



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:47 PM UTC

PDB ID : 2Z3Y / pdb_00002z3y
Title : Crystal structure of Lysine-specific demethylase1
Authors : Mimasu, S.; Sengoku, T.; Umehara, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-06-08
Resolution : 2.25 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

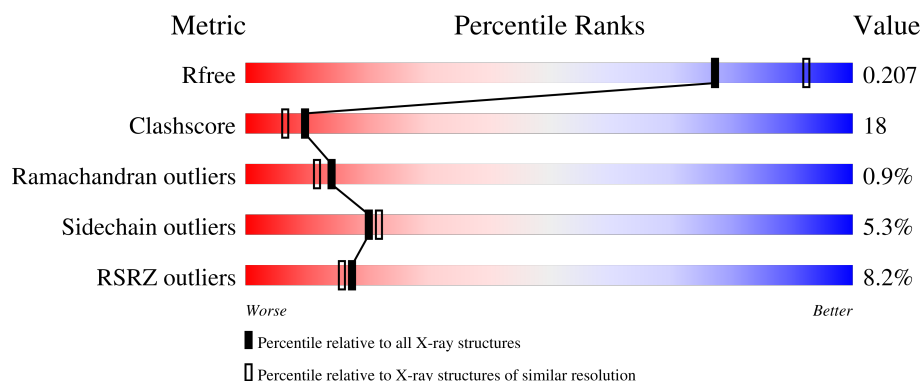
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	662	8% 67% 26% • •

2 Entry composition [i](#)

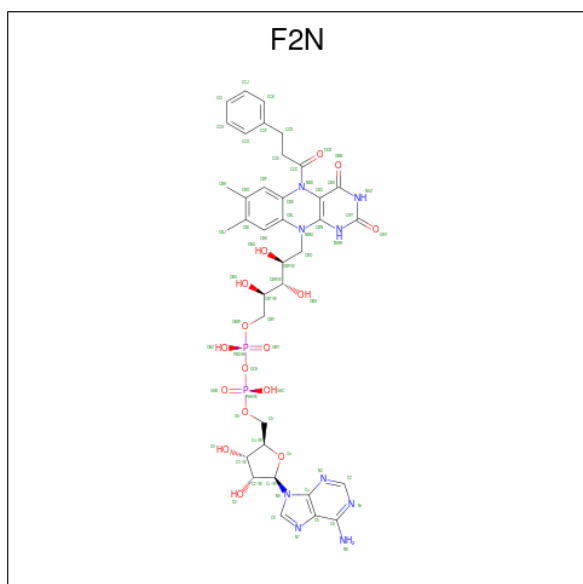
There are 3 unique types of molecules in this entry. The entry contains 5267 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysine-specific histone demethylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	643	5052	3218	878	937	19	0	0	0

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYL (2R,3S,4S)-5-[7,8-DIMETHYL-2,4-DIOXO-5-(3-PHENYLPROPANOYL)-1,3,4,5-TETRAHYDROBENZO[G]PTERIDIN-10(2H)-YL]-2,3,4-TRIHYDROXYPENTYL DIHYDROGEN DIPHOSPHATE (CCD ID: F2N) (formula: $C_{36}H_{43}N_9O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	63	36	9	16	2	0	0

