



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2016 – 06:41 PM EDT

PDB ID : 5F32
Title : Crystal structure of human KDM4A in complex with compound 40
Authors : Le Bihan, Y.-V.; Dempster, S.; Westwood, I.M.; van Montfort, R.L.M.
Deposited on : 2015-12-02
Resolution : 2.05 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

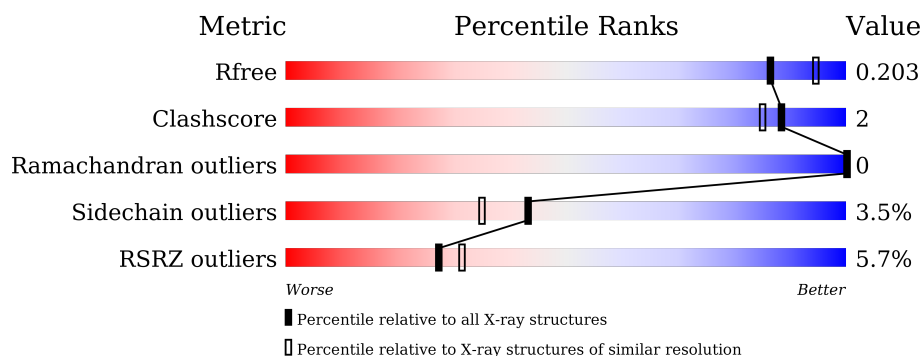
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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 $\leq 5\%$. 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	360	<div> <div>7%</div> <div>88%</div> <div>7%</div> <div>5%</div> </div>
1	B	360	<div> <div>4%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	C	360	<div> <div>7%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>
1	D	360	<div> <div>3%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	5V7	A	403	-	-	-	X
3	5V7	C	403	-	-	-	X
3	5V7	D	403	-	-	-	X
4	DMS	A	404	-	-	-	X
4	DMS	B	404	-	-	-	X
4	DMS	C	404	-	-	-	X
4	DMS	C	405	-	-	-	X
5	EDO	B	405	-	-	-	X
6	GOL	A	406	-	-	-	X
6	GOL	B	406	-	-	X	X
6	GOL	D	409	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11989 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
1	A	342	Total	C	N	O	S	0	4	0
			2719	1772	448	484	15			
1	B	344	Total	C	N	O	S	0	5	0
			2775	1810	456	493	16			
1	C	350	Total	C	N	O	S	0	2	0
			2789	1817	456	501	15			
1	D	348	Total	C	N	O	S	0	3	0
			2800	1821	462	502	15			

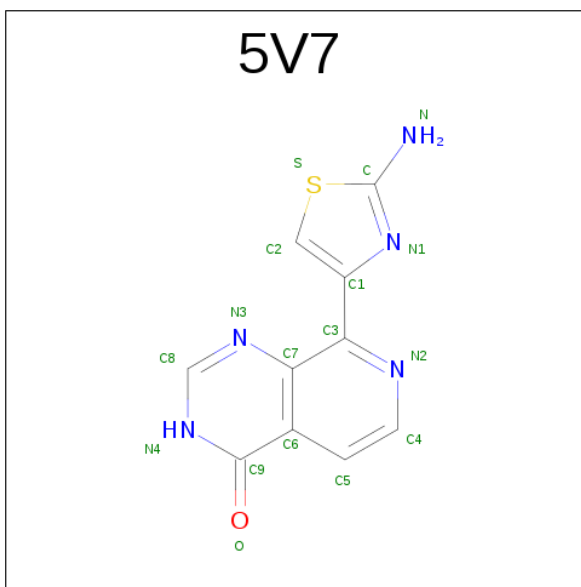
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP O75164
B	0	SER	-	expression tag	UNP O75164
C	0	SER	-	expression tag	UNP O75164
D	0	SER	-	expression tag	UNP O75164

