Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:06 AM 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 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 ⓘ symbol.

The following versions of software and data (see references ⓘ) 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
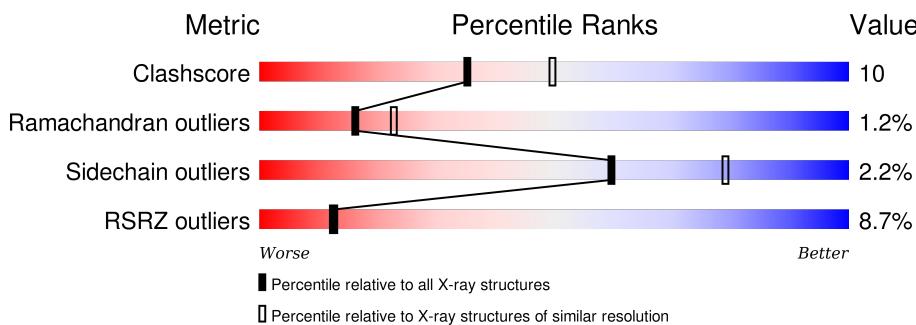
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
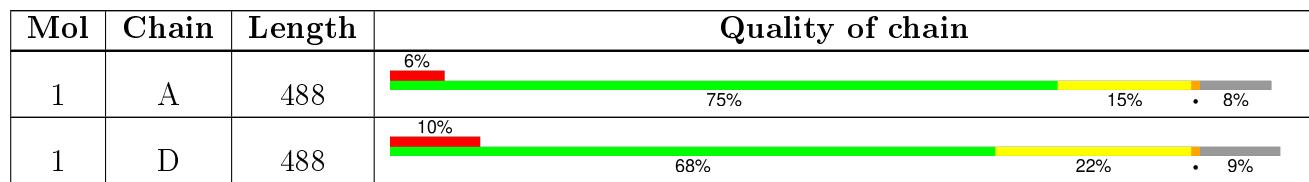
The reported resolution of this entry is 2.39 Å.

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		8.7%

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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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. 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	488	6% / 75% / 15% · 8%
1	D	488	10% / 68% / 22% · 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	OGA	A	5798	-	-	-	X

2 Entry composition (i)

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 3512	C 2260	N 591	O 635	S 26	0	0	0
1	A	447	Total 3589	C 2316	N 607	O 640	S 26	0	2	0
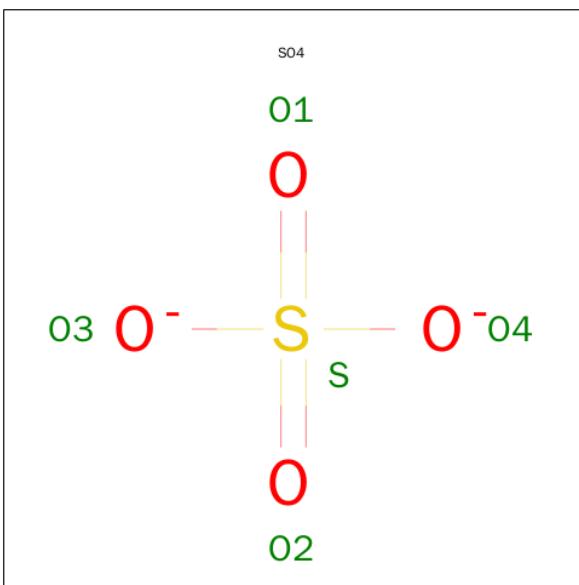
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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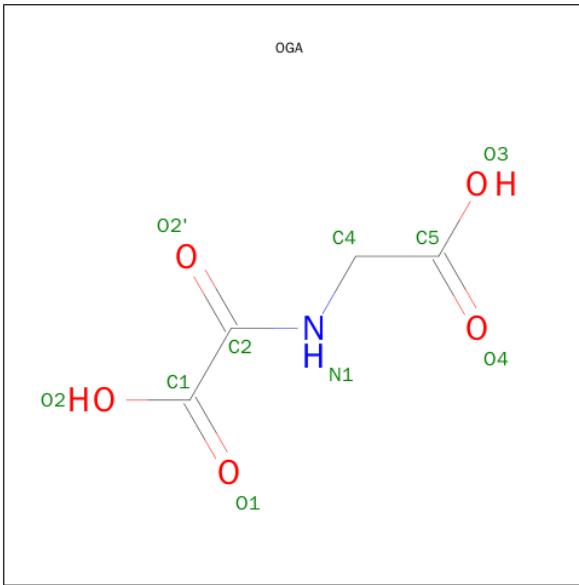
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Fe 2	0	0
3	D	1	Total 1	Fe 1	0	0

