Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 03:28 PM EDT

PDB ID	:	6CG1
Title	:	Crystal Structure of KDM4A with Compound 14
Authors	:	Hosfield, D.J.; Nie, Z.
Deposited on	:	2018-02-19
Resolution	:	2.16 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 (i) 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 (i)) were used in the production of this report:

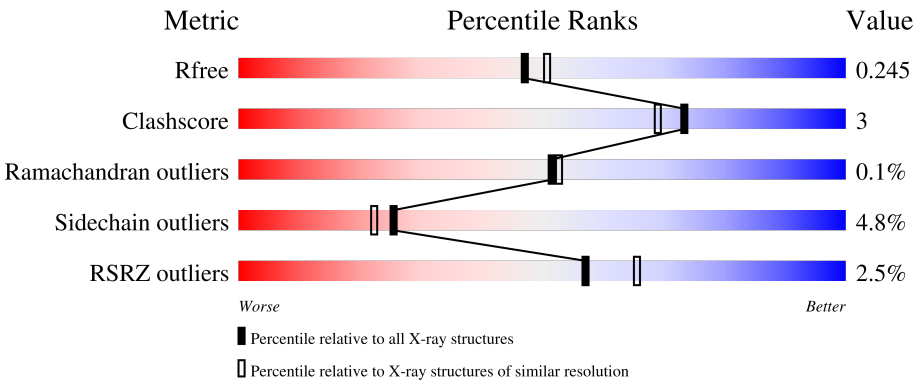
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.16 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))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 <=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	350	3% 89% 10% •
1	B	350	5% 88% 11% ••
1	C	350	2% 85% 11% •
1	D	350	89% 7% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12175 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 demethylase 4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	347	2850	1843	479	514	14	0	0	0
1	B	347	2858	1847	481	516	14	0	1	0
1	C	335	2761	1792	465	490	14	0	0	0
1	D	341	2806	1814	473	505	14	0	0	0

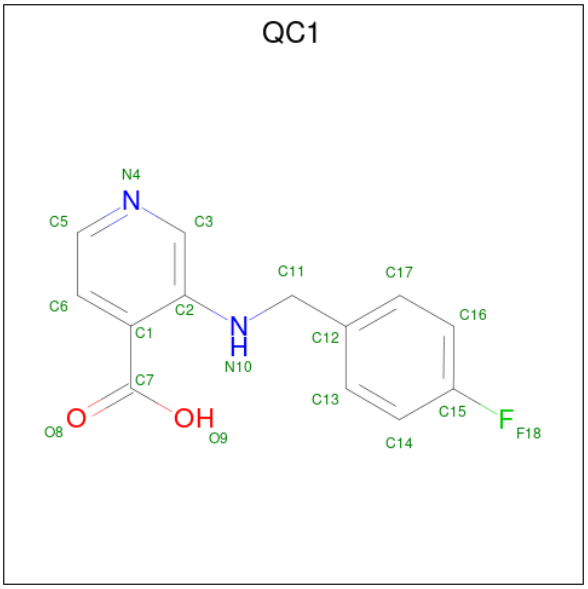
- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0

- Molecule 4 is 3-{[(4-fluorophenyl)methyl]amino}pyridine-4-carboxylic acid (three-letter code: QC1) (formula: $C_{13}H_{11}FN_2O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
4	A	1	18	13	1	2	2	0	0
4	B	1	18	13	1	2	2	0	0
4	C	1	18	13	1	2	2	0	0
4	D	1	18	13	1	2	2	0	0

- Molecule 5 is water.

