Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 07:59 PM GMT

PDB ID : 3KV5

Title : Structure of KIAA1718, human Jumonji demethylase, in complex with N-oxalylglycine

Authors : Horton, J.R.; Upadhyay, A.K.; Qi, H.H.; Zhang, X.; Shi, Y.; Cheng, X.

Deposited on : 2009-11-29

Resolution : 2.39 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html
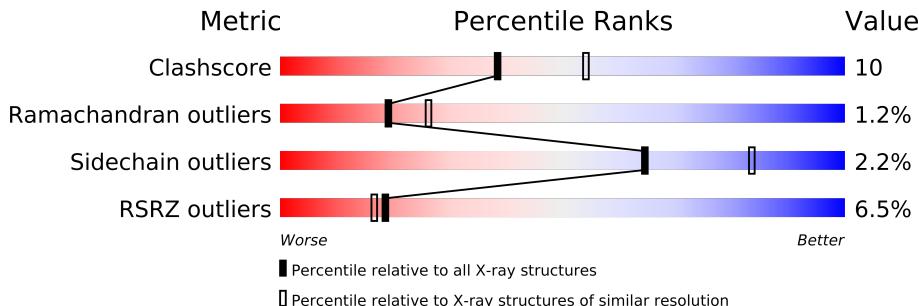
1 Overall quality at a glance ⓘ
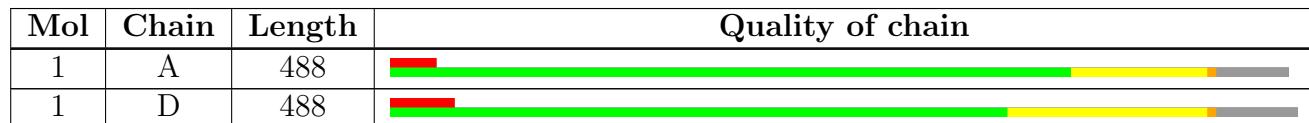
The reported resolution of this entry is 2.39 Å.

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	Percentile Ranks	Value
Clashscore		10
Ramachandran outliers		1.2%
Sidechain outliers		2.2%
RSRZ outliers		6.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	488	
1	D	488	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	FE2	A	492	-	X
3	FE2	D	491	-	X
5	OGA	A	5798	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7456 atoms, of which 0 are hydrogen and 0 are deuterium.

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 JmjC domain-containing histone demethylation protein 1D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	445	Total	C	N	O	S	0	0	0
			3512	2260	591	635	26			
1	A	447	Total	C	N	O	S	0	2	0
			3589	2316	607	640	26			
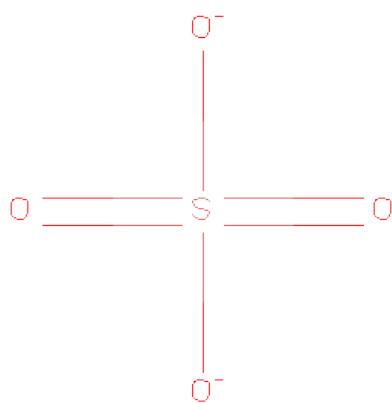
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).
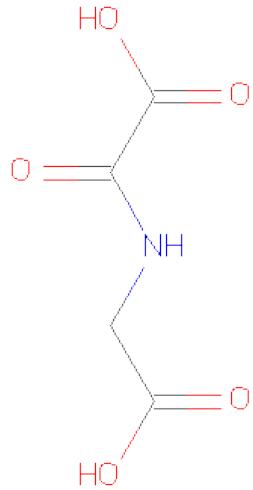
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Fe	0	0
			2	2		
3	D	1	Total	Fe	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0

- Molecule 5 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: $C_4H_5NO_5$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 10	C 4	N 1	O 5	0	0

