Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:15 PM GMT

PDB ID	:	4L03
Title	:	Crystal Structure Analysis of human IDH1 mutants in complex with NADP+ and Ca2+/alpha-Ketoglutarate
Authors	:	Concha, N.O.; Smallwood, A.M.
Deposited on	:	2013-05-30
Resolution	:	2.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

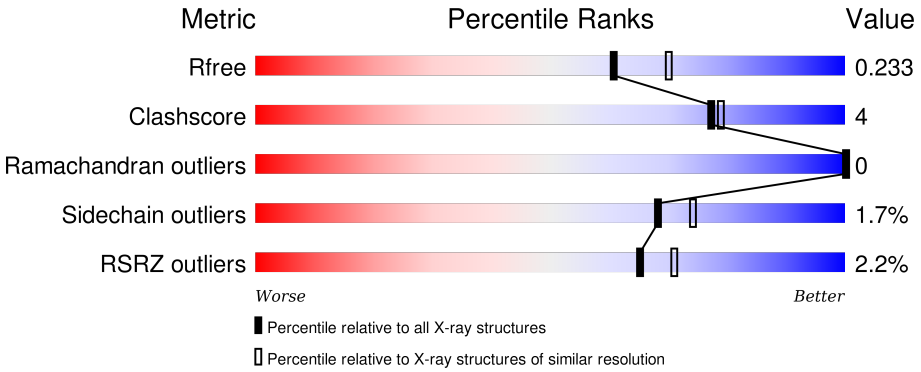
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	425	91% 6%
1	B	425	3% 91% 6%
1	C	425	3% 84% 13%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10558 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3288	2089	557	624	18			
1	B	412	Total	C	N	O	S	0	0	0
			3234	2055	547	614	18			
1	C	417	Total	C	N	O	S	0	0	0
			3274	2080	553	623	18			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ASP	GLY	CONFLICT	UNP O75874
A	415	SER	-	EXPRESSION TAG	UNP O75874
A	416	LEU	-	EXPRESSION TAG	UNP O75874
A	417	GLU	-	EXPRESSION TAG	UNP O75874
A	418	HIS	-	EXPRESSION TAG	UNP O75874
A	419	HIS	-	EXPRESSION TAG	UNP O75874
A	420	HIS	-	EXPRESSION TAG	UNP O75874
A	421	HIS	-	EXPRESSION TAG	UNP O75874
A	422	HIS	-	EXPRESSION TAG	UNP O75874
A	423	HIS	-	EXPRESSION TAG	UNP O75874
A	424	HIS	-	EXPRESSION TAG	UNP O75874
A	425	HIS	-	EXPRESSION TAG	UNP O75874
B	97	ASP	GLY	CONFLICT	UNP O75874
B	415	SER	-	EXPRESSION TAG	UNP O75874
B	416	LEU	-	EXPRESSION TAG	UNP O75874
B	417	GLU	-	EXPRESSION TAG	UNP O75874
B	418	HIS	-	EXPRESSION TAG	UNP O75874
B	419	HIS	-	EXPRESSION TAG	UNP O75874
B	420	HIS	-	EXPRESSION TAG	UNP O75874
B	421	HIS	-	EXPRESSION TAG	UNP O75874
B	422	HIS	-	EXPRESSION TAG	UNP O75874
B	423	HIS	-	EXPRESSION TAG	UNP O75874
B	424	HIS	-	EXPRESSION TAG	UNP O75874