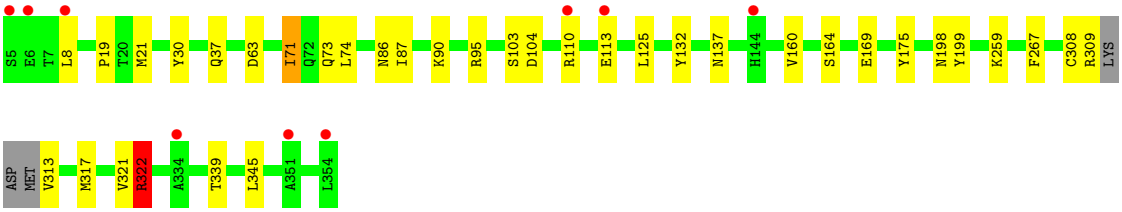
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	182	182	182	0	0
5	B	191	191	191	0	0
5	C	196	196	196	0	0
5	D	251	251	251	0	0

3 Residue-property plots (i)

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

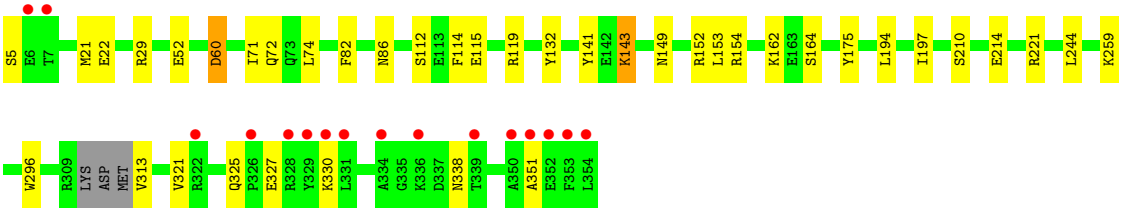
• Molecule 1: Lysine-specific demethylase 4A

Chain A:



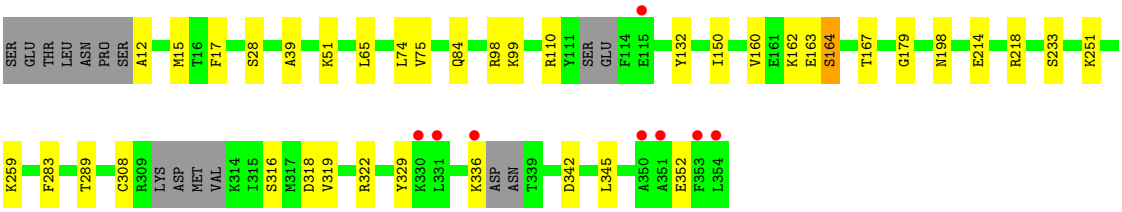
• Molecule 1: Lysine-specific demethylase 4A

Chain B:



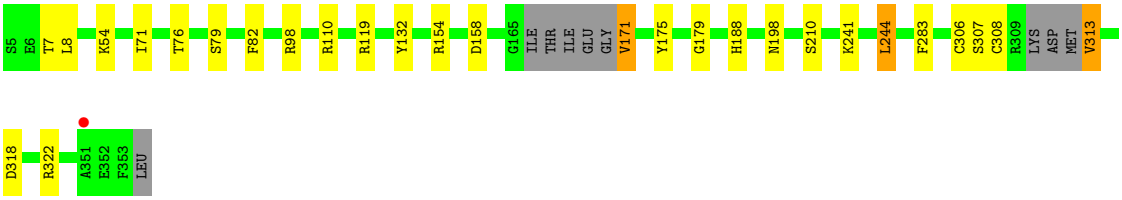
• Molecule 1: Lysine-specific demethylase 4A

Chain C:



• Molecule 1: Lysine-specific demethylase 4A

Chain D:


S5
E6
T7
L8
K54
I71
T76
S79
F82
R98
R110
R119
Y132
R154
D158
G165
ILE
THR
ILE
GLU
GLY
V171
Y175
G179
H188
N198
S210
K241
L244
F283
C306
S307
C308
R309
LYS
ASP
MET
V313
D318
R322
A351
E352
F353
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.58Å 101.65Å 142.43Å 90.00° 99.73° 90.00°	Depositor
Resolution (Å)	140.38 – 2.16 44.70 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.2 (140.38-2.16) 98.7 (44.70-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.175 , 0.240 0.183 , 0.245	Depositor DCC
R_{free} test set	4327 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12175	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.6702e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, QC1, NI