- Molecule 6 is water.
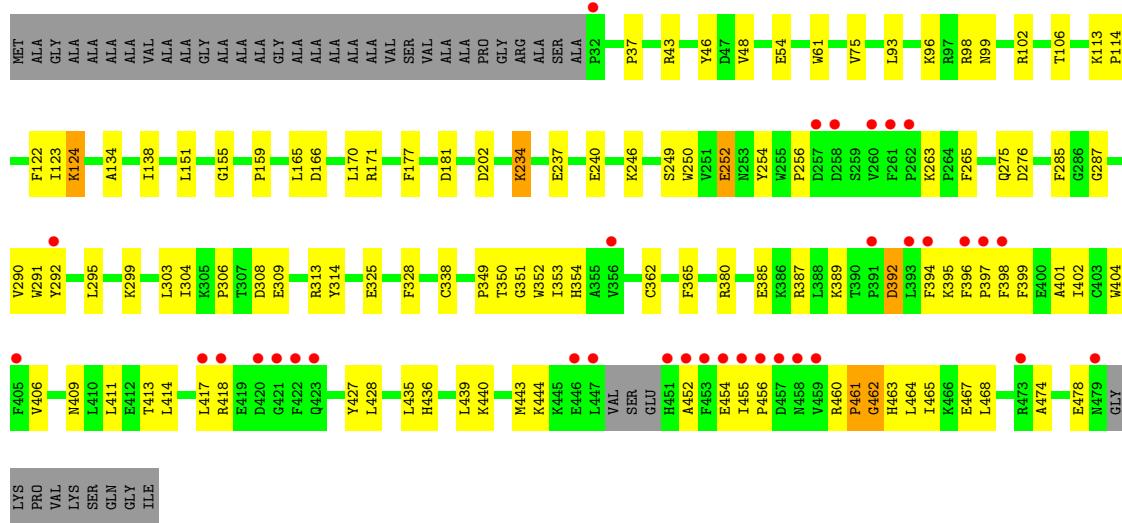
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	161	Total 161	O 161	0	0
6	A	167	Total 167	O 167	0	0

3 Residue-property plots ⓘ

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.
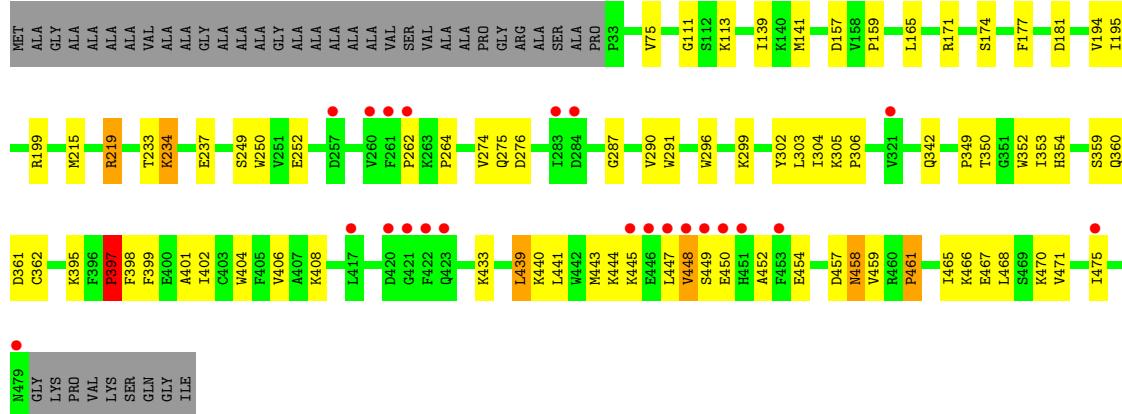
• Molecule 1: JmjC domain-containing histone demethylation protein 1D

Chain D:

• Molecule 1: JmjC domain-containing histone demethylation protein 1D

Chain A:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.70Å 125.60Å 206.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.82 – 2.39 34.82 – 2.38	Depositor EDS
% Data completeness (in resolution range)	87.7 (34.82-2.39) 86.9 (34.82-2.38)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.216 , 0.245 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 29.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.46, < L^2 > = 0.28$	Xtriage
Outliers	2 of 61928 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7456	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OGA, ZN, FE2, SO4

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	0.37	0/3694	0.61	0/5019
1	D	0.36	0/3612	0.60	0/4913
All	All	0.36	0/7306	0.61	0/9932

