
1:A:249:ARG:HG3	1:A:249:ARG:HH11	1.54	0.73
1:B:407:LEU:HD21	1:B:439:ILE:HG12	1.70	0.73
1:A:344:LEU:O	1:A:377:THR:HG21	1.88	0.73
1:B:162:ARG:O	1:B:166:LYS:HD2	1.89	0.72
1:B:260:ARG:O	1:B:261:ARG:C	2.30	0.72
1:B:319:HIS:C	1:B:321:GLY:N	2.42	0.72
1:A:137:ARG:NH2	1:B:176:ARG:HH12	1.88	0.71
1:A:381:TYR:O	2:A:501:SAH:O2'	2.03	0.71
1:A:407:LEU:HB2	1:A:419:VAL:HG22	1.72	0.71
1:A:166:LYS:HG2	1:A:175:ARG:NH2	2.06	0.71
1:A:254:ASP:HB3	1:B:149:GLN:NE2	2.05	0.71
1:A:365:GLU:HG3	1:A:366:LEU:HG	1.73	0.70
1:B:409:GLU:HB2	1:B:433:VAL:CG1	2.21	0.70
1:B:419:VAL:CG1	1:B:429:LEU:HD22	2.22	0.70
1:A:349:TYR:HD1	1:A:349:TYR:N	1.89	0.70
1:A:137:ARG:NH2	1:B:176:ARG:NH1	2.40	0.70
1:A:284:GLN:HA	1:A:287:LEU:HD21	1.73	0.69
1:A:370:ASN:HD21	1:B:370:ASN:HA	1.56	0.69
1:A:300:LYS:NZ	1:A:300:LYS:HB3	2.08	0.69
1:B:233:LEU:O	1:B:237:GLN:HG3	1.91	0.69
1:B:55:GLU:HG3	1:B:57:MET:HG2	1.75	0.68
1:B:241:GLN:O	1:B:295:ARG:HD3	1.94	0.68
1:A:403:MET:HE1	1:A:442:GLY:HA2	1.76	0.68
1:B:164:ARG:HD2	1:B:208:PHE:CE2	2.29	0.68
1:B:412:THR:H	1:B:416:GLN:HE21	1.42	0.68
1:B:284:GLN:HG3	1:B:288:ARG:HH21	1.59	0.68
1:B:66:ASP:O	1:B:69:LEU:HB2	1.93	0.67
1:A:346:HIS:CE1	1:A:347:ARG:NH2	2.60	0.67
1:A:300:LYS:HB3	1:A:300:LYS:HZ2	1.59	0.67
1:B:265:ARG:HG3	1:B:265:ARG:HH11	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:HE3	1:A:114:PRO:HD2	1.77	0.66
1:B:395:ILE:HG23	1:B:423:LEU:HD13	1.78	0.66
1:A:287:LEU:HD23	1:A:287:LEU:H	1.59	0.66
1:A:85:VAL:HG22	1:A:88:ARG:HH21	1.61	0.65
1:A:418:VAL:H	1:A:457:HIS:CE1	2.13	0.65
1:A:112:ILE:HD13	1:A:129:GLY:HA2	1.78	0.65
1:A:45:PHE:CE1	1:A:60:LEU:HD22	2.31	0.65
1:A:346:HIS:HE1	1:A:347:ARG:CD	2.01	0.65
1:B:430:ALA:C	1:B:432:GLN:H	2.05	0.65
1:A:401:ALA:O	1:A:422:VAL:HG12	1.97	0.65
1:A:123:MET:HE1	1:B:1:MET:HE2	1.78	0.65
1:B:236:LEU:HD21	1:B:240:GLN:HE21	1.62	0.65
1:B:319:HIS:O	1:B:320:ALA:C	2.37	0.65
1:B:287:LEU:HD21	1:B:320:ALA:CB	2.27	0.65
1:A:281:GLU:O	1:A:285:ILE:HG13	1.96	0.64
1:B:390:ILE:O	1:B:394:LEU:HB2	1.98	0.64
1:B:239:ILE:HD11	1:B:299:LEU:HD21	1.78	0.64
1:A:447:LEU:H	1:A:447:LEU:CD2	2.08	0.64
1:A:420:HIS:CD2	1:A:421:GLY:N	2.65	0.64
1:A:227:ASP:H	1:A:412:THR:HG23	1.61	0.64
1:B:403:MET:HE1	1:B:442:GLY:N	2.13	0.64
1:A:168:GLN:HE21	1:A:168:GLN:HA	1.62	0.64
1:B:287:LEU:O	1:B:291:GLN:HG3	1.97	0.64
1:A:177:ARG:CZ	1:A:213:ASP:HB3	2.28	0.64
1:B:346:HIS:H	1:B:350:ALA:HB2	1.62	0.64
1:A:352:SER:OG	1:B:354:ARG:HD3	1.99	0.63
1:A:444:VAL:O	1:A:447:LEU:HD23	1.99	0.63
1:B:352:SER:HB3	1:B:376:GLN:HB3	1.80	0.63
1:A:356:VAL:HG12	1:A:357:THR:N	2.13	0.63
1:A:406:ALA:O	1:A:407:LEU:HD23	1.98	0.63
1:B:228:ALA:HA	1:B:255:ILE:CD1	2.28	0.63
1:B:339:TYR:HB3	1:B:416:GLN:HE22	1.64	0.63
1:A:276:CYS:C	1:A:277:VAL:CG2	2.72	0.63
1:B:346:HIS:O	1:B:347:ARG:C	2.40	0.63
1:A:425:GLN:HA	1:A:428:GLU:HG3	1.81	0.62
1:A:117:ILE:HD13	1:A:143:LEU:CB	2.30	0.62
1:B:309:ARG:NH1	1:B:312:GLU:OE1	2.32	0.62
1:B:369:GLU:HB2	1:B:397:PHE:CD2	2.34	0.62
1:A:213:ASP:OD1	1:A:215:ARG:HG2	2.00	0.62
1:B:298:ARG:NH1	1:B:313:GLU:OE2	2.33	0.61
1:A:231:LEU:O	1:B:233:LEU:HD13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:THR:H	1:B:416:GLN:NE2	1.98	0.61
1:B:318:CYS:O	1:B:319:HIS:CD2	2.53	0.61
1:B:400:GLN:O	1:B:403:MET:HB2	2.00	0.61
1:A:118:ASP:O	1:A:119:ARG:HD3	2.01	0.61
1:B:407:LEU:CD2	1:B:439:ILE:HG12	2.31	0.61
1:B:176:ARG:O	1:B:180:GLU:HG3	2.00	0.61
1:A:171:THR:OG1	1:A:174:GLU:HG3	2.01	0.61
1:A:331:THR:CG2	1:A:334:SER:H	2.14	0.61
1:B:281:GLU:O	1:B:285:ILE:HG13	1.99	0.60
1:A:117:ILE:HD13	1:A:143:LEU:HB3	1.83	0.60
1:A:349:TYR:N	1:A:349:TYR:CD1	2.60	0.60
1:B:309:ARG:HH12	1:B:312:GLU:CD	2.09	0.60
