Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 12:33 AM EDT

PDB ID	:	5KLL
Title	:	Crystal structure of 2-hydroxymuconate-6-semialdehyde derived tautomeric intermediate in 2-aminomuconate 6-semialdehyde dehydrogenase N169D
Authors	:	Yang, Y.; Davis, I.; Ha, U.; Wang, Y.; Shin, I.; Liu, A.
Deposited on	:	2016-06-24
Resolution	:	2.17 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:

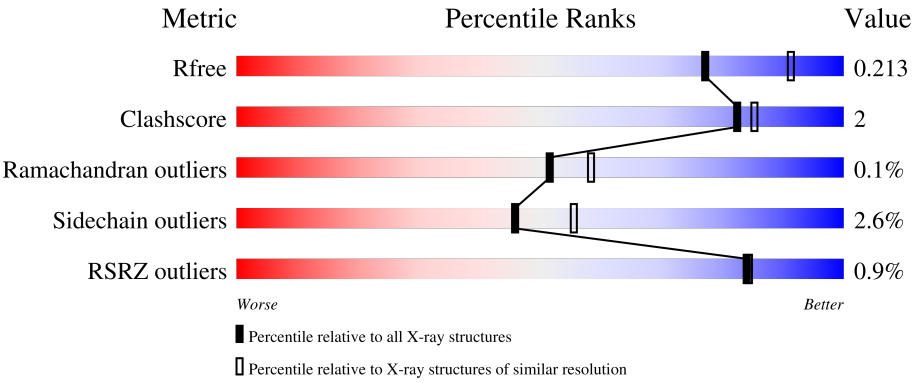
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	520	87% 5% 7%
1	B	520	88% 5% 7%
1	C	520	86% 7% 7%
1	D	520	87% 5% 7%

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
2	6UN	A	601	-	-	X	-
2	6UN	B	601	-	-	X	-
2	6UN	C	601	-	-	X	-
2	6UN	D	601	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15960 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 2-aminomuconate 6-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	2	0
			3684	2329	639	703	13			
1	B	483	Total	C	N	O	S	0	2	0
			3684	2329	639	703	13			
1	C	483	Total	C	N	O	S	0	2	0
			3684	2329	639	703	13			
1	D	483	Total	C	N	O	S	0	1	0
			3674	2323	636	702	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q83V33
A	-18	GLY	-	expression tag	UNP Q83V33
A	-17	SER	-	expression tag	UNP Q83V33
A	-16	SER	-	expression tag	UNP Q83V33
A	-15	HIS	-	expression tag	UNP Q83V33
A	-14	HIS	-	expression tag	UNP Q83V33
A	-13	HIS	-	expression tag	UNP Q83V33
A	-12	HIS	-	expression tag	UNP Q83V33
A	-11	HIS	-	expression tag	UNP Q83V33
A	-10	HIS	-	expression tag	UNP Q83V33
A	-9	SER	-	expression tag	UNP Q83V33
A	-8	SER	-	expression tag	UNP Q83V33
A	-7	GLY	-	expression tag	UNP Q83V33
A	-6	LEU	-	expression tag	UNP Q83V33
A	-5	VAL	-	expression tag	UNP Q83V33
A	-4	PRO	-	expression tag	UNP Q83V33
A	-3	ARG	-	expression tag	UNP Q83V33
A	-2	GLY	-	expression tag	UNP Q83V33
A	-1	SER	-	expression tag	UNP Q83V33
A	0	HIS	-	expression tag	UNP Q83V33
A	169	ASP	ASN	engineered mutation	UNP Q83V33

