



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:50 AM UTC

PDB ID : 3KV5 / pdb_00003kv5
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 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
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

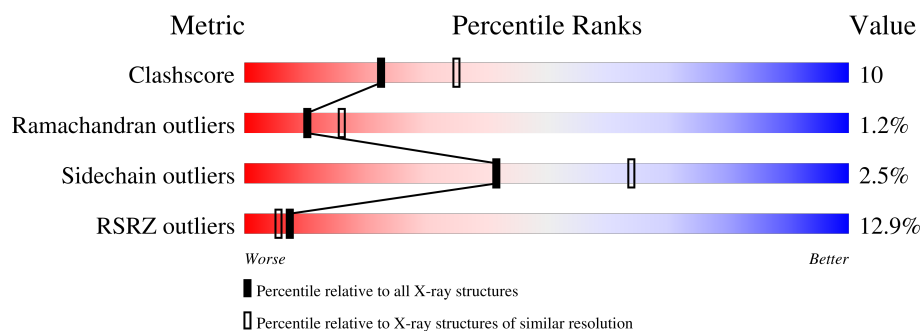
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	488	9% 72% 18% • 8%
1	D	488	15% 66% 23% • 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7456 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 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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is FE (II) ION (CCD ID: FE2) (formula: Fe).

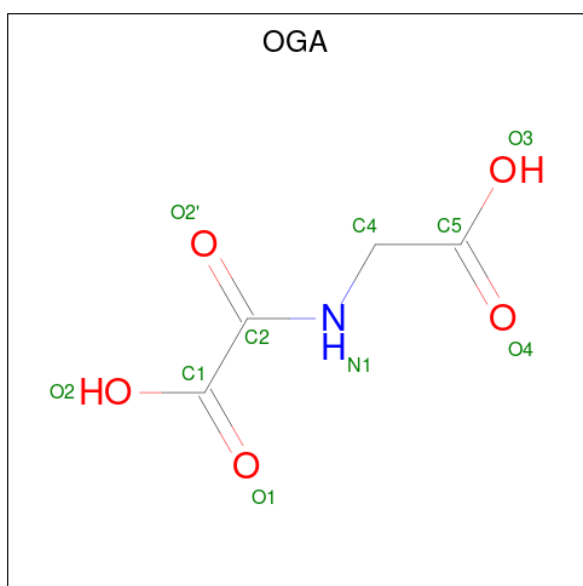
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Fe	0	0
			1	1		
3	A	2	Total	Fe	0	0
			2	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: C₄H₅NO₅).



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

- 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

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 – 2.39	Depositor EDS
% Data completeness (in resolution range)	87.7 (34.82-2.39) 87.7 (34.82-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.245 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	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 14.03% 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: ZN, OGA, SO4, FE2

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	0.42	0/3694	0.94	11/5019 (0.2%)
1	D	0.43	0/3612	0.93	11/4913 (0.2%)
All	All	0.42	0/7306	0.94	22/9932 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	362	CYS	N-CA-C	7.03	120.61	109.50
1	D	197	VAL	N-CA-C	6.98	118.58	110.62
1	A	197	VAL	N-CA-C	6.50	118.03	110.62
1	A	362	CYS	N-CA-C	6.23	119.35	109.50
1	A	162	VAL	CA-C-N	5.94	125.64	119.05
1	A	162	VAL	C-N-CA	5.94	125.64	119.05
1	D	162	VAL	CA-C-N	5.83	125.53	119.05
1	D	162	VAL	C-N-CA	5.83	125.53	119.05
1	A	158	VAL	N-CA-C	-5.67	104.54	109.19
1	D	206	THR	N-CA-C	-5.42	101.70	110.32
1	D	249	SER	N-CA-C	5.32	118.28	110.30
1	A	226	ILE	N-CA-C	5.26	118.20	113.10
1	A	132	PRO	N-CA-C	-5.24	103.06	111.38
1	D	44	GLN	N-CA-C	5.19	114.27	108.25
1	A	297	GLY	N-CA-C	-5.19	105.41	112.52
1	A	239	VAL	N-CA-C	5.15	115.89	108.48
1	A	166	ASP	N-CA-C	5.12	117.76	110.24
1	D	277	SER	N-CA-C	-5.08	103.33	110.50
1	D	253	ASN	N-CA-C	5.06	119.73	113.50
1	D	334	LYS	N-CA-C	5.04	116.63	108.26
1	A	289	SER	N-CA-C	-5.03	102.08	110.17
1	D	373	LEU	N-CA-C	5.02	117.48	111.71

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	3589	0	3463	64	0
1	D	3512	0	3340	82	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
6	D	161	0	0	3	0
All	All	7456	0	6806	146	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 10.