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

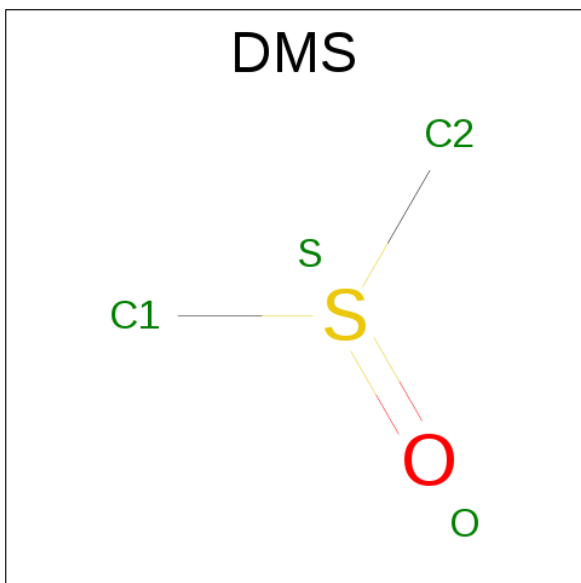
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 8-(2-azanyl-1,3-thiazol-4-yl)-3 {H}-pyrido[3,4-d]pyrimidin-4-one (three-letter code: 5V7) (formula: C₁₀H₇N₅OS).



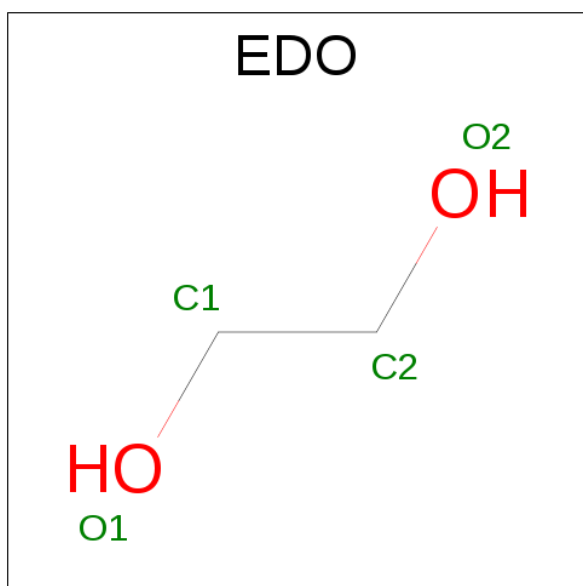
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			17	10	5	1	1		
3	B	1	Total	C	N	O	S	0	0
			17	10	5	1	1		
3	C	1	Total	C	N	O	S	0	0
			17	10	5	1	1		
3	D	1	Total	C	N	O	S	0	0
			17	10	5	1	1		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

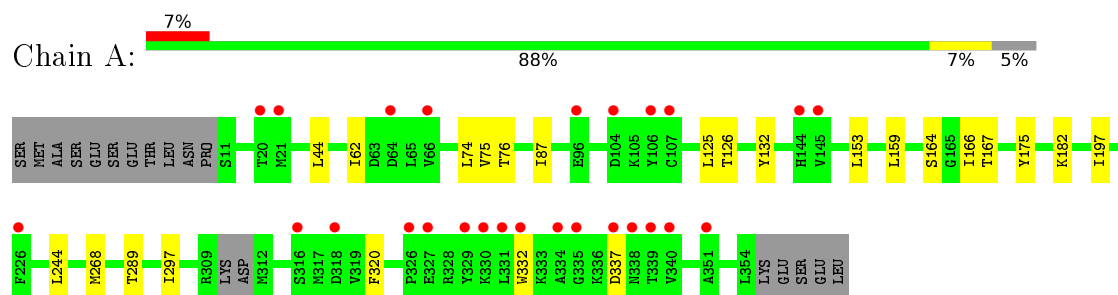
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	138	Total	O	0	0
			138	138		
7	B	184	Total	O	0	0
			184	184		
7	C	211	Total	O	0	0
			211	211		
7	D	232	Total	O	0	1
			233	233		

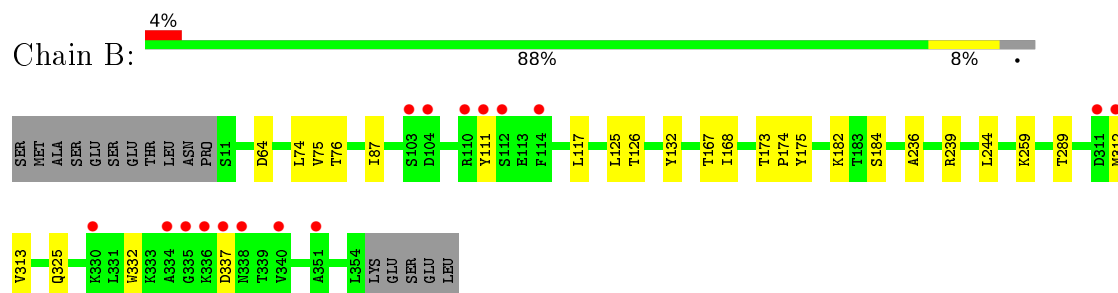
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