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	0.80	0/2936	0.91	1/3975 (0.0%)
1	B	0.82	2/2944 (0.1%)	0.88	1/3986 (0.0%)
1	C	0.85	1/2844 (0.0%)	0.89	2/3845 (0.1%)
1	D	0.87	0/2891	0.91	2/3912 (0.1%)
All	All	0.84	3/11615 (0.0%)	0.90	6/15718 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	GLU	CD-OE2	8.07	1.34	1.25
1	C	214	GLU	CD-OE2	6.19	1.32	1.25
1	B	60	ASP	CB-CG	5.88	1.64	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	98	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	119	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	119	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	322	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	110	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	98	ARG	NE-CZ-NH2	-5.13	117.74	120.30

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	2850	0	2773	14	0
1	B	2858	0	2778	21	0
1	C	2761	0	2694	21	0
1	D	2806	0	2723	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	18	0	0	0	0
4	B	18	0	0	1	0
4	C	18	0	0	0	0
4	D	18	0	0	0	0
5	A	182	0	0	5	0
5	B	191	0	0	14	0
5	C	196	0	0	8	0
5	D	251	0	0	13	0
All	All	12175	0	10968	74	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 3.

All (74) 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:B:210:SER:HB2	5:B:729:HOH:O	1.68	0.93
1:D:322:ARG:HD2	5:D:749:HOH:O	1.70	0.89
1:C:163:GLU:HG3	1:C:319:VAL:HG21	1.54	0.87
1:C:160:VAL:HG12	5:C:601:HOH:O	1.79	0.80
1:D:210:SER:HB2	5:D:717:HOH:O	1.85	0.77
1:D:313:VAL:HG22	5:D:641:HOH:O	1.84	0.76
1:B:313:VAL:N	5:B:602:HOH:O	2.19	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ILE:HG23	5:B:601:HOH:O	1.91	0.68
1:D:76:THR:HB	5:D:820:HOH:O	1.93	0.67
1:C:15:MET:CE	1:C:17:PHE:HZ	2.08	0.67
1:B:72:GLN:O	5:B:601:HOH:O	2.13	0.65
1:A:74:LEU:HD23	1:A:87:ILE:HD11	1.79	0.65
1:B:221:ARG:HD2	5:B:669:HOH:O	2.02	0.58
1:C:15:MET:HE3	1:C:17:PHE:HZ	1.69	0.57
1:D:154:ARG:HA	1:D:158:ASP:OD2	2.07	0.55
1:B:141:TYR:CE2	1:B:149:ASN:HA	2.42	0.55
1:B:29:ARG:NE	5:B:604:HOH:O	2.39	0.54
1:A:317:MET:O	1:A:321:VAL:HG23	2.08	0.54
1:D:171:VAL:HA	5:D:784:HOH:O	2.08	0.53
1:D:171:VAL:N	5:D:607:HOH:O	2.42	0.52
1:A:137:ASN:OD1	1:A:169:GLU:HG2	2.10	0.51
1:B:153:LEU:HD11	1:B:197:ILE:HG21	1.93	0.51
1:C:99:LYS:NZ	5:C:604:HOH:O	2.43	0.50
1:A:95:ARG:CZ	1:A:95:ARG:HB3	2.41	0.49
4:B:503:QC1:O8	4:B:503:QC1:N10	2.45	0.49
1:D:79:SER:N	5:D:611:HOH:O	2.46	0.49
