



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:00 PM UTC

PDB ID : 6F6J / pdb_00006f6j
Title : Crystal structure of the Fe(II)/alpha-ketoglutarate dependent dioxygenase KDO1 with Fe(II)/succinate/(3S)-3-hydroxy-L-lysine
Authors : Isabet, T.; Stura, E.A.; Legrand, P.; Zaparucha, A.; Bastard, K.
Deposited on : 2017-12-05
Resolution : 2.00 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

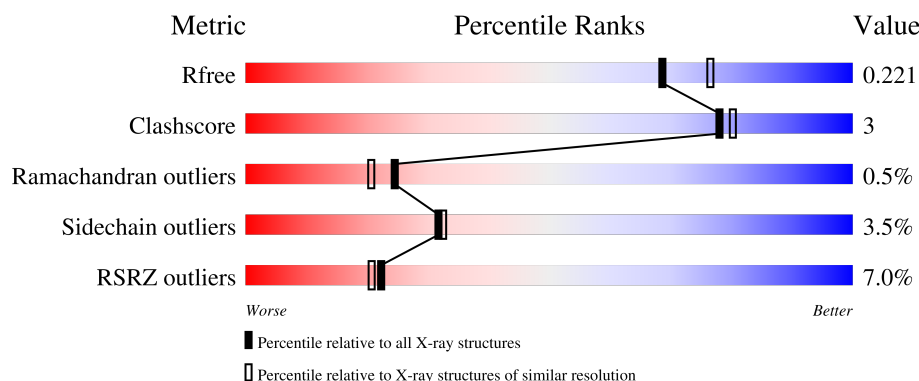
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	358	6% 80% 9% 9%
1	B	358	6% 82% 9% 9%
1	C	358	10% 82% 8% 9%
1	D	358	4% 83% 8% 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
3	SIN	A	402[A]	-	X	-	-
3	SIN	A	402[B]	-	X	-	-
3	SIN	D	402	-	X	-	-
5	ACT	A	404	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11560 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.

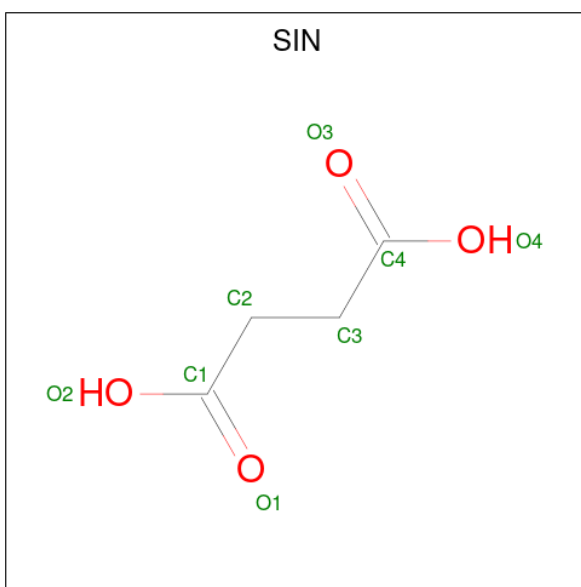
- Molecule 1 is a protein called L-lysine 3-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	6	0
			2558	1603	463	476	16			
1	B	326	Total	C	N	O	S	0	6	0
			2562	1605	463	480	14			
1	C	325	Total	C	N	O	S	0	4	0
			2539	1592	458	474	15			
1	D	326	Total	C	N	O	S	0	2	0
			2526	1585	453	474	14			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

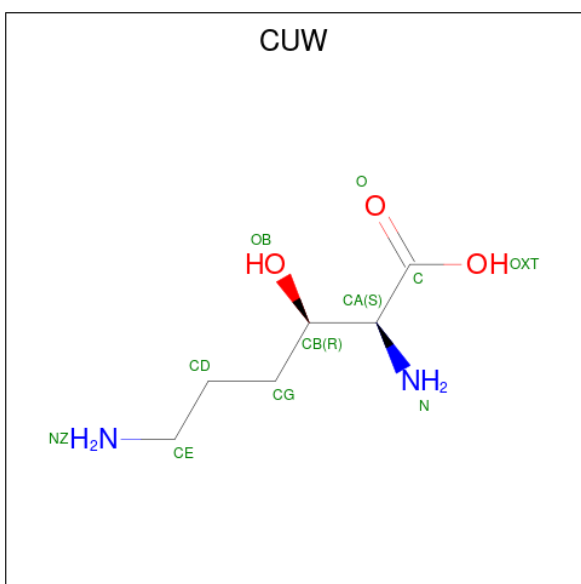
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄).



