



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:30 AM UTC

PDB ID : 2H94 / pdb_00002h94
Title : Crystal Structure and Mechanism of human Lysine-Specific Demethylase-1
Authors : Stavropoulos, P.; Blobel, G.; Hoelz, A.
Deposited on : 2006-06-08
Resolution : 2.90 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

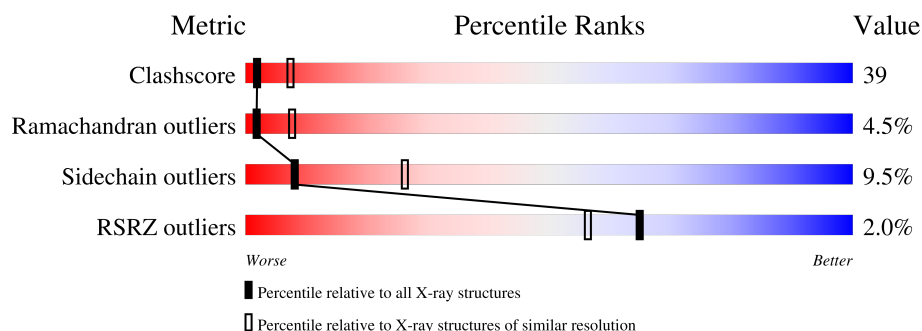
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	664	2% 40% 47% 9% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5153 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.

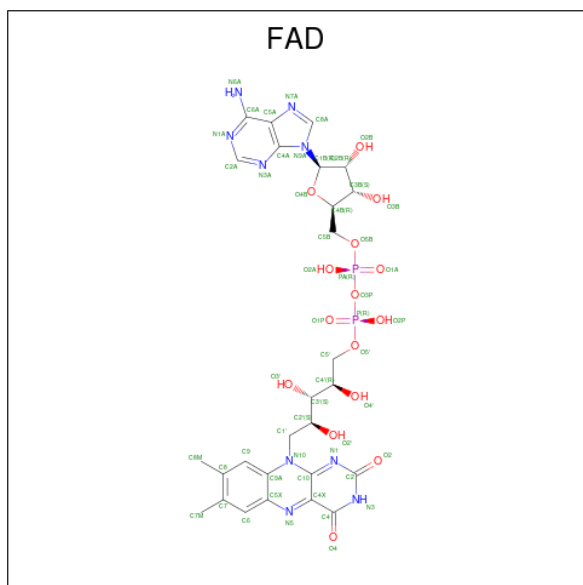
- Molecule 1 is a protein called Lysine-specific histone demethylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	647	Total	C	N	O	S	0	0	0
			5077	3232	882	943	20			

- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Hg	0	0
			3	3		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	187.94Å 187.94Å 108.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	88.8 (20.00-2.90) 88.3 (20.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.88Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.281 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5153	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: FAD, HG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/5182	1.12	43/7020 (0.6%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	640	VAL	CA-C-N	-12.39	107.62	120.38
1	A	640	VAL	C-N-CA	-12.39	107.62	120.38
1	A	793	ILE	CA-C-N	10.35	130.42	119.76
1	A	793	ILE	C-N-CA	10.35	130.42	119.76
1	A	688	ARG	N-CA-C	-8.36	103.09	113.38
1	A	562	GLY	N-CA-C	-8.04	104.31	111.95
1	A	641	PRO	N-CA-C	-7.68	101.33	110.70
1	A	434	ILE	N-CA-C	-7.54	103.45	110.53
1	A	310	ARG	N-CA-C	7.50	121.77	111.71
1	A	805	ARG	N-CA-C	7.17	119.71	111.11
1	A	754	ASP	CA-C-N	7.03	126.72	119.56
1	A	754	ASP	C-N-CA	7.03	126.72	119.56
1	A	247	VAL	N-CA-C	6.87	116.99	110.53
1	A	190	SER	N-CA-C	-6.79	103.88	111.28
1	A	208	LYS	N-CA-C	-6.48	103.33	111.11
1	A	686	ALA	N-CA-C	-6.47	99.48	109.76
1	A	551	HIS	N-CA-C	6.44	121.94	113.30
1	A	335	THR	N-CA-C	6.27	120.00	108.58
1	A	327	ALA	N-CA-C	6.18	120.41	112.12
1	A	550	LYS	N-CA-C	6.16	119.26	111.69
1	A	270	ILE	N-CA-C	-5.95	99.84	108.89
1	A	773	TYR	N-CA-C	-5.85	104.99	111.36
1	A	610	THR	N-CA-C	5.66	122.85	110.80
1	A	231	PHE	N-CA-C	-5.65	105.12	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	739	ALA	N-CA-C	-5.65	106.19	112.57
1	A	199	ILE	N-CA-C	-5.59	105.66	112.76
1	A	201	SER	N-CA-C	-5.56	106.70	112.93
1	A	598	SER	CB-CA-C	-5.46	109.20	117.07
1	A	693	LEU	N-CA-C	5.43	117.06	107.61
1	A	666	PHE	N-CA-C	5.39	118.48	109.96
1	A	271	LYS	CA-C-N	5.35	125.29	119.78
1	A	271	LYS	C-N-CA	5.35	125.29	119.78
1	A	478	PHE	N-CA-C	-5.33	106.75	113.20
1	A	429	GLU	N-CA-C	-5.29	105.62	111.71
1	A	185	HIS	N-CA-C	5.27	117.10	111.36
1	A	740	VAL	CA-C-N	5.27	126.42	119.84
1	A	740	VAL	C-N-CA	5.27	126.42	119.84
1	A	493	GLU	N-CA-C	-5.23	106.41	112.89
1	A	456	LYS	N-CA-C	-5.11	107.11	113.55
1	A	367	GLY	N-CA-C	-5.05	108.00	114.37
1	A	326	VAL	N-CA-C	-5.03	101.01	108.45
1	A	485	ARG	N-CA-C	-5.02	105.93	111.71
1	A	634	PRO	N-CA-C	5.02	116.82	110.70

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	5077	0	5100	403	0
2	A	3	0	0	0	0
3	A	53	0	31	5	0
4	A	20	0	0	4	0
All	All	5153	0	5131	403	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 39.

