



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:34 PM UTC

PDB ID : 9Y43 / pdb_00009y43
Title : 3-hydroxypropionyl-CoA Synthetase (ADP-forming) from *Nitrosopumilus maritimus*.
Authors : Johnson, J.A.; Yilmaz, M.; Tosun, B.; Wakatsuki, S.; Demirci, H.
Deposited on : 2025-09-02
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

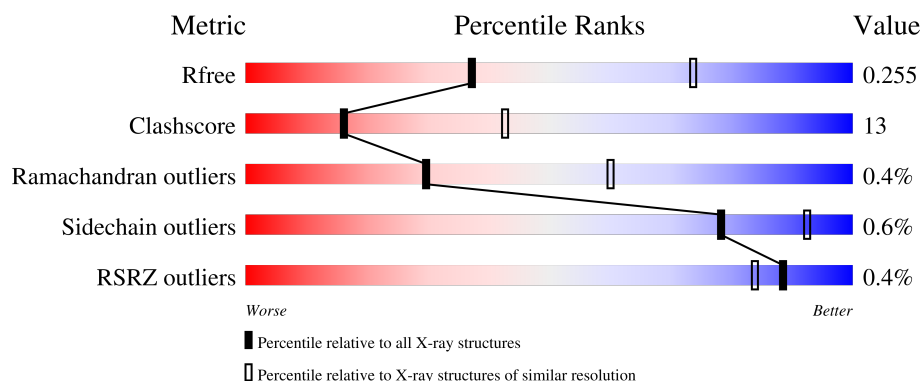
1 Overall quality at a glance

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	705	
1	B	705	

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
3	3OH	A	802[A]	-	X	-	-
3	3OH	A	802[B]	-	X	-	-
3	3OH	B	801[A]	-	X	-	-
3	3OH	B	801[B]	-	X	-	-

2 Entry composition [i](#)

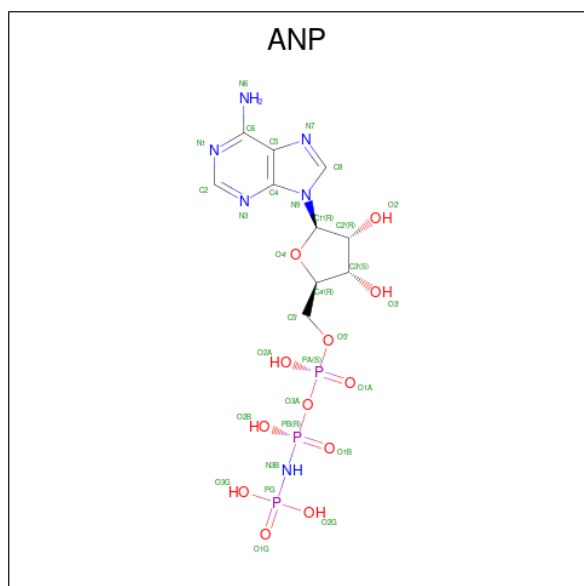
There are 6 unique types of molecules in this entry. The entry contains 10810 atoms, of which 13 are hydrogens and 0 are deuteriums.

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 3-hydroxypropionate--CoA ligase [ADP-forming].

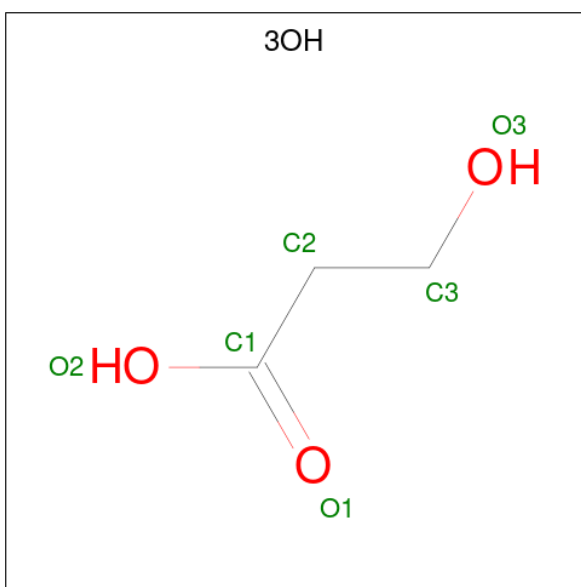
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	1	0
			5255	3370	893	960	32			
1	B	703	Total	C	N	O	S	0	2	0
			5342	3422	905	983	32			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



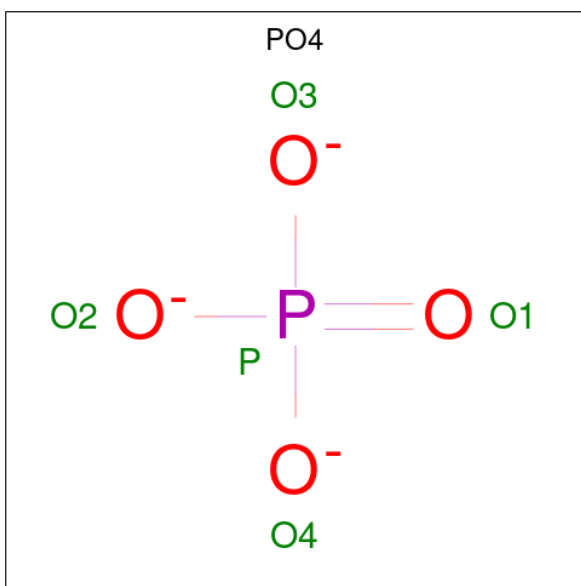
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			44	10	13	6	12		

- Molecule 3 is 3-HYDROXY-PROPANOIC ACID (CCD ID: 3OH) (formula: $C_3H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		
3	B	1	Total	C	O	0	1
			12	6	6		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0