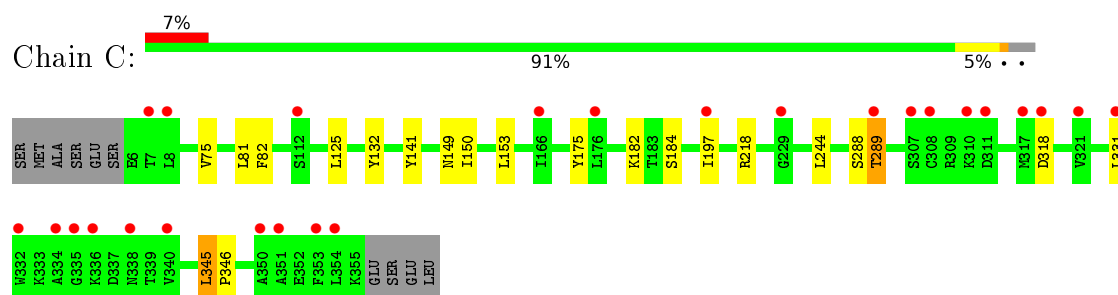
- Molecule 1: Lysine-specific demethylase 4A



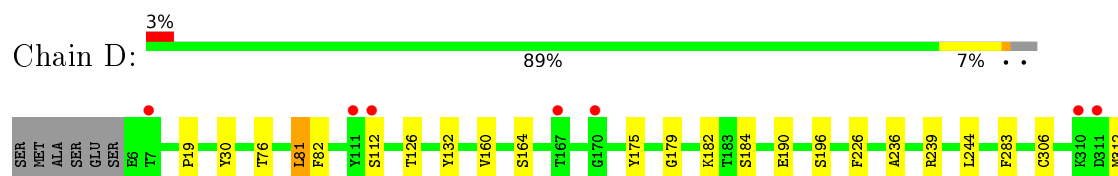
- Molecule 1: Lysine-specific demethylase 4A

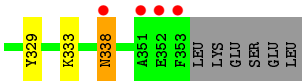


- Molecule 1: Lysine-specific demethylase 4A



- Molecule 1: Lysine-specific demethylase 4A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.22Å 102.59Å 141.74Å 90.00° 99.29° 90.00°	Depositor
Resolution (Å)	41.00 – 2.05 40.83 – 2.05	Depositor EDS
% Data completeness (in resolution range)	88.0 (41.00-2.05) 88.0 (40.83-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.05Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.168 , 0.203 0.172 , 0.203	Depositor DCC
R_{free} test set	4452 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.8	EDS
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 89166 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11989	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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 23.26 % 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 4.8289e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GOL, ZN, DMS, EDO, 5V7

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	0.49	0/2805	0.65	0/3817
1	B	0.53	0/2862	0.66	0/3887
1	C	0.51	0/2875	0.66	0/3910
1	D	0.54	0/2887	0.66	0/3923
All	All	0.52	0/11429	0.66	0/15537

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	2719	0	2511	12	0
1	B	2775	0	2608	15	0
1	C	2789	0	2614	6	0
1	D	2800	0	2634	14	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	17	0	7	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	7	2	0
3	C	17	0	7	1	0
3	D	17	0	7	2	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	8	0	12	0	0
4	D	8	0	12	0	0
5	A	4	0	6	1	0
5	B	4	0	6	0	0
5	D	8	0	12	0	0
6	A	6	0	8	3	0
6	B	6	0	8	10	0
6	D	12	0	16	0	0
7	A	138	0	0	0	0
7	B	184	0	0	1	0
7	C	211	0	0	0	0
7	D	233	0	0	0	0
All	All	11989	0	10487	54	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 2.