1:B:403:MET:HE1	1:B:442:GLY:HA2	1.83	0.60
1:B:354:ARG:NH1	1:B:371:LEU:HD23	2.17	0.60
1:A:330:ILE:HD13	1:B:330:ILE:HD13	1.84	0.60
1:A:374:GLU:HG2	1:A:375:LYS:H	1.66	0.60
1:A:400:GLN:O	1:A:403:MET:HB2	2.01	0.60
1:A:276:CYS:O	1:A:277:VAL:HG23	2.01	0.59
1:A:262:ASP:HA	1:B:26:ARG:HD3	1.84	0.59
1:A:365:GLU:OE1	1:A:368:TRP:CZ2	2.56	0.59
1:A:331:THR:HG23	1:A:334:SER:H	1.68	0.58
1:B:287:LEU:O	1:B:287:LEU:HD23	2.03	0.58
1:A:333:ALA:HB2	1:A:379:VAL:HG11	1.84	0.58
1:B:339:TYR:CD2	1:B:412:THR:HA	2.37	0.58
1:B:220:LEU:HD13	1:B:314:LEU:HD21	1.85	0.58
1:A:225:PRO:HG2	1:A:412:THR:HG21	1.86	0.58
1:A:387:ALA:HB1	1:A:426:LEU:CD2	2.33	0.58
1:A:352:SER:HB3	1:A:376:GLN:HG2	1.84	0.58
1:A:14:ASP:OD1	1:A:37:ARG:HG2	2.04	0.58
1:A:233:LEU:HD11	1:B:236:LEU:HD12	1.84	0.58
1:B:248:ASP:OD2	1:B:298:ARG:NH2	2.37	0.58
1:A:410:ASN:ND2	1:A:436:PRO:HD2	2.19	0.57
1:A:268:VAL:HG13	1:A:282:ILE:HG12	1.86	0.57
1:B:265:ARG:HG3	1:B:265:ARG:NH1	2.19	0.57
1:A:176:ARG:HH11	1:A:295:ARG:NH1	2.01	0.57
1:B:139:LEU:O	1:B:143:LEU:HG	2.05	0.57
1:B:290:ALA:HB3	1:B:322:ILE:HD13	1.86	0.57
1:A:137:ARG:HG2	1:A:137:ARG:HH21	1.70	0.57
1:B:259:VAL:HG13	1:B:265:ARG:NH2	2.19	0.57
1:A:268:VAL:HG13	1:A:277:VAL:HG23	1.85	0.57
1:A:410:ASN:HD21	1:A:436:PRO:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LEU:HG	1:B:317:LEU:HD23	1.87	0.56
1:A:365:GLU:HG3	1:A:366:LEU:N	2.20	0.56
1:A:162:ARG:HD2	4:A:518:HOH:O	2.04	0.56
1:A:411:GLY:HA2	1:A:416:GLN:HG3	1.88	0.56
1:A:277:VAL:HG12	1:A:281:GLU:CD	2.30	0.56
1:A:354:ARG:CD	1:A:371:LEU:HD23	2.36	0.56
1:A:374:GLU:HG2	1:A:375:LYS:CA	2.35	0.56
1:A:112:ILE:CD1	1:A:129:GLY:HA2	2.35	0.56
1:A:137:ARG:HH22	1:B:176:ARG:HH12	1.52	0.56
1:A:254:ASP:HB3	1:B:149:GLN:HE22	1.68	0.56
1:B:259:VAL:HG13	1:B:265:ARG:HH21	1.71	0.56
1:B:340:SER:O	1:B:448:ARG:HG3	2.06	0.56
1:A:401:ALA:O	1:A:422:VAL:CG1	2.54	0.56
1:A:74:TRP:HH2	1:B:94:GLU:HG2	1.70	0.56
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.70	0.56
1:A:2:ASP:HB2	1:B:11:ARG:HH21	1.71	0.55
1:B:279:GLN:HG2	1:B:309:ARG:NH1	2.22	0.55
1:A:176:ARG:NH1	1:A:295:ARG:NH1	2.55	0.55
1:B:219:VAL:HG21	1:B:238:GLN:HE21	1.72	0.55
1:B:287:LEU:HD21	1:B:320:ALA:HB1	1.88	0.55
1:B:429:LEU:O	1:B:432:GLN:HB3	2.07	0.55
1:B:105:ALA:HB1	1:B:108:ALA:HB2	1.88	0.55
1:A:164:ARG:HD2	1:A:208:PHE:CE2	2.41	0.55
1:B:196:ASP:O	1:B:200:VAL:HG23	2.06	0.55
1:A:244:ILE:HG13	1:A:264:ASP:HB2	1.88	0.55
1:A:387:ALA:HA	1:A:390:ILE:HD12	1.89	0.55
1:A:374:GLU:HG2	1:A:376:GLN:H	1.71	0.55
1:B:394:LEU:HD23	1:B:399:MET:SD	2.47	0.55
1:B:419:VAL:HG12	1:B:429:LEU:HD22	1.88	0.55
1:B:100:CYS:H	1:B:110:SER:HB2	1.71	0.55
1:A:354:ARG:HH22	1:B:354:ARG:HH21	1.50	0.55
1:B:148:PRO:HA	1:B:237:GLN:HE22	1.72	0.54
1:A:176:ARG:NH1	1:A:295:ARG:HH11	2.06	0.54
1:B:284:GLN:CG	1:B:288:ARG:HH21	2.20	0.54
1:A:391:GLN:HE22	1:A:424:THR:HA	1.71	0.54
1:A:366:LEU:HD12	1:A:371:LEU:CD1	2.35	0.54
1:B:360:LEU:C	1:B:360:LEU:CB	2.72	0.54
1:A:403:MET:HA	1:A:443:ARG:NH1	2.22	0.54
1:B:369:GLU:HG2	1:B:397:PHE:HB3	1.90	0.54
1:A:251:VAL:HG11	1:A:299:LEU:HD13	1.89	0.54
1:A:406:ALA:C	1:A:407:LEU:HD23	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:503:PO4:O2	4:B:552:HOH:O	2.18	0.53
1:B:291:GLN:C	1:B:293:GLY:H	2.14	0.53
1:A:85:VAL:CG2	1:A:88:ARG:HH21	2.21	0.53
1:A:354:ARG:HD3	1:A:371:LEU:HD23	1.89	0.53
1:A:2:ASP:CB	1:B:11:ARG:HH21	2.21	0.53
1:A:137:ARG:HH22	1:B:176:ARG:NH1	2.04	0.53
1:B:117:ILE:N	1:B:117:ILE:HD12	2.22	0.53
1:B:58:LEU:HD12	1:B:58:LEU:C	2.33	0.53
1:A:283:ASN:O	1:A:287:LEU:HD23	2.07	0.53
1:B:228:ALA:HA	1:B:255:ILE:HD11	1.89	0.53
1:A:425:GLN:O	1:A:429:LEU:HG	2.09	0.53
1:A:48:GLN:HG3	1:A:52:TRP:CZ3	2.44	0.53