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP Q83V33
B	-18	GLY	-	expression tag	UNP Q83V33
B	-17	SER	-	expression tag	UNP Q83V33
B	-16	SER	-	expression tag	UNP Q83V33
B	-15	HIS	-	expression tag	UNP Q83V33
B	-14	HIS	-	expression tag	UNP Q83V33
B	-13	HIS	-	expression tag	UNP Q83V33
B	-12	HIS	-	expression tag	UNP Q83V33
B	-11	HIS	-	expression tag	UNP Q83V33
B	-10	HIS	-	expression tag	UNP Q83V33
B	-9	SER	-	expression tag	UNP Q83V33
B	-8	SER	-	expression tag	UNP Q83V33
B	-7	GLY	-	expression tag	UNP Q83V33
B	-6	LEU	-	expression tag	UNP Q83V33
B	-5	VAL	-	expression tag	UNP Q83V33
B	-4	PRO	-	expression tag	UNP Q83V33
B	-3	ARG	-	expression tag	UNP Q83V33
B	-2	GLY	-	expression tag	UNP Q83V33
B	-1	SER	-	expression tag	UNP Q83V33
B	0	HIS	-	expression tag	UNP Q83V33
B	169	ASP	ASN	engineered mutation	UNP Q83V33
C	-19	MET	-	initiating methionine	UNP Q83V33
C	-18	GLY	-	expression tag	UNP Q83V33
C	-17	SER	-	expression tag	UNP Q83V33
C	-16	SER	-	expression tag	UNP Q83V33
C	-15	HIS	-	expression tag	UNP Q83V33
C	-14	HIS	-	expression tag	UNP Q83V33
C	-13	HIS	-	expression tag	UNP Q83V33
C	-12	HIS	-	expression tag	UNP Q83V33
C	-11	HIS	-	expression tag	UNP Q83V33
C	-10	HIS	-	expression tag	UNP Q83V33
C	-9	SER	-	expression tag	UNP Q83V33
C	-8	SER	-	expression tag	UNP Q83V33
C	-7	GLY	-	expression tag	UNP Q83V33
C	-6	LEU	-	expression tag	UNP Q83V33
C	-5	VAL	-	expression tag	UNP Q83V33
C	-4	PRO	-	expression tag	UNP Q83V33
C	-3	ARG	-	expression tag	UNP Q83V33
C	-2	GLY	-	expression tag	UNP Q83V33
C	-1	SER	-	expression tag	UNP Q83V33
C	0	HIS	-	expression tag	UNP Q83V33
C	169	ASP	ASN	engineered mutation	UNP Q83V33

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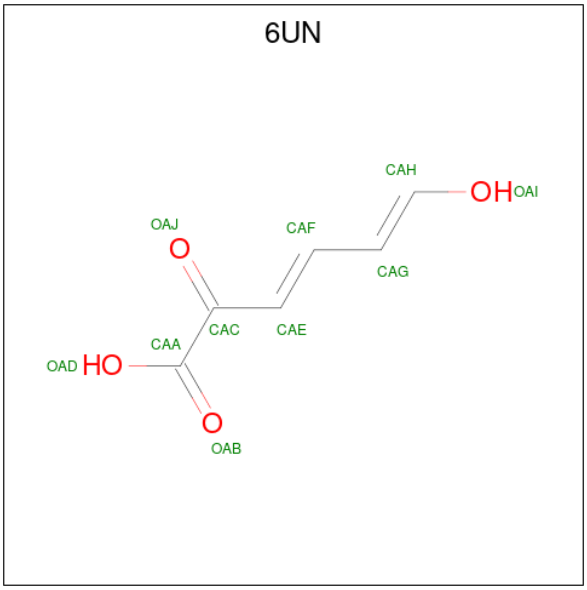
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP Q83V33
D	-18	GLY	-	expression tag	UNP Q83V33
D	-17	SER	-	expression tag	UNP Q83V33
D	-16	SER	-	expression tag	UNP Q83V33
D	-15	HIS	-	expression tag	UNP Q83V33
D	-14	HIS	-	expression tag	UNP Q83V33
D	-13	HIS	-	expression tag	UNP Q83V33
D	-12	HIS	-	expression tag	UNP Q83V33
D	-11	HIS	-	expression tag	UNP Q83V33
D	-10	HIS	-	expression tag	UNP Q83V33
D	-9	SER	-	expression tag	UNP Q83V33
D	-8	SER	-	expression tag	UNP Q83V33
D	-7	GLY	-	expression tag	UNP Q83V33
D	-6	LEU	-	expression tag	UNP Q83V33
D	-5	VAL	-	expression tag	UNP Q83V33
D	-4	PRO	-	expression tag	UNP Q83V33
D	-3	ARG	-	expression tag	UNP Q83V33
D	-2	GLY	-	expression tag	UNP Q83V33
D	-1	SER	-	expression tag	UNP Q83V33
D	0	HIS	-	expression tag	UNP Q83V33
D	169	ASP	ASN	engineered mutation	UNP Q83V33