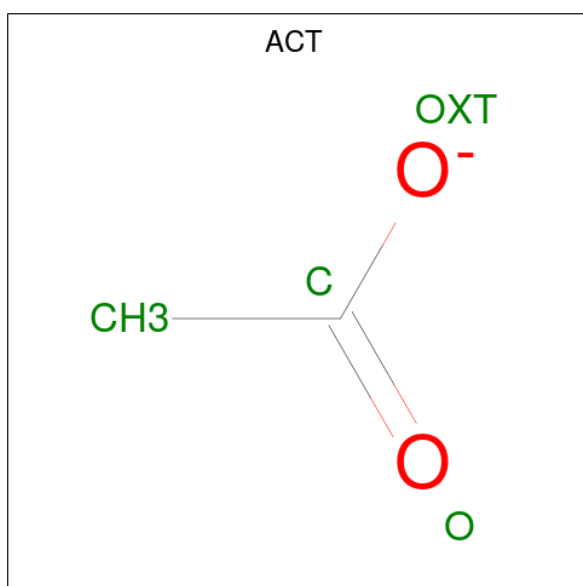
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			16	8	8		
3	B	1	Total	C	O	0	0
			8	4	4		
3	C	1	Total	C	O	0	1
			16	8	8		
3	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is (2 {S},3 {R})-2,6-bis(azanyl)-3-oxidanyl-hexanoic acid (CCD ID: CUW) (formula: C₆H₁₄N₂O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 11 6 2 3	0	0
4	B	1	Total C N O 11 6 2 3	0	0
4	C	1	Total C N O 11 6 2 3	0	0
4	D	1	Total C N O 11 6 2 3	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

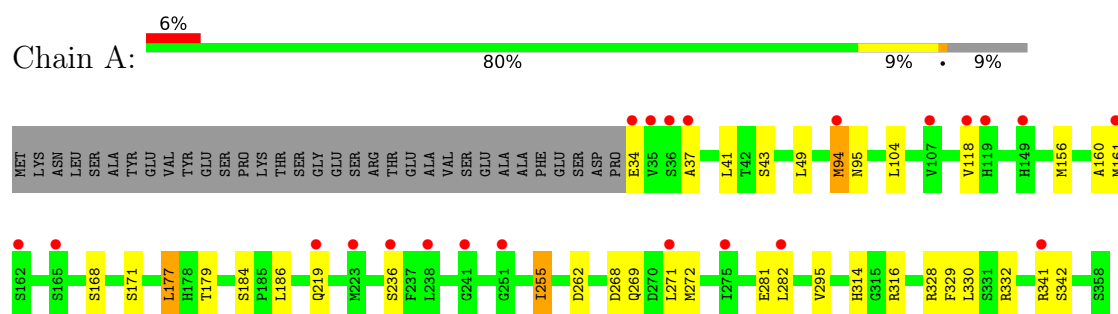
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	353	Total O 354 354	0	4
6	B	277	Total O 277 277	0	0
6	C	345	Total O 345 345	0	1
6	D	295	Total O 295 295	0	0

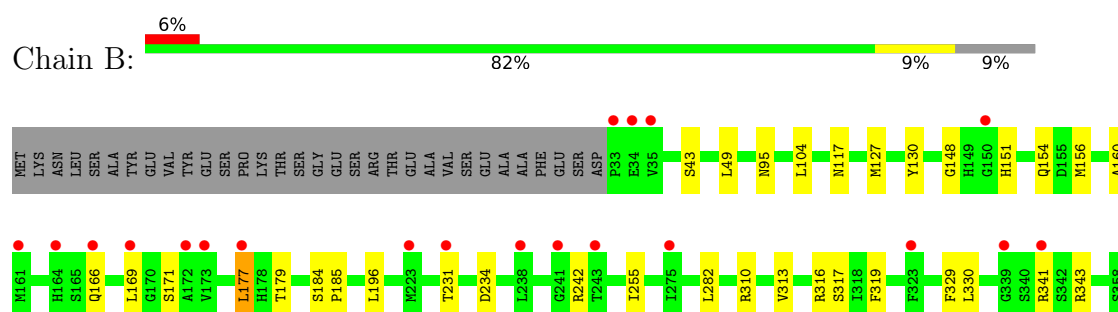
3 Residue-property plots [i](#)

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.