All (54) 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)
6:B:406:GOL:H2	1:D:126:THR:HB	1.43	1.01
1:B:76:THR:HA	6:B:406:GOL:H11	1.44	0.99
6:B:406:GOL:H31	1:D:76[A]:THR:HA	1.66	0.78
1:B:126:THR:HB	6:B:406:GOL:H32	1.66	0.78
1:A:164:SER:OG	1:A:166:ILE:HG12	1.85	0.77
6:B:406:GOL:H31	1:D:76[B]:THR:HA	1.67	0.77
1:A:74:LEU:HD23	1:A:87:ILE:HD12	1.77	0.66
1:B:126:THR:CB	6:B:406:GOL:H32	2.26	0.66
1:B:126:THR:HB	6:B:406:GOL:H12	1.79	0.65
1:A:126:THR:HB	6:A:406:GOL:H11	1.81	0.62
3:B:403:5V7:H5	3:B:403:5V7:N3	2.17	0.59
1:B:74:LEU:HD11	1:B:87:ILE:CD1	2.32	0.59
1:D:82:PHE:HB2	1:D:244[A]:LEU:HB2	1.86	0.56
3:D:403:5V7:H5	3:D:403:5V7:N3	2.20	0.55
1:A:297:ILE:HD12	1:A:320:PHE:HB3	1.88	0.55
1:C:153:LEU:HD11	1:C:197:ILE:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:VAL:HG11	1:C:125[B]:LEU:HG	1.90	0.54
1:B:75:VAL:HG11	1:B:125[B]:LEU:HG	1.92	0.52
3:A:403:5V7:N3	3:A:403:5V7:H5	2.25	0.51
3:C:403:5V7:N3	3:C:403:5V7:H5	2.25	0.51
1:B:126:THR:CB	6:B:406:GOL:H12	2.41	0.51
1:C:345:LEU:HD23	1:C:346:PRO:HD2	1.93	0.50
1:A:153:LEU:HD11	1:A:197:ILE:HG21	1.92	0.50
1:A:126:THR:CB	6:A:406:GOL:H11	2.41	0.50
1:D:82:PHE:HB2	1:D:244[B]:LEU:HB2	1.94	0.49
1:D:338:ASN:H	1:D:338:ASN:HD22	1.60	0.49
3:B:403:5V7:C2	3:B:403:5V7:N3	2.76	0.48
1:C:82:PHE:HB2	1:C:244:LEU:HB2	1.94	0.48
1:D:190:GLU:HG3	1:D:196:SER:HB3	1.97	0.47
1:D:160:VAL:O	1:D:164:SER:HB2	2.15	0.47
1:A:125[B]:LEU:HD21	1:A:244:LEU:HD13	1.96	0.47
1:B:259:LYS:HB2	7:B:614:HOH:O	2.14	0.46
3:D:403:5V7:N3	3:D:403:5V7:C2	2.78	0.46
1:B:126:THR:HB	6:B:406:GOL:C1	2.45	0.46
1:D:179:GLY:O	1:D:283:PHE:HA	2.16	0.46
1:C:150:ILE:HG23	1:C:289:THR:HG22	1.98	0.46
1:A:75:VAL:HG11	1:A:125[B]:LEU:HG	1.98	0.46
1:B:111:TYR:CD1	1:B:117:LEU:HD13	2.51	0.46
1:A:332:TRP:HA	1:A:337:ASP:HB2	1.98	0.45
3:A:403:5V7:C2	3:A:403:5V7:N3	2.80	0.45
1:A:44:LEU:HG	1:A:268:MET:CE	2.47	0.45
1:B:74:LEU:HD11	1:B:87:ILE:HD11	1.99	0.44
1:B:168:ILE:HD13	1:B:313:VAL:HG13	2.00	0.44
1:B:332:TRP:HA	1:B:337:ASP:HB2	2.02	0.42
6:B:406:GOL:H2	1:D:126:THR:CB	2.31	0.42
1:D:329:TYR:CZ	1:D:333:LYS:HD2	2.55	0.42
1:A:153:LEU:HA	5:A:405:EDO:H22	2.01	0.42
1:B:236:ALA:HB1	1:B:239:ARG:HG3	2.01	0.42
1:B:125[B]:LEU:HD21	1:B:244:LEU:HD13	2.01	0.41
1:C:141:TYR:CE2	1:C:149:ASN:HA	2.55	0.41
1:D:236:ALA:HB1	1:D:239:ARG:HG3	2.01	0.41
1:A:76:THR:HA	6:A:406:GOL:H32	2.02	0.41
1:D:19:PRO:HB3	1:D:30:TYR:CZ	2.56	0.40
1:D:81:LEU:HD11	1:D:226:PHE:CD2	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	342/360 (95%)	335 (98%)	7 (2%)	0	100	100
1	B	347/360 (96%)	343 (99%)	4 (1%)	0	100	100
1	C	350/360 (97%)	343 (98%)	7 (2%)	0	100	100
1	D	349/360 (97%)	345 (99%)	4 (1%)	0	100	100
All	All	1388/1440 (96%)	1366 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	266/316 (84%)	259 (97%)	7 (3%)	54	47
1	B	276/316 (87%)	264 (96%)	12 (4%)	35	27
1	C	276/316 (87%)	265 (96%)	11 (4%)	38	29
1	D	280/316 (89%)	271 (97%)	9 (3%)	46	38
All	All	1098/1264 (87%)	1059 (96%)	39 (4%)	43	34