All (403) 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:755:PRO:HA	1:A:758:ARG:HH12	1.10	1.12
1:A:803:THR:HG21	1:A:820:ARG:HH22	1.14	1.12
1:A:617:LYS:HD3	1:A:617:LYS:H	1.05	1.09
1:A:755:PRO:HA	1:A:758:ARG:NH1	1.69	1.06
1:A:229:LEU:HA	4:A:5004:HOH:O	1.57	1.02
1:A:803:THR:HG22	1:A:820:ARG:HH12	1.32	0.94
1:A:198:ASP:HA	1:A:201:SER:HB2	1.48	0.92
1:A:803:THR:CG2	1:A:820:ARG:HH22	1.85	0.89
1:A:251:ARG:HD3	1:A:835:THR:HG23	1.51	0.89
1:A:189:THR:HB	1:A:192:GLU:HG3	1.54	0.89
1:A:617:LYS:H	1:A:617:LYS:CD	1.86	0.88
1:A:617:LYS:HD3	1:A:617:LYS:N	1.89	0.88
1:A:613:THR:C	1:A:614:PHE:HD2	1.85	0.85
1:A:662:VAL:HB	1:A:705:ALA:HB3	1.56	0.85
1:A:189:THR:HG22	1:A:191:GLN:H	1.40	0.84
1:A:230:THR:HG22	1:A:232:GLU:H	1.39	0.84
1:A:294:ALA:HB1	1:A:582:LEU:HD22	1.61	0.83
1:A:586:LEU:O	1:A:588:THR:HG23	1.77	0.82
1:A:357:LYS:H	1:A:676:ASN:ND2	1.78	0.81
1:A:449:VAL:HA	1:A:452:LYS:HD2	1.60	0.81
1:A:441:LEU:HD21	1:A:504:LEU:HB3	1.63	0.80
1:A:660:ASN:HD21	1:A:751:TRP:H	1.25	0.80
1:A:434:ILE:O	1:A:438:GLN:HG3	1.83	0.79
1:A:794:PRO:HD2	1:A:828:GLN:NE2	1.98	0.78
1:A:509:GLN:HE21	1:A:513:ALA:HB2	1.48	0.78
1:A:200:ILE:HD12	1:A:201:SER:N	1.99	0.78
1:A:685:THR:O	1:A:688:ARG:HG2	1.85	0.77
1:A:455:ILE:HG22	1:A:490:LEU:HB3	1.67	0.77
1:A:327:ALA:O	1:A:328:ASP:HB2	1.86	0.75
1:A:760:SER:HA	3:A:5000:FAD:HM82	1.68	0.75
1:A:672:ASP:O	1:A:675:VAL:HG12	1.86	0.75
1:A:238:LEU:HB2	1:A:243:ASN:HB3	1.68	0.75
1:A:619:ASP:HB3	1:A:829:PHE:HE2	1.52	0.74
1:A:197:PRO:O	1:A:199:ILE:N	2.21	0.74
1:A:537:GLU:HG2	1:A:544:LEU:HD13	1.68	0.74
1:A:310:ARG:O	1:A:310:ARG:HG2	1.87	0.73
1:A:594:ARG:HG2	1:A:640:VAL:CG2	2.18	0.73
1:A:667:ASP:HB3	1:A:668:ARG:HH11	1.51	0.73
1:A:546:THR:HG21	1:A:763:TYR:OH	1.88	0.73
1:A:374:LYS:HE2	1:A:524:ARG:NH1	2.02	0.73
1:A:452:LYS:O	1:A:456:LYS:HB2	1.89	0.73
1:A:229:LEU:H	1:A:263:ASN:HD21	1.34	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:THR:HG22	3:A:5000:FAD:H52A	1.71	0.72
1:A:736:GLY:HA3	1:A:739:ALA:HB3	1.72	0.72
1:A:325:TYR:CE1	1:A:665:CYS:HB3	2.23	0.72
1:A:665:CYS:HB2	1:A:745:GLU:HB2	1.72	0.72
1:A:309:ALA:HB2	1:A:589:ALA:HA	1.72	0.71
1:A:199:ILE:HG21	1:A:835:THR:O	1.90	0.71
1:A:357:LYS:H	1:A:676:ASN:HD22	1.36	0.70
1:A:732:LYS:HD2	1:A:738:SER:HA	1.72	0.70
1:A:307:LEU:HD23	1:A:585:LYS:HB3	1.73	0.70
1:A:230:THR:HG22	1:A:232:GLU:N	2.07	0.70
1:A:229:LEU:N	1:A:263:ASN:HD21	1.89	0.70
1:A:240:ALA:HB3	1:A:241:PRO:HD3	1.74	0.70
1:A:320:PHE:HB3	1:A:327:ALA:HB3	1.74	0.70
1:A:660:ASN:ND2	1:A:751:TRP:H	1.91	0.69
1:A:266:ILE:HD12	1:A:580:GLU:HG2	1.74	0.69
1:A:310:ARG:HD3	1:A:312:ARG:NH1	2.08	0.69
1:A:547:LEU:HD22	1:A:552:TRP:HB2	1.75	0.68
1:A:594:ARG:HG2	1:A:640:VAL:HG21	1.74	0.67
1:A:586:LEU:O	1:A:588:THR:N	2.28	0.67
1:A:627:LEU:HD12	1:A:656:PHE:HB2	1.77	0.67
1:A:720:ASP:OD2	1:A:750:ARG:NH2	2.28	0.67
1:A:406:VAL:HA	1:A:410:GLN:OE1	1.94	0.66
1:A:251:ARG:HD3	1:A:835:THR:CG2	2.23	0.66
1:A:219:GLN:HG2	1:A:223:ASP:OD2	1.95	0.66
1:A:612:GLN:O	1:A:613:THR:OG1	2.09	0.66
1:A:197:PRO:O	1:A:199:ILE:HG13	1.96	0.66
1:A:585:LYS:HZ1	1:A:614:PHE:HE1	1.44	0.66
1:A:778:GLN:HE21	1:A:778:GLN:HA	1.61	0.66
1:A:610:THR:HG22	1:A:610:THR:O	1.96	0.66
1:A:284:ILE:O	1:A:624:THR:HB	1.95	0.66
1:A:566:THR:HG21	1:A:697:LEU:HD13	1.78	0.66
1:A:826:ALA:HB1	1:A:830:LEU:HD12	1.77	0.66
1:A:605:VAL:HG12	1:A:606:ASN:O	1.96	0.65
1:A:342:MET:HE1	1:A:815:LEU:HD13	1.77	0.65
1:A:803:THR:HG21	1:A:820:ARG:NH2	1.98	0.65
1:A:509:GLN:NE2	1:A:513:ALA:HB2	2.12	0.65
1:A:644:PRO:HD2	1:A:780:ILE:HD13	1.78	0.65
1:A:794:PRO:HD2	1:A:828:GLN:CD	2.22	0.65
1:A:802:HIS:CD2	1:A:802:HIS:H	2.13	0.65
1:A:197:PRO:C	1:A:199:ILE:H	2.04	0.64
1:A:358:GLN:CD	1:A:358:GLN:H	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:VAL:HG21	1:A:746:THR:HG21	1.78	0.64
1:A:232:GLU:HG2	1:A:236:GLN:HE21	1.61	0.63
1:A:595:TYR:HA	1:A:600:CYS:HB3	1.80	0.63
1:A:640:VAL:HG12	1:A:641:PRO:CD	2.28	0.63
1:A:807:TYR:N	1:A:808:PRO:CD	2.60	0.63
1:A:329:LEU:HD11	1:A:747:VAL:HG11	1.80	0.63
1:A:200:ILE:HD12	1:A:201:SER:H	1.64	0.63
1:A:794:PRO:HD2	1:A:828:GLN:HE22	1.63	0.63
1:A:461:GLN:O	1:A:465:ALA:HB3	1.98	0.63
1:A:475:THR:O	1:A:479:LEU:HD23	1.99	0.62
1:A:418:LEU:O	1:A:421:LYS:HB3	1.98	0.62
1:A:441:LEU:HD21	1:A:504:LEU:CB	2.29	0.62
1:A:720:ASP:O	1:A:724:VAL:HG23	1.99	0.62
1:A:640:VAL:CG1	1:A:641:PRO:HD3	2.30	0.62
1:A:283:ILE:HB	1:A:306:LEU:CD2	2.30	0.62
1:A:566:THR:CG2	1:A:697:LEU:HD13	2.30	0.61