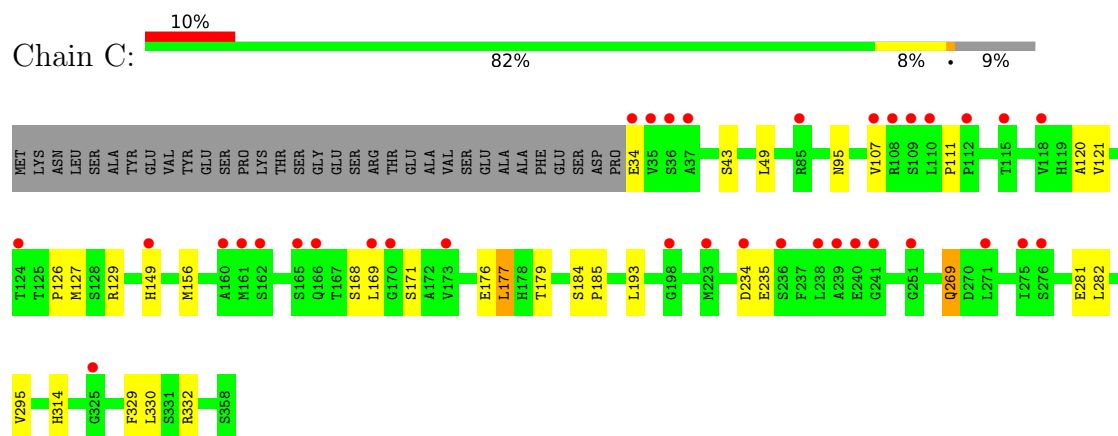
- Molecule 1: L-lysine 3-hydroxylase



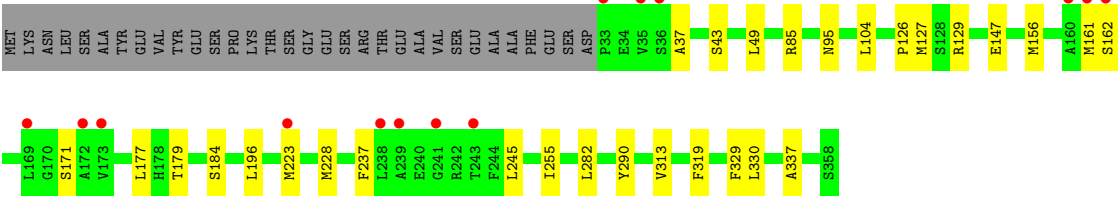
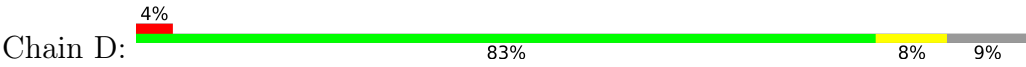
- Molecule 1: L-lysine 3-hydroxylase



- Molecule 1: L-lysine 3-hydroxylase



- Molecule 1: L-lysine 3-hydroxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.95Å 67.39Å 110.65Å 107.55° 102.87° 93.58°	Depositor
Resolution (Å)	40.00 – 2.00 40.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.00-2.00) 99.3 (40.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.194 , 0.225 0.190 , 0.221	Depositor DCC
R_{free} test set	5027 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11560	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.12% 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: ACT, FE, SIN, CUW