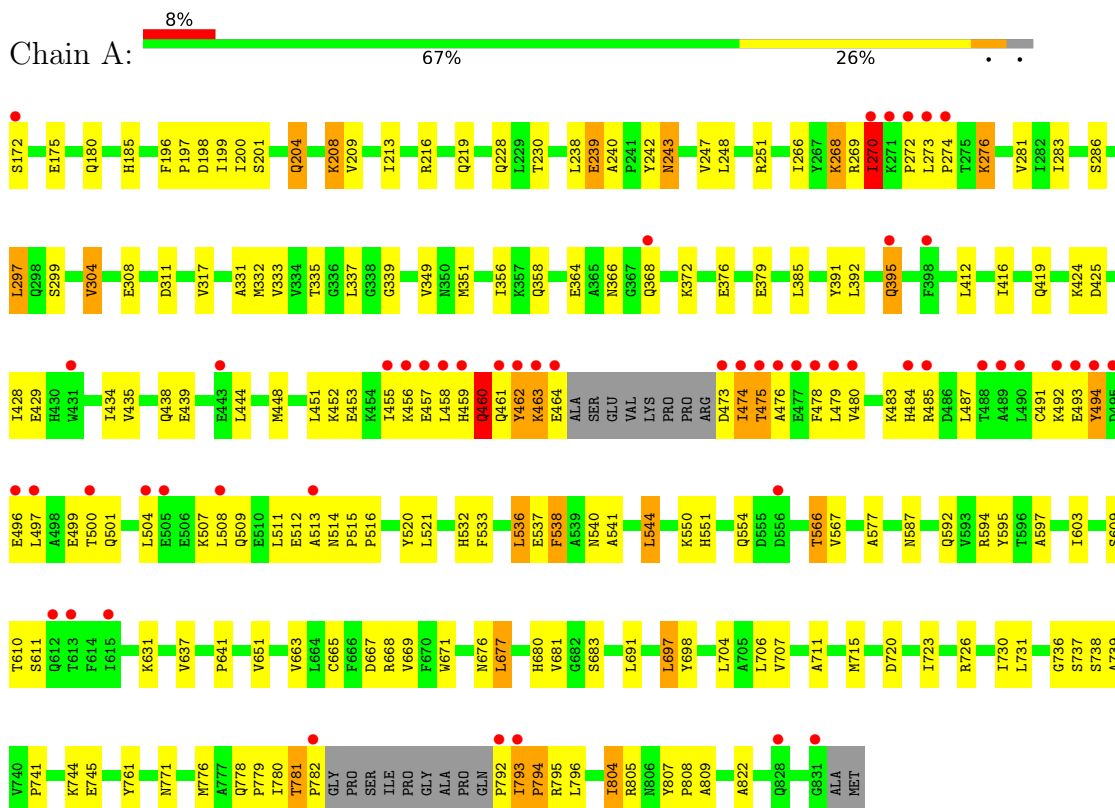
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total 152	O 152	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: Lysine-specific histone demethylase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	185.74Å 185.74Å 108.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.36 – 2.25 35.36 – 2.28	Depositor EDS
% Data completeness (in resolution range)	97.2 (35.36-2.25) 97.3 (35.36-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.255 0.219 , 0.207	Depositor DCC
R_{free} test set	2489 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.1	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	0.95	EDS
Total number of atoms	5267	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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: F2N

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	0.43	0/5157	0.96	16/6988 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	THR	N-CA-C	-9.96	101.13	113.18
1	A	781	THR	CA-C-N	-8.83	111.28	120.38
1	A	781	THR	C-N-CA	-8.83	111.28	120.38
1	A	335	THR	N-CA-C	8.57	124.86	113.20
1	A	492	LYS	N-CA-C	-8.26	103.19	113.18
1	A	805	ARG	N-CA-C	7.04	119.84	111.33
1	A	337	LEU	N-CA-C	6.79	119.69	111.82
1	A	491	CYS	N-CA-C	-6.79	105.56	114.31
1	A	474	ILE	N-CA-C	-6.71	105.57	113.42
1	A	270	ILE	N-CA-C	-6.43	103.94	113.39
1	A	698	TYR	N-CA-C	6.21	119.32	109.81
1	A	358	GLN	N-CA-C	6.18	118.09	111.36
1	A	460	GLN	N-CA-C	-5.90	98.23	110.80
1	A	335	THR	CB-CA-C	-5.61	104.26	111.22
1	A	317	VAL	N-CA-C	-5.58	98.93	106.85
1	A	550	LYS	N-CA-C	5.51	117.37	111.36

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	5052	0	5081	176	0
2	A	63	0	41	6	0
3	A	152	0	0	4	0
All	All	5267	0	5122	180	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 18.