1:B:162:ARG:O	1:B:166:LYS:CD	2.57	0.53
1:B:251:VAL:HG11	1:B:299:LEU:HD13	1.90	0.53
1:B:339:TYR:CB	1:B:416:GLN:HE22	2.21	0.53
1:A:227:ASP:H	1:A:412:THR:CG2	2.22	0.52
1:B:380:PHE:HB2	1:B:439:ILE:HB	1.91	0.52
1:A:365:GLU:OE1	1:A:368:TRP:CH2	2.63	0.52
1:A:213:ASP:CG	1:A:215:ARG:HG2	2.35	0.52
1:A:247:TYR:H	1:A:247:TYR:HD2	1.55	0.52
1:A:365:GLU:HG3	1:A:366:LEU:H	1.74	0.52
1:A:183:PHE:HZ	1:B:132:SER:HB3	1.74	0.52
1:A:411:GLY:HA2	1:A:416:GLN:HE21	1.75	0.52
1:A:447:LEU:HD23	1:A:447:LEU:N	2.15	0.52
1:B:148:PRO:HA	1:B:237:GLN:NE2	2.25	0.52
1:A:166:LYS:HG2	1:A:175:ARG:CZ	2.39	0.51
1:A:176:ARG:HH11	1:A:295:ARG:HH11	1.56	0.51
1:A:183:PHE:CZ	1:B:132:SER:HB3	2.46	0.51
1:A:87:GLN:HB3	4:A:563:HOH:O	2.11	0.51
1:A:420:HIS:HD2	1:A:421:GLY:N	2.05	0.51
1:B:368:TRP:NE1	1:B:393:LYS:HD3	2.25	0.51
1:B:401:ALA:HB1	1:B:424:THR:HG23	1.92	0.51
1:A:2:ASP:CB	1:B:11:ARG:NH2	2.73	0.51
1:A:407:LEU:HB2	1:A:419:VAL:CG2	2.40	0.51
1:A:123:MET:CE	1:B:1:MET:HE2	2.41	0.51
1:B:28:ALA:O	1:B:32:LEU:HG	2.11	0.51
1:A:420:HIS:HD2	1:A:421:GLY:H	1.57	0.51
1:B:75:LEU:HD22	1:B:111:PHE:CE1	2.45	0.51
1:B:284:GLN:HG3	1:B:288:ARG:NH2	2.23	0.51
1:A:249:ARG:HH11	1:A:249:ARG:CG	2.18	0.51
1:B:395:ILE:CG2	1:B:423:LEU:HD13	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:TRP:CH2	1:B:94:GLU:HG2	2.46	0.50
1:A:302:GLY:HA3	2:A:501:SAH:C	2.41	0.50
1:A:370:ASN:ND2	1:B:370:ASN:HA	2.26	0.50
1:B:401:ALA:HB1	1:B:424:THR:CG2	2.41	0.50
1:A:220:LEU:HD23	1:A:298:ARG:HB3	1.92	0.50
1:A:409:GLU:OE1	1:A:434:GLU:HG2	2.12	0.50
1:B:448:ARG:O	1:B:448:ARG:HG2	2.12	0.50
1:A:223:ALA:HB2	1:A:299:LEU:CD2	2.39	0.50
1:A:249:ARG:CG	1:A:249:ARG:NH1	2.75	0.50
1:A:332:ALA:N	2:A:501:SAH:OXT	2.31	0.50
1:B:150:HIS:HB3	1:B:153:GLN:HG3	1.93	0.50
1:B:169:PHE:CE2	1:B:212:LEU:HD13	2.46	0.50
1:B:180:GLU:O	1:B:184:VAL:HG22	2.12	0.49
1:B:368:TRP:HH2	1:B:390:ILE:HG12	1.76	0.49
1:A:339:TYR:HB3	1:A:416:GLN:HE22	1.77	0.49
1:B:411:GLY:HA2	1:B:416:GLN:HE21	1.77	0.49
1:A:11:ARG:HA	1:A:35:GLY:O	2.12	0.49
1:A:220:LEU:HD13	1:A:304:PRO:HB2	1.94	0.49
1:A:444:VAL:O	1:A:447:LEU:CD2	2.60	0.49
1:B:215:ARG:HD3	1:B:215:ARG:N	2.28	0.49
1:A:275:HIS:C	1:A:277:VAL:H	2.17	0.49
1:B:55:GLU:HG3	1:B:57:MET:CG	2.41	0.49
1:B:137:ARG:HD3	4:B:523:HOH:O	2.13	0.49
1:A:333:ALA:CB	1:A:379:VAL:HG11	2.42	0.49
1:A:378:LEU:HB2	1:A:441:VAL:HB	1.94	0.48
1:B:137:ARG:NH1	4:B:523:HOH:O	2.43	0.48
1:B:228:ALA:HA	1:B:255:ILE:HD13	1.95	0.48
1:B:411:GLY:HA2	1:B:416:GLN:HG3	1.94	0.48
1:A:16:LEU:HD23	1:A:70:LEU:HD23	1.93	0.48
1:A:284:GLN:HA	1:A:284:GLN:NE2	2.29	0.48
1:B:369:GLU:OE2	1:B:369:GLU:C	2.56	0.48
1:A:456:ASN:O	1:A:457:HIS:HB2	2.14	0.48
1:A:137:ARG:NH2	1:A:137:ARG:HG2	2.29	0.48
1:A:47:PRO:O	1:A:48:GLN:C	2.57	0.48
1:A:346:HIS:ND1	1:A:347:ARG:CD	2.70	0.48
1:A:356:VAL:CG1	1:A:357:THR:N	2.75	0.48
1:B:354:ARG:NH2	1:B:370:ASN:O	2.45	0.48
1:B:404:PRO:HG2	1:B:443:ARG:HA	1.95	0.48
1:B:422:VAL:HG22	1:B:425:GLN:OE1	2.13	0.48
1:A:157:TYR:CE2	1:A:161:LEU:HD11	2.49	0.48
1:A:346:HIS:CD2	1:A:447:LEU:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:GLU:HA	1:B:315:GLU:HG2	1.95	0.48
1:B:336:CYS:HB3	1:B:408:VAL:HG11	1.95	0.48
1:A:2:ASP:HB3	1:B:11:ARG:NH2	2.29	0.47
1:A:339:TYR:CD2	1:A:412:THR:HA	2.49	0.47
1:A:382:MET:HG2	2:A:501:SAH:H4'	1.96	0.47
1:A:277:VAL:O	1:A:282:ILE:HG13	2.14	0.47
1:A:289:GLU:OE2	1:A:294:LYS:HD2	2.13	0.47
1:B:287:LEU:HD23	1:B:287:LEU:C	2.39	0.47
1:B:405:VAL:HG11	1:B:426:LEU:HG	1.95	0.47
1:A:406:ALA:HB2	1:A:445:VAL:HG11	1.96	0.47
1:B:386:GLN:O	1:B:390:ILE:HG13	2.14	0.47
1:B:51:VAL:O	1:B:55:GLU:HG2	2.14	0.47
1:A:10:LEU:HD11	1:B:4:LEU:CD2	2.44	0.47