All (146) 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:D:392:ASP:HA	1:D:395:LYS:HG2	1.55	0.88
1:A:234:LYS:H	1:A:234:LYS:NZ	1.75	0.85
1:A:215:MET:HE2	1:A:215:MET:HA	1.66	0.77
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:234:LYS:H	1:A:234:LYS:HZ1	1.39	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:HH11	1:A:219:ARG:HG3	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:52:MET:HE3	1:A:63:HIS:CD2	2.33	0.63
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:D:392:ASP:C	1:D:394:PHE:H	2.09	0.59
1:A:264:PRO:HB3	1:A:397:PRO:HB2	1.85	0.58
1:D:414:LEU:HD21	1:D:428:LEU:CD2	2.35	0.57
1:A:349:PRO:HG2	1:A:352:TRP:CD1	2.40	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:D:299:LYS:HE2	1:D:362:CYS:SG	2.47	0.55
1:D:452:ALA:HA	1:D:455:ILE:CD1	2.37	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
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:A:443:MET:HE2	1:A:461:PRO:HB3	1.89	0.53
1:D:411:LEU:HD22	1:D:464:LEU:HD12	1.90	0.53
1:D:399:PHE:O	1:D:402:ILE:HG22	2.09	0.52
1:A:398:PHE:HB3	1:A:401:ALA:CB	2.39	0.52
1:A:234:LYS:H	1:A:234:LYS:HZ2	1.55	0.52
1:D:454:GLU:O	1:D:456:PRO:HD3	2.09	0.52
1:D:392:ASP:C	1:D:394:PHE:N	2.68	0.52
1:A:359:SER:C	1:A:360:GLN:HG2	2.35	0.52
1:D:428:LEU:HD23	1:D:428:LEU:C	2.34	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:450:GLU:C	1:A:452:ALA:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:275:GLN:O	1:A:276:ASP:HB2	2.11	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:461:PRO:O	1:D:462:GLY:C	2.53	0.50
1:D:387:ARG:C	1:D:389:LYS:H	2.18	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:A:311:LEU:HD22	1:A:384:MET:HE1	1.94	0.48
1:D:413:THR:O	1:D:417:LEU:HD23	2.13	0.48
1:A:443:MET:O	1:A:444:LYS:C	2.56	0.48
1:D:414:LEU:HD21	1:D:428:LEU:HD22	1.95	0.48
1:A:159:PRO:HG2	1:A:303:LEU:HD13	1.95	0.48
1:D:411:LEU:HD21	1:D:467:GLU:HG2	1.96	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:A:441:LEU:O	1:A:447:LEU:HD12	2.15	0.46
1:D:440:LYS:CG	1:D:465:ILE:HD11	2.45	0.46
1:A:194:VAL:HG12	1:A:195:ILE:N	2.31	0.46
1:A:452:ALA:C	1:A:454:GLU:H	2.23	0.46
1:D:124:LYS:HD2	6:D:635:HOH:O	2.15	0.46
1:A:360:GLN:O	1:A:361:ASP:C	2.56	0.45
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:151:LEU:O	1:D:155:GLY:N	2.48	0.45
1:D:165:LEU:CD2	1:D:170:LEU:HD23	2.47	0.45
1:D:308:ASP:OD1	1:D:380:ARG:NH2	2.48	0.45
1:D:418:ARG:HH11	1:D:418:ARG:HG3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ASN:ND2	1:D:102:ARG:H	2.15	0.44
1:D:290:VAL:HG12	1:D:291:TRP:N	2.33	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:D:285:PHE:HB2	1:D:396:PHE:H	1.83	0.43
1:D:360:GLN:O	1:D:361:ASP:C	2.60	0.43
1:D:440:LYS:O	1:D:443:MET:HB2	2.17	0.43
1:D:252:GLU:HA	1:D:252:GLU:OE1	2.19	0.43
1:D:303:LEU:HD23	1:D:354:HIS:HB3	2.00	0.43
1:D:460:ARG:O	1:D:461:PRO:O	2.36	0.43
1:D:315:GLU:HB2	1:D:384:MET:HE2	2.01	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:452:ALA:C	1:A:454:GLU:N	2.77	0.43
1:A:219:ARG:NH1	1:A:274:VAL:HB	2.34	0.43
1:A:249:SER:CB	1:A:252:GLU:HB2	2.48	0.43
1:A:290:VAL:CG2	1:A:291:TRP:N	2.81	0.43
1:D:165:LEU:HD21	1:D:170:LEU:HD23	2.01	0.42
1:D:427:TYR:CG	1:D:428:LEU:N	2.87	0.42
1:A:233:THR:HB	1:A:234:LYS:HZ1	1.84	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:D:387:ARG:C	1:D:389:LYS:N	2.77	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:395:LYS:HB3	6:A:518:HOH:O	2.19	0.42
1:A:440:LYS:HA	1:A:465:ILE:HD13	2.01	0.42
1:D:138:ILE:HG22	1:D:159:PRO:HB2	2.02	0.42
1:D:411:LEU:HD13	1:D:468:LEU:HD12	2.01	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
1:A:219:ARG:HG3	1:A:219:ARG:NH1	2.31	0.41
1:D:246:LYS:HE3	1:D:246:LYS:HB2	1.75	0.41
1:A:443:MET:HE2	1:A:461:PRO:CB	2.50	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:HG22	1:D:75:VAL:O	2.20	0.41
1:A:233:THR:HB	1:A:234:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:306:PRO:HB3	1:D:351:GLY:O	2.21	0.40
1:D:436:HIS:CE1	1:D:440:LYS:HD3	2.56	0.40
1:D:159:PRO:HG2	1:D:303:LEU:HD13	2.02	0.40
1:A:387:ARG:C	1:A:389:LYS:H	2.29	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 [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	447/488 (92%)	418 (94%)	23 (5%)	6 (1%)	9	14
1	D	441/488 (90%)	407 (92%)	29 (7%)	5 (1%)	11	18
All	All	888/976 (91%)	825 (93%)	52 (6%)	11 (1%)	10	16