All (180) 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:276:LYS:HD3	1:A:276:LYS:H	1.17	1.09
1:A:566:THR:HG21	1:A:697:LEU:HG	1.48	0.94
1:A:172:SER:HB2	1:A:175:GLU:HB3	1.53	0.91
1:A:792:PRO:HG2	1:A:793:ILE:HG22	1.56	0.87
1:A:668:ARG:HH21	1:A:741:PRO:HB3	1.39	0.85
1:A:715:MET:HE3	1:A:723:ILE:HD13	1.56	0.85
1:A:781:THR:HG22	1:A:794:PRO:HA	1.58	0.84
1:A:651:VAL:HG23	1:A:776:MET:HE1	1.61	0.82
1:A:537:GLU:HG2	1:A:544:LEU:HD13	1.61	0.80
1:A:270:ILE:H	1:A:270:ILE:HD13	1.47	0.80
1:A:230:THR:HG23	1:A:270:ILE:HD11	1.65	0.79
1:A:462:TYR:CD2	1:A:483:LYS:HB3	2.18	0.79
1:A:462:TYR:O	1:A:463:LYS:HB2	1.83	0.77
1:A:332:MET:HE1	1:A:704:LEU:HD12	1.66	0.76
1:A:460:GLN:O	1:A:461:GLN:HB3	1.84	0.76
1:A:458:LEU:C	1:A:460:GLN:H	1.94	0.76
1:A:476:ALA:HA	1:A:479:LEU:HB3	1.68	0.76
1:A:283:ILE:HD13	1:A:304:VAL:HG23	1.72	0.72
1:A:507:LYS:O	1:A:511:LEU:HD13	1.89	0.71
1:A:268:LYS:NZ	1:A:268:LYS:HB3	2.07	0.69
1:A:276:LYS:HD3	1:A:276:LYS:N	2.01	0.67
1:A:239:GLU:CD	1:A:239:GLU:H	2.02	0.67
2:A:1:F2N:HCD1	2:A:1:F2N:CBA	2.25	0.67
1:A:274:PRO:HB2	1:A:276:LYS:HE3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:MET:CE	1:A:723:ILE:HD13	2.25	0.66
1:A:464:GLU:C	1:A:473:ASP:HA	2.21	0.65
1:A:458:LEU:HD22	1:A:462:TYR:CE1	2.32	0.65
1:A:276:LYS:H	1:A:276:LYS:CD	1.99	0.64
1:A:273:LEU:HD21	1:A:299:SER:HA	1.78	0.64
1:A:711:ALA:O	1:A:715:MET:HG2	1.98	0.64
1:A:434:ILE:O	1:A:438:GLN:HG3	1.98	0.63
1:A:513:ALA:C	1:A:515:PRO:HD3	2.23	0.63
1:A:597:ALA:CB	1:A:792:PRO:HD3	2.28	0.63
1:A:228:GLN:OE1	1:A:270:ILE:HD13	1.98	0.63
1:A:458:LEU:HD22	1:A:462:TYR:CZ	2.34	0.63
1:A:487:LEU:O	1:A:487:LEU:HD23	1.99	0.63
1:A:592:GLN:NE2	1:A:594:ARG:HH11	1.96	0.62
1:A:208:LYS:HB2	1:A:208:LYS:NZ	2.14	0.62
1:A:230:THR:CG2	1:A:270:ILE:HD11	2.29	0.62
2:A:1:F2N:CBN	2:A:1:F2N:HCE2	2.19	0.61
1:A:243:ASN:HD22	1:A:243:ASN:N	1.97	0.61
1:A:266:ILE:HD12	1:A:349:VAL:HG12	1.82	0.61
1:A:781:THR:CG2	1:A:794:PRO:HA	2.29	0.61
1:A:726:ARG:O	1:A:730:ILE:HG12	2.01	0.61
1:A:311:ASP:HB3	1:A:587:ASN:HD21	1.66	0.60
1:A:458:LEU:C	1:A:460:GLN:N	2.55	0.60
1:A:500:THR:O	1:A:504:LEU:HD13	2.01	0.60
1:A:781:THR:HG21	1:A:794:PRO:HG3	1.84	0.59
1:A:474:ILE:HD12	1:A:475:THR:N	2.18	0.58
1:A:668:ARG:NH2	1:A:741:PRO:HB3	2.15	0.58
1:A:196:PHE:HB3	1:A:199:ILE:HD13	1.84	0.58
1:A:665:CYS:HB2	1:A:745:GLU:HB2	1.85	0.58
1:A:269:ARG:HH21	1:A:299:SER:HB2	1.68	0.58
1:A:663:VAL:HG22	1:A:704:LEU:CD2	2.33	0.58
1:A:452:LYS:HG2	1:A:494:TYR:HE2	1.69	0.57
1:A:434:ILE:HD11	1:A:511:LEU:HB3	1.87	0.57
1:A:537:GLU:CG	1:A:544:LEU:HD13	2.35	0.57
1:A:266:ILE:HD13	1:A:577:ALA:HB1	1.85	0.57
1:A:782:PRO:HG2	1:A:792:PRO:CD	2.35	0.57
1:A:197:PRO:HA	1:A:200:ILE:HG22	1.87	0.56