1:A:122:LEU:HD23	1:B:128:ALA:HB2	1.96	0.47
1:A:276:CYS:C	1:A:277:VAL:HG23	2.40	0.47
1:B:205:GLU:O	1:B:206:ARG:C	2.57	0.47
1:B:223:ALA:HB2	1:B:299:LEU:HD22	1.96	0.47
1:A:58:LEU:C	1:A:58:LEU:HD12	2.40	0.47
1:A:168:GLN:HA	1:A:168:GLN:NE2	2.29	0.47
1:B:146:LEU:HD22	1:B:240:GLN:NE2	2.30	0.47
1:B:309:ARG:NH1	1:B:312:GLU:CD	2.73	0.47
1:A:37:ARG:HH21	1:A:37:ARG:CG	2.27	0.47
1:A:117:ILE:HD11	1:A:140:ARG:HA	1.96	0.47
1:A:289:GLU:O	1:A:294:LYS:HB2	2.15	0.47
1:B:67:GLU:HG2	1:B:96:ARG:HH12	1.80	0.47
1:A:194:ASN:O	1:A:195:ALA:C	2.57	0.46
1:B:309:ARG:HH11	1:B:309:ARG:CB	2.22	0.46
1:B:309:ARG:HB3	1:B:309:ARG:NH1	2.24	0.46
1:B:349:TYR:H	1:B:349:TYR:HD1	1.55	0.46
1:A:168:GLN:HG2	1:A:208:PHE:HD2	1.81	0.46
1:B:352:SER:HB3	1:B:376:GLN:CB	2.45	0.46
1:A:406:ALA:HB2	1:A:445:VAL:CG1	2.45	0.46
1:A:17:ILE:HG13	1:A:38:LEU:HD21	1.98	0.46
1:B:187:ARG:HE	1:B:217:GLU:CD	2.24	0.46
1:B:361:LYS:HE3	4:B:548:HOH:O	2.15	0.46
1:A:233:LEU:HD11	1:B:236:LEU:CD1	2.46	0.46
1:A:277:VAL:C	1:A:278:PRO:O	2.59	0.46
1:A:278:PRO:O	1:A:281:GLU:N	2.49	0.46
1:A:268:VAL:CG1	1:A:282:ILE:HG12	2.45	0.46
1:A:38:LEU:HD22	1:A:39:THR:N	2.31	0.45
1:A:48:GLN:O	1:A:51:VAL:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:CD1	1:A:143:LEU:HB2	2.46	0.45
1:B:132:SER:O	1:B:133:PRO:C	2.60	0.45
1:B:236:LEU:HD23	1:B:236:LEU:C	2.41	0.45
1:B:291:GLN:HG2	1:B:322:ILE:HD11	1.98	0.45
1:A:16:LEU:HD23	1:A:70:LEU:CD2	2.47	0.45
1:A:10:LEU:HD11	1:B:4:LEU:HD22	1.98	0.45
1:A:268:VAL:HG13	1:A:277:VAL:CG2	2.46	0.45
1:A:159:GLY:O	1:A:162:ARG:HB2	2.16	0.45
1:B:346:HIS:O	1:B:350:ALA:CB	2.64	0.45
1:B:356:VAL:HG12	1:B:357:THR:N	2.31	0.45
1:B:408:VAL:O	2:B:502:SAH:H2	2.15	0.45
1:A:391:GLN:NE2	1:A:424:THR:HA	2.30	0.45
1:A:7:PHE:CE2	1:B:114:PRO:HB3	2.52	0.45
1:A:33:GLU:O	1:B:1:MET:HB3	2.16	0.45
1:B:42:ALA:O	1:B:62:GLU:HA	2.17	0.45
1:B:188:LEU:HB2	1:B:203:THR:HG21	1.99	0.45
1:B:234:LYS:HA	1:B:237:GLN:OE1	2.17	0.45
1:B:287:LEU:C	1:B:287:LEU:CD2	2.90	0.45
1:A:169:PHE:HB3	1:A:174:GLU:HB2	1.99	0.45
1:B:236:LEU:CD2	1:B:240:GLN:HE21	2.28	0.45
1:B:291:GLN:C	1:B:293:GLY:N	2.71	0.45
1:B:23:VAL:HG11	1:B:103:VAL:HG11	1.99	0.45
1:B:164:ARG:HD2	1:B:208:PHE:CD2	2.51	0.45
1:B:401:ALA:C	1:B:403:MET:H	2.25	0.45
1:B:171:THR:O	1:B:174:GLU:HB2	2.18	0.44
1:B:433:VAL:HG12	1:B:434:GLU:H	1.82	0.44
1:B:67:GLU:HG2	1:B:96:ARG:NH1	2.33	0.44
1:A:52:TRP:HB3	1:A:58:LEU:HG	1.99	0.44
1:A:407:LEU:CD2	1:A:439:ILE:HG23	2.47	0.44
1:A:176:ARG:CZ	1:A:295:ARG:HD2	2.47	0.44
1:A:286:LEU:HD23	1:A:296:VAL:HG11	1.99	0.44
1:A:291:GLN:C	1:A:293:GLY:H	2.23	0.44
1:A:308:GLY:C	1:A:310:GLY:H	2.26	0.44
1:A:117:ILE:HD13	1:A:143:LEU:HB2	1.99	0.44
1:A:249:ARG:O	1:A:249:ARG:HG2	2.16	0.44
1:A:400:GLN:HB3	1:A:402:ASP:OD2	2.18	0.44
1:B:41:ASN:ND2	1:B:61:VAL:O	2.44	0.44
1:B:119:ARG:HG2	1:B:119:ARG:HH11	1.83	0.44
1:B:206:ARG:O	1:B:210:GLU:HG2	2.18	0.44
1:A:374:GLU:CG	1:A:375:LYS:N	2.65	0.44
1:A:279:GLN:HG2	1:A:309:ARG:HE	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LEU:HG	1:A:381:TYR:HE1	1.82	0.44
1:B:99:PHE:HB3	1:B:111:PHE:CD1	2.53	0.44
1:B:341:GLY:O	1:B:343:PRO:HD3	2.18	0.44
1:A:5:PRO:HD2	1:B:116:ILE:HD13	2.01	0.43
1:A:333:ALA:O	1:A:337:SER:HB3	2.18	0.43
1:B:31:LEU:HD23	1:B:38:LEU:HD13	2.00	0.43
1:B:161:LEU:O	1:B:162:ARG:C	2.60	0.43
1:A:314:LEU:O	1:A:316:THR:N	2.45	0.43
1:A:330:ILE:CG2	1:A:334:SER:HB3	2.49	0.43
1:A:134:VAL:O	1:A:138:LEU:HG	2.19	0.43
1:A:168:GLN:HE21	1:A:168:GLN:CA	2.27	0.43
1:A:391:GLN:O	1:A:395:ILE:HG13	2.18	0.43
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.80	0.43
1:A:228:ALA:HB3	1:B:149:GLN:NE2	2.34	0.43
1:A:354:ARG:NH1	1:B:354:ARG:CZ	2.74	0.43