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	A	132	TYR

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Mol	Chain	Res	Type
1	A	159	LEU
1	A	167	THR
1	A	175	TYR
1	A	182	LYS
1	A	289	THR
1	B	64	ASP
1	B	132	TYR
1	B	167	THR
1	B	173	THR
1	B	174	PRO
1	B	175	TYR
1	B	182	LYS
1	B	184	SER
1	B	289	THR
1	B	312[A]	MET
1	B	312[B]	MET
1	B	325	GLN
1	C	81	LEU
1	C	132	TYR
1	C	175	TYR
1	C	182	LYS
1	C	184	SER
1	C	218	ARG
1	C	288	SER
1	C	289	THR
1	C	318	ASP
1	C	331	LEU
1	C	345	LEU
1	D	81	LEU
1	D	112	SER
1	D	132	TYR
1	D	175	TYR
1	D	182	LYS
1	D	184	SER
1	D	306	CYS
1	D	312	MET
1	D	338	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	338	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	5V7	A	403	2	14,19,19	1.30	1 (7%)	14,27,27	2.33	6 (42%)
4	DMS	A	404	-	3,3,3	0.28	0	3,3,3	0.30	0
5	EDO	A	405	-	3,3,3	0.55	0	2,2,2	0.29	0
6	GOL	A	406	-	5,5,5	0.23	0	5,5,5	0.55	0
3	5V7	B	403	2	14,19,19	1.29	2 (14%)	14,27,27	2.40	7 (50%)
4	DMS	B	404	-	3,3,3	0.26	0	3,3,3	0.22	0
5	EDO	B	405	-	3,3,3	0.55	0	2,2,2	0.33	0
6	GOL	B	406	-	5,5,5	0.48	0	5,5,5	0.85	0
3	5V7	C	403	2	14,19,19	1.35	2 (14%)	14,27,27	2.29	5 (35%)
4	DMS	C	404	-	3,3,3	0.28	0	3,3,3	0.46	0
4	DMS	C	405	-	3,3,3	0.31	0	3,3,3	0.25	0
3	5V7	D	403	2	14,19,19	1.34	2 (14%)	14,27,27	2.27	5 (35%)
4	DMS	D	404	-	3,3,3	0.26	0	3,3,3	0.24	0
4	DMS	D	405	-	3,3,3	0.30	0	3,3,3	0.26	0
5	EDO	D	406	-	3,3,3	0.64	0	2,2,2	0.07	0
5	EDO	D	407	-	3,3,3	0.59	0	2,2,2	0.10	0
6	GOL	D	408	-	5,5,5	0.08	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	D	409	-	5,5,5	0.22	0	5,5,5	0.24	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
3	5V7	A	403	2	-	0/1/4/4	0/3/3/3
4	DMS	A	404	-	-	0/0/0/0	0/0/0/0
5	EDO	A	405	-	-	0/1/1/1	0/0/0/0
6	GOL	A	406	-	-	0/4/4/4	0/0/0/0
3	5V7	B	403	2	-	0/1/4/4	0/3/3/3
4	DMS	B	404	-	-	0/0/0/0	0/0/0/0
5	EDO	B	405	-	-	0/1/1/1	0/0/0/0
6	GOL	B	406	-	-	0/4/4/4	0/0/0/0
3	5V7	C	403	2	-	0/1/4/4	0/3/3/3
4	DMS	C	404	-	-	0/0/0/0	0/0/0/0
4	DMS	C	405	-	-	0/0/0/0	0/0/0/0
3	5V7	D	403	2	-	0/1/4/4	0/3/3/3
4	DMS	D	404	-	-	0/0/0/0	0/0/0/0
4	DMS	D	405	-	-	0/0/0/0	0/0/0/0
5	EDO	D	406	-	-	0/1/1/1	0/0/0/0
5	EDO	D	407	-	-	0/1/1/1	0/0/0/0
6	GOL	D	408	-	-	0/4/4/4	0/0/0/0
6	GOL	D	409	-	-	0/4/4/4	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	5V7	C3-N2	2.08	1.34	1.32