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	0.90	0/2613	1.17	7/3545 (0.2%)
1	B	0.83	0/2617	1.20	9/3552 (0.3%)
1	C	0.85	0/2594	1.18	7/3521 (0.2%)
1	D	0.83	0/2581	1.20	6/3505 (0.2%)
All	All	0.85	0/10405	1.19	29/14123 (0.2%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	95	ASN	CA-CB-CG	7.46	120.06	112.60
1	D	329	PHE	CA-CB-CG	7.22	121.02	113.80
1	C	329	PHE	CA-CB-CG	7.20	121.00	113.80
1	B	329	PHE	CA-CB-CG	7.17	120.97	113.80
1	A	329	PHE	CA-CB-CG	7.15	120.95	113.80
1	B	95	ASN	CA-CB-CG	6.87	119.47	112.60
1	A	255	ILE	N-CA-C	-6.68	105.24	111.45
1	C	95	ASN	CA-CB-CG	6.48	119.08	112.60
1	A	95	ASN	CA-CB-CG	6.47	119.07	112.60
1	D	179	THR	N-CA-C	-5.89	100.07	109.96
1	B	179	THR	N-CA-C	-5.80	100.21	109.96
1	A	179	THR	N-CA-C	-5.76	100.28	109.96
1	B	184	SER	N-CA-C	5.72	117.92	109.62
1	D	184	SER	N-CA-C	5.70	117.88	109.62
1	A	268	ASP	CA-C-N	5.61	128.11	120.54
1	A	268	ASP	C-N-CA	5.61	128.11	120.54
1	A	184	SER	N-CA-C	5.54	117.65	109.62
1	B	234	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	184	SER	N-CA-C	5.49	117.58	109.62
1	B	319	PHE	CA-CB-CG	5.45	119.25	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	255	ILE	N-CA-C	-5.45	105.80	111.58
1	C	179	THR	N-CA-C	-5.39	100.90	109.96
1	B	160	ALA	CA-C-N	5.33	127.42	120.28
1	B	160	ALA	C-N-CA	5.33	127.42	120.28
1	B	255	ILE	N-CA-C	-5.23	106.03	111.58
1	C	120	ALA	CA-C-N	5.11	127.46	120.46
1	C	120	ALA	C-N-CA	5.11	127.46	120.46
1	C	234	ASP	CA-CB-CG	5.09	117.69	112.60
1	D	319	PHE	CA-CB-CG	5.06	118.86	113.80