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3589	0	3463	58	0
1	D	3512	0	3340	79	0
2	A	2	0	0	0	0
2	D	2	0	0	0	0
3	A	2	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	A	10	0	3	0	0
6	A	167	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	161	0	0	3	0
All	All	7456	0	6806	137	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (137) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:234:LYS:HZ1	1:A:234:LYS:H	1.16	0.94
1:D:392:ASP:HA	1:D:395:LYS:HG2	1.55	0.88
1:A:234:LYS:NZ	1:A:234:LYS:H	1.75	0.85
1:A:458:ASN:HD22	1:A:458:ASN:H	1.36	0.72
1:D:171:ARG:HB3	1:D:240:GLU:HB2	1.72	0.71
1:A:306:PRO:HG3	1:A:352:TRP:HA	1.73	0.71
1:A:398:PHE:HB3	1:A:401:ALA:HB3	1.74	0.69
1:A:287:GLY:O	1:A:350:THR:HG23	1.93	0.68
1:A:249:SER:HB3	1:A:252:GLU:HB2	1.76	0.66
1:A:408:LYS:HD2	1:A:459:VAL:HG12	1.77	0.66
1:A:458:ASN:HD22	1:A:458:ASN:N	1.94	0.65
1:A:219:ARG:HG3	1:A:219:ARG:HH11	1.60	0.65
1:D:435:LEU:O	1:D:439:LEU:HB2	1.97	0.64
1:A:75:VAL:HG11	1:A:199:ARG:HD2	1.80	0.64
1:A:402:ILE:O	1:A:406:VAL:HG23	1.99	0.63
1:A:459:VAL:O	1:A:461:PRO:HD3	2.00	0.62
1:D:349:PRO:HG2	1:D:352:TRP:CD1	2.35	0.61
1:D:122:PHE:HD2	1:D:123:ILE:HD12	1.66	0.61
1:D:452:ALA:HA	1:D:455:ILE:HG13	1.82	0.60
1:A:399:PHE:O	1:A:402:ILE:HG22	2.02	0.60
1:A:264:PRO:HB3	1:A:397:PRO:HB2	1.85	0.58
1:A:349:PRO:HG2	1:A:352:TRP:CD1	2.40	0.57
1:D:414:LEU:HD21	1:D:428:LEU:CD2	2.35	0.57
1:A:404:TRP:CZ3	1:A:439:LEU:HG	2.40	0.56
1:D:404:TRP:CH2	1:D:439:LEU:HG	2.41	0.56
1:D:249:SER:HB3	1:D:252:GLU:HB2	1.88	0.55
1:A:234:LYS:N	1:A:234:LYS:HZ1	1.96	0.55
1:D:452:ALA:HA	1:D:455:ILE:CD1	2.37	0.55
1:D:299:LYS:HE2	1:D:362:CYS:SG	2.47	0.55
1:D:392:ASP:C	1:D:394:PHE:H	2.09	0.55
1:A:445:LYS:O	1:A:448:VAL:HG12	2.08	0.55
1:D:263:LYS:HD3	1:D:265:PHE:CZ	2.42	0.54
1:D:295:LEU:HD22	1:D:365:PHE:HE1	1.72	0.54
1:D:428:LEU:HD23	1:D:428:LEU:O	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:98:ARG:HD2	1:D:106:THR:O	2.08	0.54
1:D:452:ALA:HA	1:D:455:ILE:CG1	2.37	0.53
1:A:471:VAL:O	1:A:475:ILE:HD13	2.07	0.53
1:D:398:PHE:HB3	1:D:401:ALA:HB3	1.89	0.53
1:D:250:TRP:HB3	1:D:402:ILE:HD11	1.89	0.53
1:D:254:TYR:O	1:D:256:PRO:HD3	2.08	0.53