1:A:448:MET:CG	1:A:497:LEU:HD23	2.31	0.61
1:A:198:ASP:HA	1:A:201:SER:CB	2.25	0.61
1:A:781:THR:OG1	1:A:794:PRO:HG3	2.00	0.61
1:A:801:GLU:CG	1:A:809:ALA:HA	2.31	0.60
1:A:476:ALA:HA	1:A:480:VAL:HG23	1.82	0.60
1:A:477:GLU:HG3	1:A:478:PHE:H	1.66	0.60
1:A:189:THR:HG22	1:A:191:GLN:N	2.13	0.60
1:A:803:THR:HG22	1:A:820:ARG:NH1	2.12	0.60
1:A:640:VAL:HG12	1:A:641:PRO:HD3	1.84	0.59
1:A:633:GLN:HA	1:A:633:GLN:OE1	2.02	0.59
1:A:778:GLN:HE21	1:A:779:PRO:HD2	1.67	0.59
1:A:776:MET:HE2	1:A:776:MET:HA	1.82	0.59
1:A:663:VAL:HG22	1:A:704:LEU:HD11	1.83	0.59
1:A:283:ILE:HG12	1:A:622:LEU:HB3	1.84	0.59
1:A:248:LEU:HA	1:A:251:ARG:HD2	1.84	0.59
1:A:650:ALA:O	1:A:654:MET:HG3	2.03	0.59
1:A:757:ALA:O	1:A:758:ARG:HB2	2.03	0.59
1:A:835:THR:O	1:A:835:THR:HG22	2.02	0.59
1:A:457:GLU:HG3	1:A:461:GLN:HE21	1.68	0.58
1:A:551:HIS:HB2	1:A:764:VAL:HG11	1.84	0.58
1:A:610:THR:O	1:A:611:SER:OG	2.15	0.58
1:A:294:ALA:HB2	1:A:306:LEU:HD21	1.86	0.58
1:A:308:GLU:OE1	1:A:310:ARG:HB3	2.03	0.58
1:A:406:VAL:HG13	1:A:410:GLN:OE1	2.03	0.58
1:A:485:ARG:HG2	1:A:485:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:THR:C	1:A:614:PHE:CD2	2.75	0.58
1:A:196:PHE:O	1:A:200:ILE:HD11	2.04	0.58
1:A:407:SER:HB2	1:A:545:SER:O	2.04	0.58
1:A:283:ILE:HB	1:A:306:LEU:HD23	1.84	0.57
1:A:357:LYS:CB	1:A:676:ASN:HD22	2.17	0.57
1:A:520:TYR:CD2	1:A:521:LEU:HG	2.39	0.57
1:A:640:VAL:HB	1:A:641:PRO:HD3	1.86	0.57
1:A:695:TRP:HD1	1:A:697:LEU:HG	1.70	0.57
1:A:695:TRP:CD1	1:A:697:LEU:HG	2.39	0.57
1:A:568:ARG:HG3	1:A:568:ARG:HH11	1.70	0.56
1:A:585:LYS:NZ	1:A:614:PHE:HE1	2.01	0.56
1:A:194:ALA:O	1:A:197:PRO:HD3	2.05	0.56
1:A:199:ILE:HD12	1:A:835:THR:HB	1.87	0.56
1:A:269:ARG:NH1	1:A:273:LEU:HD21	2.19	0.56
1:A:426:GLU:HA	1:A:429:GLU:OE1	2.05	0.56
1:A:340:ASN:OD1	1:A:342:MET:HB2	2.06	0.56
1:A:289:SER:OG	1:A:624:THR:HG23	2.06	0.56
1:A:425:ASP:C	1:A:427:GLN:H	2.14	0.56
1:A:603:ILE:HG13	1:A:615:ILE:HG12	1.86	0.56
1:A:778:GLN:HE21	1:A:778:GLN:CA	2.17	0.56
1:A:730:ILE:O	1:A:734:ILE:HG23	2.06	0.56
1:A:546:THR:HG21	1:A:763:TYR:CZ	2.41	0.55
1:A:448:MET:O	1:A:452:LYS:HG3	2.07	0.55
1:A:494:TYR:CD2	1:A:494:TYR:O	2.59	0.55
1:A:728:LEU:O	1:A:732:LYS:HG2	2.06	0.55
1:A:803:THR:CG2	1:A:820:ARG:NH2	2.64	0.55
1:A:624:THR:HG22	1:A:624:THR:O	2.06	0.55
1:A:640:VAL:HG12	1:A:641:PRO:N	2.20	0.55
1:A:794:PRO:CD	1:A:828:GLN:HE22	2.19	0.55
1:A:231:PHE:HA	1:A:253:HIS:CD2	2.42	0.55
1:A:232:GLU:HG2	1:A:236:GLN:NE2	2.21	0.54
1:A:424:LYS:O	1:A:428:ILE:HG13	2.07	0.54
1:A:508:LEU:HG	1:A:508:LEU:O	2.07	0.54
1:A:455:ILE:CG2	1:A:490:LEU:HB3	2.35	0.54
1:A:594:ARG:CG	1:A:640:VAL:HG21	2.36	0.54
1:A:686:ALA:O	1:A:687:SER:OG	2.22	0.54
1:A:357:LYS:HB2	1:A:676:ASN:HD22	1.71	0.54
1:A:659:LEU:HG	1:A:659:LEU:O	2.06	0.54
1:A:778:GLN:NE2	1:A:779:PRO:HD2	2.23	0.54
1:A:668:ARG:HD3	1:A:668:ARG:N	2.22	0.54
1:A:651:VAL:HG23	1:A:776:MET:HE1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ILE:O	1:A:432:LYS:HB2	2.07	0.54
1:A:594:ARG:HG2	1:A:640:VAL:HG23	1.90	0.53
1:A:188:MET:HE1	1:A:200:ILE:HD13	1.91	0.53
1:A:197:PRO:C	1:A:199:ILE:N	2.66	0.53
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.44	0.53
1:A:389:THR:HG22	1:A:390:SER:N	2.24	0.53
1:A:546:THR:HG22	1:A:763:TYR:CE1	2.44	0.53
1:A:220:LEU:HD22	1:A:237:GLN:OE1	2.08	0.53
1:A:228:GLN:HA	1:A:263:ASN:ND2	2.25	0.53
1:A:684:THR:HB	1:A:686:ALA:O	2.09	0.53
1:A:775:LEU:O	1:A:778:GLN:HB2	2.09	0.53
1:A:181:SER:OG	1:A:218:LEU:HG	2.09	0.52
1:A:606:ASN:OD1	1:A:607:THR:N	2.41	0.52
1:A:198:ASP:CA	1:A:201:SER:HB2	2.30	0.52
1:A:633:GLN:O	1:A:634:PRO:C	2.51	0.52
1:A:367:GLY:HA2	1:A:734:ILE:HG22	1.91	0.52
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.74	0.52
1:A:455:ILE:HG22	1:A:490:LEU:CB	2.39	0.52
1:A:669:VAL:HG11	1:A:673:PRO:HG3	1.92	0.52
1:A:614:PHE:HD2	1:A:614:PHE:N	2.07	0.52
1:A:665:CYS:CB	1:A:745:GLU:HB2	2.39	0.52
1:A:183:LEU:HD11	1:A:261:LEU:HD13	1.91	0.52
1:A:448:MET:HG3	1:A:497:LEU:HD23	1.91	0.52
1:A:446:ASN:O	1:A:450:ASN:HB2	2.10	0.51
1:A:801:GLU:HB2	3:A:5000:FAD:H5'2	1.91	0.51
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.92	0.51
1:A:306:LEU:HD12	1:A:584:ILE:HG12	1.92	0.51
1:A:614:PHE:CD2	1:A:614:PHE:N	2.78	0.51
1:A:640:VAL:CB	1:A:641:PRO:HD3	2.39	0.51
1:A:537:GLU:CD	1:A:688:ARG:HH11	2.19	0.51
1:A:695:TRP:CZ3	1:A:706:LEU:HD11	2.46	0.51
1:A:715:MET:HE2	1:A:718:ILE:HD12	1.93	0.51
1:A:726:ARG:O	1:A:730:ILE:HG13	2.11	0.51
1:A:755:PRO:CA	1:A:758:ARG:HH12	2.02	0.50
1:A:806:ASN:O	1:A:807:TYR:CG	2.64	0.50