1:B:21:MET:HE1	5:B:691:HOH:O	2.13	0.48
1:B:221:ARG:CD	5:B:669:HOH:O	2.59	0.48
1:A:313:VAL:N	5:A:605:HOH:O	2.45	0.48
1:B:154:ARG:HD2	1:C:164:SER:HA	1.96	0.48
1:A:71:ILE:HD11	1:A:73:GLN:HG2	1.96	0.48
1:B:71:ILE:HD11	5:B:661:HOH:O	2.13	0.48
1:B:71:ILE:CG2	5:B:601:HOH:O	2.55	0.47
1:A:198:ASN:HB2	5:A:721:HOH:O	2.14	0.47
1:D:198:ASN:ND2	5:D:613:HOH:O	2.47	0.47
1:D:198:ASN:HB2	5:D:751:HOH:O	2.14	0.47
1:C:15:MET:HE2	1:C:17:PHE:HZ	1.80	0.47
1:C:218:ARG:CD	5:C:732:HOH:O	2.62	0.47
1:C:15:MET:HE3	1:C:17:PHE:CZ	2.48	0.46
1:C:65:LEU:HD12	5:C:721:HOH:O	2.15	0.46
1:A:37:GLN:NE2	5:A:608:HOH:O	2.48	0.46
1:B:86:ASN:HA	5:B:601:HOH:O	2.15	0.46
1:C:336:LYS:C	5:C:602:HOH:O	2.53	0.45
1:B:5:SER:HB3	5:B:720:HOH:O	2.15	0.45
1:B:82:PHE:HB2	1:B:244:LEU:HB2	1.98	0.45
1:B:143:LYS:O	1:B:152:ARG:NH1	2.50	0.45
1:D:322:ARG:CD	5:D:749:HOH:O	2.45	0.45
1:C:15:MET:HE1	1:C:39:ALA:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:ASP:OD2	1:C:345:LEU:HD13	2.17	0.44
1:B:194:LEU:HD23	1:B:296:TRP:CE2	2.53	0.44
1:C:15:MET:CE	1:C:17:PHE:CZ	2.96	0.43
1:A:160:VAL:O	1:A:164:SER:HB2	2.18	0.43
1:C:198:ASN:HB2	5:C:718:HOH:O	2.17	0.43
1:A:19:PRO:HB3	1:A:30:TYR:CZ	2.54	0.43
1:C:12:ALA:N	5:C:613:HOH:O	2.51	0.43
1:B:112:SER:HB3	5:B:769:HOH:O	2.19	0.42
1:C:150:ILE:HG23	1:C:289:THR:HG22	2.01	0.42
1:D:82:PHE:HB2	1:D:244:LEU:HB2	2.00	0.42
1:C:75:VAL:HG22	1:C:84:GLN:HG3	2.01	0.42
1:C:179:GLY:O	1:C:283:PHE:HA	2.18	0.42
1:D:198:ASN:HB2	5:D:770:HOH:O	2.20	0.42
1:A:322:ARG:NH1	5:A:610:HOH:O	2.52	0.42
1:A:71:ILE:HD13	1:A:86:ASN:CG	2.40	0.42
1:C:322:ARG:HG3	1:C:329:TYR:CD1	2.55	0.42
1:B:114:PHE:HB3	5:B:780:HOH:O	2.19	0.41
1:B:321:VAL:HG13	1:B:325:GLN:HB2	2.02	0.41
1:A:199:TYR:HB2	1:A:267:PHE:CE1	2.56	0.41
1:A:322:ARG:HD3	5:A:610:HOH:O	2.21	0.41
1:D:179:GLY:O	1:D:283:PHE:HA	2.21	0.41
1:D:318:ASP:OD1	1:D:322:ARG:HD3	2.20	0.41
1:D:79:SER:CA	5:D:611:HOH:O	2.69	0.41
1:C:316:SER:HB2	5:C:689:HOH:O	2.21	0.40
1:D:188:HIS:CD2	1:D:241:LYS:HE3	2.55	0.40
1:D:313:VAL:CG2	5:D:641:HOH:O	2.57	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	343/350 (98%)	334 (97%)	9 (3%)	0	100	100
1	B	344/350 (98%)	335 (97%)	8 (2%)	1 (0%)	41	37
1	C	327/350 (93%)	318 (97%)	9 (3%)	0	100	100
1	D	335/350 (96%)	329 (98%)	5 (2%)	1 (0%)	41	37
All	All	1349/1400 (96%)	1316 (98%)	31 (2%)	2 (0%)	51	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	351	ALA
1	D	308	CYS