1:D:411:LEU:HD22	1:D:464:LEU:HD12	1.90	0.53
1:A:398:PHE:HB3	1:A:401:ALA:CB	2.39	0.52
1:D:399:PHE:O	1:D:402:ILE:HG22	2.09	0.52
1:D:454:GLU:O	1:D:456:PRO:HD3	2.09	0.52
1:A:443:MET:O	1:A:448:VAL:HB	2.09	0.51
1:A:304:ILE:HB	1:A:353:ILE:HB	1.91	0.51
1:A:275:GLN:O	1:A:276:ASP:HB2	2.11	0.51
1:D:240:GLU:OE1	1:D:246:LYS:NZ	2.44	0.51
1:A:262:PRO:HG2	1:A:398:PHE:HE2	1.76	0.51
1:D:402:ILE:O	1:D:406:VAL:HG23	2.11	0.51
1:D:309:GLU:HG2	1:D:313:ARG:HE	1.75	0.50
1:D:440:LYS:HG2	1:D:465:ILE:CD1	2.41	0.50
1:D:37:PRO:HD2	6:D:620:HOH:O	2.11	0.50
1:D:418:ARG:NH2	1:D:474:ALA:HB1	2.27	0.50
1:D:275:GLN:O	1:D:276:ASP:HB2	2.11	0.50
1:D:452:ALA:HA	1:D:455:ILE:HD12	1.93	0.50
1:D:285:PHE:HA	1:D:385:GLU:OE2	2.12	0.49
1:D:440:LYS:HG2	1:D:465:ILE:HD11	1.93	0.49
1:D:404:TRP:CZ3	1:D:439:LEU:HG	2.47	0.49
1:D:234:LYS:HE3	1:D:237:GLU:OE1	2.12	0.49
1:A:466:LYS:O	1:A:470:LYS:HG3	2.13	0.48
1:D:413:THR:O	1:D:417:LEU:HD23	2.13	0.48
1:D:414:LEU:HD21	1:D:428:LEU:HD22	1.95	0.48
1:A:450:GLU:C	1:A:452:ALA:H	2.18	0.48
1:A:159:PRO:HG2	1:A:303:LEU:HD13	1.95	0.48
1:D:392:ASP:C	1:D:394:PHE:N	2.68	0.47
1:D:411:LEU:HD21	1:D:467:GLU:HG2	1.96	0.47
1:D:428:LEU:HD23	1:D:428:LEU:C	2.34	0.47
1:D:54:GLU:HB2	1:D:61:TRP:CE2	2.49	0.47
1:D:461:PRO:O	1:D:463:HIS:N	2.47	0.46
1:D:387:ARG:C	1:D:389:LYS:H	2.18	0.46
1:D:461:PRO:O	1:D:462:GLY:C	2.53	0.46
1:A:441:LEU:O	1:A:447:LEU:HD12	2.15	0.46
1:A:359:SER:C	1:A:360:GLN:HG2	2.35	0.46
1:D:440:LYS:CG	1:D:465:ILE:HD11	2.45	0.46
1:A:215:MET:CE	1:A:215:MET:HA	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:194:VAL:HG12	1:A:195:ILE:N	2.31	0.46
1:D:124:LYS:HD2	6:D:635:HOH:O	2.15	0.46
1:D:177:PHE:CE1	1:D:181:ASP:HB3	2.51	0.45
1:A:467:GLU:O	1:A:471:VAL:HG23	2.16	0.45
1:D:165:LEU:CD2	1:D:170:LEU:HD23	2.47	0.45
1:D:151:LEU:O	1:D:155:GLY:N	2.48	0.45
1:D:418:ARG:HH11	1:D:418:ARG:HG3	1.81	0.45
1:D:308:ASP:OD1	1:D:380:ARG:NH2	2.48	0.45
1:D:96:LYS:O	1:D:106:THR:HG22	2.17	0.44
1:A:290:VAL:HG22	1:A:291:TRP:N	2.32	0.44
1:D:304:ILE:HB	1:D:353:ILE:HB	2.00	0.44
1:A:171:ARG:NH1	1:A:237:GLU:O	2.51	0.44
1:D:290:VAL:HG12	1:D:291:TRP:N	2.33	0.44
1:D:99:ASN:ND2	1:D:102:ARG:H	2.15	0.44
1:D:114:PRO:HG2	1:D:325:GLU:OE2	2.17	0.44