1:A:100:CYS:O	1:A:109:ALA:HB1	2.18	0.43
1:B:405:VAL:HG12	1:B:406:ALA:N	2.33	0.43
1:A:37:ARG:CG	1:A:37:ARG:NH2	2.82	0.43
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.85	0.43
1:A:348:ASP:HB2	1:A:375:LYS:NZ	2.34	0.43
1:B:391:GLN:HG3	1:B:423:LEU:O	2.19	0.43
1:B:404:PRO:HG2	1:B:442:GLY:O	2.19	0.43
1:A:322:ILE:HA	1:A:323:PRO:HD3	1.87	0.43
1:A:290:ALA:O	1:A:293:GLY:N	2.46	0.42
1:B:197:GLU:O	1:B:201:ASN:ND2	2.52	0.42
1:B:348:ASP:O	1:B:349:TYR:C	2.61	0.42
1:A:119:ARG:HG3	4:A:565:HOH:O	2.19	0.42
1:B:306:ILE:O	1:B:306:ILE:HG22	2.19	0.42
1:B:404:PRO:CG	1:B:443:ARG:HA	2.49	0.42
1:B:346:HIS:O	1:B:350:ALA:HB2	2.19	0.42
1:B:303:ASP:HA	1:B:304:PRO:HD3	1.85	0.42
1:B:430:ALA:C	1:B:432:GLN:N	2.73	0.42
1:A:11:ARG:HB3	4:A:502:HOH:O	2.19	0.42
1:A:231:LEU:HD23	1:A:232:THR:H	1.84	0.42
1:A:412:THR:H	1:A:416:GLN:NE2	2.17	0.42
1:B:10:LEU:O	1:B:11:ARG:C	2.62	0.42
1:B:164:ARG:HD2	1:B:208:PHE:CZ	2.54	0.42
1:B:245:VAL:HG21	1:B:259:VAL:HG21	2.00	0.42
1:B:391:GLN:HG3	1:B:423:LEU:CD2	2.49	0.42
1:A:38:LEU:CD2	1:A:39:THR:N	2.83	0.42
1:A:408:VAL:O	1:A:437:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:VAL:CG1	1:B:103:VAL:HG11	2.49	0.42
1:B:69:LEU:HD12	1:B:69:LEU:HA	1.85	0.42
1:A:187:ARG:HG3	1:A:187:ARG:HH11	1.83	0.42
1:A:213:ASP:OD2	1:A:215:ARG:HG2	2.19	0.42
1:A:216:GLY:O	1:A:323:PRO:HD2	2.20	0.42
1:A:365:GLU:CG	1:A:366:LEU:N	2.83	0.42
1:A:179:TRP:HA	1:A:182:PHE:HB3	2.01	0.42
1:A:194:ASN:O	1:A:196:ASP:N	2.52	0.42
1:B:53:ALA:C	1:B:55:GLU:H	2.27	0.42
1:B:96:ARG:HG3	1:B:98:ILE:HD12	2.02	0.42
1:B:305:PHE:CZ	1:B:326:VAL:HG21	2.54	0.42
1:A:177:ARG:NH1	1:A:213:ASP:CB	2.78	0.42
1:A:287:LEU:HD23	1:A:287:LEU:N	2.30	0.42
1:A:354:ARG:HB2	1:A:378:LEU:HD23	2.02	0.42
1:A:366:LEU:HD12	1:A:366:LEU:O	2.19	0.42
1:A:13:ARG:HD3	1:A:74:TRP:CD2	2.55	0.41
1:B:423:LEU:C	1:B:425:GLN:H	2.28	0.41
1:A:132:SER:HB3	1:A:135:LEU:CB	2.46	0.41
1:A:211:PRO:HG2	1:A:211:PRO:O	2.20	0.41
1:B:433:VAL:HG12	1:B:434:GLU:N	2.35	0.41
1:A:347:ARG:NH2	1:B:315:GLU:CD	2.66	0.41
1:B:99:PHE:HB3	1:B:111:PHE:HD1	1.85	0.41
1:B:146:LEU:HD22	1:B:240:GLN:HE22	1.85	0.41
1:B:41:ASN:OD1	1:B:65:PHE:HA	2.20	0.41
1:B:165:VAL:HG22	1:B:178:PHE:CE2	2.56	0.41
1:A:354:ARG:NH2	1:B:354:ARG:NH2	2.62	0.41
1:A:426:LEU:C	1:A:426:LEU:HD23	2.46	0.41
1:B:346:HIS:HB3	1:B:349:TYR:CD1	2.56	0.41
1:A:7:PHE:HB3	1:B:3:HIS:HB3	2.03	0.41
1:A:276:CYS:C	1:A:277:VAL:HG22	2.43	0.41
1:A:348:ASP:C	1:A:375:LYS:CE	2.82	0.41
1:A:354:ARG:HH12	1:B:354:ARG:NE	2.19	0.41
1:B:48:GLN:HG3	1:B:52:TRP:CZ3	2.56	0.41
1:B:358:GLY:N	1:B:381:TYR:O	2.46	0.41
1:B:425:GLN:O	1:B:426:LEU:C	2.63	0.41
1:A:37:ARG:HH21	1:A:37:ARG:HG3	1.86	0.41
1:B:70:LEU:O	1:B:73:CYS:HB2	2.21	0.41
1:B:314:LEU:C	1:B:316:THR:N	2.77	0.41
1:A:124:VAL:HG21	1:A:147:LEU:HD11	2.03	0.40
1:A:249:ARG:CG	1:A:249:ARG:O	2.69	0.40
1:A:279:GLN:OE1	1:A:279:GLN:HA	2.13	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ASP:O	1:B:371:LEU:HG	2.21	0.40
1:A:119:ARG:NH2	1:A:147:LEU:O	2.46	0.40
1:A:41:ASN:OD1	1:A:65:PHE:HA	2.22	0.40
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.95	0.40
1:A:354:ARG:NH1	1:B:354:ARG:NE	2.70	0.40
1:A:412:THR:H	1:A:416:GLN:HE21	1.70	0.40
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.91	0.40
1:B:378:LEU:HB2	1:B:441:VAL:HB	2.03	0.40
1:B:384:LEU:HD12	1:B:384:LEU:HA	1.98	0.40
1:A:351:GLN:NE2	1:B:367:ASP:OD1	2.55	0.40
1:B:457:HIS:ND1	1:B:457:HIS:N	2.70	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	442/457 (97%)	393 (89%)	40 (9%)	9 (2%)	6	21
1	B	451/457 (99%)	405 (90%)	41 (9%)	5 (1%)	11	36
All	All	893/914 (98%)	798 (89%)	81 (9%)	14 (2%)	7	27