3	D	403	5V7	C3-N2	2.16	1.34	1.32
3	C	403	5V7	C3-N2	2.19	1.34	1.32
3	B	403	5V7	C9-C6	3.14	1.46	1.41
3	D	403	5V7	C9-C6	3.24	1.46	1.41
3	C	403	5V7	C9-C6	3.24	1.46	1.41
3	A	403	5V7	C9-C6	3.25	1.46	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	5V7	N3-C8-N4	-4.73	125.16	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	5V7	N3-C8-N4	-4.72	125.17	128.87
3	A	403	5V7	N3-C8-N4	-4.71	125.17	128.87
3	D	403	5V7	N3-C8-N4	-4.67	125.20	128.87
3	B	403	5V7	C4-C5-C6	-3.36	116.58	119.70
3	A	403	5V7	C4-C5-C6	-3.22	116.71	119.70
3	A	403	5V7	C6-C9-N4	-3.15	114.98	123.90
3	B	403	5V7	C6-C9-N4	-3.14	114.99	123.90
3	C	403	5V7	C6-C9-N4	-3.14	114.99	123.90
3	D	403	5V7	C6-C9-N4	-3.14	115.00	123.90
3	C	403	5V7	C4-C5-C6	-3.11	116.81	119.70
3	D	403	5V7	C4-C5-C6	-3.06	116.86	119.70
3	B	403	5V7	C7-C3-N2	-2.07	120.12	122.96
3	A	403	5V7	C4-N2-C3	2.12	119.44	117.94
3	D	403	5V7	C5-C6-C7	2.17	120.18	118.06
3	A	403	5V7	C5-C6-C7	2.25	120.27	118.06
3	C	403	5V7	C5-C6-C7	2.27	120.28	118.06
3	B	403	5V7	C5-C6-C7	2.39	120.41	118.06
3	B	403	5V7	C4-N2-C3	2.52	119.73	117.94
3	D	403	5V7	C8-N4-C9	3.85	122.77	116.13
3	B	403	5V7	C8-N4-C9	3.88	122.81	116.13
3	A	403	5V7	C8-N4-C9	3.88	122.81	116.13
3	C	403	5V7	C8-N4-C9	3.89	122.82	116.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	5V7	2	0
5	A	405	EDO	1	0
6	A	406	GOL	3	0
3	B	403	5V7	2	0
6	B	406	GOL	10	0
3	C	403	5V7	1	0
3	D	403	5V7	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	342/360 (95%)	0.28	26 (7%) 17 19	38, 61, 93, 110	0
1	B	344/360 (95%)	-0.01	16 (4%) 35 41	32, 53, 87, 102	0
1	C	350/360 (97%)	0.38	26 (7%) 17 20	35, 54, 88, 122	0
1	D	348/360 (96%)	0.10	11 (3%) 51 58	34, 50, 80, 94	0
All	All	1384/1440 (96%)	0.19	79 (5%) 27 31	32, 55, 89, 122	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	ALA	5.7
1	B	334	ALA	5.3
1	A	104	ASP	4.9
1	B	340	VAL	4.7
1	C	354	LEU	4.7
1	C	331	LEU	4.6
1	A	339	THR	4.1
1	D	167	THR	4.1
1	B	335	GLY	4.0
1	B	111	TYR	3.9
1	B	338	ASN	3.9
1	C	318	ASP	3.8
1	D	7	THR	3.8
1	C	351	ALA	3.8
1	D	311	ASP	3.7
1	A	326	PRO	3.7
1	C	311	ASP	3.7
1	C	307	SER	3.7
1	D	112	SER	3.6
1	C	350	ALA	3.6
1	A	107	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	308	CYS	3.5
1	A	337	ASP	3.5
1	C	353	PHE	3.5
1	C	335	GLY	3.5
1	B	114[A]	PHE	3.4
1	C	334	ALA	3.3
1	A	335	GLY	3.3