1:A:631:LYS:HE3	3:A:928:HOH:O	2.04	0.56
1:A:366:ASN:OD1	1:A:368:GLN:HG2	2.05	0.56
1:A:448:MET:HE3	1:A:497:LEU:CB	2.37	0.55
1:A:597:ALA:HB1	1:A:792:PRO:HG3	1.89	0.55
1:A:566:THR:HG22	3:A:902:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:O	1:A:272:PRO:HD3	2.07	0.55
1:A:175:GLU:HG3	1:A:185:HIS:CG	2.41	0.54
1:A:180:GLN:NE2	1:A:339:GLY:H	2.04	0.54
1:A:514:ASN:N	1:A:515:PRO:HD3	2.23	0.54
1:A:175:GLU:HG3	1:A:185:HIS:CD2	2.42	0.54
1:A:458:LEU:O	1:A:460:GLN:O	2.26	0.54
1:A:508:LEU:O	1:A:512:GLU:HG2	2.08	0.54
1:A:476:ALA:C	1:A:478:PHE:N	2.65	0.54
1:A:592:GLN:HE21	1:A:594:ARG:HD2	1.73	0.53
1:A:391:TYR:CE1	1:A:395:GLN:HG2	2.43	0.53
1:A:198:ASP:CG	1:A:199:ILE:HD12	2.33	0.53
1:A:297:LEU:HD13	1:A:822:ALA:HB1	1.89	0.53
1:A:680:HIS:CE1	1:A:730:ILE:HD12	2.43	0.53
2:A:1:F2N:CBA	2:A:1:F2N:CCE	2.83	0.53
1:A:804:ILE:O	1:A:804:ILE:HG23	2.10	0.52
1:A:609:SER:C	1:A:611:SER:H	2.17	0.52
1:A:372:LYS:O	1:A:376:GLU:HG3	2.09	0.52
1:A:448:MET:HE3	1:A:497:LEU:HB3	1.92	0.52
1:A:462:TYR:CZ	1:A:483:LYS:HD2	2.45	0.52
1:A:493:GLU:O	1:A:497:LEU:HD13	2.10	0.52
1:A:804:ILE:C	1:A:804:ILE:HD13	2.34	0.51
1:A:676:ASN:HB3	1:A:677:LEU:HD23	1.92	0.51
1:A:603:ILE:N	1:A:603:ILE:HD12	2.25	0.51
1:A:216:ARG:HE	1:A:219:GLN:HE21	1.59	0.50
1:A:474:ILE:HD12	1:A:474:ILE:C	2.35	0.50
1:A:707:VAL:HG11	1:A:715:MET:HG3	1.93	0.50
1:A:286:SER:HB2	1:A:308:GLU:HB2	1.94	0.50
1:A:435:VAL:O	1:A:439:GLU:HG3	2.12	0.49
1:A:509:GLN:HA	1:A:512:GLU:CG	2.42	0.49
1:A:715:MET:HB2	3:A:910:HOH:O	2.10	0.49
1:A:452:LYS:O	1:A:456:LYS:HG3	2.12	0.49
1:A:554:GLN:HG2	3:A:837:HOH:O	2.13	0.49
1:A:332:MET:HE1	1:A:704:LEU:CD1	2.41	0.49
1:A:412:LEU:O	1:A:416:ILE:HG12	2.12	0.49
1:A:476:ALA:HB1	1:A:480:VAL:HG23	1.95	0.49
1:A:459:HIS:CD2	1:A:487:LEU:HD11	2.49	0.48
1:A:780:ILE:HB	1:A:796:LEU:HB3	1.95	0.48
1:A:597:ALA:HA	1:A:792:PRO:CD	2.44	0.48
1:A:736:GLY:O	1:A:739:ALA:HB3	2.14	0.48
1:A:485:ARG:HH21	1:A:485:ARG:HG3	1.78	0.48
1:A:541:ALA:HB2	1:A:761:TYR:CZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LYS:C	1:A:464:GLU:HG3	2.40	0.47
1:A:462:TYR:CE1	1:A:483:LYS:HD2	2.49	0.47
1:A:669:VAL:HG13	1:A:671:TRP:CE2	2.50	0.47
1:A:452:LYS:HG2	1:A:494:TYR:CE2	2.48	0.47
1:A:597:ALA:HA	1:A:792:PRO:HD3	1.97	0.46
1:A:458:LEU:HB3	1:A:462:TYR:CE2	2.50	0.46
1:A:533:PHE:O	1:A:537:GLU:HG3	2.15	0.46
1:A:463:LYS:O	1:A:463:LYS:HG2	2.15	0.46
1:A:479:LEU:O	1:A:483:LYS:HG2	2.15	0.46
1:A:592:GLN:NE2	1:A:594:ARG:HD2	2.30	0.46
1:A:737:SER:C	1:A:739:ALA:H	2.24	0.46
1:A:720:ASP:O	1:A:723:ILE:HG22	2.15	0.46
2:A:1:F2N:CBA	2:A:1:F2N:CCD	2.93	0.46
1:A:180:GLN:HE22	1:A:339:GLY:H	1.64	0.46
1:A:243:ASN:N	1:A:243:ASN:ND2	2.64	0.46
1:A:457:GLU:C	1:A:458:LEU:HD23	2.41	0.46