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	GLU
1	A	367	ASP
1	A	375	LYS
1	B	320	ALA
1	B	350	ALA
1	B	373	ALA
1	A	195	ALA

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Mol	Chain	Res	Type
1	A	347	ARG
1	B	261	ARG
1	B	370	ASN
1	A	270	LYS
1	A	47	PRO
1	A	277	VAL
1	A	307	PHE

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	367/372 (99%)	335 (91%)	32 (9%)	9	30
1	B	371/372 (100%)	336 (91%)	35 (9%)	8	27
All	All	738/744 (99%)	671 (91%)	67 (9%)	9	28

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	38	LEU
1	A	43	LEU
1	A	44	THR
1	A	50	THR
1	A	111	PHE
1	A	119	ARG
1	A	120	SER
1	A	135	LEU
1	A	151	LEU
1	A	156	ARG
1	A	162	ARG
1	A	188	LEU
1	A	231	LEU
1	A	270	LYS
1	A	277	VAL

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Mol	Chain	Res	Type
1	A	278	PRO
1	A	279	GLN
1	A	287	LEU
1	A	300	LYS
1	A	347	ARG
1	A	348	ASP
1	A	349	TYR
1	A	355	LEU
1	A	370	ASN
1	A	403	MET
1	A	413	SER
1	A	423	LEU
1	A	428	GLU
1	A	438	LEU
1	A	443	ARG
1	A	447	LEU
1	B	9	GLN
1	B	73	CYS
1	B	81	ASP
1	B	90	SER
1	B	94	GLU
1	B	97	ARG
1	B	107	LYS
1	B	120	SER
1	B	124	VAL
1	B	132	SER
1	B	135	LEU
1	B	147	LEU
1	B	151	LEU
1	B	164	ARG
1	B	172	MET
1	B	209	SER
1	B	215	ARG
1	B	220	LEU
1	B	233	LEU
1	B	241	GLN
1	B	261	ARG
1	B	262	ASP
1	B	298	ARG
1	B	309	ARG
1	B	316	THR
1	B	334	SER

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Mol	Chain	Res	Type
1	B	349	TYR
1	B	351	GLN
1	B	360	LEU
1	B	369	GLU
1	B	394	LEU
1	B	423	LEU
1	B	426	LEU
1	B	435	SER
1	B	455	SER

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	160	GLN
1	A	168	GLN
1	A	190	GLN
1	A	240	GLN
1	A	241	GLN
1	A	279	GLN
1	A	284	GLN
1	A	346	HIS
1	A	351	GLN
1	A	391	GLN
1	A	400	GLN
1	A	410	ASN
1	A	416	GLN
1	A	420	HIS
1	A	431	GLN
1	A	452	ASN
1	B	9	GLN
1	B	54	ASN
1	B	86	ASN
1	B	149	GLN
1	B	150	HIS
1	B	190	GLN
1	B	238	GLN
1	B	240	GLN
1	B	284	GLN
1	B	346	HIS
1	B	351	GLN
1	B	385	ASN

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Mol	Chain	Res	Type
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 ⓘ

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 ⓘ

3 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$
2	SAH	A	501	-	27,28,28	1.17	3 (11%)	36,40,40	1.96	9 (25%)
3	PO4	B	503	-	4,4,4	1.95	1 (25%)	6,6,6	0.81	0
2	SAH	B	502	-	27,28,28	1.21	2 (7%)	36,40,40	1.84	8 (22%)

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	SAH	A	501	-	-	0/15/31/31	0/3/3/3
2	SAH	B	502	-	-	0/15/31/31	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	SAH	C5-N7	-3.22	1.33	1.39
2	A	501	SAH	C5-N7	-3.13	1.33	1.39
2	B	502	SAH	O4'-C1'	3.08	1.49	1.42
3	B	503	PO4	P-O2	-2.66	1.46	1.54
2	A	501	SAH	C4-N9	-2.52	1.32	1.37
2	A	501	SAH	O4'-C1'	2.43	1.47	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	SAH	N3-C2-N1	-5.45	120.33	128.58
2	B	502	SAH	N3-C2-N1	-5.11	120.85	128.58
2	B	502	SAH	C5-C4-N3	-5.09	119.70	126.72
2	A	501	SAH	C5-C4-N3	-4.71	120.24	126.72
2	A	501	SAH	C2-N3-C4	3.68	120.83	111.83
2	A	501	SAH	N9-C8-N7	-3.62	108.80	113.94
2	B	502	SAH	C2-N3-C4	3.53	120.46	111.83
2	B	502	SAH	N3-C4-N9	3.46	133.06	127.17
2	A	501	SAH	C2'-C1'-N9	-3.39	104.88	113.30
2	B	502	SAH	N9-C8-N7	-3.05	109.61	113.94
2	A	501	SAH	N3-C4-N9	2.89	132.08	127.17
2	B	502	SAH	C5-N7-C8	2.75	107.77	103.45
2	A	501	SAH	C5-N7-C8	2.72	107.73	103.45
2	A	501	SAH	C4-C5-N7	-2.49	107.73	110.58
2	B	502	SAH	C4-C5-N7	-2.46	107.78	110.58
2	A	501	SAH	C4-N9-C8	2.23	108.08	105.74
2	B	502	SAH	O4'-C4'-C5'	2.02	114.03	108.83

There are no chirality outliers.

There are no torsion outliers.