1:A:232:GLU:O	1:A:236:GLN:HG2	2.12	0.50
1:A:639:PHE:O	1:A:640:VAL:C	2.54	0.50
1:A:640:VAL:O	1:A:641:PRO:C	2.47	0.50
1:A:423:VAL:O	1:A:427:GLN:HB2	2.12	0.50
1:A:632:GLN:NE2	1:A:758:ARG:NH2	2.59	0.50
1:A:357:LYS:N	1:A:676:ASN:HD22	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LYS:O	1:A:440:GLU:HG3	2.10	0.50
1:A:553:ASP:O	1:A:555:ASP:N	2.43	0.50
1:A:548:SER:HB2	1:A:766:ALA:HA	1.94	0.50
1:A:731:LEU:C	1:A:733:GLY:H	2.18	0.50
1:A:379:GLU:O	1:A:382:PHE:HB3	2.12	0.50
1:A:310:ARG:HD2	4:A:5010:HOH:O	2.12	0.49
1:A:833:MET:HA	1:A:833:MET:HE3	1.93	0.49
1:A:558:PHE:CD1	1:A:806:ASN:HB3	2.47	0.49
1:A:753:ALA:O	1:A:754:ASP:C	2.54	0.49
1:A:585:LYS:HE3	1:A:616:TYR:OH	2.11	0.49
1:A:187:ARG:O	1:A:211:LEU:HD21	2.12	0.49
1:A:425:ASP:C	1:A:427:GLN:N	2.68	0.49
1:A:448:MET:HG2	1:A:497:LEU:HD23	1.94	0.49
1:A:182:ARG:HD2	1:A:807:TYR:OH	2.12	0.49
1:A:188:MET:HE1	1:A:200:ILE:CD1	2.42	0.49
1:A:444:LEU:HD23	1:A:444:LEU:C	2.37	0.49
1:A:435:VAL:O	1:A:439:GLU:HG3	2.13	0.49
1:A:568:ARG:HG3	1:A:568:ARG:NH1	2.27	0.49
1:A:230:THR:HG22	1:A:231:PHE:N	2.27	0.48
1:A:335:THR:HG22	1:A:564:HIS:CD2	2.49	0.48
1:A:538:PHE:CE1	1:A:706:LEU:HD13	2.48	0.48
1:A:426:GLU:HA	1:A:429:GLU:CD	2.38	0.48
1:A:650:ALA:HA	1:A:653:ARG:NH1	2.28	0.48
1:A:826:ALA:O	1:A:830:LEU:HB2	2.13	0.48
1:A:807:TYR:H	1:A:808:PRO:HD3	1.78	0.48
1:A:180:GLN:HA	1:A:339:GLY:HA2	1.96	0.48
1:A:477:GLU:HG3	1:A:478:PHE:N	2.29	0.48
1:A:637:VAL:HG23	1:A:639:PHE:CE1	2.49	0.48
1:A:534:ALA:HA	1:A:537:GLU:HG3	1.95	0.48
1:A:667:ASP:CB	1:A:668:ARG:HH11	2.23	0.48
1:A:736:GLY:O	1:A:738:SER:N	2.47	0.48
1:A:829:PHE:O	1:A:830:LEU:HD23	2.13	0.48
1:A:204:GLN:HG2	1:A:205:GLN:H	1.79	0.47
1:A:198:ASP:C	1:A:200:ILE:N	2.71	0.47
1:A:310:ARG:HD3	1:A:312:ARG:HH11	1.79	0.47
1:A:631:LYS:NZ	1:A:654:MET:O	2.31	0.47
1:A:731:LEU:C	1:A:733:GLY:N	2.71	0.47
1:A:627:LEU:CD1	1:A:656:PHE:HB2	2.43	0.47
1:A:807:TYR:H	1:A:808:PRO:CD	2.26	0.47
1:A:374:LYS:HE2	1:A:524:ARG:HH11	1.73	0.47
1:A:667:ASP:O	1:A:668:ARG:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLU:C	1:A:366:ASN:H	2.23	0.47
1:A:643:LEU:O	1:A:644:PRO:O	2.32	0.47
1:A:225:PRO:CB	1:A:344:VAL:HG13	2.45	0.47
1:A:661:LYS:HG2	1:A:706:LEU:CD2	2.45	0.47
1:A:258:ARG:HD3	1:A:827:ASP:OD1	2.15	0.47
1:A:529:LEU:O	1:A:532:HIS:HB2	2.16	0.46
1:A:342:MET:O	1:A:346:SER:HB2	2.14	0.46
1:A:732:LYS:HB3	1:A:740:VAL:CG2	2.46	0.46
1:A:389:THR:HG21	1:A:408:LEU:HD11	1.96	0.46
1:A:419:GLN:HA	1:A:422:HIS:CD2	2.50	0.46
1:A:327:ALA:O	1:A:328:ASP:CB	2.60	0.46
1:A:349:VAL:HG12	1:A:349:VAL:O	2.16	0.46
1:A:716:GLU:HG2	1:A:750:ARG:HG2	1.97	0.46
1:A:808:PRO:O	1:A:810:THR:HG23	2.16	0.46
1:A:829:PHE:N	1:A:829:PHE:CD1	2.84	0.46
1:A:382:PHE:CD1	1:A:532:HIS:HB3	2.51	0.46
1:A:663:VAL:CG1	1:A:702:ILE:HD11	2.46	0.46
1:A:803:THR:CG2	1:A:820:ARG:HH12	2.15	0.46
1:A:189:THR:HG22	1:A:190:SER:N	2.31	0.45
1:A:778:GLN:HA	1:A:778:GLN:NE2	2.30	0.45
1:A:807:TYR:N	1:A:808:PRO:HD3	2.30	0.45
1:A:331:ALA:HA	3:A:5000:FAD:C4X	2.47	0.45
1:A:509:GLN:O	1:A:513:ALA:HB3	2.16	0.45
1:A:639:PHE:CD1	1:A:639:PHE:N	2.84	0.45
1:A:655:GLY:O	1:A:762:SER:HA	2.16	0.45
1:A:296:GLN:HB2	1:A:822:ALA:HB1	1.99	0.45
1:A:310:ARG:O	1:A:311:ASP:OD1	2.35	0.45
1:A:558:PHE:CE1	1:A:806:ASN:HB3	2.52	0.45
1:A:695:TRP:NE1	1:A:697:LEU:HD11	2.32	0.45
1:A:229:LEU:H	1:A:263:ASN:ND2	2.07	0.45
1:A:619:ASP:HB3	1:A:829:PHE:CE2	2.43	0.45
1:A:376:GLU:O	1:A:380:GLN:HG3	2.17	0.45
1:A:624:THR:O	1:A:624:THR:CG2	2.65	0.45
1:A:625:LEU:HD11	1:A:637:VAL:HG21	1.98	0.45
1:A:671:TRP:HB2	4:A:5009:HOH:O	2.15	0.45
1:A:182:ARG:HH11	1:A:182:ARG:HG3	1.82	0.44
1:A:248:LEU:O	1:A:251:ARG:HB2	2.17	0.44
1:A:424:LYS:HD3	1:A:427:GLN:OE1	2.17	0.44
1:A:640:VAL:HB	1:A:641:PRO:CD	2.48	0.44
1:A:722:VAL:O	1:A:726:ARG:HG3	2.17	0.44
1:A:668:ARG:NH2	1:A:741:PRO:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:HB2	1:A:304:VAL:HG11	1.99	0.44
1:A:309:ALA:HB1	1:A:589:ALA:HB2	2.00	0.44
1:A:340:ASN:OD1	1:A:342:MET:N	2.42	0.44
1:A:691:LEU:HA	1:A:706:LEU:O	2.17	0.44
1:A:742:GLN:NE2	1:A:743:PRO:HD2	2.32	0.44
1:A:731:LEU:O	1:A:734:ILE:HG12	2.17	0.44
1:A:304:VAL:HG23	1:A:304:VAL:O	2.17	0.44
1:A:695:TRP:CE3	1:A:706:LEU:HD11	2.52	0.44
1:A:794:PRO:HD2	1:A:828:GLN:OE1	2.17	0.44
1:A:355:LYS:HG2	1:A:565:LEU:CD2	2.46	0.44
1:A:509:GLN:C	1:A:511:LEU:H	2.25	0.44
1:A:718:ILE:HG22	1:A:719:SER:N	2.33	0.44
1:A:718:ILE:CG2	1:A:722:VAL:HB	2.48	0.44
1:A:196:PHE:O	1:A:200:ILE:CD1	2.64	0.44