1:A:496:GLU:OE2	1:A:496:GLU:HA	2.16	0.45
1:A:458:LEU:HD23	1:A:458:LEU:N	2.32	0.45
1:A:494:TYR:C	1:A:496:GLU:N	2.75	0.45
1:A:216:ARG:HE	1:A:219:GLN:NE2	2.15	0.45
1:A:458:LEU:HD13	1:A:462:TYR:CZ	2.52	0.45
1:A:332:MET:HG3	1:A:333:VAL:HG23	1.99	0.45
1:A:200:ILE:HG23	1:A:201:SER:N	2.31	0.45
1:A:667:ASP:OD2	1:A:668:ARG:HG3	2.17	0.44
1:A:209:VAL:O	1:A:213:ILE:HG12	2.18	0.44
1:A:520:TYR:CD2	1:A:521:LEU:HG	2.53	0.44
1:A:283:ILE:HD12	1:A:283:ILE:N	2.33	0.44
1:A:247:VAL:O	1:A:251:ARG:HG3	2.18	0.44
1:A:778:GLN:HA	1:A:779:PRO:HD3	1.90	0.44
1:A:476:ALA:C	1:A:478:PHE:H	2.25	0.43
1:A:592:GLN:HE22	1:A:594:ARG:HH11	1.66	0.43
1:A:609:SER:C	1:A:611:SER:N	2.76	0.43
1:A:425:ASP:O	1:A:429:GLU:HG3	2.19	0.43
1:A:761:TYR:CD2	1:A:809:ALA:HB1	2.53	0.43
1:A:499:GLU:C	1:A:501:GLN:H	2.27	0.43
1:A:737:SER:O	1:A:738:SER:CB	2.66	0.43
1:A:208:LYS:HB2	1:A:208:LYS:HZ2	1.83	0.43
1:A:379:GLU:HG3	1:A:532:HIS:CE1	2.53	0.43
1:A:676:ASN:CB	1:A:677:LEU:HD23	2.49	0.43
1:A:463:LYS:O	1:A:464:GLU:HG3	2.19	0.43
1:A:676:ASN:C	1:A:677:LEU:HD23	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LYS:O	1:A:428:ILE:HG12	2.19	0.42
1:A:691:LEU:HA	1:A:706:LEU:O	2.18	0.42
1:A:461:GLN:NE2	1:A:462:TYR:HE1	2.17	0.42
1:A:676:ASN:HD22	1:A:676:ASN:HA	1.67	0.42
1:A:204:GLN:HE21	1:A:204:GLN:HB2	1.56	0.42
1:A:240:ALA:HA	1:A:243:ASN:ND2	2.34	0.42
1:A:462:TYR:CE2	1:A:483:LYS:HD2	2.55	0.42
1:A:213:ILE:HD11	1:A:242:TYR:HB3	2.02	0.42
1:A:356:ILE:CG2	1:A:677:LEU:HD21	2.49	0.42
1:A:228:GLN:HE22	1:A:269:ARG:HH12	1.68	0.42
1:A:243:ASN:HD22	1:A:243:ASN:H	1.68	0.42
1:A:268:LYS:HB3	1:A:268:LYS:HZ2	1.80	0.42
1:A:494:TYR:C	1:A:496:GLU:H	2.28	0.42
1:A:515:PRO:HA	1:A:516:PRO:HD3	1.97	0.42
1:A:595:TYR:CZ	1:A:641:PRO:HD2	2.54	0.41
1:A:480:VAL:O	1:A:484:HIS:HB2	2.20	0.41
1:A:216:ARG:HG2	1:A:238:LEU:HD23	2.03	0.41
1:A:782:PRO:HG2	1:A:792:PRO:HD2	2.02	0.41
1:A:268:LYS:HB3	1:A:268:LYS:HZ3	1.85	0.41
1:A:351:MET:HE2	1:A:567:VAL:CG1	2.51	0.41
1:A:364:GLU:HA	1:A:681:VAL:HB	2.02	0.41
1:A:451:LEU:O	1:A:455:ILE:HG13	2.20	0.41
1:A:331:ALA:HA	2:A:1:F2N:CBC	2.52	0.40
1:A:597:ALA:CA	1:A:792:PRO:HD3	2.51	0.40
1:A:419:GLN:NE2	1:A:419:GLN:HA	2.36	0.40
1:A:538:PHE:CD1	1:A:538:PHE:C	3.00	0.40
1:A:551:HIS:O	1:A:554:GLN:HB2	2.21	0.40
1:A:453:GLU:O	1:A:457:GLU:HG3	2.21	0.40
1:A:511:LEU:C	1:A:513:ALA:H	2.30	0.40
1:A:536:LEU:HD22	1:A:540:ASN:ND2	2.36	0.40
1:A:331:ALA:HA	2:A:1:F2N:NBD	2.37	0.40
1:A:444:LEU:C	1:A:444:LEU:HD13	2.46	0.40
1:A:807:TYR:N	1:A:808:PRO:CD	2.84	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	637/662 (96%)	600 (94%)	31 (5%)	6 (1%)	14 12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	LYS
1	A	462	TYR
1	A	610	THR
1	A	395	GLN
1	A	460	GLN
1	A	494	TYR