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	304/307 (99%)	286 (94%)	18 (6%)	19	15
1	B	305/307 (99%)	291 (95%)	14 (5%)	27	23
1	C	292/307 (95%)	279 (96%)	13 (4%)	27	24
1	D	299/307 (97%)	287 (96%)	12 (4%)	31	29
All	All	1200/1228 (98%)	1143 (95%)	57 (5%)	25	22

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	21	MET
1	A	63	ASP
1	A	71	ILE
1	A	90	LYS
1	A	103	SER
1	A	104	ASP
1	A	110	ARG
1	A	113	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	125	LEU
1	A	132	TYR
1	A	175	TYR
1	A	259	LYS
1	A	308	CYS
1	A	309	ARG
1	A	322	ARG
1	A	339	THR
1	A	345	LEU
1	B	22	GLU
1	B	52	GLU
1	B	60	ASP
1	B	74	LEU
1	B	115	GLU
1	B	132	TYR
1	B	143	LYS
1	B	162	LYS
1	B	164	SER
1	B	175	TYR
1	B	259	LYS
1	B	327	GLU
1	B	330	LYS
1	B	338	ASN
1	C	28	SER
1	C	51	LYS
1	C	74	LEU
1	C	132	TYR
1	C	162	LYS
1	C	164	SER
1	C	167	THR
1	C	233	SER
1	C	251	LYS
1	C	259	LYS
1	C	308	CYS
1	C	318	ASP
1	C	352	GLU
1	D	7	THR
1	D	8	LEU
1	D	54	LYS
1	D	71	ILE
1	D	110	ARG
1	D	132	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	171	VAL
1	D	175	TYR
1	D	244	LEU
1	D	306	CYS
1	D	307	SER
1	D	313	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	B	37	GLN
1	C	84	GLN
1	C	215	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	QC1	D	503	2	19,19,19	1.32	1 (5%)	23,25,25	1.68	6 (26%)
4	QC1	A	503	2	19,19,19	1.75	4 (21%)	23,25,25	1.35	5 (21%)
4	QC1	C	503	2	19,19,19	1.30	2 (10%)	23,25,25	1.99	11 (47%)
4	QC1	B	503	2	19,19,19	1.73	3 (15%)	23,25,25	1.55	5 (21%)

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	QC1	D	503	2	-	0/9/9/9	0/2/2/2
4	QC1	A	503	2	-	0/9/9/9	0/2/2/2
4	QC1	C	503	2	-	0/9/9/9	0/2/2/2
4	QC1	B	503	2	-	0/9/9/9	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	QC1	C11-N10	-4.81	1.29	1.45
4	A	503	QC1	C11-N10	-4.61	1.30	1.45
4	D	503	QC1	C11-N10	-4.37	1.30	1.45
4	C	503	QC1	C11-N10	-4.08	1.31	1.45
4	B	503	QC1	O8-C7	3.84	1.34	1.22
4	A	503	QC1	O9-C7	-3.30	1.20	1.30
4	A	503	QC1	O8-C7	2.68	1.30	1.22
4	C	503	QC1	C3-C2	2.45	1.43	1.39
4	B	503	QC1	O9-C7	-2.43	1.23	1.30
4	A	503	QC1	C3-C2	2.11	1.42	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	503	QC1	C13-C14-C15	3.63	122.11	118.36
4	C	503	QC1	C11-C12-C17	-3.60	113.45	120.91
4	D	503	QC1	C11-C12-C17	-3.42	113.81	120.91
4	D	503	QC1	C5-N4-C3	3.01	122.06	116.85
4	D	503	QC1	F18-C15-C14	2.94	123.53	118.54
4	C	503	QC1	O9-C7-O8	-2.94	116.82	123.35
4	B	503	QC1	C11-C12-C17	-2.83	115.05	120.91
4	C	503	QC1	F18-C15-C14	2.74	123.19	118.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	503	QC1	C6-C5-N4	-2.71	118.91	123.62
4	D	503	QC1	C11-C12-C13	2.66	126.43	120.91
4	B	503	QC1	C5-N4-C3	2.63	121.40	116.85
4	C	503	QC1	C11-C12-C13	2.59	126.30	120.91
4	C	503	QC1	C16-C15-C14	-2.58	119.40	122.83
4	A	503	QC1	C6-C5-N4	-2.58	119.13	123.62
4	A	503	QC1	O9-C7-O8	-2.55	117.68	123.35
4	C	503	QC1	C1-C2-N10	2.49	124.15	121.25
4	A	503	QC1	C11-C12-C17	-2.43	115.87	120.91
4	B	503	QC1	C6-C1-C2	2.36	121.49	118.81
4	B	503	QC1	C6-C5-N4	-2.31	119.60	123.62
4	C	503	QC1	C14-C13-C12	-2.29	117.88	121.03
4	D	503	QC1	F18-C15-C16	-2.24	114.74	118.54
4	C	503	QC1	C5-N4-C3	2.21	120.67	116.85
4	C	503	QC1	O9-C7-C1	2.17	121.56	115.31
4	C	503	QC1	C6-C5-N4	-2.16	119.86	123.62
4	B	503	QC1	F18-C15-C14	2.14	122.18	118.54
4	A	503	QC1	O9-C7-C1	2.09	121.33	115.31
4	A	503	QC1	C5-N4-C3	2.02	120.34	116.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	QC1	1	0