1	B	103	SER	3.3
1	C	340	VAL	3.2
1	C	336	LYS	3.2
1	A	331	LEU	3.2
1	C	338	ASN	3.2
1	C	310	LYS	3.0
1	A	144[A]	HIS	3.0
1	D	351	ALA	3.0
1	C	8	LEU	3.0
1	C	112	SER	2.9
1	D	338	ASN	2.9
1	D	353	PHE	2.8
1	A	64	ASP	2.8
1	A	329	TYR	2.8
1	B	311	ASP	2.7
1	A	351	ALA	2.7
1	D	310	LYS	2.7
1	C	7	THR	2.7
1	A	96	GLU	2.7
1	A	330	LYS	2.6
1	A	20	THR	2.6
1	B	110	ARG	2.6
1	A	21	MET	2.6
1	A	66	VAL	2.6
1	B	336	LYS	2.5
1	A	332	TRP	2.5
1	A	340	VAL	2.5
1	A	226	PHE	2.5
1	B	104	ASP	2.4
1	C	321	VAL	2.4
1	B	337	ASP	2.4
1	A	106	TYR	2.4
1	B	112	SER	2.3
1	A	145	VAL	2.3
1	B	330	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	229	GLY	2.2
1	D	170	GLY	2.2
1	C	176	LEU	2.2
1	D	111	TYR	2.2
1	B	312[A]	MET	2.2
1	A	318	ASP	2.1
1	C	317	MET	2.1
1	A	316	SER	2.1
1	D	352	GLU	2.1
1	B	351	ALA	2.1
1	A	338	ASN	2.1
1	C	332	TRP	2.1
1	A	327	GLU	2.0
1	C	166	ILE	2.0
1	C	197	ILE	2.0
1	C	289	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 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
6	GOL	A	406	6/6	0.84	0.32	12.44	34,37,38,39	6
4	DMS	C	404	4/4	0.92	0.42	8.73	88,88,89,89	0
3	5V7	C	403	17/17	0.94	0.31	5.73	33,36,43,44	17
6	GOL	D	409	6/6	0.85	0.26	4.97	43,44,46,49	6
5	EDO	B	405	4/4	0.85	0.22	4.10	72,74,78,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	5V7	D	403	17/17	0.95	0.24	3.96	30,35,40,41	17
4	DMS	B	404	4/4	0.94	0.23	3.91	88,89,89,90	0
6	GOL	B	406	6/6	0.93	0.21	3.77	30,34,36,36	6
3	5V7	A	403	17/17	0.95	0.21	3.04	36,42,44,44	17
4	DMS	A	404	4/4	0.95	0.23	2.27	94,94,96,96	0
4	DMS	C	405	4/4	0.82	0.26	2.07	96,97,97,97	4
4	DMS	D	404	4/4	0.93	0.22	1.39	96,96,97,97	0
3	5V7	B	403	17/17	0.95	0.16	1.17	37,40,43,44	17
5	EDO	A	405	4/4	0.82	0.15	0.44	67,69,70,72	0
2	ZN	A	402	1/1	0.99	0.11	-0.41	48,48,48,48	1
2	ZN	B	402	1/1	0.98	0.09	-0.54	42,42,42,42	1
5	EDO	D	407	4/4	0.91	0.10	-0.69	63,64,64,64	4
2	ZN	D	402	1/1	1.00	0.09	-0.71	41,41,41,41	1
2	ZN	C	402	1/1	0.99	0.07	-1.32	56,56,56,56	1
5	EDO	D	406	4/4	0.85	0.16	-	69,70,70,70	0
2	ZN	A	401	1/1	0.99	0.17	-	43,43,43,43	1
2	ZN	B	401	1/1	1.00	0.15	-	39,39,39,39	1
6	GOL	D	408	6/6	0.53	0.55	-	105,107,108,109	0
4	DMS	D	405	4/4	0.85	0.16	-	129,129,130,130	0
2	ZN	C	401	1/1	1.00	0.16	-	43,43,43,43	1
2	ZN	D	401	1/1	1.00	0.15	-	43,43,43,43	0

6.5 Other polymers

There are no such residues in this entry.