Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:27 AM GMT

PDB ID	:	2H94
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

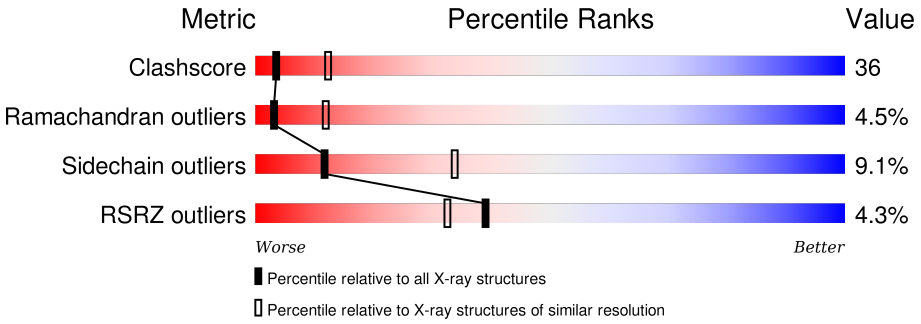
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	4% 46% 44% 6%

2 Entry composition

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.

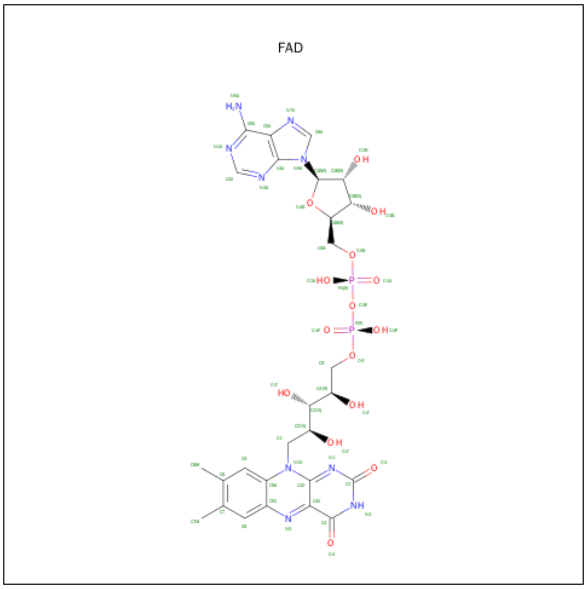
- Molecule 1 is a protein called Lysine-specific histone demethylase 1.

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 (three-letter code: HG) (formula: Hg).

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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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.