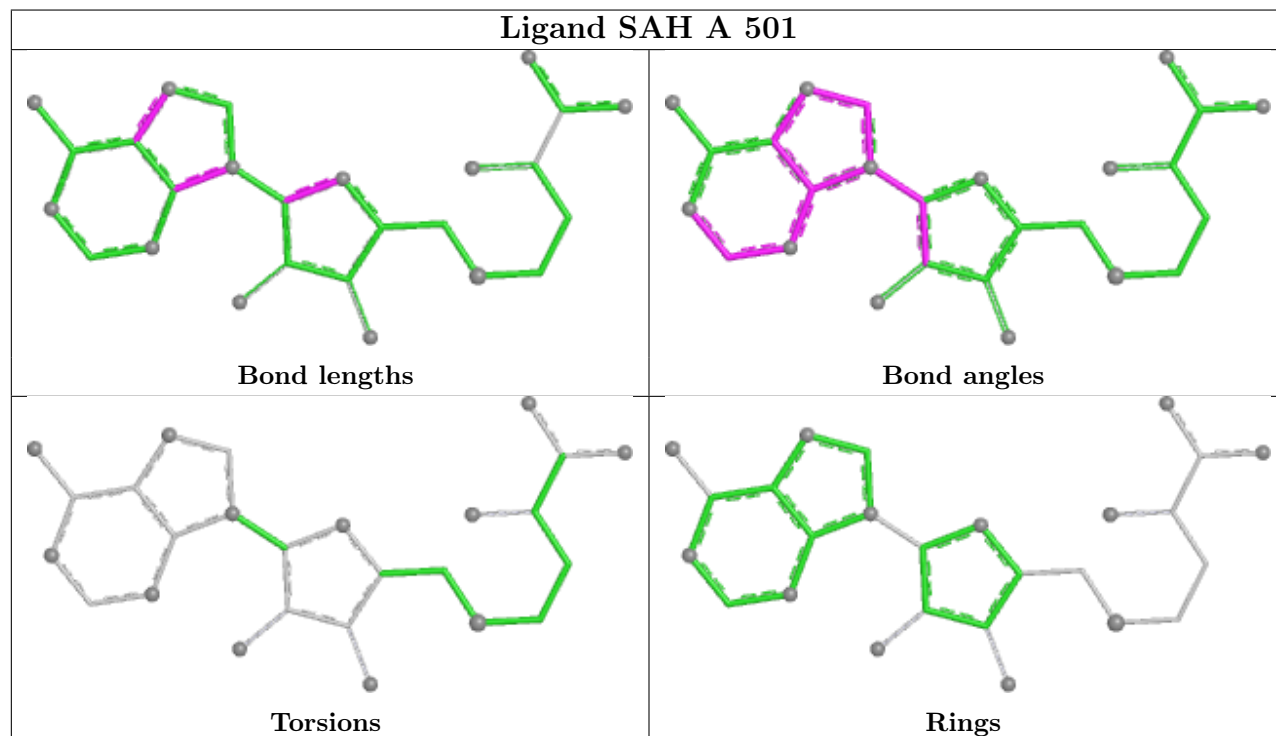
There are no ring outliers.

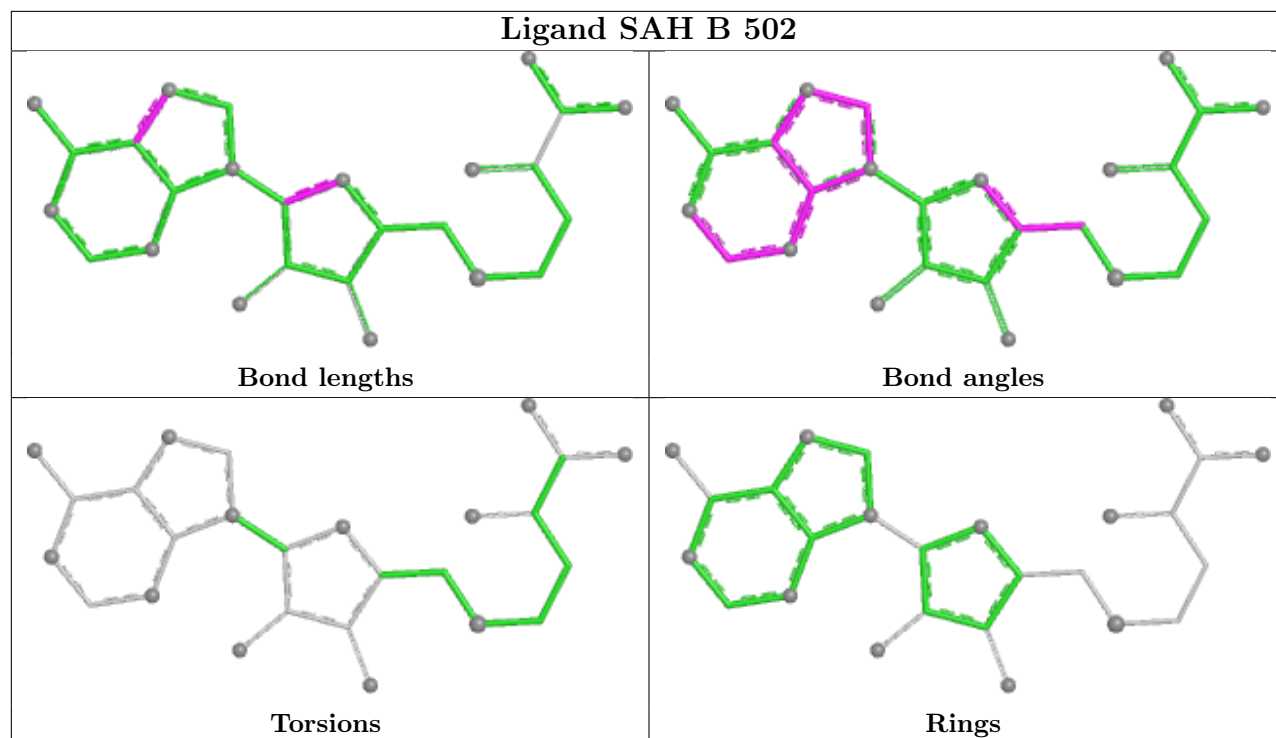
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SAH	4	0
3	B	503	PO4	1	0
2	B	502	SAH	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](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	448/457 (98%)	-0.04	4 (0%) 81 74	14, 37, 62, 91	0
1	B	455/457 (99%)	-0.11	9 (1%) 65 56	13, 35, 63, 94	0
All	All	903/914 (98%)	-0.08	13 (1%) 73 64	13, 36, 63, 94	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	CYS	5.1
1	B	360	LEU	3.8
1	B	367	ASP	3.5
1	B	363	GLY	3.3
1	A	364	GLY	3.1
1	B	275	HIS	3.1
1	A	357	THR	2.9
1	B	361	LYS	2.4
1	B	359	HIS	2.4
1	B	351	GLN	2.3
1	B	364	GLY	2.1
1	B	449	ASP	2.1
1	A	365	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