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	444	LYS
1	D	461	PRO
1	D	462	GLY
1	A	397	PRO
1	A	448	VAL
1	D	392	ASP
1	A	113	LYS

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Mol	Chain	Res	Type
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%)	381 (97%)	10 (3%)	40	63
1	D	376/424 (89%)	367 (98%)	9 (2%)	43	65
All	All	767/848 (90%)	748 (98%)	19 (2%)	42	64

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	87	VAL
1	D	93	LEU
1	D	124	LYS
1	D	202	ASP
1	D	234	LYS
1	D	252	GLU
1	D	409	ASN
1	D	465	ILE
1	D	478	GLU
1	A	108	ILE
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
1	A	458	ASN
1	A	468	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	49	ASN
1	D	72	HIS
1	D	99	ASN
1	D	142	HIS
1	D	200	GLN
1	D	253	ASN
1	D	354	HIS
1	D	425	GLN
1	D	430	GLN
1	D	436	HIS
1	A	148	GLN
1	A	209	ASN
1	A	253	ASN
1	A	360	GLN
1	A	425	GLN
1	A	430	GLN
1	A	436	HIS
1	A	458	ASN

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 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	$\# Z > 2$
5	OGA	A	5798	3	9,9,9	1.36	1 (11%)	8,11,11	2.34	5 (62%)
4	SO4	A	493	-	4,4,4	0.35	0	6,6,6	0.12	0
4	SO4	D	492	-	4,4,4	0.36	0	6,6,6	0.14	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
5	OGA	A	5798	3	-	0/8/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5798	OGA	C2-C1	-3.05	1.50	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	5798	OGA	C4-N1-C2	3.58	126.82	121.29
5	A	5798	OGA	O2-C1-O1	-3.19	116.30	123.90
5	A	5798	OGA	O3-C5-O4	-2.95	115.74	123.33
5	A	5798	OGA	O2'-C2-C1	-2.35	118.27	121.36
5	A	5798	OGA	O3-C5-C4	2.21	121.21	112.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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%)	0.47	44 (9%) 13 10	13, 34, 77, 91	2 (0%)
1	D	445/488 (91%)	0.77	71 (15%) 5 4	16, 36, 87, 99	0
All	All	892/976 (91%)	0.62	115 (12%) 7 5	13, 35, 84, 99	2 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	451	HIS	8.5
1	D	452	ALA	8.1
1	D	394	PHE	6.7
1	D	32	PRO	6.5
1	A	479	ASN	6.4
1	D	479	ASN	6.4
1	D	458	ASN	6.2
1	D	396	PHE	6.0
1	D	457	ASP	5.4
1	D	446	GLU	5.3
1	D	393	LEU	5.2
1	D	472	ILE	5.2
1	D	422	PHE	5.1
1	D	391	PRO	5.0
1	A	33	PRO	5.0
1	D	447	LEU	4.9
1	D	459	VAL	4.8
1	D	455	ILE	4.8
1	D	475	ILE	4.7