- Molecule 2 is (3 {E},5 {E})-6-oxidanyl-2-oxidanylidene-hexa-3,5-dienoic acid (three-letter code: 6UN) (formula: $C_6H_6O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 6 4	0	0
2	B	1	Total C O 10 6 4	0	0
2	C	1	Total C O 10 6 4	0	0
2	D	1	Total C O 10 6 4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is water.

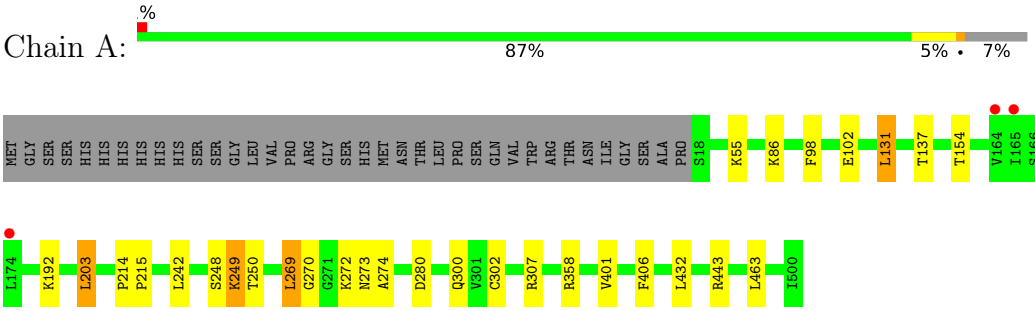
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	331	Total O 331 331	0	0
4	B	302	Total O 302 302	0	0
4	C	277	Total O 277 277	0	0
4	D	280	Total O 280 280	0	0

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.

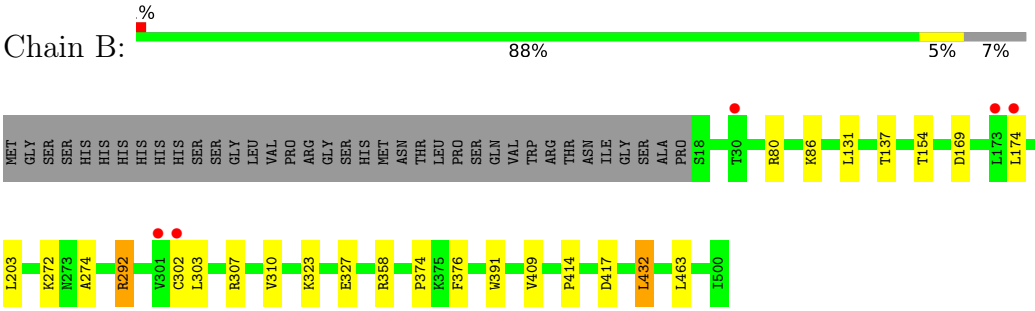
• Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

Chain A:



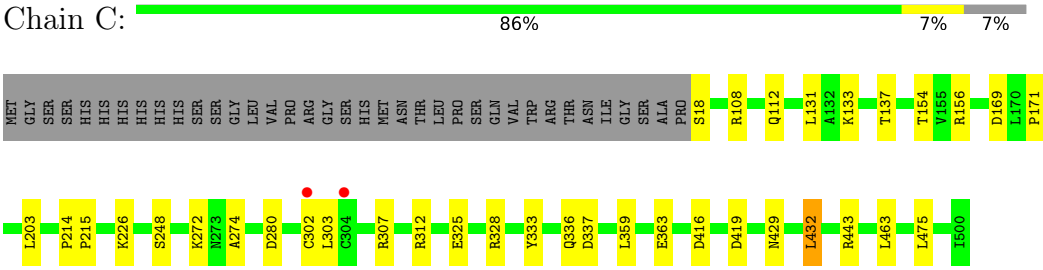
• Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

Chain B:



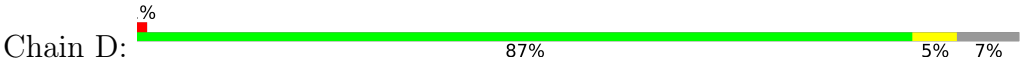
• Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

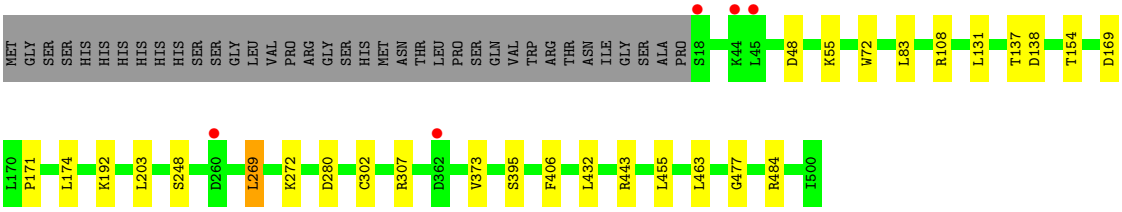
Chain C:



• Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

Chain D:




MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ASN THR LEU PRO SER GLN VAL TRP ARG THR ASN ILE GLY SER ALA PRO S18 K44 L45 D48 K55 W72 L83 R108 L131 T137 D138 T154 D169
L170 P171 L174 K192 L203 S248 D260 L269 K272 D280 C302 R307 D362 V373 S396 F406 L432 R443 L455 L463 G477 R484 I500

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.36Å 143.06Å 174.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.15 – 2.17 35.15 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.7 (35.15-2.17) 95.7 (35.15-2.17)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 2.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.170 , 0.218 0.166 , 0.213	Depositor DCC
R_{free} test set	2000 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15960	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 6UN

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	0.43	0/3767	0.55	0/5121
1	B	0.40	0/3767	0.52	0/5121
1	C	0.42	0/3767	0.55	0/5121
1	D	0.40	0/3756	0.53	0/5106
All	All	0.41	0/15057	0.54	0/20469