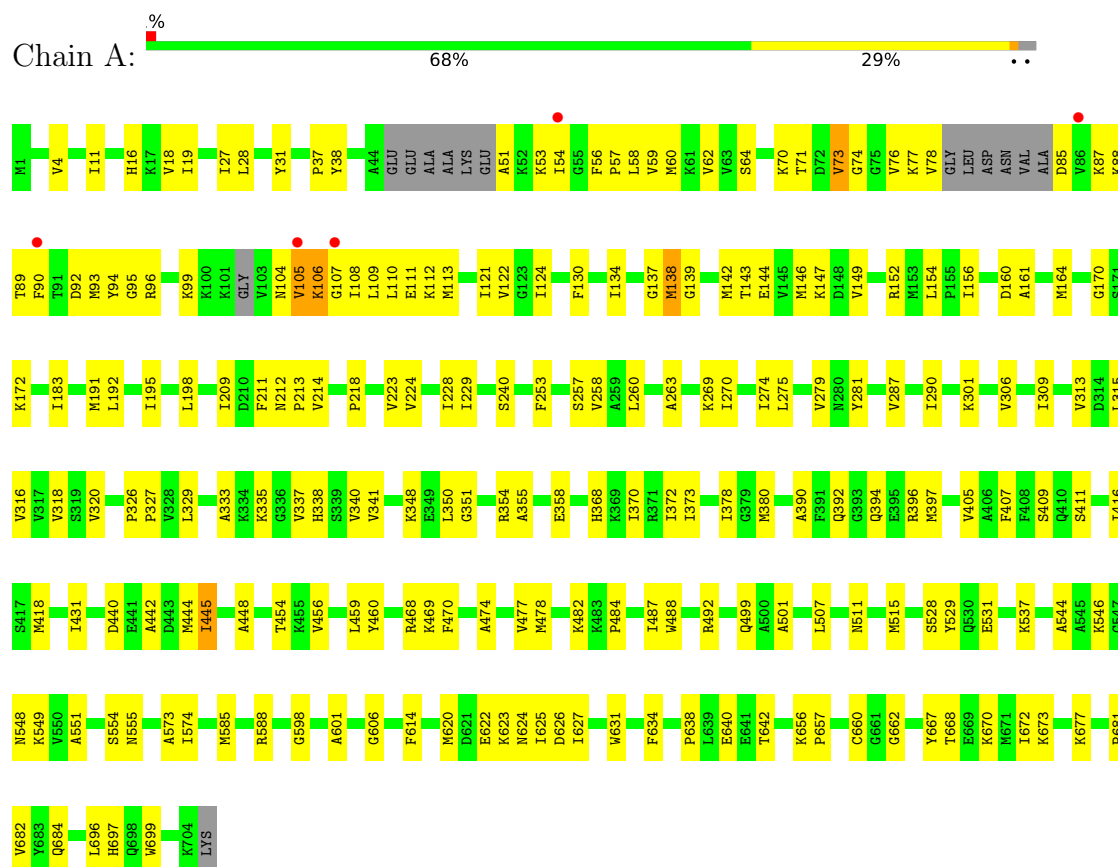
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	61	Total 61	O 61	0	0
6	B	73	Total 73	O 73	0	0

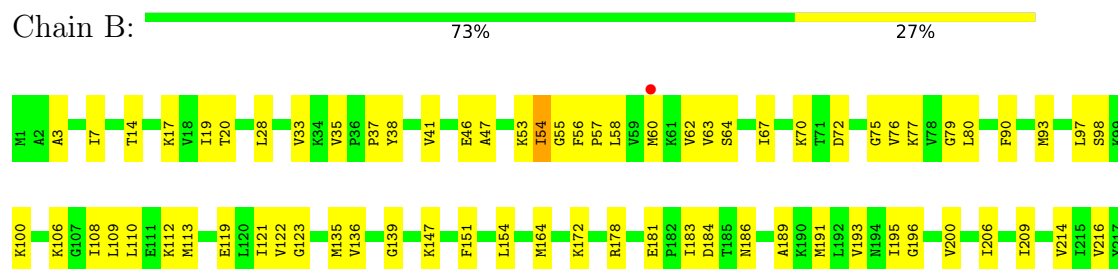
3 Residue-property plots

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: 3-hydroxypropionate--CoA ligase [ADP-forming]



- Molecule 1: 3-hydroxypropionate--CoA ligase [ADP-forming]



P637	N511	Q392	P218
P638	A512	R396	H221
K653	I513	M397	V222
K656	I514	K401	V223
P657	Y529	F408	K232
L658	A538	S409	F253
L659	A545	Q410	V251
C660	V550	M414	P267
G661	A551	L419	N272
T668	M552	K429	S273
K673	T553	M430	I274
L674	S554	I431	L275
I675	M560	S432	I290
E676	I564	F433	K296
K677	L567	D438	I297
V680	E568	V439	F298
P681	K569	D440	I309
V682	F570	E441	P310
A692	S571	A442	G311
L696	L572	D443	K312
H697	L581	M444	V313
S703	M585	Y447	V316
LYS	G598	A448	V317
LYS	N599	T454	V318
	P600	K455	S319
	A601	V456	V320
	G606	F470	P326
	F614	V473	E330
	Q618	V477	V337
	F619	P484	E358
	M620	L485	A359
	D621	V486	E360
	E622	I487	V361
	W623	W488	L364
	K624	K489	I372
	I625	R492	G379
	D626	T493	R386
	I627	A494	L387
	A628	K498	D388
	M629	A501	C389
	P630	T504	A390
	W631	L507	F391
	F634		
	Q635		
	D636		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.88Å 127.59Å 137.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 2.80 48.72 – 2.80	Depositor EDS
% Data completeness (in resolution range)	73.2 (48.72-2.80) 73.3 (48.72-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.210 , 0.250 0.212 , 0.255	Depositor DCC
R_{free} test set	1296 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10810	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: ANP, MG, PO4, 3OH

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	0.21	0/5351	0.66	5/7201 (0.1%)
1	B	0.19	0/5441	0.64	7/7329 (0.1%)
All	All	0.20	0/10792	0.65	12/14530 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	GLY	CA-C-N	6.79	134.19	121.97
1	B	75	GLY	C-N-CA	6.79	134.19	121.97
1	B	296	LYS	CA-C-N	6.08	132.92	121.97
1	B	296	LYS	C-N-CA	6.08	132.92	121.97
1	A	105	VAL	CA-C-N	5.99	132.58	122.15
1	A	105	VAL	C-N-CA	5.99	132.58	122.15
1	A	138	MET	CA-CB-CG	-5.93	102.24	114.10
1	A	106	LYS	CA-C-N	5.48	132.15	121.41
1	A	106	LYS	C-N-CA	5.48	132.15	121.41
1	B	72	ASP	CA-C-N	5.47	131.82	121.97
1	B	72	ASP	C-N-CA	5.47	131.82	121.97
1	B	98	SER	CB-CA-C	-5.19	102.03	110.85

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	5255	0	5467	155	0
1	B	5342	0	5544	133	0
2	A	31	13	13	2	0
3	A	12	0	3	0	0
3	B	12	0	3	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	1	0	0	0	0
6	A	61	0	0	1	0
6	B	73	0	0	0	0
All	All	10797	13	11030	284	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 13.