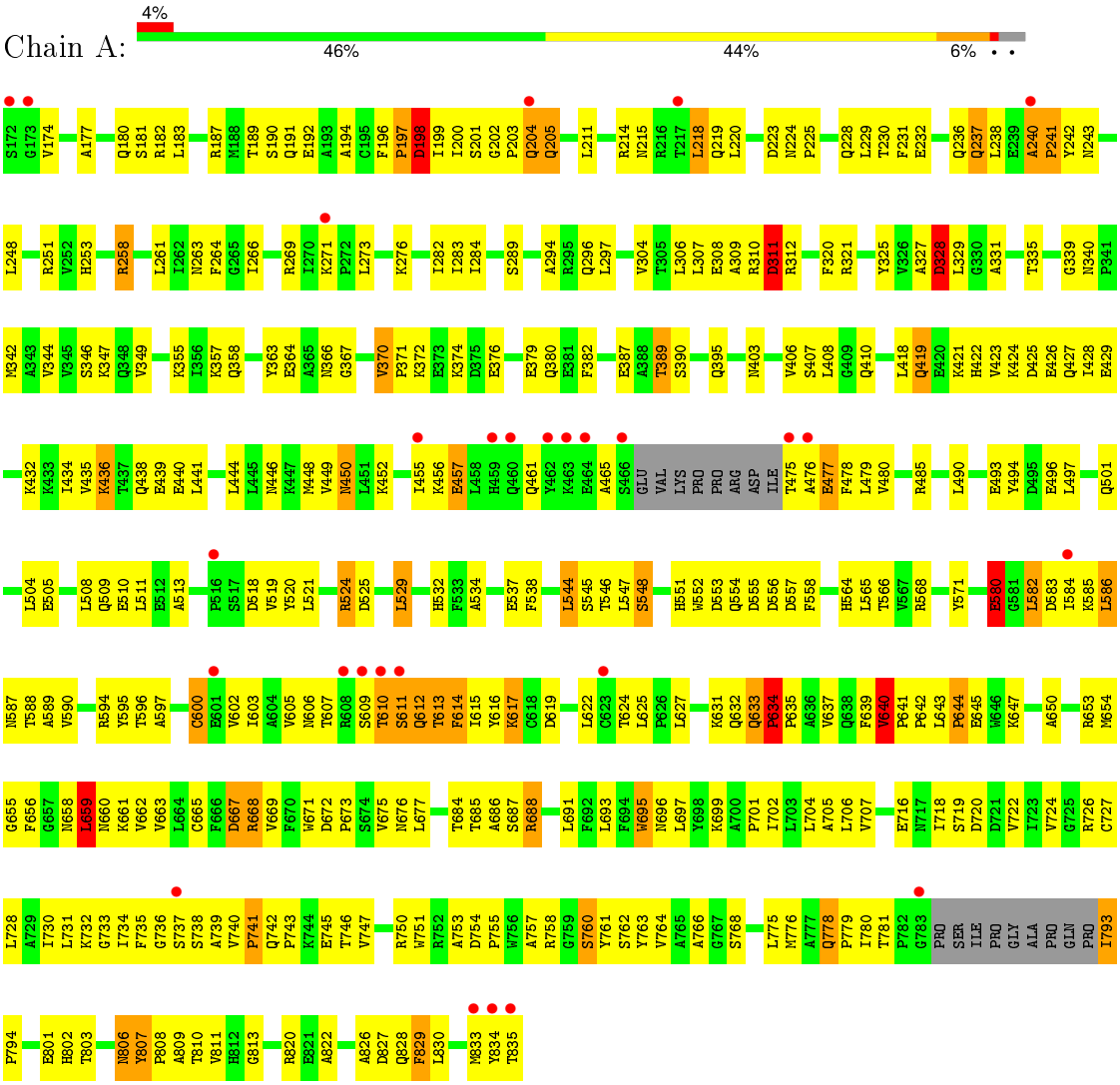
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	20	Total O 20 20	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain A:



4 Data and refinement statistics (i)

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 19.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	88.8 (20.00-2.90) 88.6 (19.91-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.67 (at 2.88Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.281 0.236 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	73.9	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 24948 reflections	Xtriage
F_o,F_c correlation	0.93	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 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: HG, FAD

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	0.44	0/5182	0.69	2/7020 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	640	VAL	C-N-CD	5.91	140.82	128.40
1	A	611	SER	CB-CA-C	5.32	120.21	110.10

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	371	0
2	A	3	0	0	0	0
3	A	53	0	31	7	0
4	A	20	0	0	4	0
All	All	5153	0	5131	371	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 36.