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	2558	0	2514	20	0
1	B	2562	0	2513	15	0
1	C	2539	0	2494	15	0
1	D	2526	0	2483	11	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	16	0	8	2	0
3	B	8	0	4	0	0
3	C	16	0	8	3	0
3	D	8	0	4	0	0
4	A	11	0	0	0	0
4	B	11	0	0	0	0
4	C	11	0	0	0	0
4	D	11	0	0	0	0
5	A	4	0	3	2	0
5	D	4	0	3	0	0
6	A	354	0	0	1	0
6	B	277	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	345	0	0	1	0
6	D	295	0	0	1	0
All	All	11560	0	10034	57	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 (57) 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:328:ARG:HH12	3:A:402[B]:SIN:H21	1.50	0.76
1:D:177:LEU:HD13	1:D:290:TYR:CE1	2.27	0.69
1:A:177:LEU:HD23	1:A:269:GLN:OE1	1.93	0.67
1:A:255:ILE:HG12	1:A:272:MET:HE1	1.76	0.67
1:D:177:LEU:HD11	1:D:313:VAL:HG23	1.78	0.65
1:A:41:LEU:CD1	1:A:104:LEU:HD23	2.27	0.65
1:A:94[A]:MET:HE1	1:A:262:ASP:HB2	1.80	0.64
1:D:337:ALA:HB2	6:D:552:HOH:O	2.03	0.58
1:C:107:VAL:HG21	1:C:127:MET:HB2	1.85	0.58
1:A:94[A]:MET:CE	1:B:343:ARG:HH21	2.18	0.57
1:B:154[A]:GLN:HG2	6:B:532:HOH:O	2.05	0.56
1:A:156[A]:MET:HE2	1:A:168:SER:HB2	1.87	0.55
1:C:156[B]:MET:HE2	1:C:168:SER:HB3	1.87	0.55
1:A:41:LEU:HD11	1:A:104:LEU:HD23	1.87	0.55
1:A:342:SER:HB3	5:A:404:ACT:H1	1.89	0.55
1:A:160:ALA:HB1	1:D:223:MET:HG3	1.88	0.55
1:C:185:PRO:HD2	6:C:554:HOH:O	2.06	0.54
1:C:314:HIS:HD2	3:C:402[A]:SIN:C4	2.20	0.54
1:C:156[B]:MET:HE1	1:C:332:ARG:HD3	1.91	0.52
1:B:185:PRO:HD2	6:B:535:HOH:O	2.11	0.51
1:A:161:MET:HE3	1:D:228:MET:HG2	1.93	0.50
1:B:148:GLY:HA3	1:B:154[A]:GLN:CD	2.37	0.49
1:A:34:GLU:HB3	1:A:295:VAL:HB	1.94	0.49
1:A:94[A]:MET:HE1	1:B:343:ARG:HH21	1.76	0.48
1:C:156[B]:MET:HB3	1:C:330:LEU:HB2	1.95	0.48
1:D:147:GLU:HB2	1:D:237:PHE:CE1	2.48	0.48
1:D:127:MET:HG2	1:D:196:LEU:CD2	2.43	0.48
1:A:156[B]:MET:HB2	1:A:330:LEU:HB2	1.95	0.48
1:D:156:MET:HB2	1:D:330:LEU:HB2	1.95	0.47
1:B:127:MET:HG2	1:B:196:LEU:HD21	1.97	0.47
1:C:156[A]:MET:HB2	1:C:330:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:MET:HG2	1:B:196:LEU:CD2	2.45	0.47
1:D:127:MET:HG2	1:D:196:LEU:HD21	1.97	0.46
1:B:156:MET:HB2	1:B:330:LEU:HB2	1.96	0.46
1:C:176:GLU:HB3	1:C:269:GLN:HG2	1.97	0.46
1:C:34:GLU:HB3	1:C:295:VAL:HB	1.96	0.46
1:D:177:LEU:HD11	1:D:313:VAL:CG2	2.44	0.46
1:A:186:LEU:HB3	5:A:404:ACT:H3	1.98	0.45
1:C:177:LEU:HD23	1:C:269:GLN:HE21	1.82	0.44
1:B:117:ASN:HB2	1:B:154[A]:GLN:HE21	1.82	0.44
1:A:156[A]:MET:HB3	1:A:330:LEU:HB2	2.01	0.43
1:A:156[A]:MET:HE1	1:A:332:ARG:HD3	2.00	0.43
1:C:193:LEU:HD11	3:C:402[B]:SIN:H31	1.99	0.43
1:B:127:MET:HA	1:B:130:TYR:CD2	2.54	0.42
1:D:126:PRO:HB3	1:D:129:ARG:HH21	1.84	0.42
1:A:156[B]:MET:SD	1:A:168:SER:HB2	2.59	0.42
1:B:117:ASN:HB3	1:B:169:LEU:HD21	2.02	0.42
1:B:316:ARG:HD2	1:B:317:SER:O	2.20	0.42
1:C:126:PRO:HA	1:C:129:ARG:NH2	2.35	0.41
1:B:177:LEU:HD12	1:B:313:VAL:HG21	2.01	0.41
1:C:156[B]:MET:SD	3:C:402[B]:SIN:H32	2.61	0.41
1:B:151:HIS:HB2	1:B:154[A]:GLN:OE1	2.21	0.41
1:A:316:ARG:HG3	3:A:402[B]:SIN:O3	2.20	0.41
1:C:176:GLU:HB3	1:C:269:GLN:CG	2.51	0.41
1:B:310:ARG:NH2	6:B:501:HOH:O	2.53	0.41
1:C:111:PRO:HG2	1:C:121:VAL:CG1	2.51	0.41
1:A:314:HIS:HD2	6:A:702[B]:HOH:O	2.04	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	329/358 (92%)	325 (99%)	2 (1%)	2 (1%)	21	17
1	B	330/358 (92%)	327 (99%)	2 (1%)	1 (0%)	36	35
1	C	327/358 (91%)	323 (99%)	3 (1%)	1 (0%)	36	35
1	D	326/358 (91%)	321 (98%)	3 (1%)	2 (1%)	21	17
All	All	1312/1432 (92%)	1296 (99%)	10 (1%)	6 (0%)	24	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ALA
1	A	171	SER
1	C	171	SER
1	D	171	SER
1	B	171	SER
1	D	37	ALA