All (284) 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:A:56:PHE:HB2	1:A:57:PRO:HD3	1.41	1.03
1:B:54:ILE:HG23	1:B:112:LYS:HD2	1.55	0.87
1:B:470:PHE:HZ	1:B:487:ILE:HD11	1.47	0.79
1:A:253:PHE:HZ	1:A:431:ILE:HD11	1.48	0.78
1:B:390:ALA:HB1	1:B:392:GLN:HE21	1.49	0.77
1:B:93:MET:HE3	1:B:108:ILE:HD13	1.67	0.76
1:A:76:VAL:HG11	1:A:93:MET:HG3	1.66	0.76
1:A:89:THR:HA	1:A:92:ASP:HB3	1.68	0.75
1:A:640:GLU:HB2	1:A:642:THR:HG22	1.70	0.74
1:B:316:VAL:HG23	1:B:337:VAL:HG11	1.69	0.73
1:A:56:PHE:HB2	1:A:57:PRO:CD	2.18	0.72
1:A:445:ILE:HD11	1:A:459:LEU:HD11	1.70	0.72
1:B:290:ILE:HD11	1:B:309:ILE:HD11	1.71	0.71
1:B:119:GLU:HG3	1:B:139:GLY:HA3	1.71	0.71
1:B:41:VAL:HG23	1:B:46:GLU:HG2	1.71	0.71
1:B:550:VAL:HG23	1:B:627:ILE:HB	1.75	0.69
1:B:191:MET:HE1	1:B:216:VAL:HG12	1.75	0.68
1:B:56:PHE:CD1	1:B:57:PRO:HD2	2.30	0.67
1:B:634:PHE:HD2	1:B:668:THR:HG23	1.61	0.65
1:B:20:THR:HG21	1:B:106:LYS:HE3	1.77	0.65
1:B:191:MET:HE2	1:B:221:HIS:CB	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLY:HA2	1:A:355:ALA:HB2	1.79	0.64
1:B:390:ALA:CB	1:B:392:GLN:HE21	2.10	0.64
1:B:392:GLN:HG3	1:B:397:MET:SD	2.36	0.64
1:B:470:PHE:CZ	1:B:487:ILE:HD11	2.31	0.64
1:A:470:PHE:HZ	1:A:487:ILE:HD11	1.61	0.64
1:B:309:ILE:HG22	1:B:311:GLY:H	1.63	0.64
1:A:240:SER:H	1:A:468[B]:ARG:HD2	1.63	0.64
1:B:550:VAL:HG21	1:B:629:MET:HE2	1.78	0.63
1:A:470:PHE:CZ	1:A:487:ILE:HD11	2.34	0.63
1:B:58:LEU:HD21	1:B:110:LEU:HD12	1.81	0.63
1:A:445:ILE:HG22	1:A:477:VAL:HG21	1.81	0.62
1:A:59:VAL:HG23	1:A:111:GLU:HB2	1.81	0.62
1:B:275:LEU:HD23	1:B:297:ILE:HG21	1.80	0.62
1:A:62:VAL:HG12	1:A:64:SER:H	1.63	0.62
1:B:136:VAL:HG12	1:B:164:MET:HE2	1.80	0.62
1:A:440:ASP:O	1:A:444:MET:HG3	2.00	0.61
1:B:659:LEU:HD21	1:B:696:LEU:HD12	1.81	0.61
1:B:191:MET:HE2	1:B:221:HIS:CG	2.35	0.61
1:A:456:VAL:HG13	1:A:484:PRO:HG2	1.83	0.60
1:A:350:LEU:HD11	1:A:354:ARG:HB2	1.84	0.59
1:A:57:PRO:HB2	1:A:113:MET:HB3	1.84	0.59
1:B:121:ILE:HD13	1:B:135:MET:HE3	1.85	0.59
1:A:554:SER:HB2	1:A:631:TRP:HB3	1.84	0.59
1:B:196:GLY:O	1:B:200:VAL:HG23	2.04	0.58
1:B:183:ILE:HA	1:B:218:PRO:HA	1.86	0.58
1:B:267:PRO:HA	1:B:272:ASN:ND2	2.19	0.58
1:A:112:LYS:O	1:A:112:LYS:HG2	2.04	0.57
1:A:137:GLY:HA3	1:A:149:VAL:HG12	1.86	0.57
1:B:55:GLY:O	1:B:112:LYS:HE2	2.05	0.57
1:B:191:MET:HE2	1:B:221:HIS:HB2	1.86	0.57
1:B:554:SER:HB3	1:B:631:TRP:HB3	1.87	0.56
1:B:620:MET:HA	1:B:656:LYS:HD2	1.86	0.56
1:A:95:GLY:O	1:A:99:LYS:HG3	2.06	0.56
1:A:606:GLY:HA2	1:A:638:PRO:HG2	1.88	0.56
1:A:405:VAL:HG22	1:A:456:VAL:HB	1.88	0.56
1:A:622:GLU:HG2	1:A:625:ILE:HD13	1.87	0.56
1:A:183:ILE:HA	1:A:218:PRO:HA	1.88	0.55
1:A:548:ASN:HB3	1:A:697:HIS:CE1	2.42	0.55
1:A:77:LYS:O	1:A:78:VAL:HG23	2.07	0.55
1:A:442:ALA:HB2	1:A:470:PHE:HA	1.89	0.55
1:A:270:ILE:O	1:A:274:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:PHE:O	1:B:618:GLN:HG2	2.08	0.54
1:A:341:VAL:HG21	1:A:380:MET:HE1	1.90	0.54
1:B:567:LEU:HD22	1:B:572:LEU:HB2	1.90	0.54
1:A:474:ALA:O	1:A:478:MET:HG3	2.08	0.53
1:A:122:VAL:HG11	1:A:195:ILE:HD12	1.90	0.53
1:A:214:VAL:HG22	1:A:223:VAL:HG13	1.90	0.53
1:B:64:SER:HB3	1:B:67:ILE:HG12	1.90	0.53
1:A:142:MET:O	1:A:146:MET:HG3	2.09	0.53
1:A:56:PHE:CB	1:A:57:PRO:HD3	2.27	0.53
1:B:297:ILE:HG22	1:B:298:PHE:H	1.74	0.53
1:B:552:MET:HE3	1:B:629:MET:HE3	1.91	0.53
1:B:477:VAL:HG21	1:B:485:ILE:HD11	1.91	0.53
1:A:378:ILE:HG21	1:A:416:ILE:HD11	1.91	0.53
1:B:97:LEU:HA	1:B:100:LYS:HG3	1.90	0.53
1:A:154:LEU:HD23	1:A:156:ILE:HG23	1.90	0.53
1:A:442:ALA:HB3	1:A:469:LYS:HE2	1.90	0.52
1:B:37:PRO:HG2	1:B:112:LYS:HD3	1.89	0.52
1:B:456:VAL:HG13	1:B:484:PRO:HG2	1.91	0.52
1:B:326:PRO:O	1:B:330:GLU:HG2	2.09	0.52
1:A:281:TYR:CZ	1:A:394:GLN:HG3	2.44	0.52
1:B:473:VAL:O	1:B:477:VAL:HG13	2.10	0.52
1:A:138:MET:HE3	1:A:170:GLY:C	2.35	0.51
1:B:214:VAL:HG22	1:B:223:VAL:HG13	1.92	0.51
1:B:675:ILE:HG22	1:B:680:VAL:HB	1.93	0.51
1:A:191:MET:O	1:A:195:ILE:HG13	2.11	0.51
1:B:206:ILE:HD13	1:B:209:ILE:HD11	1.93	0.51
1:B:275:LEU:CD2	1:B:297:ILE:HG21	2.40	0.51
1:B:564:ILE:HD11	1:B:600:PRO:HG2	1.92	0.51
1:A:448:ALA:HB1	1:A:454:THR:HG21	1.93	0.51
1:A:627:ILE:HG23	1:A:657:PRO:HB2	1.93	0.51
1:A:544:ALA:HB2	1:A:699:TRP:CD1	2.46	0.51
1:A:390:ALA:HB1	1:A:392:GLN:OE1	2.11	0.51
1:A:37:PRO:HG2	1:A:112:LYS:HD2	1.92	0.50
1:A:625:ILE:O	1:A:656:LYS:HE3	2.11	0.50
1:B:37:PRO:HB2	1:B:54:ILE:HG12	1.94	0.50
1:B:598:GLY:O	1:B:601:ALA:HB2	2.11	0.50
1:A:161:ALA:HA	1:A:164:MET:HE2	1.93	0.50
1:A:51:ALA:N	1:A:87:LYS:HZ3	2.09	0.50
1:A:213:PRO:HD3	2:A:801:ANP:H5'2	1.93	0.50
1:B:41:VAL:HG12	1:B:108:ILE:O	2.12	0.50
1:A:622:GLU:HG3	1:A:624:ASN:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ILE:HG23	1:A:682:VAL:HB	1.93	0.50
1:A:16:HIS:H	1:A:16:HIS:CD2	2.29	0.50
1:A:51:ALA:HB3	1:A:90:PHE:HE2	1.76	0.50
1:A:634:PHE:HD2	1:A:668:THR:HG23	1.77	0.50
1:A:290:ILE:HD11	1:A:309:ILE:HD11	1.94	0.49
1:B:408:PHE:HB3	1:B:444:MET:HE3	1.94	0.49
1:A:59:VAL:HG12	1:A:77:LYS:HA	1.94	0.49
1:B:386:ARG:NH2	1:B:401:LYS:HA	2.27	0.49
1:B:154:LEU:HB3	1:B:200:VAL:HG22	1.95	0.49
1:A:620:MET:HA	1:A:656:LYS:HD2	1.95	0.49
1:B:410:GLN:HG2	1:B:504:THR:HG21	1.95	0.49
1:B:581:LEU:HD12	1:B:622:GLU:HB2	1.93	0.49
1:A:88:LYS:HD3	1:A:89:THR:OG1	2.13	0.49
1:A:501:ALA:HB2	1:A:507:LEU:HD23	1.95	0.49
1:A:106:LYS:HG2	1:A:107:GLY:H	1.78	0.48
1:A:209:ILE:HG23	1:A:228:ILE:HG22	1.95	0.48
1:A:38:TYR:HA	1:A:110:LEU:O	2.13	0.48
1:B:28[B]:LEU:HG	1:B:33:VAL:CG2	2.43	0.48
1:A:94:TYR:HD1	1:A:108:ILE:HG13	1.78	0.48
1:A:263:ALA:HB1	1:A:275:LEU:HD22	1.95	0.48
1:B:379:GLY:HA3	1:B:389:CYS:SG	2.54	0.48
1:A:318:VAL:HG13	1:A:320:VAL:HG12	1.95	0.48
1:A:139:GLY:HA2	1:A:143:THR:HG23	1.95	0.48
1:A:113:MET:HA	2:A:801:ANP:N1	2.29	0.48
1:A:574:ILE:O	1:A:574:ILE:HD12	2.13	0.48
1:A:89:THR:HG22	1:A:93:MET:HG2	1.96	0.47
1:A:253:PHE:CZ	1:A:431:ILE:HD11	2.37	0.47
1:A:392:GLN:HG3	1:B:636:ASP:HA	1.96	0.47
1:A:392:GLN:HB2	1:A:397:MET:HE3	1.95	0.47
1:B:433:PHE:CD1	1:B:444:MET:HE1	2.48	0.47
1:B:626:ASP:O	1:B:657:PRO:HD2	2.14	0.47
1:A:626:ASP:O	1:A:657:PRO:HD2	2.14	0.47
1:B:441:GLU:HA	1:B:444:MET:HE2	1.97	0.47
1:A:281:TYR:CE1	1:A:394:GLN:HG3	2.50	0.47
1:B:414:MET:HE3	1:B:488:TRP:CZ3	2.49	0.47
1:A:537:LYS:HE3	1:A:681:PRO:HB3	1.96	0.47
1:B:390:ALA:HB1	1:B:392:GLN:HG2	1.96	0.47
1:A:657:PRO:HB3	1:A:696:LEU:HD13	1.95	0.47
1:B:62:VAL:HG12	1:B:70:LYS:HG3	1.96	0.47
1:B:261:VAL:HA	1:B:290:ILE:HB	1.96	0.47