- 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
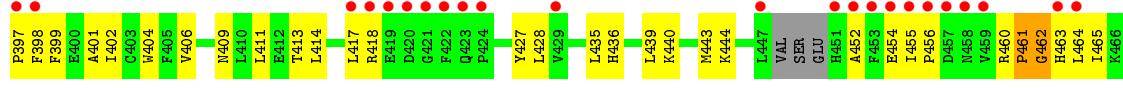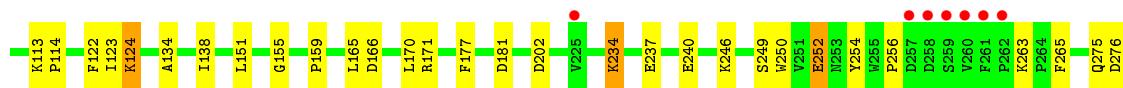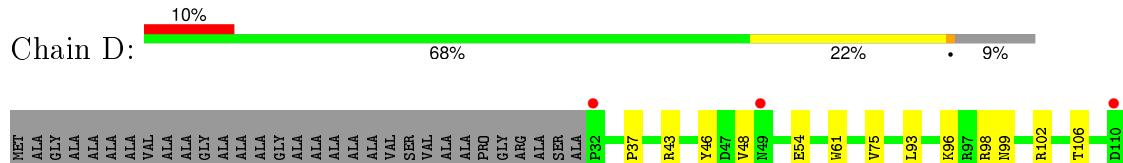
• Molecule 6 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	161	Total O 161 161	0	0
6	A	167	Total O 167 167	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

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

4 Data and refinement statistics (i)

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 0.214　,　(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)	0.32 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.46$, $<L^2> = 0.28$	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.

[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 (i)

5.1 Standard geometry (i)

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 Too-close contacts (i)

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	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
6	D	161	0	0	3	0
All	All	7456	0	6806	137	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 (137) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:219:ARG:HG3	1:A:219:ARG:NH1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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%)	15	21
1	D	441/488 (90%)	407 (92%)	29 (7%)	5 (1%)	17	25
All	All	888/976 (91%)	825 (93%)	52 (6%)	11 (1%)	16	23

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
1	A	461	PRO
1	D	397	PRO
1	A	457	ASP
1	A	111	GLY

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	391/424 (92%)	382 (98%)	9 (2%)	58	78
1	D	376/424 (89%)	368 (98%)	8 (2%)	61	80
All	All	767/848 (90%)	750 (98%)	17 (2%)	60	79