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	347/350 (99%)	0.03	9 (2%)	56	64	21, 41, 76, 122	1 (0%)
1	B	347/350 (99%)	-0.00	16 (4%)	32	42	19, 37, 82, 106	0
1	C	335/350 (95%)	-0.09	8 (2%)	59	67	17, 36, 74, 98	0
1	D	341/350 (97%)	-0.23	1 (0%)	94	95	19, 32, 65, 95	0
All	All	1370/1400 (97%)	-0.07	34 (2%)	57	65	17, 36, 74, 122	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	353	PHE	4.5
1	C	354	LEU	4.3
1	A	5	SER	4.1
1	A	6	GLU	4.0
1	A	354	LEU	3.8
1	C	351	ALA	3.7
1	B	354	LEU	3.6
1	B	334	ALA	3.6
1	D	351	ALA	3.5
1	B	351	ALA	3.4
1	B	353	PHE	3.2
1	B	330	LYS	3.1
1	C	336	LYS	3.1
1	C	115	GLU	2.9
1	C	350	ALA	2.7
1	B	336	LYS	2.6
1	B	350	ALA	2.5
1	A	113	GLU	2.5
1	B	328	ARG	2.4
1	C	330	LYS	2.4
1	A	334	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	322	ARG	2.4
1	B	331	LEU	2.4
1	A	144	HIS	2.3
1	B	329	TYR	2.3
1	A	8	LEU	2.3
1	C	331	LEU	2.3
1	B	7	THR	2.2
1	B	326	PRO	2.2
1	A	351	ALA	2.2
1	B	352	GLU	2.2
1	B	6	GLU	2.1
1	A	110	ARG	2.1
1	B	339	THR	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 monosaccharides 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(Å^2)	Q<0.9
4	QC1	A	503	18/18	0.95	0.13	28,34,42,46	0
4	QC1	D	503	18/18	0.96	0.10	19,25,36,39	0
4	QC1	C	503	18/18	0.97	0.10	26,30,35,38	0
4	QC1	B	503	18/18	0.97	0.12	25,30,40,48	0
3	ZN	A	502	1/1	0.99	0.08	37,37,37,37	0
3	ZN	C	502	1/1	0.99	0.08	37,37,37,37	0
2	NI	C	501	1/1	0.99	0.13	25,25,25,25	0
3	ZN	D	502	1/1	1.00	0.09	30,30,30,30	0
2	NI	D	501	1/1	1.00	0.10	21,21,21,21	0
2	NI	B	501	1/1	1.00	0.11	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	B	502	1/1	1.00	0.10	41,41,41,41	0
2	NI	A	501	1/1	1.00	0.12	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.