1:A:396:ARG:HB3	1:B:635:GLN:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:GLY:O	1:A:684:GLN:HG2	2.15	0.47
1:A:335:LYS:HG3	1:A:337:VAL:HG23	1.98	0.46
1:B:17:LYS:HE2	1:B:232:LYS:HA	1.98	0.46
1:B:121:ILE:CD1	1:B:135:MET:HE3	2.46	0.46
1:B:442:ALA:HB2	1:B:470:PHE:HA	1.97	0.46
1:A:60:MET:HG2	1:A:110:LEU:HD23	1.97	0.46
1:A:478:MET:HE3	1:A:484:PRO:HA	1.97	0.46
1:A:240:SER:H	1:A:468[A]:ARG:HD2	1.81	0.46
1:A:551:ALA:HB2	1:A:625:ILE:HG12	1.97	0.46
1:A:53:LYS:HG3	1:A:58:LEU:HD13	1.96	0.46
1:B:606:GLY:HA2	1:B:638:PRO:HG2	1.98	0.46
1:B:60:MET:HA	1:B:109:LEU:O	2.16	0.46
1:B:551:ALA:HB2	1:B:625:ILE:HG12	1.97	0.46
1:A:588:ARG:HD2	1:A:614:PHE:CD2	2.50	0.46
1:A:667:TYR:CG	1:B:396:ARG:HA	2.51	0.46
1:B:56:PHE:O	1:B:57:PRO:C	2.59	0.46
1:B:57:PRO:HB2	1:B:113:MET:HE2	1.98	0.46
1:B:419:LEU:HD21	1:B:430:MET:SD	2.56	0.46
1:A:93:MET:HE3	1:A:93:MET:HA	1.96	0.46
1:B:569:LYS:HE2	1:B:570:PHE:CZ	2.51	0.46
1:A:418:MET:HE2	1:A:418:MET:HB2	1.79	0.45
1:A:27:ILE:HG22	1:A:198:LEU:HD21	1.96	0.45
1:B:37:PRO:HG2	1:B:112:LYS:CD	2.47	0.45
1:B:184:ASP:OD1	1:B:186:ASN:HB2	2.16	0.45
1:B:214:VAL:HG13	1:B:223:VAL:HG22	1.98	0.45
1:A:58:LEU:HD11	1:A:110:LEU:HD22	1.98	0.45
1:A:335:LYS:HE2	1:A:335:LYS:HA	1.97	0.45
1:B:360:GLU:O	1:B:364:LEU:HD12	2.17	0.45
1:B:433:PHE:CE1	1:B:444:MET:HE1	2.52	0.45
1:B:622:GLU:HG2	1:B:625:ILE:HD13	1.97	0.45
1:A:670:LYS:HA	1:A:670:LYS:HE2	1.98	0.45
1:A:144:GLU:O	1:A:147:LYS:HG3	2.17	0.45
1:B:20:THR:OG1	1:B:63:VAL:HG13	2.17	0.45
1:A:329:LEU:CD2	1:A:372:ILE:HD11	2.47	0.45
1:B:358:GLU:O	1:B:361:VAL:HG22	2.17	0.44
1:A:18:VAL:HG22	1:A:229:ILE:HG13	1.99	0.44
1:A:58:LEU:HD21	1:A:110:LEU:HD23	2.00	0.44
1:B:14:THR:O	1:B:17:LYS:HG3	2.17	0.44
1:A:515:MET:HE3	1:A:515:MET:HB3	1.75	0.44
1:B:53:LYS:O	1:B:54:ILE:HB	2.16	0.44
1:B:123:GLY:HA3	1:B:135:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:PHE:CD1	1:B:513:ILE:HG12	2.52	0.44
1:A:191:MET:HE2	1:A:195:ILE:HD11	1.99	0.44
1:A:549:LYS:HA	1:A:573:ALA:O	2.17	0.44
1:B:492:ARG:HG2	1:B:511:ASN:OD1	2.18	0.44
1:A:482:LYS:HD3	1:A:482:LYS:HA	1.74	0.44
1:A:499:GLN:HG3	1:B:564:ILE:HD13	2.00	0.44
1:A:598:GLY:O	1:A:601:ALA:HB2	2.17	0.44
1:B:64:SER:HB3	1:B:67:ILE:CG1	2.47	0.44
1:B:673:LYS:O	1:B:677:LYS:HG2	2.18	0.44
1:A:257:SER:OG	1:A:313:VAL:HA	2.17	0.43
1:A:326:PRO:HB2	1:A:327:PRO:HD3	2.00	0.43
1:A:407:PHE:CE2	1:A:409:SER:HB2	2.53	0.43
1:B:122:VAL:HG11	1:B:195:ILE:HG21	2.00	0.43
1:B:660:CYS:HB2	1:B:682:VAL:HG22	2.00	0.43
1:B:79:GLY:O	1:B:80:LEU:HD23	2.17	0.43
1:B:623:LYS:HB2	1:B:623:LYS:HE2	1.87	0.43
1:B:545:ALA:HB3	1:B:697:HIS:HA	1.99	0.43
1:A:673:LYS:O	1:A:677:LYS:HD3	2.18	0.43
1:B:448:ALA:HB1	1:B:454:THR:HG21	1.99	0.43
1:A:130:PHE:HA	1:A:468[B]:ARG:HG3	2.00	0.43
1:A:528:SER:HB3	1:A:531:GLU:HG3	2.00	0.43
1:A:634:PHE:CD2	1:A:668:THR:HG23	2.54	0.43
1:A:28:LEU:HD21	1:A:211:PHE:CZ	2.54	0.43
1:A:134:ILE:HG21	1:A:156:ILE:HD13	2.01	0.43
1:A:316:VAL:O	1:A:340:VAL:HA	2.18	0.43
1:A:585:MET:HA	1:A:614:PHE:HZ	1.84	0.43
1:B:477:VAL:CG2	1:B:485:ILE:HD11	2.48	0.43
1:B:551:ALA:HA	1:B:599:ASN:HD21	1.82	0.43
1:A:124:ILE:HB	1:A:209:ILE:HB	2.01	0.43
1:A:333:ALA:HB2	1:A:368:HIS:CG	2.54	0.43
1:B:90:PHE:CD1	1:B:90:PHE:C	2.97	0.43
1:B:253:PHE:CZ	1:B:431:ILE:HD11	2.54	0.43
1:B:318:VAL:HG13	1:B:320:VAL:HG22	2.00	0.43
1:B:189:ALA:O	1:B:193:VAL:HG23	2.19	0.43
1:B:489:LYS:HE3	1:B:514:ILE:HD13	2.00	0.43
1:B:538:ALA:HB2	1:B:692:ALA:HB1	2.00	0.43
1:A:213:PRO:O	1:A:224:VAL:HG22	2.18	0.42
1:B:181:GLU:H	1:B:181:GLU:HG2	1.62	0.42
1:B:440:ASP:O	1:B:444:MET:HG3	2.19	0.42
1:A:445:ILE:HD12	1:A:470:PHE:HE1	1.83	0.42
1:B:253:PHE:HZ	1:B:431:ILE:HD11	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ASP:O	1:A:164:MET:HG3	2.18	0.42
1:B:253:PHE:CD1	1:B:429:LYS:HG2	2.54	0.42
1:B:554:SER:CB	1:B:631:TRP:HB3	2.49	0.42
1:A:109:LEU:HD23	1:A:109:LEU:HA	1.84	0.42
1:B:585:MET:HA	1:B:614:PHE:HE2	1.84	0.42
1:A:260:LEU:HG	1:A:263:ALA:HB2	2.02	0.42
1:A:546:LYS:HZ1	1:A:623:LYS:HD3	1.85	0.42
1:A:152:ARG:HG2	1:A:164:MET:SD	2.59	0.42
1:A:622:GLU:C	1:A:624:ASN:H	2.27	0.42
1:A:104:ASN:CG	1:A:105:VAL:H	2.28	0.42
1:A:341:VAL:HG22	1:A:373:ILE:HB	2.00	0.42
1:A:660:CYS:HB2	1:A:682:VAL:HG22	2.02	0.42
1:B:494:ALA:O	1:B:498:LYS:HG3	2.19	0.42
1:B:653:LYS:HB3	1:B:653:LYS:HE3	1.77	0.42
1:B:372:ILE:H	1:B:438:ASP:HB3	1.84	0.42
1:A:258:VAL:HA	1:A:315:LEU:O	2.20	0.42
1:B:631:TRP:CE3	1:B:661:GLY:HA3	2.55	0.42
1:A:170:GLY:C	1:A:172:LYS:N	2.78	0.41
1:A:445:ILE:CG2	1:A:477:VAL:HG21	2.49	0.41
1:B:560:MET:HE3	1:B:600:PRO:HB2	2.02	0.41
1:A:411:SER:HB3	1:A:460:TYR:CE1	2.54	0.41
1:A:551:ALA:HB2	1:A:625:ILE:CG1	2.50	0.41
1:B:3:ALA:O	1:B:7:ILE:HD12	2.20	0.41
1:B:38:TYR:HA	1:B:110:LEU:O	2.20	0.41
1:B:274:ILE:HG23	1:B:389:CYS:C	2.45	0.41
1:A:445:ILE:HD12	1:A:470:PHE:CE1	2.56	0.41
1:A:11:ILE:HG21	1:A:19:ILE:HG12	2.01	0.41
1:A:70:LYS:H	1:A:70:LYS:HG2	1.59	0.41
1:B:429:LYS:HD3	1:B:447:TYR:HE1	1.85	0.41
1:A:4:VAL:HG11	1:A:31:TYR:HE1	1.86	0.41
1:A:290:ILE:HG12	1:A:306:VAL:HG12	2.03	0.41
1:B:147:LYS:CG	1:B:147:LYS:O	2.69	0.41
1:A:60:MET:HE1	1:A:93:MET:HB2	2.02	0.41
1:A:96:ARG:HA	1:A:99:LYS:HD2	2.02	0.41
1:A:348:LYS:HB3	1:A:358:GLU:HG2	2.01	0.41
1:B:501:ALA:HB2	1:B:507:LEU:HA	2.02	0.41
1:A:73:VAL:HB	1:A:74:GLY:H	1.79	0.41
1:A:154:LEU:HD23	1:A:154:LEU:HA	1.93	0.41
1:B:41:VAL:HG21	1:B:47:ALA:CA	2.51	0.41
1:B:77:LYS:HG3	1:B:80:LEU:HD21	2.03	0.41
1:A:53:LYS:C	1:A:54:ILE:HG13	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:HG13	1:A:212:ASN:HB2	2.02	0.41
1:A:269:LYS:NZ	6:A:904:HOH:O	2.53	0.41
1:A:338:HIS:HA	1:A:370:ILE:HG23	2.02	0.41
1:A:672:ILE:HG12	1:A:682:VAL:HG11	2.03	0.41
1:B:488:TRP:CZ3	1:B:529:TYR:HB2	2.56	0.41
1:A:492:ARG:HG2	1:A:511:ASN:OD1	2.21	0.40
1:B:560:MET:O	1:B:564:ILE:HG13	2.21	0.40
1:A:191:MET:HG3	1:A:192:LEU:N	2.36	0.40
1:A:341:VAL:HG21	1:A:380:MET:CE	2.51	0.40
1:B:58:LEU:HD21	1:B:110:LEU:CD1	2.50	0.40
1:B:28[B]:LEU:HD23	1:B:35:VAL:HG12	2.02	0.40
1:B:387:LEU:HD12	1:B:388:ASP:N	2.36	0.40
1:A:58:LEU:HD11	1:A:110:LEU:CD2	2.51	0.40
1:A:85:ASP:HB2	1:A:88:LYS:HB3	2.03	0.40
1:A:279:VAL:HG12	1:A:287:VAL:HB	2.03	0.40
1:A:488:TRP:CZ3	1:A:529:TYR:HB2	2.57	0.40
1:B:232:LYS:HA	1:B:232:LYS:HD2	1.87	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	684/705 (97%)	673 (98%)	9 (1%)	2 (0%)	36	66
1	B	703/705 (100%)	685 (97%)	15 (2%)	3 (0%)	30	60
All	All	1387/1410 (98%)	1358 (98%)	24 (2%)	5 (0%)	30	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	VAL