1:A:305:LYS:HA	1:A:306:PRO:HD3	1.78	0.43
1:A:443:MET:O	1:A:444:LYS:C	2.56	0.43
1:D:285:PHE:HB2	1:D:396:PHE:H	1.83	0.43
1:D:440:LYS:O	1:D:443:MET:HB2	2.17	0.43
1:D:252:GLU:OE1	1:D:252:GLU:HA	2.19	0.43
1:D:460:ARG:O	1:D:461:PRO:O	2.36	0.43
1:D:303:LEU:HD23	1:D:354:HIS:HB3	2.00	0.43
1:A:302:TYR:O	1:A:354:HIS:HA	2.18	0.43
1:D:134:ALA:CB	1:D:338:CYS:HB2	2.48	0.43
1:A:249:SER:CB	1:A:252:GLU:HB2	2.48	0.43
1:A:219:ARG:NH1	1:A:274:VAL:HB	2.34	0.43
1:A:290:VAL:CG2	1:A:291:TRP:N	2.81	0.43
1:D:427:TYR:CG	1:D:428:LEU:N	2.87	0.42
1:D:165:LEU:HD21	1:D:170:LEU:HD23	2.01	0.42
1:A:475:ILE:HD12	1:A:475:ILE:N	2.34	0.42
1:A:262:PRO:HG2	1:A:398:PHE:CE2	2.53	0.42
1:A:433:LYS:HE3	1:A:433:LYS:HB2	1.87	0.42
1:D:113:LYS:HA	1:D:114:PRO:HD3	1.78	0.42
1:A:177:PHE:CE1	1:A:181:ASP:HB3	2.54	0.42
1:D:287:GLY:O	1:D:350:THR:HG23	2.19	0.42
1:A:250:TRP:CD2	1:A:406:VAL:HG21	2.55	0.42
1:A:440:LYS:HA	1:A:465:ILE:HD13	2.01	0.42
1:A:395:LYS:HB3	6:A:518:HOH:O	2.19	0.42
1:D:411:LEU:HD13	1:D:468:LEU:HD12	2.01	0.42
1:D:138:ILE:HG22	1:D:159:PRO:HB2	2.02	0.42
1:A:139:ILE:HG22	1:A:141:MET:HG3	2.02	0.42
1:D:392:ASP:OD1	1:D:395:LYS:HD3	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:219:ARG:HG3	1:A:219:ARG:NH1	2.31	0.41
1:D:246:LYS:HB2	1:D:246:LYS:HE3	1.75	0.41
1:D:314:TYR:HA	1:D:328:PHE:CE1	2.55	0.41
1:A:296:TRP:HA	1:A:342:GLN:HB3	2.02	0.41
1:D:75:VAL:O	1:D:75:VAL:HG22	2.20	0.41
1:A:233:THR:HB	1:A:234:LYS:NZ	2.35	0.41
1:A:458:ASN:ND2	1:A:458:ASN:N	2.65	0.41
1:A:452:ALA:C	1:A:454:GLU:H	2.23	0.41
1:A:447:LEU:O	1:A:449:SER:N	2.54	0.41
1:A:299:LYS:NZ	1:A:362:CYS:SG	2.80	0.41
1:D:290:VAL:HG11	1:D:292:TYR:CE2	2.56	0.41
1:D:46:TYR:CE1	1:D:48:VAL:HG22	2.56	0.41
1:D:46:TYR:HE1	1:D:48:VAL:HG22	1.86	0.41
1:D:436:HIS:CE1	1:D:440:LYS:HD3	2.56	0.40
1:A:360:GLN:O	1:A:361:ASP:C	2.56	0.40
1:D:306:PRO:HB3	1:D:351:GLY:O	2.21	0.40
1:D:159:PRO:HG2	1:D:303:LEU:HD13	2.02	0.40
1:D:43:ARG:NH1	6:D:493:HOH:O	2.52	0.40
1:A:404:TRP:CH2	1:A:439:LEU:HG	2.56	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	447/488 (92%)	418 (94%)	23 (5%)	6 (1%)	18	24
1	D	441/488 (90%)	407 (92%)	29 (7%)	5 (1%)	21	29
All	All	888/976 (91%)	825 (93%)	52 (6%)	11 (1%)	19	26