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	271/293 (92%)	258 (95%)	13 (5%)	23	21
1	B	271/293 (92%)	261 (96%)	10 (4%)	30	30
1	C	269/293 (92%)	259 (96%)	10 (4%)	30	30
1	D	268/293 (92%)	260 (97%)	8 (3%)	36	38
All	All	1079/1172 (92%)	1038 (96%)	41 (4%)	32	29

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	A	49	LEU
1	A	94[A]	MET
1	A	94[B]	MET
1	A	118	VAL

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Mol	Chain	Res	Type
1	A	177	LEU
1	A	219	GLN
1	A	236	SER
1	A	271	LEU
1	A	281	GLU
1	A	282	LEU
1	A	341[A]	ARG
1	A	341[B]	ARG
1	B	43	SER
1	B	49	LEU
1	B	104	LEU
1	B	166	GLN
1	B	177	LEU
1	B	231	THR
1	B	242	ARG
1	B	282	LEU
1	B	341[A]	ARG
1	B	341[B]	ARG
1	C	43	SER
1	C	49	LEU
1	C	149[A]	HIS
1	C	149[B]	HIS
1	C	169	LEU
1	C	177	LEU
1	C	235	GLU
1	C	269	GLN
1	C	281	GLU
1	C	282	LEU
1	D	43	SER
1	D	49	LEU
1	D	85	ARG
1	D	104	LEU
1	D	161	MET
1	D	162	SER
1	D	245	LEU
1	D	282	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	283	GLN

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Mol	Chain	Res	Type
1	B	106	GLN
1	B	117	ASN
1	B	131	GLN
1	C	131	GLN
1	C	269	GLN
1	C	314	HIS
1	D	131	GLN
1	D	280	GLN

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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	CUW	C	403	-	9,10,10	0.34	0	9,12,12	0.53	0
3	SIN	C	402[A]	-	7,7,7	0.15	0	8,8,8	0.32	0
3	SIN	C	402[B]	2	7,7,7	0.21	0	8,8,8	0.20	0
3	SIN	A	402[A]	2	7,7,7	2.18	4 (57%)	8,8,8	2.13	4 (50%)
3	SIN	A	402[B]	-	7,7,7	2.12	4 (57%)	8,8,8	2.00	4 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SIN	D	402	2	7,7,7	1.47	2 (28%)	8,8,8	1.56	2 (25%)
4	CUW	A	403	2	9,10,10	1.42	2 (22%)	9,12,12	1.17	2 (22%)
3	SIN	B	402	2	7,7,7	0.29	0	8,8,8	0.21	0
5	ACT	A	404	-	3,3,3	1.11	0	3,3,3	0.71	0
4	CUW	D	403	-	9,10,10	0.34	0	9,12,12	0.31	0
5	ACT	D	404	-	3,3,3	0.90	0	3,3,3	0.99	0
4	CUW	B	403	-	9,10,10	0.44	0	9,12,12	0.57	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	CUW	C	403	-	-	1/12/12/12	-
3	SIN	C	402[A]	-	-	2/5/5/5	-
3	SIN	C	402[B]	2	-	3/5/5/5	-
3	SIN	A	402[A]	2	-	5/5/5/5	-
3	SIN	A	402[B]	-	-	4/5/5/5	-
3	SIN	D	402	2	-	4/5/5/5	-
4	CUW	A	403	2	-	3/12/12/12	-
3	SIN	B	402	2	-	4/5/5/5	-
4	CUW	D	403	-	-	1/12/12/12	-
4	CUW	B	403	-	-	3/12/12/12	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[A]	SIN	O3-C4	3.22	1.32	1.22
4	A	403	CUW	O-C	3.00	1.31	1.22
3	A	402[A]	SIN	O4-C4	-2.99	1.20	1.30
3	A	402[B]	SIN	O4-C4	-2.97	1.21	1.30
4	A	403	CUW	OXT-C	-2.89	1.21	1.30
3	A	402[B]	SIN	O1-C1	2.88	1.31	1.22
3	A	402[B]	SIN	O2-C1	-2.85	1.21	1.30
3	D	402	SIN	O3-C4	2.83	1.31	1.22
3	A	402[A]	SIN	O1-C1	2.81	1.31	1.22
3	D	402	SIN	O4-C4	-2.66	1.22	1.30
3	A	402[B]	SIN	O3-C4	2.49	1.30	1.22
3	A	402[A]	SIN	O2-C1	-2.45	1.22	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402[A]	SIN	O1-C1-C2	-3.36	112.44	123.09
3	D	402	SIN	O3-C4-C3	-3.20	112.93	123.09
3	A	402[A]	SIN	O2-C1-C2	3.13	123.90	114.00
3	D	402	SIN	O4-C4-C3	3.01	123.50	114.00
3	A	402[B]	SIN	O3-C4-C3	-2.96	113.72	123.09
3	A	402[B]	SIN	O4-C4-C3	2.91	123.21	114.00
3	A	402[A]	SIN	O3-C4-C3	-2.84	114.07	123.09
3	A	402[B]	SIN	O1-C1-C2	-2.79	114.25	123.09
3	A	402[A]	SIN	O4-C4-C3	2.63	122.30	114.00
3	A	402[B]	SIN	O2-C1-C2	2.60	122.22	114.00
4	A	403	CUW	O-C-CA	-2.34	113.78	121.72
4	A	403	CUW	OXT-C-CA	2.21	121.77	114.15