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Mol	Chain	Res	Type
1	B	178	ARG
1	A	71	THR
1	B	54	ILE
1	B	313	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	569/577 (99%)	566 (100%)	3 (0%)	81	93
1	B	577/577 (100%)	573 (99%)	4 (1%)	76	91
All	All	1146/1154 (99%)	1139 (99%)	7 (1%)	78	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	LYS
1	A	445	ILE
1	A	555	ASN
1	B	19	ILE
1	B	76	VAL
1	B	172	LYS
1	B	386	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	166	ASN
1	A	338	HIS
1	A	697	HIS
1	B	186	ASN
1	B	202	ASN
1	B	272	ASN

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Mol	Chain	Res	Type
1	B	392	GLN
1	B	624	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 1 is 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	3OH	A	802[A]	-	5,5,5	23.80	4 (80%)	5,5,5	30.02	5 (100%)
3	3OH	B	801[A]	-	5,5,5	23.71	4 (80%)	5,5,5	28.54	4 (80%)
3	3OH	A	802[B]	-	5,5,5	23.93	4 (80%)	5,5,5	28.61	4 (80%)
4	PO4	B	802	-	4,4,4	1.50	1 (25%)	6,6,6	0.39	0
2	ANP	A	801	-	33,33,33	1.09	5 (15%)	45,52,52	0.97	4 (8%)
4	PO4	A	803	-	4,4,4	1.44	1 (25%)	6,6,6	0.54	0
3	3OH	B	801[B]	-	5,5,5	23.87	4 (80%)	5,5,5	28.69	5 (100%)