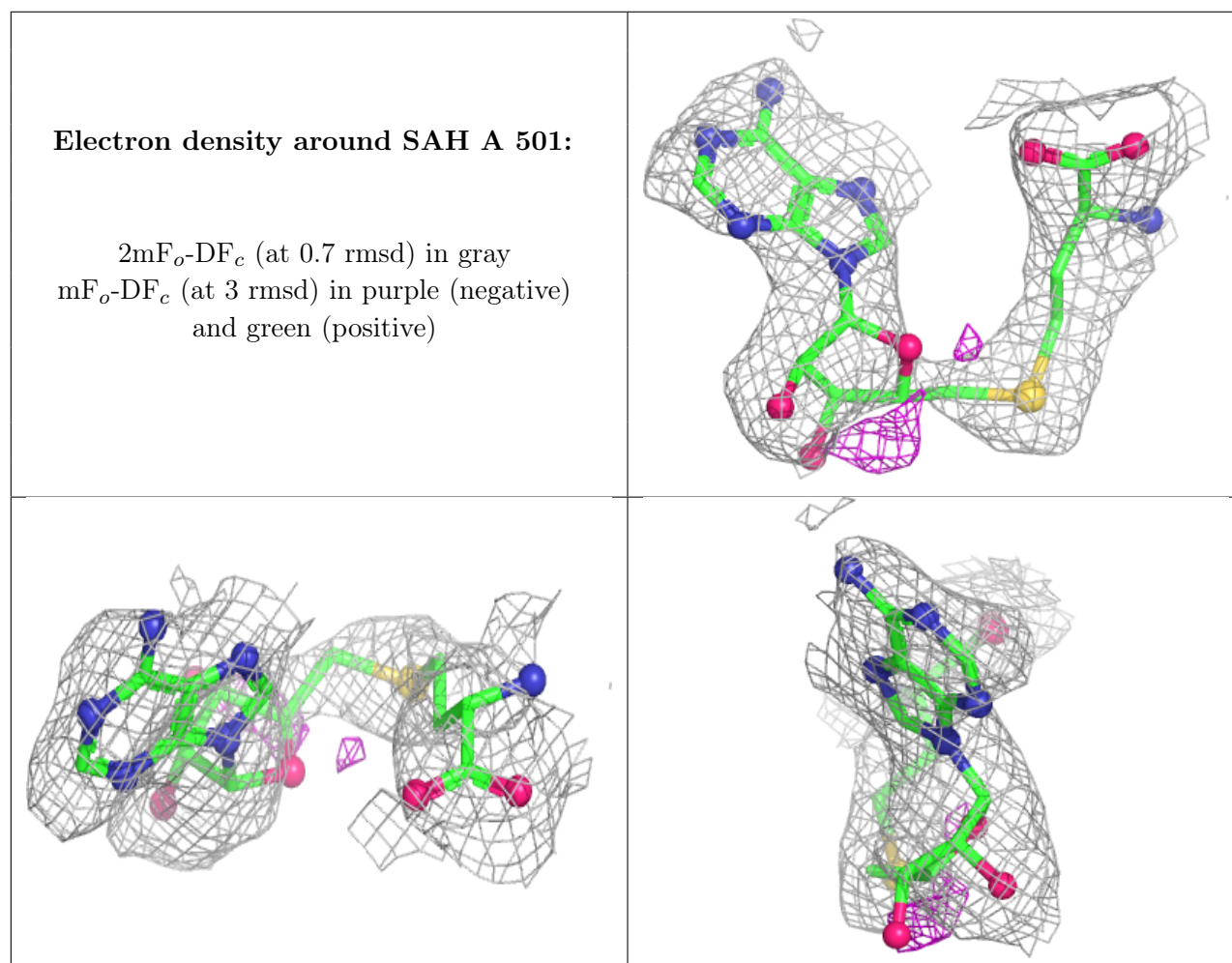
There are no oligosaccharides in this entry.

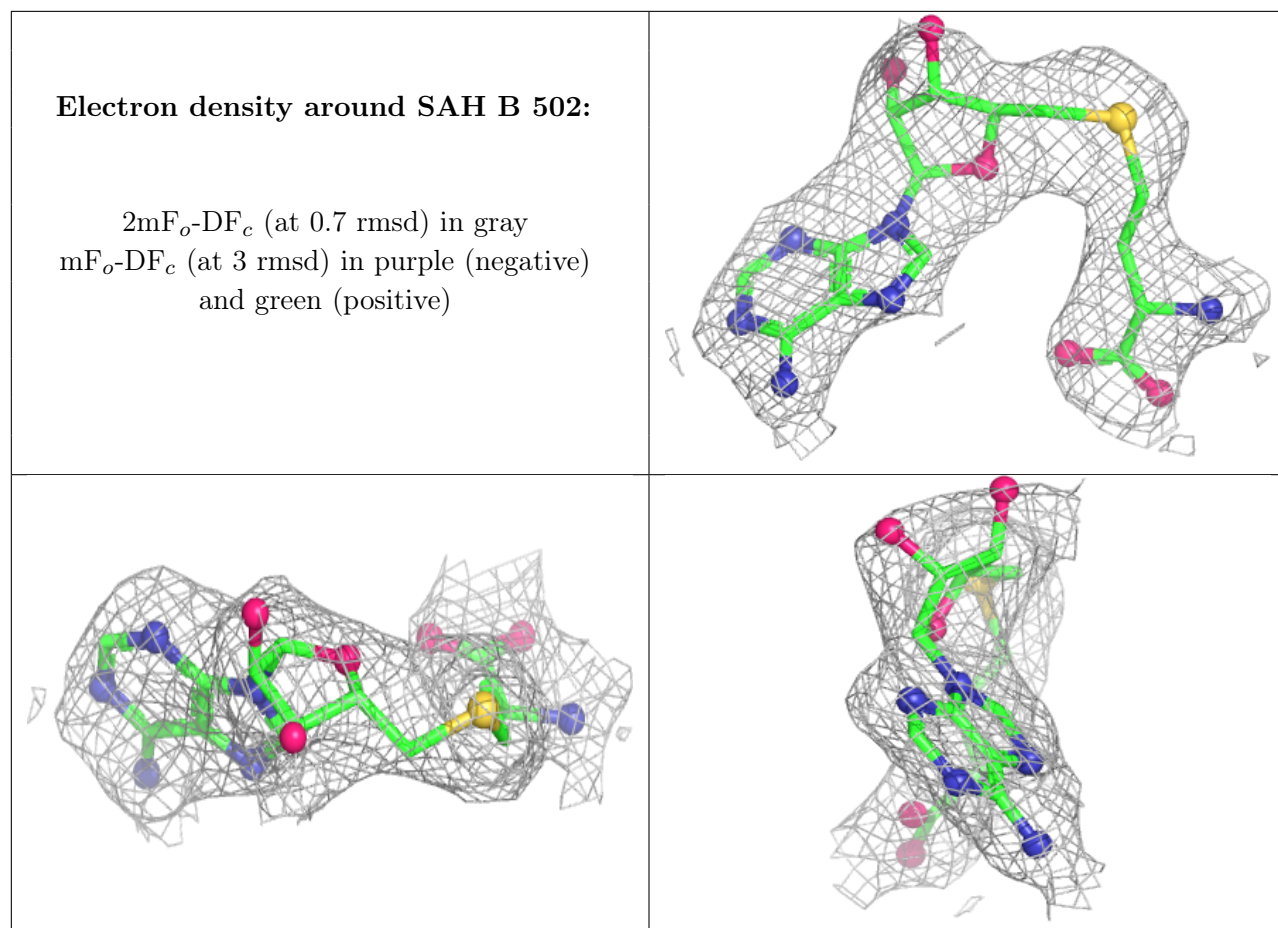
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SAH	A	501	26/26	0.85	0.12	36,65,68,68	0
3	PO4	B	503	5/5	0.92	0.10	52,54,55,56	0
2	SAH	B	502	26/26	0.95	0.08	28,41,46,46	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.