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	CUW	OXT-C-CA-CB
4	B	403	CUW	O-C-CA-CB
4	A	403	CUW	CA-CB-CG-CD
3	C	402[B]	SIN	C1-C2-C3-C4
3	A	402[A]	SIN	C1-C2-C3-C4
4	A	403	CUW	O-C-CA-N
4	A	403	CUW	OXT-C-CA-N
4	B	403	CUW	OXT-C-CA-N
4	C	403	CUW	CE-CD-CG-CB
3	C	402[B]	SIN	O1-C1-C2-C3
3	C	402[A]	SIN	O2-C1-C2-C3
3	A	402[A]	SIN	C2-C3-C4-O4
3	A	402[A]	SIN	C2-C3-C4-O3
3	B	402	SIN	C2-C3-C4-O3
3	B	402	SIN	C2-C3-C4-O4
3	C	402[B]	SIN	O2-C1-C2-C3
3	A	402[A]	SIN	O1-C1-C2-C3
3	A	402[B]	SIN	O2-C1-C2-C3
3	C	402[A]	SIN	O1-C1-C2-C3
3	D	402	SIN	O2-C1-C2-C3
3	D	402	SIN	C2-C3-C4-O4
3	A	402[B]	SIN	C2-C3-C4-O3
3	A	402[B]	SIN	C2-C3-C4-O4
3	D	402	SIN	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	402[A]	SIN	O2-C1-C2-C3
3	A	402[B]	SIN	O1-C1-C2-C3
3	D	402	SIN	C2-C3-C4-O3
4	D	403	CUW	CA-CB-CG-CD
3	B	402	SIN	O2-C1-C2-C3
3	B	402	SIN	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402[A]	SIN	1	0
3	C	402[B]	SIN	2	0
3	A	402[B]	SIN	2	0
5	A	404	ACT	2	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 ⓘ