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

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	3684	0	3614	20	0
1	B	3684	0	3614	18	0
1	C	3684	0	3614	21	0
1	D	3674	0	3608	13	0
2	A	10	0	0	4	0
2	B	10	0	0	4	0
2	C	10	0	0	4	0
2	D	10	0	0	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	331	0	0	2	0
4	B	302	0	0	5	0
4	C	277	0	0	4	0
4	D	280	0	0	1	0
All	All	15960	0	14450	72	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 (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302[A]:CYS:SG	2:D:601:6UN:CAH	2.31	1.19
1:A:302[A]:CYS:SG	2:A:601:6UN:CAH	2.32	1.18
1:B:302[A]:CYS:SG	2:B:601:6UN:CAH	2.42	1.08
1:C:302[A]:CYS:SG	2:C:601:6UN:CAH	2.44	1.05
1:D:302[A]:CYS:SG	2:D:601:6UN:CAG	2.61	0.87
1:C:156:ARG:NH1	4:C:701:HOH:O	2.07	0.87
1:A:280:ASP:OD2	1:A:443:ARG:NH1	2.08	0.86
1:B:292:ARG:NH2	4:B:701:HOH:O	2.09	0.83
1:A:358:ARG:NH2	4:A:701:HOH:O	2.15	0.79
1:C:302[A]:CYS:SG	2:C:601:6UN:CAG	2.76	0.72
1:D:248:SER:HA	1:D:269:LEU:HG	1.72	0.69
1:A:272:LYS:HG3	1:A:307:ARG:HD2	1.75	0.69
1:D:272:LYS:HG3	1:D:307:ARG:HD2	1.77	0.67
1:C:312:ARG:HD2	1:C:416:ASP:OD1	1.96	0.66
1:A:302[A]:CYS:SG	2:A:601:6UN:CAG	2.84	0.65
1:A:248:SER:HA	1:A:269:LEU:HG	1.78	0.62
1:C:272:LYS:HG3	1:C:307:ARG:HD2	1.81	0.62
1:D:302[A]:CYS:SG	2:D:601:6UN:OAI	2.57	0.62
1:C:18:SER:N	4:C:704:HOH:O	2.32	0.62
1:B:272:LYS:HG3	1:B:307:ARG:HD2	1.83	0.60
1:B:302[A]:CYS:SG	2:B:601:6UN:CAG	2.91	0.59
1:C:280:ASP:OD2	1:C:443:ARG:NH1	2.40	0.55
1:B:169:ASP:OD2	2:B:601:6UN:OAI	2.24	0.55
1:C:429:ASN:HB3	1:C:475:LEU:HD12	1.89	0.54
1:C:302[A]:CYS:SG	2:C:601:6UN:OAI	2.66	0.54
1:C:303:LEU:HD23	1:C:432:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASP:OD2	2:A:601:6UN:OAI	2.28	0.52
1:B:303:LEU:HD23	1:B:432:LEU:HD13	1.92	0.52
1:B:358:ARG:NH2	4:B:711:HOH:O	2.44	0.51
1:C:359:LEU:O	1:C:363:GLU:HG2	2.11	0.51
1:B:86:LYS:HD3	4:B:894:HOH:O	2.11	0.49
1:B:302[B]:CYS:SG	4:B:925:HOH:O	2.60	0.49
1:D:169:ASP:OD2	2:D:601:6UN:OAI	2.29	0.49
1:D:280:ASP:OD2	1:D:443:ARG:NH1	2.46	0.48
1:D:269:LEU:HD22	1:D:477:GLY:HA2	1.96	0.48
1:C:137:THR:HB	1:C:154:THR:OG1	2.14	0.47
1:A:302[A]:CYS:SG	2:A:601:6UN:OAI	2.70	0.47
1:C:133:LYS:NZ	4:C:707:HOH:O	2.39	0.47
1:C:108:ARG:NH1	1:C:112:GLN:OE1	2.49	0.46
1:D:108:ARG:NH2	4:D:714:HOH:O	2.47	0.46
1:A:137:THR:HB	1:A:154:THR:OG1	2.16	0.46
1:A:169:ASP:HB2	1:A:300:GLN:O	2.15	0.46
1:A:86:LYS:HE2	1:A:86:LYS:HB3	1.60	0.46
1:B:302[A]:CYS:SG	2:B:601:6UN:OAI	2.73	0.45
1:A:214:PRO:HA	1:A:215:PRO:HD3	1.90	0.44
1:A:274:ALA:HA	1:A:307:ARG:O	2.17	0.44
1:C:169:ASP:OD2	2:C:601:6UN:OAI	2.34	0.44
1:D:72:TRP:HZ3	1:D:83:LEU:HD23	1.82	0.44
1:C:274:ALA:HA	1:C:307:ARG:O	2.18	0.44
1:C:333:TYR:HB2	1:C:336:GLN:HB2	1.98	0.44
1:B:323:LYS:NZ	1:B:327:GLU:OE2	2.51	0.44
1:B:391:TRP:CH2	1:B:409:VAL:HG21	2.52	0.44
1:B:374:PRO:HG2	1:B:376:PHE:CE2	2.53	0.44
1:A:98:PHE:CE1	1:A:203:LEU:HB3	2.54	0.43
1:D:137:THR:HB	1:D:154:THR:OG1	2.19	0.43
1:C:419:ASP:HB2	4:C:884:HOH:O	2.19	0.43
1:B:174:LEU:HD23	1:B:174:LEU:HA	1.91	0.42
1:C:214:PRO:HA	1:C:215:PRO:HD3	1.89	0.42
1:A:249:LYS:HG3	1:A:250:THR:N	2.33	0.42
1:B:137:THR:HB	1:B:154:THR:OG1	2.20	0.42
1:C:325:GLU:OE2	1:C:328:ARG:NH1	2.52	0.42
1:B:274:ALA:HA	1:B:307:ARG:O	2.20	0.41
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.92	0.41
1:D:174:LEU:HA	1:D:174:LEU:HD23	1.87	0.41
1:C:174:LEU:HD23	1:C:174:LEU:HA	1.89	0.41
1:A:269:LEU:HB3	1:A:270:GLY:H	1.69	0.41
1:B:310:VAL:O	1:B:414:PRO:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302[B]:CYS:SG	4:A:920:HOH:O	2.62	0.41
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.92	0.40
1:B:80:ARG:NH1	4:B:721:HOH:O	2.52	0.40
1:D:137:THR:HB	1:D:138:ASP:H	1.79	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	483/520 (93%)	469 (97%)	14 (3%)	0	100	100
1	B	483/520 (93%)	464 (96%)	19 (4%)	0	100	100
1	C	483/520 (93%)	466 (96%)	16 (3%)	1 (0%)	47	52
1	D	482/520 (93%)	465 (96%)	16 (3%)	1 (0%)	47	52
All	All	1931/2080 (93%)	1864 (96%)	65 (3%)	2 (0%)	51	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	171	PRO
1	C	171	PRO