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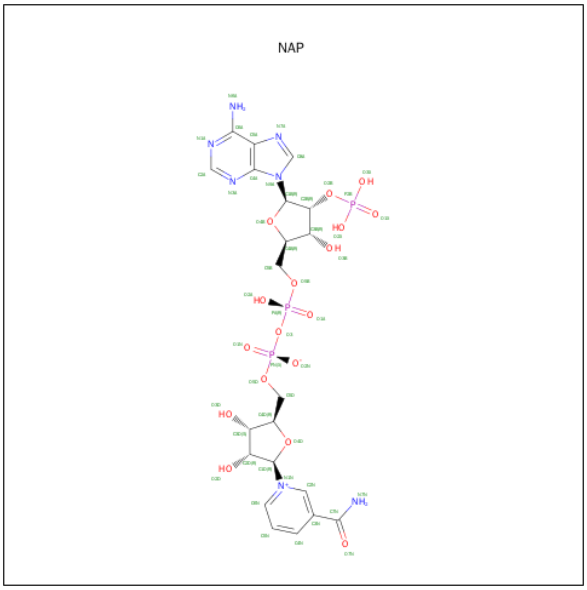
Chain	Residue	Modelled	Actual	Comment	Reference
B	425	HIS	-	EXPRESSION TAG	UNP O75874
C	97	ASP	GLY	CONFLICT	UNP O75874
C	415	SER	-	EXPRESSION TAG	UNP O75874
C	416	LEU	-	EXPRESSION TAG	UNP O75874
C	417	GLU	-	EXPRESSION TAG	UNP O75874
C	418	HIS	-	EXPRESSION TAG	UNP O75874
C	419	HIS	-	EXPRESSION TAG	UNP O75874
C	420	HIS	-	EXPRESSION TAG	UNP O75874
C	421	HIS	-	EXPRESSION TAG	UNP O75874
C	422	HIS	-	EXPRESSION TAG	UNP O75874
C	423	HIS	-	EXPRESSION TAG	UNP O75874
C	424	HIS	-	EXPRESSION TAG	UNP O75874
C	425	HIS	-	EXPRESSION TAG	UNP O75874

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

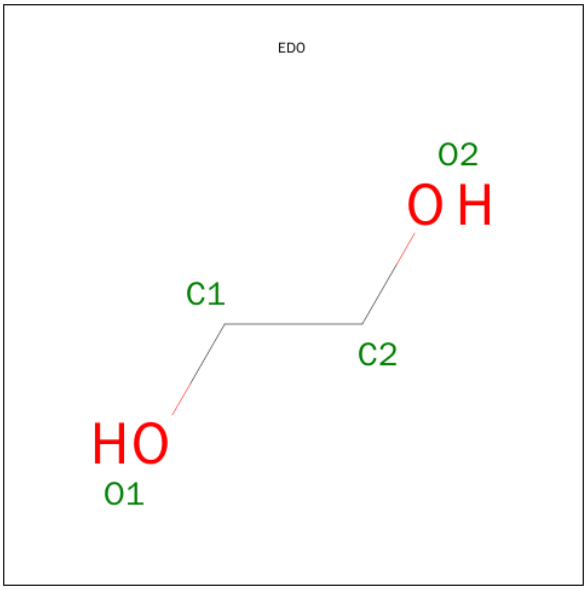


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

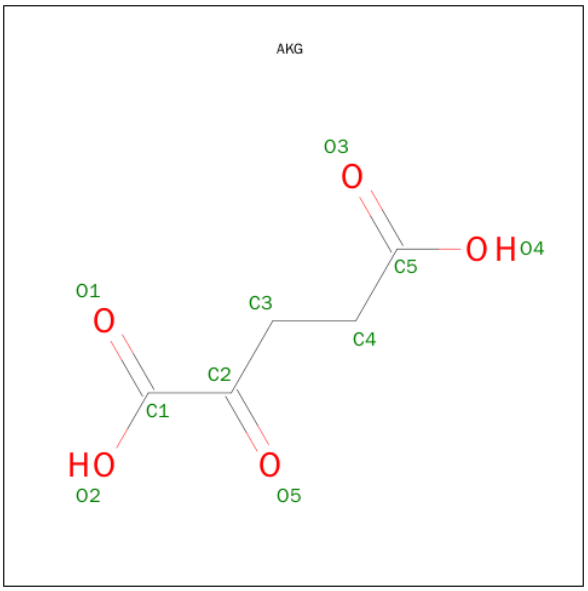
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 5 5	0	0
5	B	1	Total C O 10 5 5	0	0
5	C	1	Total C O 10 5 5	0	0

- Molecule 6 is water.

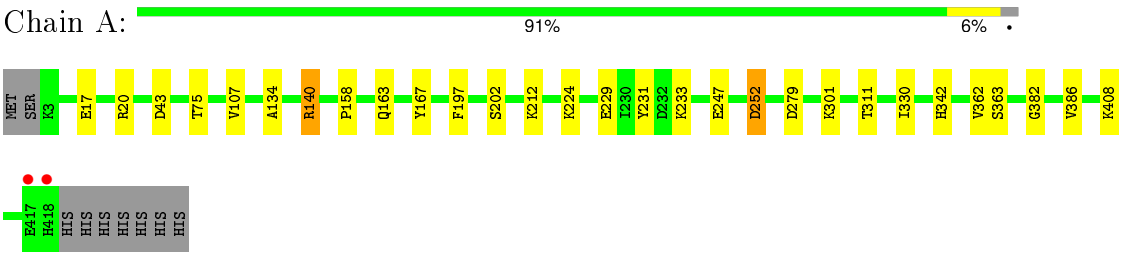
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	255	Total O 255 255	0	0
6	B	184	Total O 184 184	0	0
6	C	142	Total O 142 142	0	0

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.