All (371) 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: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:613:THR:C	1:A:614:PHE:HD2	1.85	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: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:HG2	1:A:310:ARG:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:H	1:A:263:ASN:HD21	1.34	0.72
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:320:PHE:HB3	1:A:327:ALA:HB3	1.74	0.70
1:A:240:ALA:HB3	1:A:241:PRO:HD3	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: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:O	1:A:610:THR:HG22	1.96	0.66
1:A:826:ALA:HB1	1:A:830:LEU:HD12	1.77	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:605:VAL:HG12	1:A:606:ASN:O	1.96	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:802:HIS:H	1:A:802:HIS:CD2	2.13	0.65
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:640:VAL:HG12	1:A:641:PRO:CD	2.28	0.63
1:A:595:TYR:HA	1:A:600:CYS:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:TYR:N	1:A:808:PRO:CD	2.60	0.63
1:A:612:GLN:O	1:A:613:THR:OG1	2.09	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: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:418:LEU:O	1:A:421:LYS:HB3	1.98	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:794:PRO:HD2	1:A:828:GLN:CD	2.22	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:197:PRO:C	1:A:199:ILE:H	2.04	0.60
1:A:358:GLN:CD	1:A:358:GLN:H	2.05	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:778:GLN:HE21	1:A:779:PRO:HD2	1.67	0.59
1:A:633:GLN:OE1	1:A:633:GLN:HA	2.02	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:HG22	1:A:835:THR:O	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
1:A:196:PHE:O	1:A:200:ILE:HD11	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:585:LYS:NZ	1:A:614:PHE:HE1	2.01	0.56
1:A:568:ARG:HG3	1:A:568:ARG:HH11	1.70	0.56
1:A:199:ILE:HD12	1:A:835:THR:HB	1.87	0.56
1:A:194:ALA:O	1:A:197:PRO:HD3	2.05	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:778:GLN:HE21	1:A:778:GLN:CA	2.17	0.56
1:A:603:ILE:HG13	1:A:615:ILE:HG12	1.86	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:728:LEU:O	1:A:732:LYS:HG2	2.06	0.55
1:A:494:TYR:CD2	1:A:494:TYR:O	2.59	0.55
1:A:803:THR:CG2	1:A:820:ARG:NH2	2.64	0.55
1:A:794:PRO:CD	1:A:828:GLN:HE22	2.19	0.55
1:A:640:VAL:HG12	1:A:641:PRO:N	2.20	0.55
1:A:624:THR:HG22	1:A:624:THR:O	2.06	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: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:761:TYR:CD1	1:A:809:ALA:HB1	2.44	0.53
1:A:546:THR:HG22	1:A:763:TYR:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:THR:HG22	1:A:390:SER:N	2.24	0.53
1:A:228:GLN:HA	1:A:263:ASN:ND2	2.25	0.53
1:A:775:LEU:O	1:A:778:GLN:HB2	2.09	0.53
1:A:684:THR:HB	1:A:686:ALA:O	2.09	0.53
1:A:220:LEU:HD22	1:A:237:GLN:OE1	2.08	0.53
1:A:606:ASN:OD1	1:A:607:THR:N	2.41	0.52
1:A:181:SER:OG	1:A:218:LEU:HG	2.09	0.52
1:A:198:ASP:CA	1:A:201:SER:HB2	2.30	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:448:MET:HG3	1:A:497:LEU:HD23	1.91	0.52
1:A:183:LEU:HD11	1:A:261:LEU:HD13	1.91	0.52
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:446:ASN:O	1:A:450:ASN:HB2	2.10	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:695:TRP:CZ3	1:A:706:LEU:HD11	2.46	0.51
1:A:613:THR:C	1:A:614:PHE:CD2	2.75	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:632:GLN:NE2	1:A:758:ARG:NH2	2.59	0.50