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	394/424 (93%)	382 (97%)	12 (3%)	41 49
1	B	394/424 (93%)	387 (98%)	7 (2%)	59 70
1	C	394/424 (93%)	386 (98%)	8 (2%)	55 66
1	D	393/424 (93%)	380 (97%)	13 (3%)	38 46
All	All	1575/1696 (93%)	1535 (98%)	40 (2%)	46 57

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	102	GLU
1	A	131	LEU
1	A	192	LYS
1	A	203	LEU
1	A	242	LEU
1	A	249	LYS
1	A	269	LEU
1	A	401	VAL
1	A	406	PHE
1	A	432	LEU
1	A	463	LEU
1	B	131	LEU
1	B	192	LYS
1	B	203	LEU
1	B	292	ARG
1	B	417	ASP
1	B	432	LEU
1	B	463	LEU
1	C	131	LEU
1	C	192	LYS
1	C	203	LEU
1	C	226	LYS
1	C	248	SER
1	C	337	ASP
1	C	432	LEU
1	C	463	LEU
1	D	48	ASP
1	D	55	LYS
1	D	131	LEU
1	D	192	LYS
1	D	203	LEU
1	D	269	LEU

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Mol	Chain	Res	Type
1	D	373	VAL
1	D	395	SER
1	D	406	PHE
1	D	432	LEU
1	D	455	LEU
1	D	463	LEU
1	D	484	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 8 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
2	6UN	C	601	-	9,9,9	2.79	3 (33%)	8,10,10	1.80	2 (25%)
2	6UN	B	601	-	9,9,9	2.88	3 (33%)	8,10,10	1.64	2 (25%)
2	6UN	D	601	-	9,9,9	2.90	3 (33%)	8,10,10	1.76	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	6UN	A	601	-	9,9,9	2.82	3 (33%)	8,10,10	1.77	2 (25%)