1:A:434:ILE:HG12	1:A:511:LEU:HB3	1.99	0.44
1:A:742:GLN:CD	1:A:743:PRO:HD2	2.42	0.44
1:A:177:ALA:HB1	1:A:218:LEU:HB3	1.99	0.44
1:A:242:TYR:C	1:A:244:SER:H	2.25	0.44
1:A:449:VAL:HA	1:A:452:LYS:CD	2.41	0.44
1:A:502:GLY:O	1:A:503:LYS:C	2.61	0.44
1:A:546:THR:CG2	1:A:763:TYR:CE1	3.01	0.44
1:A:611:SER:O	1:A:612:GLN:CB	2.65	0.44
1:A:282:ILE:HG21	1:A:602:VAL:HG21	2.00	0.43
1:A:634:PRO:HB2	1:A:635:PRO:C	2.43	0.43
1:A:308:GLU:HG3	1:A:310:ARG:H	1.82	0.43
1:A:344:VAL:HA	1:A:347:LYS:HE2	1.99	0.43
1:A:374:LYS:HE2	1:A:524:ARG:HH12	1.81	0.43
1:A:509:GLN:C	1:A:511:LEU:N	2.76	0.43
1:A:432:LYS:O	1:A:436:LYS:HD3	2.18	0.43
1:A:566:THR:HG21	1:A:697:LEU:HB3	2.01	0.43
1:A:653:ARG:O	1:A:768:SER:HB2	2.19	0.43
1:A:239:GLU:N	1:A:239:GLU:CD	2.76	0.43
1:A:363:TYR:HD2	1:A:367:GLY:O	2.01	0.43
1:A:633:GLN:OE1	1:A:633:GLN:CA	2.66	0.43
1:A:644:PRO:CD	1:A:780:ILE:HD13	2.48	0.43
1:A:199:ILE:HD13	1:A:835:THR:O	2.18	0.43
1:A:815:LEU:C	1:A:815:LEU:HD23	2.43	0.43
1:A:200:ILE:C	1:A:202:GLY:H	2.26	0.43
1:A:430:HIS:O	1:A:431:TRP:C	2.62	0.43
1:A:441:LEU:HD11	1:A:505:GLU:HA	1.99	0.43
1:A:572:SER:C	1:A:575:PRO:HD2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASN:OD1	1:A:342:MET:CB	2.67	0.43
1:A:639:PHE:O	1:A:640:VAL:O	2.37	0.43
1:A:668:ARG:HA	1:A:701:PRO:HB3	2.01	0.43
1:A:693:LEU:HD23	1:A:706:LEU:HD12	2.00	0.43
1:A:715:MET:C	1:A:717:ASN:H	2.27	0.43
1:A:834:TYR:CD1	1:A:834:TYR:C	2.96	0.43
1:A:611:SER:HB3	1:A:614:PHE:CE2	2.54	0.42
1:A:695:TRP:CD1	1:A:697:LEU:CG	3.01	0.42
1:A:266:ILE:CD1	1:A:580:GLU:HG2	2.45	0.42
1:A:475:THR:O	1:A:479:LEU:HB3	2.19	0.42
1:A:493:GLU:C	1:A:495:ASP:H	2.27	0.42
1:A:590:VAL:O	1:A:637:VAL:HG12	2.19	0.42
1:A:399:ASN:C	1:A:406:VAL:HG23	2.45	0.42
1:A:485:ARG:HG2	1:A:485:ARG:NH1	2.34	0.42
1:A:596:THR:HG22	1:A:597:ALA:H	1.84	0.42
1:A:658:ASN:ND2	1:A:659:LEU:H	2.18	0.42
1:A:611:SER:HB3	1:A:614:PHE:HE2	1.83	0.42
1:A:715:MET:HE2	1:A:718:ILE:CD1	2.49	0.42
1:A:834:TYR:HD1	1:A:835:THR:N	2.17	0.42
1:A:696:ASN:C	1:A:696:ASN:ND2	2.77	0.42
1:A:174:VAL:O	1:A:215:ASN:HB3	2.20	0.42
1:A:230:THR:CG2	1:A:231:PHE:N	2.82	0.42
1:A:695:TRP:HE1	1:A:697:LEU:HD21	1.85	0.42
1:A:801:GLU:HG2	1:A:809:ALA:HA	2.01	0.42
1:A:603:ILE:N	1:A:603:ILE:HD12	2.35	0.42
1:A:189:THR:CG2	1:A:191:GLN:HB2	2.50	0.41
1:A:355:LYS:HA	1:A:565:LEU:CD2	2.50	0.41
1:A:407:SER:CB	1:A:545:SER:O	2.67	0.41
1:A:183:LEU:HD12	1:A:218:LEU:HD21	2.01	0.41
1:A:427:GLN:HE21	1:A:518:ASP:HA	1.84	0.41
1:A:456:LYS:HD2	1:A:456:LYS:HA	1.94	0.41
1:A:477:GLU:CG	1:A:478:PHE:H	2.25	0.41
1:A:207:GLN:O	1:A:208:LYS:C	2.62	0.41
1:A:293:ALA:O	1:A:294:ALA:C	2.63	0.41
1:A:192:GLU:OE2	1:A:214:ARG:HD2	2.20	0.41
1:A:402:ASN:C	1:A:404:LYS:N	2.76	0.41
1:A:402:ASN:C	1:A:404:LYS:H	2.28	0.41
1:A:640:VAL:CB	1:A:641:PRO:CD	2.96	0.41
1:A:448:MET:CG	1:A:497:LEU:HB3	2.51	0.41
1:A:224:ASN:C	1:A:224:ASN:ND2	2.79	0.41
1:A:634:PRO:HB2	1:A:635:PRO:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:TYR:CD1	1:A:763:TYR:C	2.98	0.41
1:A:807:TYR:O	1:A:813:GLY:HA3	2.20	0.41
1:A:198:ASP:OD1	1:A:201:SER:O	2.39	0.41
1:A:204:GLN:H	1:A:204:GLN:CD	2.27	0.41
1:A:510:GLU:HG2	1:A:510:GLU:O	2.21	0.41
1:A:552:TRP:CE2	1:A:553:ASP:OD2	2.74	0.41
1:A:198:ASP:OD1	1:A:202:GLY:HA2	2.20	0.41
1:A:264:PHE:HA	1:A:296:GLN:HE22	1.86	0.41
1:A:276:LYS:HD2	1:A:276:LYS:HA	1.82	0.41
1:A:419:GLN:HA	1:A:422:HIS:HD2	1.85	0.41
1:A:501:GLN:O	1:A:505:GLU:CB	2.69	0.41
1:A:518:ASP:O	1:A:519:VAL:HG23	2.21	0.41
1:A:544:LEU:HA	1:A:544:LEU:HD12	1.85	0.41
1:A:546:THR:HG22	1:A:546:THR:O	2.20	0.41
1:A:660:ASN:HD21	1:A:751:TRP:N	2.04	0.41
1:A:735:PHE:HZ	4:A:5009:HOH:O	2.04	0.41
1:A:735:PHE:HB3	1:A:736:GLY:H	1.53	0.41
1:A:762:SER:OG	1:A:801:GLU:OE2	2.30	0.41
1:A:793:ILE:HA	1:A:794:PRO:HD3	1.72	0.41
1:A:821:GLU:O	1:A:822:ALA:C	2.62	0.41
1:A:224:ASN:C	1:A:224:ASN:HD22	2.28	0.41
1:A:314:GLY:O	1:A:315:GLY:C	2.63	0.41
1:A:321:ARG:HG2	1:A:321:ARG:NH1	2.36	0.41
1:A:627:LEU:HB3	1:A:656:PHE:CD1	2.56	0.41
1:A:370:VAL:HA	1:A:371:PRO:HD2	1.86	0.40
1:A:662:VAL:HG11	1:A:727:CYS:SG	2.61	0.40
1:A:633:GLN:HB3	1:A:634:PRO:HD3	2.02	0.40
1:A:640:VAL:O	1:A:642:PRO:N	2.54	0.40
1:A:667:ASP:CG	1:A:744:LYS:HE3	2.45	0.40
1:A:811:VAL:HG23	3:A:5000:FAD:C2	2.51	0.40
1:A:196:PHE:HB3	1:A:200:ILE:CG1	2.51	0.40
1:A:418:LEU:HD23	1:A:418:LEU:HA	1.84	0.40
1:A:432:LYS:HG3	1:A:436:LYS:NZ	2.36	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	641/664 (96%)	532 (83%)	80 (12%)	29 (4%)	2 8