1	D	454	GLU	4.6
1	D	453	PHE	4.6
1	D	261	PHE	4.5
1	A	394	PHE	4.5
1	D	398	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	262	PRO	4.4
1	A	393	LEU	4.3
1	D	397	PRO	4.2
1	D	463	HIS	4.2
1	D	471	VAL	4.0
1	A	260	VAL	3.8
1	D	260	VAL	3.8
1	A	453	PHE	3.6
1	D	33	PRO	3.6
1	D	395	LYS	3.6
1	D	390	THR	3.6
1	D	473	ARG	3.6
1	D	444	LYS	3.5
1	D	465	ILE	3.5
1	D	464	LEU	3.5
1	A	418	ARG	3.4
1	D	263	LYS	3.4
1	D	468	LEU	3.4
1	A	447	LEU	3.3
1	D	462	GLY	3.3
1	A	457	ASP	3.2
1	D	417	LEU	3.2
1	A	455	ILE	3.1
1	D	445	LYS	3.1
1	A	261	PHE	3.1
1	A	459	VAL	3.1
1	D	477	GLU	3.1
1	D	423	GLN	3.0
1	A	142	HIS	3.0
1	D	442	TRP	3.0
1	A	449	SER	3.0
1	A	478	GLU	3.0
1	D	456	PRO	3.0
1	A	422	PHE	2.9
1	D	265	PHE	2.9
1	D	441	LEU	2.8
1	A	34	PRO	2.7
1	D	418	ARG	2.7
1	D	474	ALA	2.7
1	A	452	ALA	2.7
1	D	34	PRO	2.7
1	D	432	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	460	ARG	2.6
1	A	397	PRO	2.6
1	A	477	GLU	2.6
1	A	398	PHE	2.6
1	A	465	ILE	2.6
1	A	444	LYS	2.6
1	D	256	PRO	2.6
1	A	475	ILE	2.6
1	D	254	TYR	2.6
1	D	414	LEU	2.5
1	D	419	GLU	2.5
1	A	446	GLU	2.5
1	A	450	GLU	2.4
1	D	476	GLU	2.4
1	D	285	PHE	2.4
1	A	448	VAL	2.4
1	D	466	LYS	2.3
1	A	464	LEU	2.3
1	A	232	ASP	2.3
1	A	445	LYS	2.3
1	A	421	GLY	2.3
1	A	468	LEU	2.3
1	D	202	ASP	2.3
1	D	257	ASP	2.3
1	A	111	GLY	2.3
1	D	438	ALA	2.3
1	A	414	LEU	2.2
1	D	412	GLU	2.2
1	D	392	ASP	2.2
1	D	264	PRO	2.2
1	D	461	PRO	2.1
1	A	391	PRO	2.1
1	D	258	ASP	2.1
1	A	392	ASP	2.1
1	D	255	TRP	2.1
1	A	423	GLN	2.1
1	D	403	CYS	2.1
1	A	412	GLU	2.1
1	A	262	PRO	2.1
1	D	401	ALA	2.1
1	A	417	LEU	2.1
1	D	232	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	461	PRO	2.1
1	A	474	ALA	2.0
1	A	202	ASP	2.0
1	D	321	VAL	2.0
1	D	322	THR	2.0
1	A	451	HIS	2.0
1	D	428	LEU	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
3	FE2	D	491	1/1	0.78	0.15	120,120,120,120	0
5	OGA	A	5798	10/10	0.81	0.30	106,107,107,107	0
3	FE2	A	491	1/1	0.82	0.18	112,112,112,112	0
3	FE2	A	492	1/1	0.87	0.24	112,112,112,112	0
4	SO4	D	492	5/5	0.95	0.10	51,52,52,52	0
4	SO4	A	493	5/5	0.96	0.07	52,52,53,54	0
2	ZN	D	489	1/1	0.99	0.02	28,28,28,28	0
2	ZN	A	489	1/1	0.99	0.02	26,26,26,26	0
2	ZN	D	490	1/1	1.00	0.01	29,29,29,29	0
2	ZN	A	490	1/1	1.00	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.