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	548/562 (98%)	519 (95%)	29 (5%)	20 22

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	208	LYS
1	A	239	GLU
1	A	243	ASN
1	A	248	LEU

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Mol	Chain	Res	Type
1	A	268	LYS
1	A	270	ILE
1	A	276	LYS
1	A	281	VAL
1	A	297	LEU
1	A	304	VAL
1	A	385	LEU
1	A	392	LEU
1	A	460	GLN
1	A	536	LEU
1	A	538	PHE
1	A	544	LEU
1	A	566	THR
1	A	637	VAL
1	A	677	LEU
1	A	683	SER
1	A	697	LEU
1	A	731	LEU
1	A	744	LYS
1	A	771	ASN
1	A	793	ILE
1	A	794	PRO
1	A	795	ARG
1	A	804	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	185	HIS
1	A	191	GLN
1	A	204	GLN
1	A	205	GLN
1	A	207	GLN
1	A	219	GLN
1	A	243	ASN
1	A	259	HIS
1	A	296	GLN
1	A	350	ASN
1	A	368	GLN
1	A	395	GLN
1	A	410	GLN

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Mol	Chain	Res	Type
1	A	417	GLN
1	A	419	GLN
1	A	430	HIS
1	A	438	GLN
1	A	450	ASN
1	A	459	HIS
1	A	461	GLN
1	A	509	GLN
1	A	535	ASN
1	A	540	ASN
1	A	551	HIS
1	A	587	ASN
1	A	592	GLN
1	A	638	GLN
1	A	658	ASN
1	A	696	ASN
1	A	717	ASN
1	A	828	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	F2N	A	1	-	68,69,69	1.80	10 (14%)	90,104,104	1.90	18 (20%)

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	F2N	A	1	-	-	8/43/59/59	0/7/7/7

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	F2N	CBE-NBD	-6.44	1.34	1.42
2	A	1	F2N	OCB-CCC	6.35	1.36	1.23
2	A	1	F2N	CCE-CCC	-5.79	1.39	1.51
2	A	1	F2N	CCD-CCF	-4.23	1.39	1.51
2	A	1	F2N	CCC-NBD	-4.22	1.33	1.40
2	A	1	F2N	C5-N7	-3.02	1.33	1.39
2	A	1	F2N	CCD-CCE	-2.77	1.39	1.52
2	A	1	F2N	C8-N9	-2.31	1.33	1.37
2	A	1	F2N	CBC-NBD	-2.14	1.34	1.39
2	A	1	F2N	C4-N9	-2.08	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	F2N	CCD-CCE-CCC	8.86	122.41	112.33
2	A	1	F2N	CBC-CBA-NAZ	5.56	120.72	110.94
2	A	1	F2N	C5-C4-N3	-5.31	119.41	126.72
2	A	1	F2N	N3-C2-N1	-4.61	121.61	128.58
2	A	1	F2N	CBA-NAZ-CAY	-4.38	120.33	126.37
2	A	1	F2N	N3-C4-N9	3.70	133.47	127.17
2	A	1	F2N	CBE-NBD-CCC	-3.68	112.65	121.65
2	A	1	F2N	C2-N3-C4	3.60	120.61	111.83
2	A	1	F2N	OBB-CBA-CBC	-3.24	119.67	127.62
2	A	1	F2N	N9-C8-N7	-3.01	109.67	113.94
2	A	1	F2N	C4-C5-N7	-2.83	107.34	110.58
2	A	1	F2N	C5-N7-C8	2.78	107.82	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	F2N	CBF-CBE-NBD	-2.66	118.71	122.70
2	A	1	F2N	CBL-CBE-NBD	2.56	122.50	118.19
2	A	1	F2N	O4'-C1'-C2'	-2.33	101.62	106.62
2	A	1	F2N	NAW-CAY-NAZ	2.25	119.28	115.74
2	A	1	F2N	CBV-CBT-CBR	-2.25	107.97	112.22
2	A	1	F2N	C4-N9-C8	2.19	108.04	105.74

There are no chirality outliers.