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	3OH	A	802[A]	-	-	3/3/3/3	-
3	3OH	B	801[A]	-	-	3/3/3/3	-
3	3OH	A	802[B]	-	-	3/3/3/3	-
2	ANP	A	801	-	-	8/18/38/38	0/3/3/3
3	3OH	B	801[B]	-	-	2/3/3/3	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802[B]	3OH	O1-C1	36.16	2.40	1.22
3	B	801[B]	3OH	O1-C1	36.06	2.39	1.22
3	A	802[A]	3OH	O1-C1	36.04	2.39	1.22
3	B	801[A]	3OH	O1-C1	35.57	2.38	1.22
3	A	802[B]	3OH	O2-C1	33.64	2.42	1.30
3	B	801[A]	3OH	O2-C1	33.61	2.41	1.30
3	B	801[B]	3OH	O2-C1	33.58	2.41	1.30
3	A	802[A]	3OH	O2-C1	33.52	2.41	1.30
3	A	802[B]	3OH	C2-C3	20.34	2.50	1.51
3	B	801[B]	3OH	C2-C3	20.25	2.50	1.51
3	B	801[A]	3OH	C2-C3	20.14	2.49	1.51
3	A	802[A]	3OH	C2-C3	19.96	2.49	1.51
3	B	801[B]	3OH	O3-C3	-3.10	1.26	1.42
3	B	801[A]	3OH	O3-C3	-3.10	1.26	1.42
3	A	802[B]	3OH	O3-C3	-3.09	1.26	1.42
3	A	802[A]	3OH	O3-C3	-3.08	1.26	1.42
2	A	801	ANP	PB-O1B	2.96	1.50	1.46
2	A	801	ANP	PG-O1G	2.81	1.50	1.46
4	B	802	PO4	P-O1	2.70	1.56	1.50
4	A	803	PO4	P-O1	2.48	1.56	1.50
2	A	801	ANP	PG-O2G	-2.33	1.50	1.56
2	A	801	ANP	PB-O2B	-2.33	1.50	1.56
2	A	801	ANP	PG-O3G	-2.22	1.50	1.56