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	242	TYR
1	A	554	GLN
1	A	587	ASN
1	A	610	THR
1	A	612	GLN
1	A	634	PRO
1	A	640	VAL
1	A	644	PRO
1	A	241	PRO
1	A	580	GLU
1	A	586	LEU
1	A	613	THR
1	A	737	SER
1	A	311	ASP
1	A	328	ASP
1	A	647	LYS
1	A	760	SER
1	A	240	ALA
1	A	370	VAL
1	A	372	LYS
1	A	477	GLU
1	A	659	LEU
1	A	807	TYR
1	A	403	ASN
1	A	741	PRO
1	A	197	PRO
1	A	271	LYS

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Mol	Chain	Res	Type
1	A	203	PRO

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	549/564 (97%)	497 (90%)	52 (10%)	8 26

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	GLU
1	A	198	ASP
1	A	200	ILE
1	A	204	GLN
1	A	208	LYS
1	A	218	LEU
1	A	227	ILE
1	A	258	ARG
1	A	328	ASP
1	A	386	LEU
1	A	387	GLU
1	A	389	THR
1	A	395	GLN
1	A	400	VAL
1	A	419	GLN
1	A	437	THR
1	A	457	GLU
1	A	475	THR
1	A	496	GLU
1	A	519	VAL
1	A	524	ARG
1	A	525	ASP
1	A	529	LEU
1	A	544	LEU
1	A	548	SER