1:A:423:VAL:O	1:A:427:GLN:HB2	2.12	0.50
1:A:357:LYS:N	1:A:676:ASN:HD22	2.09	0.50
1:A:553:ASP:O	1:A:555:ASP:N	2.43	0.50
1:A:436:LYS:O	1:A:440:GLU:HG3	2.10	0.50
1:A:548:SER:HB2	1:A:766:ALA:HA	1.94	0.50
1:A:379:GLU:O	1:A:382:PHE:HB3	2.12	0.50
1:A:425:ASP:C	1:A:427:GLN:H	2.14	0.50
1:A:310:ARG:HD2	4:A:5010:HOH:O	2.12	0.49
1:A:558:PHE:CD1	1:A:806:ASN:HB3	2.47	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:448:MET:HG2	1:A:497:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:HD2	1:A:807:TYR:OH	2.12	0.49
1:A:435:VAL:O	1:A:439:GLU:HG3	2.13	0.49
1:A:568:ARG:NH1	1:A:568:ARG:HG3	2.27	0.49
1:A:230:THR:HG22	1:A:231:PHE:N	2.27	0.48
1:A:538:PHE:CE1	1:A:706:LEU:HD13	2.48	0.48
1:A:335:THR:HG22	1:A:564:HIS:CD2	2.49	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:637:VAL:HG23	1:A:639:PHE:CE1	2.49	0.48
1:A:477:GLU:HG3	1:A:478:PHE:N	2.29	0.48
1:A:534:ALA:HA	1:A:537:GLU:HG3	1.95	0.48
1:A:829:PHE:O	1:A:830:LEU:HD23	2.13	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:633:GLN:O	1:A:634:PRO:C	2.51	0.48
1:A:204:GLN:HG2	1:A:205:GLN:H	1.79	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: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:667:ASP:O	1:A:668:ARG:HB3	2.15	0.47
1:A:374:LYS:HE2	1:A:524:ARG:HH11	1.73	0.47
1:A:425:ASP:C	1:A:427:GLN:N	2.68	0.47
1:A:643:LEU:O	1:A:644:PRO:O	2.32	0.47
1:A:661:LYS:HG2	1:A:706:LEU:CD2	2.45	0.47
1:A:225:PRO:CB	1:A:344:VAL:HG13	2.45	0.47
1:A:640:VAL:O	1:A:641:PRO:C	2.47	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:537:GLU:CD	1:A:688:ARG:HH11	2.19	0.46
1:A:732:LYS:HB3	1:A:740:VAL:CG2	2.46	0.46
1:A:342:MET:O	1:A:346:SER:HB2	2.14	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: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:349:VAL:HG12	1:A:349:VAL:O	2.16	0.46
1:A:829:PHE:CD1	1:A:829:PHE:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:THR:CG2	1:A:820:ARG:HH12	2.15	0.46
1:A:639:PHE:O	1:A:640:VAL:C	2.54	0.46
1:A:663:VAL:CG1	1:A:702:ILE:HD11	2.46	0.46
1:A:382:PHE:CD1	1:A:532:HIS:HB3	2.51	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:731:LEU:C	1:A:733:GLY:H	2.18	0.45
1:A:331:ALA:HA	3:A:5000:FAD:C4X	2.47	0.45
1:A:794:PRO:HD2	1:A:828:GLN:OE1	2.17	0.45
1:A:509:GLN:O	1:A:513:ALA:HB3	2.16	0.45
1:A:639:PHE:N	1:A:639:PHE:CD1	2.84	0.45
1:A:655:GLY:O	1:A:762:SER:HA	2.16	0.45
1:A:304:VAL:HG23	1:A:304:VAL:O	2.17	0.45
1:A:310:ARG:O	1:A:311:ASP:OD1	2.35	0.45
1:A:695:TRP:NE1	1:A:697:LEU:HD11	2.32	0.45
1:A:558:PHE:CE1	1:A:806:ASN:HB3	2.52	0.45
1:A:296:GLN:HB2	1:A:822:ALA:HB1	1.99	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:753:ALA:O	1:A:754:ASP:C	2.54	0.45
1:A:625:LEU:HD11	1:A:637:VAL:HG21	1.98	0.45
1:A:624:THR:CG2	1:A:624:THR:O	2.65	0.45
1:A:671:TRP:HB2	4:A:5009:HOH:O	2.15	0.45
1:A:248:LEU:O	1:A:251:ARG:HB2	2.17	0.44
1:A:611:SER:O	1:A:612:GLN:CB	2.65	0.44
1:A:640:VAL:HB	1:A:641:PRO:CD	2.48	0.44
1:A:182:ARG:HG3	1:A:182:ARG:HH11	1.82	0.44
1:A:722:VAL:O	1:A:726:ARG:HG3	2.17	0.44
1:A:424:LYS:HD3	1:A:427:GLN:OE1	2.17	0.44
1:A:668:ARG:NH2	1:A:741:PRO:HG3	2.32	0.44
1:A:309:ALA:HB1	1:A:589:ALA:HB2	2.00	0.44
1:A:691:LEU:HA	1:A:706:LEU:O	2.17	0.44
1:A:340:ASN:OD1	1:A:342:MET:N	2.42	0.44
1:A:297:LEU:HB2	1:A:304:VAL:HG11	1.99	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:444:LEU:HD23	1:A:444:LEU:C	2.37	0.44
1:A:695:TRP:CE3	1:A:706:LEU:HD11	2.52	0.44