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	325/358 (90%)	0.48	22 (6%)	23 22	18, 44, 69, 90	6 (1%)
1	B	326/358 (91%)	0.61	20 (6%)	27 26	20, 52, 79, 105	6 (1%)
1	C	325/358 (90%)	0.59	35 (10%)	11 10	19, 47, 72, 99	4 (1%)
1	D	326/358 (91%)	0.55	14 (4%)	40 39	20, 52, 80, 108	2 (0%)
All	All	1302/1432 (90%)	0.56	91 (6%)	22 21	18, 49, 76, 108	18 (1%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	VAL	5.7
1	C	36	SER	5.3
1	C	118	VAL	5.0
1	A	118	VAL	4.2
1	B	35	VAL	4.2
1	A	36	SER	4.1
1	C	107	VAL	4.0
1	C	37	ALA	3.9
1	D	33	PRO	3.8
1	C	110	LEU	3.7
1	B	172	ALA	3.7
1	A	271	LEU	3.7
1	A	251	GLY	3.6
1	C	170	GLY	3.3
1	B	341[A]	ARG	3.2
1	C	160	ALA	3.2
1	A	149[A]	HIS	3.2
1	A	162	SER	3.2
1	B	33	PRO	3.1
1	D	35	VAL	3.0
1	C	115	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	35	VAL	2.9
1	D	36	SER	2.9
1	A	107	VAL	2.8
1	C	251	GLY	2.8
1	D	172	ALA	2.8
1	C	238	LEU	2.8
1	A	37	ALA	2.8
1	B	339	GLY	2.8
1	A	236	SER	2.7
1	C	276	SER	2.7
1	C	169	LEU	2.7
1	C	271	LEU	2.7
1	D	243	THR	2.7
1	B	177	LEU	2.7
1	C	34	GLU	2.7
1	C	236	SER	2.7
1	C	124	THR	2.6
1	C	85[A]	ARG	2.6
1	D	161	MET	2.5
1	D	239	ALA	2.5
1	D	169	LEU	2.5
1	B	161	MET	2.5
1	B	238	LEU	2.5
1	D	241	GLY	2.5
1	D	173	VAL	2.4
1	A	219	GLN	2.4
1	B	243	THR	2.4
1	C	325	GLY	2.4
1	C	162	SER	2.4
1	B	150	GLY	2.4
1	B	231	THR	2.4
1	A	119	HIS	2.4
1	A	238	LEU	2.4
1	C	198	GLY	2.4
1	D	162	SER	2.4
1	C	241	GLY	2.3
1	B	223	MET	2.3
1	C	161	MET	2.3
1	C	240	GLU	2.3
1	A	223	MET	2.3
1	C	109	SER	2.3
1	C	112	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	241	GLY	2.3
1	C	223	MET	2.3
1	C	149[A]	HIS	2.2
1	C	165	SER	2.2
1	C	108	ARG	2.2
1	C	275	ILE	2.2
1	A	161	MET	2.2
1	A	341[A]	ARG	2.2
1	C	239	ALA	2.2
1	B	164	HIS	2.2
1	A	94[A]	MET	2.2
1	B	166	GLN	2.1
1	C	166	GLN	2.1
1	D	160	ALA	2.1
1	A	165	SER	2.1
1	C	234	ASP	2.1
1	C	173	VAL	2.1
1	A	282	LEU	2.1
1	A	34	GLU	2.1
1	B	275	ILE	2.1
1	B	173	VAL	2.1
1	B	34	GLU	2.1
1	B	323	PHE	2.1
1	D	223	MET	2.0
1	B	169	LEU	2.0
1	D	238	LEU	2.0
1	A	241	GLY	2.0
1	A	275	ILE	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(Å ²)	Q<0.9
4	CUW	B	403	11/11	0.66	0.21	75,80,84,86	0
4	CUW	A	403	11/11	0.71	0.24	80,84,85,87	0
3	SIN	B	402	8/8	0.76	0.20	66,74,79,81	0
4	CUW	C	403	11/11	0.76	0.20	64,68,72,74	0
5	ACT	D	404	4/4	0.82	0.21	43,48,51,53	0
4	CUW	D	403	11/11	0.83	0.14	54,62,68,71	0
3	SIN	D	402	8/8	0.85	0.15	59,75,83,86	0
3	SIN	A	402[B]	8/8	0.87	0.19	82,83,84,84	8
3	SIN	A	402[A]	8/8	0.87	0.19	32,47,55,58	8
5	ACT	A	404	4/4	0.90	0.24	56,57,57,60	0
3	SIN	C	402[B]	8/8	0.91	0.15	65,68,70,72	8
3	SIN	C	402[A]	8/8	0.91	0.15	38,48,50,51	8
2	FE	B	401	1/1	0.92	0.16	103,103,103,103	0
2	FE	C	401	1/1	0.94	0.07	78,78,78,78	1
2	FE	D	401	1/1	0.95	0.15	103,103,103,103	0
2	FE	A	401	1/1	0.98	0.05	76,76,76,76	1

6.5 Other polymers [i](#)

There are no such residues in this entry.