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
2	6UN	C	601	-	-	0/8/9/9	-
2	6UN	B	601	-	-	0/8/9/9	-
2	6UN	D	601	-	-	0/8/9/9	-
2	6UN	A	601	-	-	0/8/9/9	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	6UN	CAF-CAE	5.96	1.49	1.34
2	D	601	6UN	CAF-CAE	5.84	1.49	1.34
2	A	601	6UN	CAF-CAE	5.67	1.49	1.34
2	C	601	6UN	CAF-CAE	5.63	1.49	1.34
2	D	601	6UN	CAA-CAC	-4.85	1.48	1.54
2	A	601	6UN	CAA-CAC	-4.78	1.48	1.54
2	C	601	6UN	CAA-CAC	-4.66	1.48	1.54
2	B	601	6UN	CAA-CAC	-4.55	1.48	1.54
2	B	601	6UN	CAG-CAH	2.46	1.50	1.34
2	D	601	6UN	CAG-CAH	2.42	1.49	1.34
2	C	601	6UN	CAG-CAH	2.40	1.49	1.34
2	A	601	6UN	CAG-CAH	2.32	1.49	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	6UN	CAG-CAF-CAE	-3.82	115.14	124.67
2	A	601	6UN	CAG-CAF-CAE	-3.81	115.15	124.67
2	D	601	6UN	CAG-CAF-CAE	-3.43	116.11	124.67
2	B	601	6UN	CAG-CAF-CAE	-2.99	117.19	124.67
2	B	601	6UN	OAD-CAA-CAC	2.58	120.15	113.19
2	D	601	6UN	OAD-CAA-CAC	2.44	119.77	113.19
2	C	601	6UN	CAF-CAE-CAC	-2.27	117.71	122.27
2	A	601	6UN	OAD-CAA-CAC	2.11	118.89	113.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	6UN	4	0
2	B	601	6UN	4	0
2	D	601	6UN	4	0
2	A	601	6UN	4	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, 95^{th} 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	483/520 (92%)	-0.32	4 (0%)	86	86	22, 32, 45, 60	0
1	B	483/520 (92%)	-0.29	6 (1%)	79	79	23, 36, 48, 67	0
1	C	483/520 (92%)	-0.26	2 (0%)	92	92	23, 35, 46, 58	0
1	D	483/520 (92%)	-0.27	5 (1%)	82	82	23, 37, 49, 65	0
All	All	1932/2080 (92%)	-0.28	17 (0%)	84	84	22, 35, 48, 67	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	LEU	2.8
1	D	18	SER	2.6
1	B	173	LEU	2.5
1	A	164	VAL	2.5
1	B	302[A]	CYS	2.4
1	C	302[A]	CYS	2.4
1	D	45	LEU	2.3
1	A	167	PRO	2.3
1	A	174	LEU	2.2
1	B	30	THR	2.2
1	B	301	VAL	2.2
1	D	362	ASP	2.1
1	A	165	ILE	2.1
1	D	260	ASP	2.1
1	D	44	LYS	2.1
1	B	177	TRP	2.1
1	C	304	CYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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
3	NA	D	602	1/1	0.90	0.26	39,39,39,39	0
2	6UN	B	601	10/10	0.95	0.17	32,36,46,49	0
3	NA	C	602	1/1	0.96	0.14	35,35,35,35	0
2	6UN	D	601	10/10	0.97	0.18	32,37,51,53	0
3	NA	B	602	1/1	0.97	0.25	34,34,34,34	0
2	6UN	C	601	10/10	0.98	0.14	29,35,49,53	0
2	6UN	A	601	10/10	0.98	0.14	29,33,40,45	0
3	NA	A	602	1/1	0.98	0.12	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.