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Mol	Chain	Res	Type
1	A	556	ASP
1	A	557	ASP
1	A	580	GLU
1	A	582	LEU
1	A	583	ASP
1	A	586	LEU
1	A	600	CYS
1	A	609	SER
1	A	614	PHE
1	A	617	LYS
1	A	633	GLN
1	A	634	PRO
1	A	644	PRO
1	A	645	GLU
1	A	659	LEU
1	A	667	ASP
1	A	677	LEU
1	A	688	ARG
1	A	695	TRP
1	A	699	LYS
1	A	707	VAL
1	A	723	ILE
1	A	746	THR
1	A	771	ASN
1	A	778	GLN
1	A	793	ILE
1	A	806	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	224	ASN
1	A	236	GLN
1	A	263	ASN
1	A	296	GLN
1	A	395	GLN
1	A	419	GLN
1	A	422	HIS
1	A	427	GLN
1	A	430	HIS
1	A	438	GLN

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Mol	Chain	Res	Type
1	A	461	GLN
1	A	509	GLN
1	A	564	HIS
1	A	612	GLN
1	A	632	GLN
1	A	658	ASN
1	A	660	ASN
1	A	676	ASN
1	A	742	GLN
1	A	771	ASN
1	A	778	GLN
1	A	802	HIS
1	A	812	HIS

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](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	FAD	A	5000	-	58,58,58	1.60	9 (15%)	85,89,89	1.83	8 (9%)

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	FAD	A	5000	-	-	10/34/50/50	0/6/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5000	FAD	C4X-N5	4.82	1.41	1.30
3	A	5000	FAD	C9-C8	4.43	1.45	1.39
3	A	5000	FAD	P-O3P	3.81	1.63	1.59
3	A	5000	FAD	C4A-N3A	3.72	1.41	1.34
3	A	5000	FAD	C6-C5X	2.92	1.44	1.40
3	A	5000	FAD	C9A-N10	2.57	1.45	1.41
3	A	5000	FAD	C9A-C5X	2.54	1.45	1.41
3	A	5000	FAD	C10-N1	2.48	1.38	1.33
3	A	5000	FAD	O4-C4	2.14	1.27	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5000	FAD	O2A-PA-O3P	-11.33	76.64	107.27
3	A	5000	FAD	O3P-PA-O1A	-6.62	90.80	110.70
3	A	5000	FAD	O2A-PA-O1A	4.01	131.12	112.44
3	A	5000	FAD	O5B-C5B-C4B	3.49	120.89	108.99
3	A	5000	FAD	PA-O5B-C5B	2.59	136.19	121.35
3	A	5000	FAD	O2A-PA-O5B	2.59	119.30	107.57
3	A	5000	FAD	O3P-P-O1P	-2.54	103.05	110.70
3	A	5000	FAD	C4A-N9A-C8A	-2.37	103.25	105.74

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5000	FAD	C5B-O5B-PA-O2A
3	A	5000	FAD	C4B-C5B-O5B-PA
3	A	5000	FAD	C3B-C4B-C5B-O5B
3	A	5000	FAD	O4B-C4B-C5B-O5B
3	A	5000	FAD	C2B-C1B-N9A-C8A
3	A	5000	FAD	P-O3P-PA-O1A