1:A:718:ILE:HG22	1:A:719:SER:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:ILE:CG2	1:A:722:VAL:HB	2.48	0.44
1:A:355:LYS:HG2	1:A:565:LEU:CD2	2.46	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:426:GLU:HA	1:A:429:GLU:CD	2.38	0.44
1:A:177:ALA:HB1	1:A:218:LEU:HB3	1.99	0.44
1:A:449:VAL:HA	1:A:452:LYS:CD	2.41	0.44
1:A:546:THR:CG2	1:A:763:TYR:CE1	3.01	0.44
1:A:282:ILE:HG21	1:A:602:VAL:HG21	2.00	0.43
1:A:776:MET:HA	1:A:776:MET:HE2	2.00	0.43
1:A:308:GLU:HG3	1:A:310:ARG:H	1.82	0.43
1:A:760:SER:HA	3:A:5000:FAD:C8M	2.49	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: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:432:LYS:O	1:A:436:LYS:HD3	2.18	0.43
1:A:644:PRO:CD	1:A:780:ILE:HD13	2.48	0.43
1:A:633:GLN:OE1	1:A:633:GLN:CA	2.66	0.43
1:A:363:TYR:HD2	1:A:367:GLY:O	2.01	0.43
1:A:199:ILE:HD13	1:A:835:THR:O	2.18	0.43
1:A:198:ASP:C	1:A:200:ILE:N	2.71	0.43
1:A:441:LEU:HD11	1:A:505:GLU:HA	1.99	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:340:ASN:OD1	1:A:342:MET:CB	2.67	0.43
1:A:693:LEU:HD23	1:A:706:LEU:HD12	2.00	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:731:LEU:C	1:A:733:GLY:N	2.71	0.42
1:A:590:VAL:O	1:A:637:VAL:HG12	2.19	0.42
1:A:760:SER:HA	3:A:5000:FAD:HM83	2.01	0.42
1:A:658:ASN:ND2	1:A:659:LEU:H	2.18	0.42
1:A:485:ARG:NH1	1:A:485:ARG:HG2	2.34	0.42
1:A:596:THR:HG22	1:A:597:ALA:H	1.84	0.42
1:A:834:TYR:HD1	1:A:835:THR:N	2.17	0.42
1:A:611:SER:HB3	1:A:614:PHE:HE2	1.83	0.42
1:A:364:GLU:C	1:A:366:ASN:H	2.23	0.42
1:A:230:THR:CG2	1:A:231:PHE:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:GLU:HG2	1:A:809:ALA:HA	2.01	0.42
1:A:695:TRP:HE1	1:A:697:LEU:HD21	1.85	0.42
1:A:174:VAL:O	1:A:215:ASN:HB3	2.20	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:407:SER:CB	1:A:545:SER:O	2.67	0.41
1:A:355:LYS:HA	1:A:565:LEU:CD2	2.50	0.41
1:A:197:PRO:C	1:A:199:ILE:N	2.66	0.41
1:A:456:LYS:HA	1:A:456:LYS:HD2	1.94	0.41
1:A:477:GLU:CG	1:A:478:PHE:H	2.25	0.41
1:A:427:GLN:HE21	1:A:518:ASP:HA	1.84	0.41
1:A:183:LEU:HD12	1:A:218:LEU:HD21	2.01	0.41
1:A:192:GLU:OE2	1:A:214:ARG:HD2	2.20	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:659:LEU:HG	3:A:5000:FAD:HM73	2.03	0.41
1:A:807:TYR:O	1:A:813:GLY:HA3	2.20	0.41
1:A:634:PRO:HB2	1:A:635:PRO:CA	2.51	0.41
1:A:198:ASP:OD1	1:A:201:SER:O	2.39	0.41
1:A:552:TRP:CE2	1:A:553:ASP:OD2	2.74	0.41
1:A:510:GLU:HG2	1:A:510:GLU:O	2.21	0.41
1:A:198:ASP:OD1	1:A:202:GLY:HA2	2.20	0.41
1:A:501:GLN:O	1:A:505:GLU:CB	2.69	0.41
1:A:660:ASN:HD21	1:A:751:TRP:N	2.04	0.41
1:A:793:ILE:HA	1:A:794:PRO:HD3	1.72	0.41
1:A:544:LEU:HD12	1:A:544:LEU:HA	1.85	0.41
1:A:546:THR:O	1:A:546:THR:HG22	2.20	0.41
1:A:762:SER:OG	1:A:801:GLU:OE2	2.30	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:518:ASP:O	1:A:519:VAL:HG23	2.21	0.41
1:A:419:GLN:HA	1:A:422:HIS:HD2	1.85	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:627:LEU:HB3	1:A:656:PHE:CD1	2.56	0.41
1:A:321:ARG:NH1	1:A:321:ARG:HG2	2.36	0.41
1:A:662:VAL:HG11	1:A:727:CYS:SG	2.61	0.40
1:A:370:VAL:HA	1:A:371:PRO:HD2	1.86	0.40
1:A:640:VAL:O	1:A:642:PRO:N	2.54	0.40
1:A:633:GLN:HB3	1:A:634:PRO:HD3	2.02	0.40
1:A:811:VAL:HG23	3:A:5000:FAD:C2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PHE:HB3	1:A:200:ILE:CG1	2.51	0.40
1:A:418:LEU:HA	1:A:418:LEU:HD23	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	641/664 (96%)	532 (83%)	80 (12%)	29 (4%)	3 12