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802[B]	3OH	C3-C2-C1	-56.94	34.96	113.11
3	B	801[B]	3OH	C3-C2-C1	-56.91	34.99	113.11
3	B	801[A]	3OH	C3-C2-C1	-56.80	35.14	113.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802[A]	3OH	C3-C2-C1	-56.57	35.46	113.11
3	A	802[B]	3OH	O1-C1-C2	-28.28	33.38	123.09
3	B	801[B]	3OH	O1-C1-C2	-28.27	33.43	123.09
3	A	802[A]	3OH	O1-C1-C2	-28.25	33.49	123.09
3	B	801[A]	3OH	O1-C1-C2	-28.14	33.84	123.09
3	A	802[A]	3OH	O2-C1-O1	-16.29	81.43	123.33
3	A	802[A]	3OH	O3-C3-C2	11.82	155.26	110.96
3	A	802[A]	3OH	O2-C1-C2	-10.06	82.22	114.00
3	B	801[B]	3OH	O2-C1-C2	-5.78	95.75	114.00
3	B	801[B]	3OH	O3-C3-C2	5.21	130.50	110.96
3	B	801[A]	3OH	O3-C3-C2	-5.19	91.53	110.96
3	A	802[B]	3OH	O3-C3-C2	-5.13	91.72	110.96
3	A	802[B]	3OH	O2-C1-C2	4.90	129.47	114.00
3	B	801[A]	3OH	O2-C1-C2	4.73	128.96	114.00
3	B	801[B]	3OH	O2-C1-O1	-4.03	112.98	123.33
2	A	801	ANP	O2B-PB-O1B	3.80	118.02	109.87
2	A	801	ANP	O2G-PG-O1G	-2.53	107.10	113.45
2	A	801	ANP	O3A-PB-N3B	-2.45	99.79	106.59
2	A	801	ANP	O3G-PG-O1G	-2.29	107.70	113.45

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ANP	PB-N3B-PG-O1G
2	A	801	ANP	O4'-C4'-C5'-O5'
2	A	801	ANP	C3'-C4'-C5'-O5'
3	A	802[A]	3OH	C1-C2-C3-O3
3	A	802[B]	3OH	C1-C2-C3-O3
3	B	801[A]	3OH	C1-C2-C3-O3
2	A	801	ANP	PB-O3A-PA-O1A
3	A	802[B]	3OH	O1-C1-C2-C3
2	A	801	ANP	C4'-C5'-O5'-PA
3	B	801[A]	3OH	O1-C1-C2-C3
3	B	801[B]	3OH	O1-C1-C2-C3
3	A	802[A]	3OH	O1-C1-C2-C3
3	A	802[B]	3OH	O2-C1-C2-C3
3	B	801[A]	3OH	O2-C1-C2-C3
3	B	801[B]	3OH	O2-C1-C2-C3
2	A	801	ANP	PB-O3A-PA-O2A
2	A	801	ANP	PG-N3B-PB-O1B
2	A	801	ANP	PA-O3A-PB-O2B

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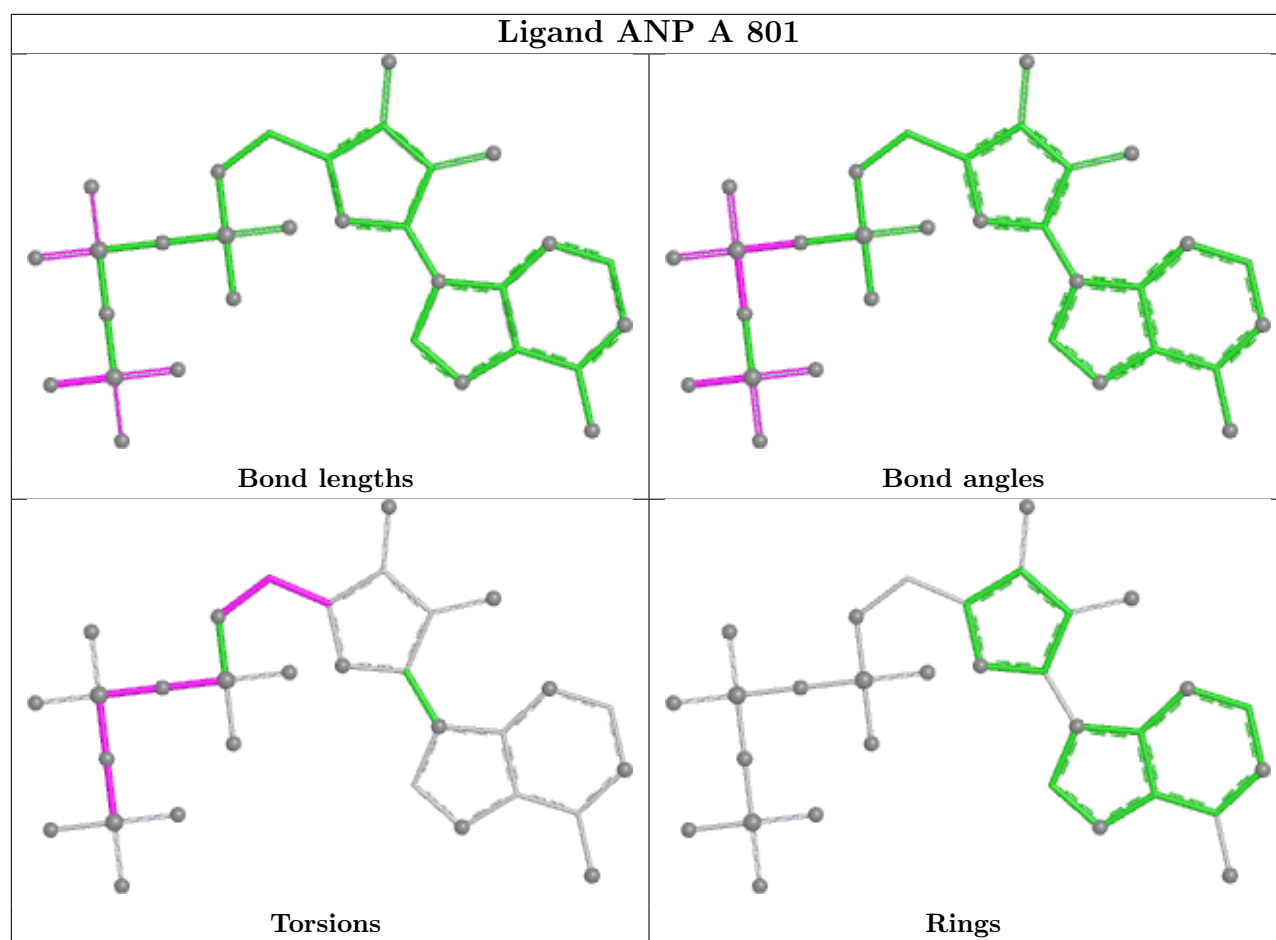
Mol	Chain	Res	Type	Atoms
3	A	802[A]	3OH	O2-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ANP	2	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	691/705 (98%)	0.06	5 (0%)	84 77	21, 52, 88, 123	1 (0%)
1	B	703/705 (99%)	-0.09	1 (0%)	92 90	18, 48, 74, 95	2 (0%)
All	All	1394/1410 (98%)	-0.02	6 (0%)	88 84	18, 50, 81, 123	3 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	VAL	2.5
1	B	60	MET	2.5
1	A	107	GLY	2.1
1	A	54	ILE	2.1
1	A	105	VAL	2.0
1	A	90	PHE	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](#)