All (8) torsion outliers are listed below:

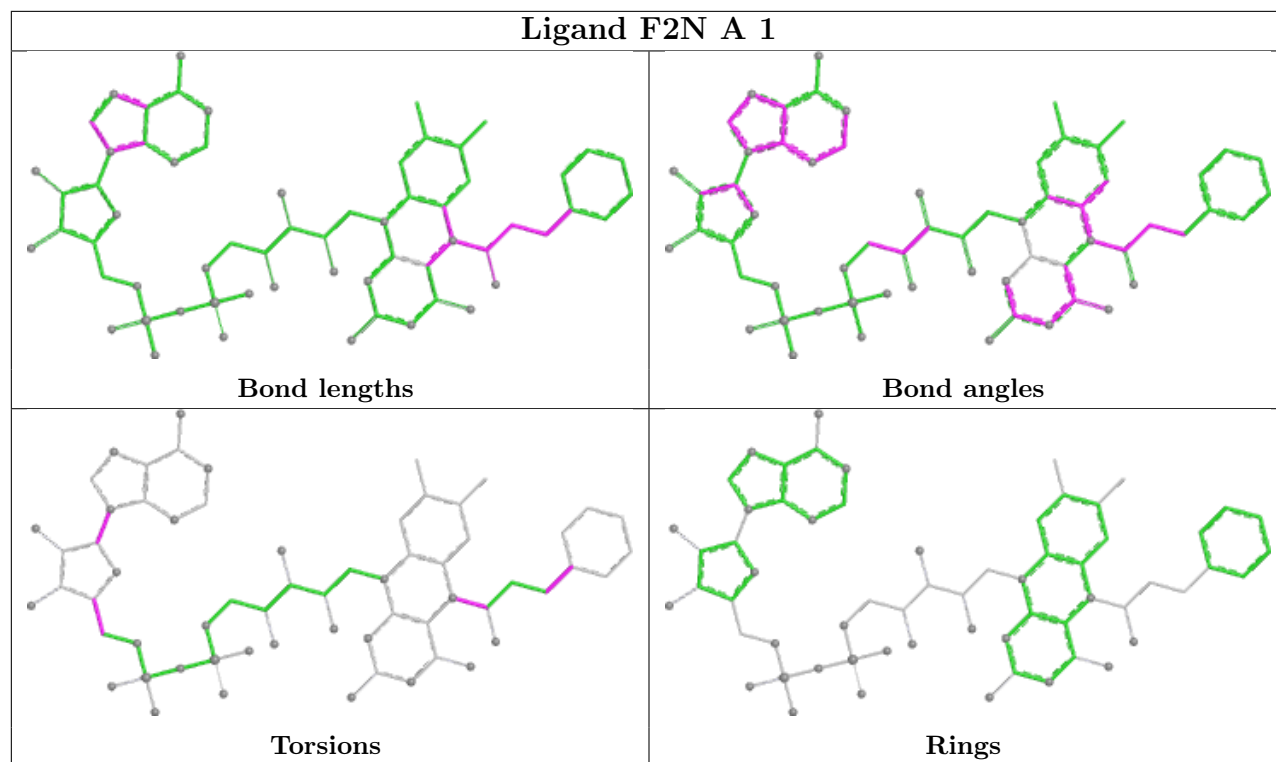
Mol	Chain	Res	Type	Atoms
2	A	1	F2N	CCE-CCC-NBD-CBE
2	A	1	F2N	OCB-CCC-NBD-CBE
2	A	1	F2N	OCB-CCC-NBD-CBC
2	A	1	F2N	CCE-CCD-CCF-CCG
2	A	1	F2N	C2'-C1'-N9-C8
2	A	1	F2N	CCE-CCC-NBD-CBC
2	A	1	F2N	CCE-CCD-CCF-CCK
2	A	1	F2N	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	F2N	6	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