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

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Mol	Chain	Res	Type
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
1	A	203	PRO

5.3.2 Protein sidechains (i)

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%)	499 (91%)	50 (9%)	12 34

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	204	GLN
1	A	205	GLN
1	A	218	LEU
1	A	224	ASN
1	A	237	GLN
1	A	258	ARG
1	A	311	ASP
1	A	328	ASP
1	A	387	GLU
1	A	389	THR
1	A	395	GLN
1	A	419	GLN
1	A	436	LYS
1	A	450	ASN

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Mol	Chain	Res	Type
1	A	457	GLU
1	A	493	GLU
1	A	496	GLU
1	A	524	ARG
1	A	525	ASP
1	A	529	LEU
1	A	544	LEU
1	A	548	SER
1	A	556	ASP
1	A	557	ASP
1	A	571	TYR
1	A	580	GLU
1	A	582	LEU
1	A	583	ASP
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	645	GLU
1	A	659	LEU
1	A	667	ASP
1	A	668	ARG
1	A	677	LEU
1	A	688	ARG
1	A	695	TRP
1	A	696	ASN
1	A	699	LYS
1	A	707	VAL
1	A	778	GLN
1	A	793	ILE
1	A	806	ASN
1	A	829	PHE
1	A	833	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	205	GLN
1	A	224	ASN

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Mol	Chain	Res	Type
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	461	GLN
1	A	509	GLN
1	A	592	GLN
1	A	632	GLN
1	A	658	ASN
1	A	660	ASN
1	A	676	ASN
1	A	742	GLN
1	A	778	GLN
1	A	802	HIS
1	A	812	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

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	-	48,58,58	1.74	8 (16%)	54,89,89	2.60	10 (18%)

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	-	-	0/30/50/50	0/6/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5000	FAD	C4X-C10	2.03	1.44	1.41
3	A	5000	FAD	O4B-C1B	2.13	1.43	1.41
3	A	5000	FAD	C2A-N3A	2.28	1.36	1.32
3	A	5000	FAD	C9-C8	2.85	1.45	1.37
3	A	5000	FAD	C4A-N3A	3.90	1.41	1.35
3	A	5000	FAD	C4-N3	4.29	1.41	1.33
3	A	5000	FAD	C9A-N10	4.95	1.45	1.38
3	A	5000	FAD	C4X-N5	4.98	1.41	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	5000	FAD	O3P-PA-O5B	-7.69	82.53	102.94
3	A	5000	FAD	O2A-PA-O3P	-6.27	76.64	105.09
3	A	5000	FAD	C4X-C4-N3	-6.15	115.18	123.59
3	A	5000	FAD	C4X-C10-N10	-2.40	119.11	120.52
3	A	5000	FAD	O2A-PA-O5B	2.15	119.30	108.46
3	A	5000	FAD	O5B-C5B-C4B	3.19	120.89	109.12
3	A	5000	FAD	O2A-PA-O1A	3.43	131.12	112.53
3	A	5000	FAD	O3P-P-O5'	3.84	113.12	102.94
3	A	5000	FAD	P-O3P-PA	5.19	147.29	132.73
3	A	5000	FAD	C4-N3-C2	10.88	124.65	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5000	FAD	7	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.07	28 (4%) 39 32	48, 78, 119, 163	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	610	THR	11.9
1	A	609	SER	11.4
1	A	475	THR	7.2
1	A	611	SER	7.0
1	A	835	THR	6.9
1	A	834	TYR	5.3
1	A	476	ALA	5.0
1	A	463	LYS	4.6
1	A	608	ARG	4.0
1	A	462	TYR	3.9
1	A	172	SER	3.8
1	A	459	HIS	3.1
1	A	516	PRO	3.0
1	A	464	GLU	2.9
1	A	737	SER	2.7
1	A	455	ILE	2.7
1	A	173	GLY	2.6
1	A	466	SER	2.6
1	A	204	GLN	2.6
1	A	460	GLN	2.5
1	A	783	GLY	2.5
1	A	833	MET	2.4
1	A	240	ALA	2.4
1	A	601	GLU	2.4
1	A	623	CYS	2.3
1	A	584	ILE	2.2
1	A	217	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	271	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	FAD	A	5000	53/53	0.97	0.23	0.94	52,65,77,79	0
2	HG	A	2	1/1	0.84	0.07	-	182,182,182,182	0
2	HG	A	3	1/1	0.94	0.08	-	189,189,189,189	0
2	HG	A	1	1/1	0.95	0.08	-	171,171,171,171	0

6.5 Other polymers (i)

There are no such residues in this entry.