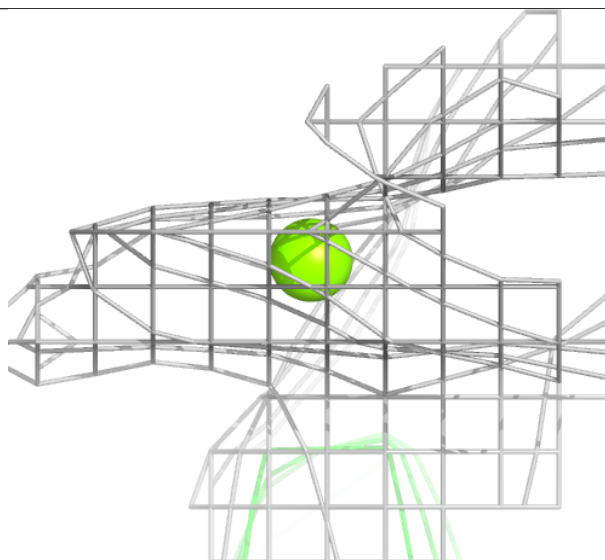
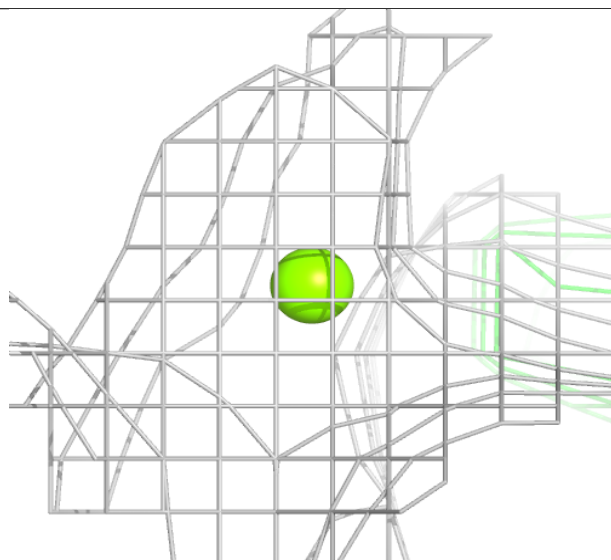
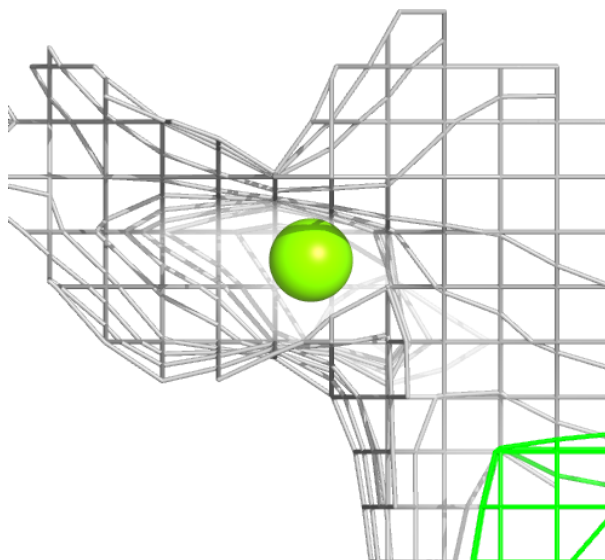
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

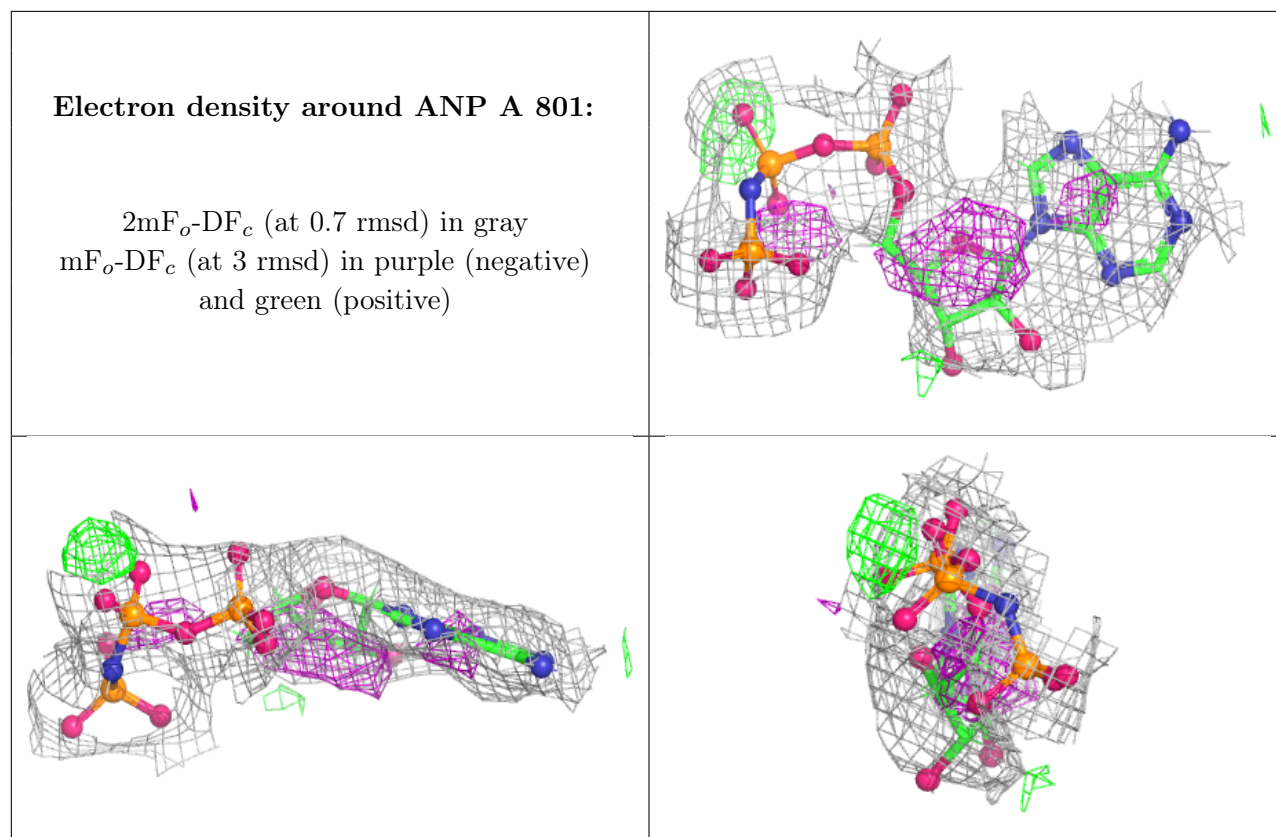
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	A	804	1/1	0.65	0.17	108,108,108,108	0
2	ANP	A	801	31/31	0.67	0.12	64,86,128,181	0
3	3OH	B	801[B]	6/6	0.88	0.12	39,41,44,44	6
3	3OH	B	801[A]	6/6	0.88	0.12	38,42,49,49	0
3	3OH	A	802[B]	6/6	0.93	0.09	55,57,58,60	6
3	3OH	A	802[A]	6/6	0.93	0.09	57,57,58,58	6
4	PO4	B	802	5/5	0.95	0.09	38,46,47,61	0
4	PO4	A	803	5/5	0.98	0.06	27,33,43,50	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 MG A 804:

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.