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

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Mol	Chain	Res	Type
1	A	397	PRO
1	A	439	LEU
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 (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 carbohydrates 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	#$|Z| > 2$
4	SO4	A	493	-	4,4,4	0.17	0	6,6,6	0.16	0
5	OGA	A	5798	3	3,9,9	0.71	0	3,11,11	1.22	0
4	SO4	D	492	-	4,4,4	0.19	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	-	0/3/9/9	0/0/0/0
4	SO4	D	492	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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 (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	447/488 (91%)	0.35	30 (6%)	21	21	16, 34, 77, 91	0
1	D	445/488 (91%)	0.55	48 (10%)	8	8	16, 36, 87, 99	0
All	All	892/976 (91%)	0.45	78 (8%)	13	12	16, 35, 84, 99	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	451	HIS	11.9
1	D	452	ALA	7.7
1	D	260	VAL	6.3
1	A	422	PHE	6.1
1	D	447	LEU	6.0
1	D	261	PHE	5.5
1	D	422	PHE	5.5
1	A	447	LEU	5.4
1	D	396	PHE	5.4
1	D	32	PRO	5.3
1	D	262	PRO	5.1
1	A	421	GLY	5.0
1	A	450	GLU	4.9
1	D	417	LEU	4.9
1	D	391	PRO	4.8
1	D	393	LEU	4.6
1	D	423	GLN	4.6
1	D	394	PHE	4.5
1	D	421	GLY	4.2
1	D	458	ASN	3.9
1	D	453	PHE	3.9
1	D	454	GLU	3.9
1	D	459	VAL	3.7
1	D	420	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	418	ARG	3.7
1	A	260	VAL	3.7
1	D	473	ARG	3.6
1	A	446	GLU	3.6
1	D	397	PRO	3.6
1	D	257	ASP	3.6
1	D	456	PRO	3.5
1	A	449	SER	3.5
1	A	445	LYS	3.4
1	A	261	PHE	3.4
1	A	451	HIS	3.3
1	A	420	ASP	3.3
1	D	258	ASP	3.1
1	D	398	PHE	3.0
1	D	356	VAL	3.0
1	A	475	ILE	3.0
1	A	479	ASN	3.0
1	D	474	ALA	3.0
1	A	417	LEU	2.9
1	A	448	VAL	2.8
1	A	262	PRO	2.7
1	D	479	ASN	2.7
1	A	423	GLN	2.7
1	D	292	TYR	2.7
1	D	455	ILE	2.6
1	D	429	VAL	2.6
1	A	257	ASP	2.6
1	D	49	ASN	2.6
1	D	419	GLU	2.6
1	A	321	VAL	2.6
1	A	283	ILE	2.5
1	D	424	PRO	2.5
1	A	258	ASP	2.4
1	D	259	SER	2.4
1	D	457	ASP	2.4
1	D	392	ASP	2.3
1	D	464	LEU	2.3
1	A	289	SER	2.2
1	D	225	VAL	2.2
1	A	356	VAL	2.2
1	D	477	GLU	2.2
1	A	424	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	390	THR	2.2
1	D	283	ILE	2.2
1	A	284	ASP	2.1
1	D	478	GLU	2.1
1	A	273	GLY	2.1
1	A	49	ASN	2.1
1	A	452	ALA	2.1
1	D	463	HIS	2.1
1	A	459	VAL	2.1
1	D	364	ALA	2.1
1	A	453	PHE	2.0
1	D	110	ASP	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, 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	LLDF	B-factors(Å^2)	Q<0.9
5	OGA	A	5798	10/10	0.69	0.55	10.31	106,107,107,107	0
4	SO4	D	492	5/5	0.99	0.15	0.15	51,52,52,52	0
4	SO4	A	493	5/5	0.98	0.10	-0.61	52,52,53,54	0
2	ZN	D	489	1/1	0.99	0.07	-1.13	28,28,28,28	0
2	ZN	D	490	1/1	1.00	0.07	-1.56	29,29,29,29	0
2	ZN	A	490	1/1	1.00	0.06	-2.11	28,28,28,28	0
2	ZN	A	489	1/1	0.99	0.07	-2.49	26,26,26,26	0
3	FE2	A	492	1/1	0.90	0.21	-	112,112,112,112	0
3	FE2	D	491	1/1	0.69	0.39	-	120,120,120,120	0
3	FE2	A	491	1/1	0.81	0.17	-	112,112,112,112	0

6.5 Other polymers (i)

There are no such residues in this entry.