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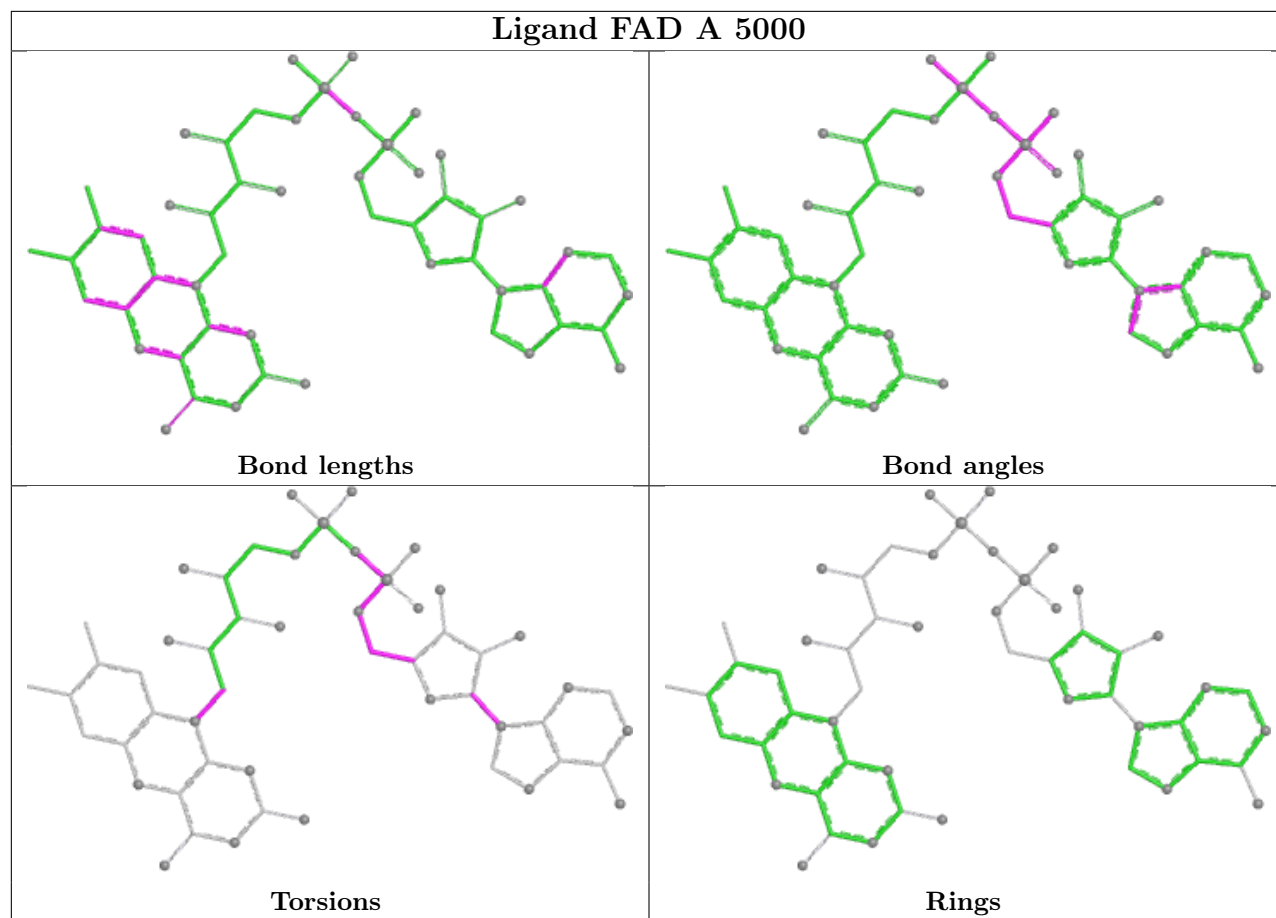
Mol	Chain	Res	Type	Atoms
3	A	5000	FAD	C2'-C1'-N10-C10
3	A	5000	FAD	C2B-C1B-N9A-C4A
3	A	5000	FAD	O4B-C1B-N9A-C8A
3	A	5000	FAD	P-O3P-PA-O2A

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5000	FAD	5	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	647/664 (97%)	0.04	13 (2%) 65 56	48, 78, 119, 163	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	609	SER	5.8
1	A	455	ILE	4.4
1	A	610	THR	3.4
1	A	462	TYR	3.3
1	A	612	GLN	3.1
1	A	611	SER	3.0
1	A	463	LYS	3.0
1	A	835	THR	3.0
1	A	454	LYS	2.6
1	A	459	HIS	2.5
1	A	584	ILE	2.3
1	A	607	THR	2.2
1	A	478	PHE	2.1

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](#)

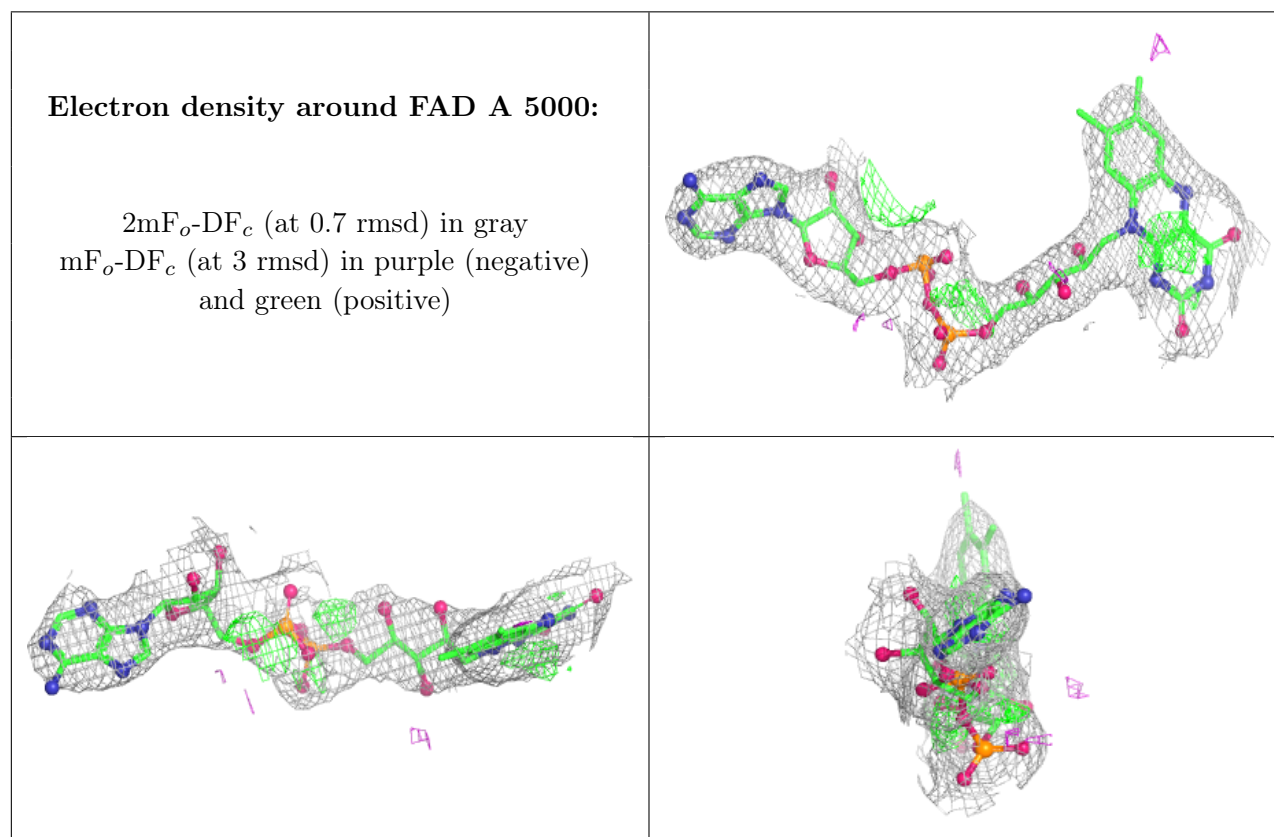
There are no oligosaccharides in this entry.

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	HG	A	2	1/1	0.94	0.08	182,182,182,182	0
2	HG	A	3	1/1	0.94	0.05	189,189,189,189	0
3	FAD	A	5000	53/53	0.95	0.10	52,65,77,79	0
2	HG	A	1	1/1	0.98	0.07	171,171,171,171	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.