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	444	LYS

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Mol	Chain	Res	Type
1	D	461	PRO
1	D	462	GLY
1	A	397	PRO
1	A	448	VAL
1	D	392	ASP
1	A	113	LYS
1	A	461	PRO
1	D	397	PRO
1	A	457	ASP
1	A	111	GLY

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	391/424 (92%)	382 (98%)	9 (2%)	63	82
1	D	376/424 (89%)	368 (98%)	8 (2%)	66	84
All	All	767/848 (90%)	750 (98%)	17 (2%)	64	83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	93	LEU
1	D	124	LYS
1	D	166	ASP
1	D	202	ASP
1	D	234	LYS
1	D	252	GLU
1	D	409	ASN
1	D	478	GLU
1	A	157	ASP
1	A	165	LEU
1	A	174	SER
1	A	219	ARG
1	A	234	LYS
1	A	397	PRO
1	A	439	LEU

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Mol	Chain	Res	Type
1	A	458	ASN
1	A	468	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	44	GLN
1	D	49	ASN
1	D	72	HIS
1	D	99	ASN
1	D	200	GLN
1	D	354	HIS
1	D	368	ASN
1	D	430	GLN
1	D	436	HIS
1	A	209	ASN
1	A	436	HIS
1	A	458	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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	#$|Z| > 2$
4	SO4	A	493	-	4,4,4	0.21	0	6,6,6	0.15	0
5	OGA	A	5798	3	9,9,9	1.23	1 (11%)	11,11,11	2.33	7 (63%)
4	SO4	D	492	-	4,4,4	0.23	0	6,6,6	0.10	0

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
4	SO4	A	493	-	-	0/0/0/0	0/0/0/0
5	OGA	A	5798	3	-	0/9/9/9	0/0/0/0
4	SO4	D	492	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5798	OGA	C2-C1	-2.68	1.50	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	5798	OGA	C4-N1-C2	3.43	126.82	121.02
5	A	5798	OGA	C1-C2-N1	3.22	120.72	113.34
5	A	5798	OGA	O2-C1-O1	-3.09	116.30	123.62
5	A	5798	OGA	O3-C5-O4	-2.97	115.74	123.30
5	A	5798	OGA	O2-C1-C2	2.89	122.43	116.64
5	A	5798	OGA	O3-C5-C4	2.26	121.21	112.98
5	A	5798	OGA	O2'-C2-C1	-2.07	118.27	121.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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, 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	447/488 (91%)	0.18	22 (4%)	28	26	16, 34, 77, 91	0
1	D	445/488 (91%)	0.36	34 (7%)	14	12	16, 36, 87, 99	0
All	All	892/976 (91%)	0.27	56 (6%)	18	18	16, 35, 84, 99	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	451	HIS	10.7
1	D	452	ALA	6.3
1	D	447	LEU	5.9
1	D	32	PRO	5.6
1	D	396	PHE	5.6
1	D	260	VAL	5.1
1	D	422	PHE	5.0
1	A	447	LEU	4.8
1	A	422	PHE	4.7
1	D	393	LEU	4.6
1	D	459	VAL	4.4
1	D	261	PHE	4.3
1	D	262	PRO	4.3
1	D	454	GLU	4.0
1	D	391	PRO	3.9
1	D	421	GLY	3.9
1	D	394	PHE	3.9
1	A	450	GLU	3.8
1	D	417	LEU	3.8
1	A	421	GLY	3.7
1	D	458	ASN	3.7
1	D	397	PRO	3.5
1	D	423	GLN	3.5
1	A	261	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	260	VAL	3.3
1	D	257	ASP	3.3
1	D	398	PHE	3.2
1	A	475	ILE	3.1
1	D	258	ASP	3.1
1	D	479	ASN	3.0
1	D	420	ASP	2.9
1	A	420	ASP	2.9
1	A	449	SER	2.8
1	D	418	ARG	2.8
1	A	446	GLU	2.7
1	A	445	LYS	2.7
1	A	451	HIS	2.6
1	D	292	TYR	2.5
1	A	479	ASN	2.5
1	A	284	ASP	2.4
1	A	417	LEU	2.4
1	D	455	ILE	2.4
1	A	262	PRO	2.4
1	D	457	ASP	2.4
1	D	453	PHE	2.3
1	D	473	ARG	2.3
1	A	257	ASP	2.3
1	A	283	ILE	2.3
1	D	446	GLU	2.3
1	A	448	VAL	2.2
1	A	453	PHE	2.2
1	A	423	GLN	2.2
1	D	456	PRO	2.1
1	D	356	VAL	2.1
1	D	405	PHE	2.0
1	A	321	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	OGA	A	5798	10/10	0.48	7.33	106,107,107,107	0
3	FE2	D	491	1/1	0.35	3.48	120,120,120,120	0
3	FE2	A	492	1/1	0.20	2.32	112,112,112,112	0
4	SO4	D	492	5/5	0.12	-0.36	51,52,52,52	0
2	ZN	D	489	1/1	0.07	-0.76	28,28,28,28	0
3	FE2	A	491	1/1	0.16	-0.79	112,112,112,112	0
2	ZN	D	490	1/1	0.07	-1.04	29,29,29,29	0
4	SO4	A	493	5/5	0.08	-1.12	52,52,53,54	0
2	ZN	A	490	1/1	0.06	-1.56	28,28,28,28	0
2	ZN	A	489	1/1	0.07	-2.07	26,26,26,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.