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	643/662 (97%)	0.51	53 (8%) 17 16	28, 46, 89, 147	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	474	ILE	12.7
1	A	462	TYR	9.1
1	A	473	ASP	8.9
1	A	477	GLU	8.4
1	A	475	THR	8.4
1	A	459	HIS	5.8
1	A	463	LYS	5.5
1	A	792	PRO	5.5
1	A	495	ASP	5.3
1	A	782	PRO	4.8
1	A	478	PHE	4.7
1	A	500	THR	4.2
1	A	398	PHE	4.1
1	A	793	ILE	4.1
1	A	476	ALA	3.9
1	A	497	LEU	3.7
1	A	496	GLU	3.5
1	A	273	LEU	3.5
1	A	457	GLU	3.3
1	A	504	LEU	3.2
1	A	464	GLU	3.2
1	A	480	VAL	3.1
1	A	270	ILE	3.1
1	A	831	GLY	3.1
1	A	368	GLN	3.1
1	A	494	TYR	3.0
1	A	431	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	488	THR	2.7
1	A	461	GLN	2.7
1	A	484	HIS	2.6
1	A	395	GLN	2.6
1	A	490	LEU	2.6
1	A	479	LEU	2.5
1	A	492	LYS	2.5
1	A	455	ILE	2.5
1	A	508	LEU	2.5
1	A	172	SER	2.4
1	A	443	GLU	2.4
1	A	272	PRO	2.3
1	A	489	ALA	2.3
1	A	513	ALA	2.3
1	A	556	ASP	2.2
1	A	493	GLU	2.2
1	A	828	GLN	2.2
1	A	612	GLN	2.2
1	A	458	LEU	2.1
1	A	274	PRO	2.1
1	A	505	GLU	2.1
1	A	613	THR	2.1
1	A	615	ILE	2.1
1	A	271	LYS	2.1
1	A	485	ARG	2.1
1	A	456	LYS	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](#)

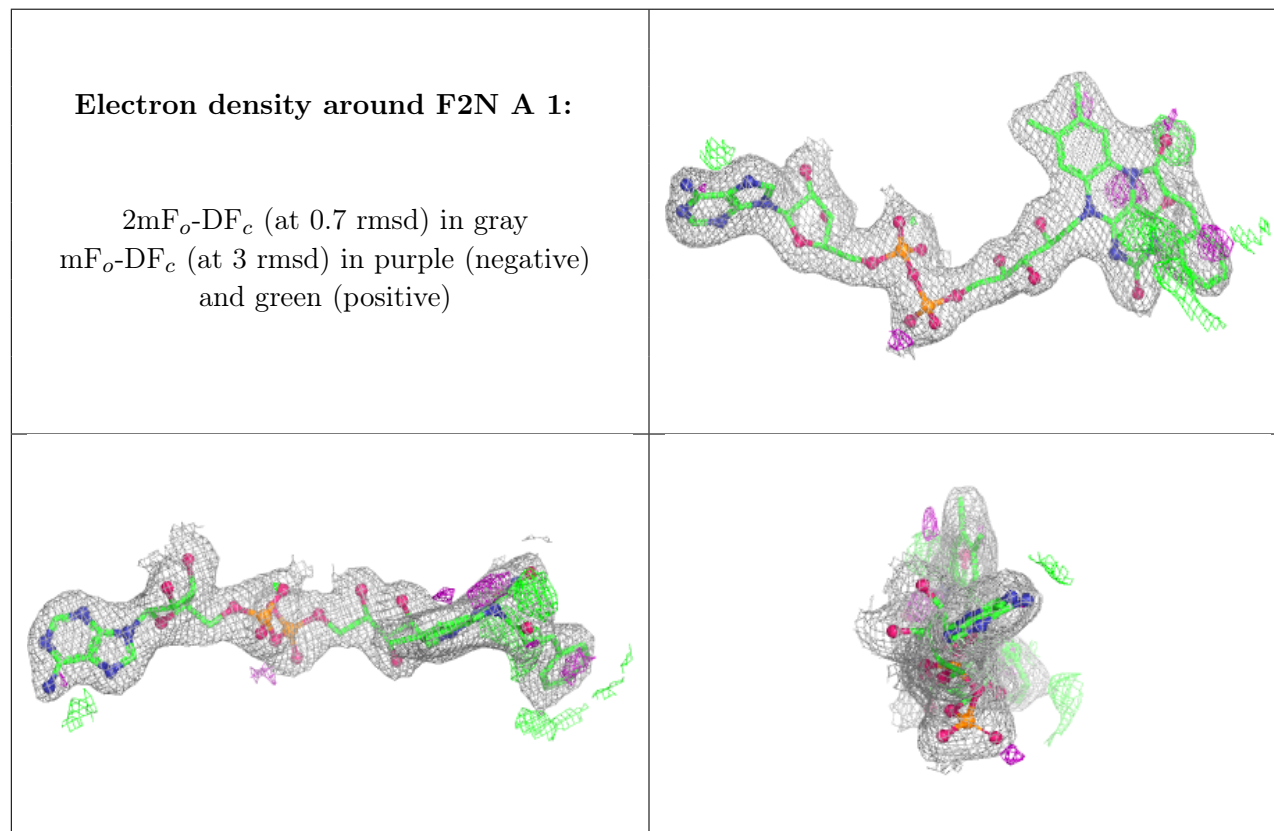
There are no oligosaccharides in this entry.

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
2	F2N	A	1	63/63	0.96	0.09	28,35,54,56	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 [i](#)

There are no such residues in this entry.