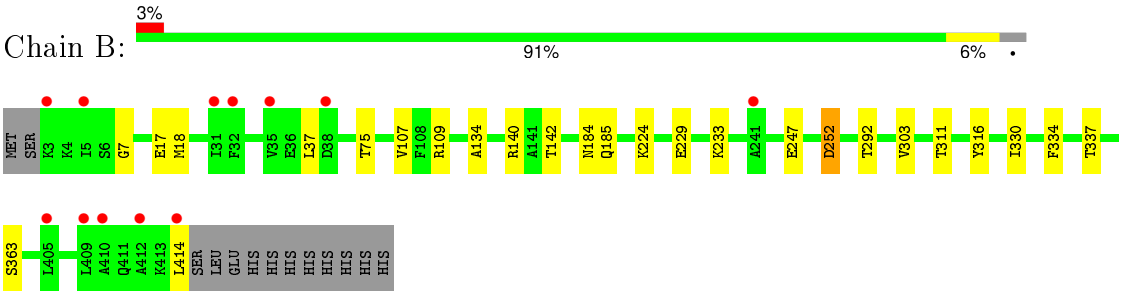
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain A:



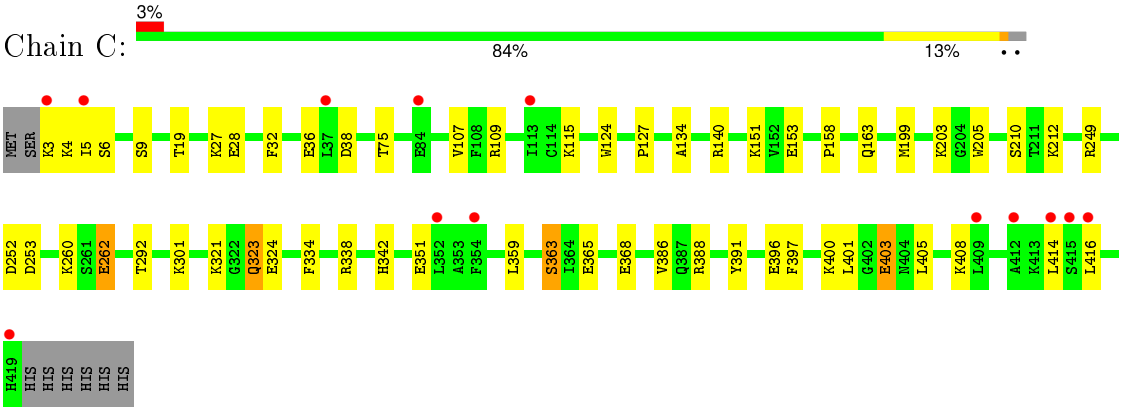
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain B:



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	96.19Å 275.38Å 116.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 2.10 48.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.98-2.10) 99.2 (48.98-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.189 , 0.230 0.194 , 0.233	Depositor DCC
R_{free} test set	4501 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 89674 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10558	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, AKG, NAP, EDO

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	0.30	0/3357	0.51	0/4531
1	B	0.28	0/3302	0.50	0/4462
1	C	0.29	0/3343	0.52	0/4517
All	All	0.29	0/10002	0.51	0/13510

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	262	GLU	Peptide

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	3288	0	3234	20	0
1	B	3234	0	3160	15	0
1	C	3274	0	3197	37	0
2	A	48	0	25	1	0
2	B	48	0	25	2	0
2	C	48	0	25	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	6	0	0
5	A	10	0	4	0	0
5	B	10	0	4	0	0
5	C	10	0	4	0	0
6	A	255	0	0	3	3
6	B	184	0	0	5	0
6	C	142	0	0	5	6
All	All	10558	0	9684	72	9

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 4.

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:C:3:LYS:O	1:C:36:GLU:HG3	1.75	0.84
1:C:301:LYS:O	1:C:342:HIS:NE2	2.23	0.71
1:A:212:LYS:NZ	1:A:252:ASP:OD2	2.24	0.71
1:C:124:TRP:HA	1:C:262:GLU:O	1.93	0.69
1:C:253:ASP:OD1	6:C:734:HOH:O	2.11	0.68
1:C:212:LYS:NZ	1:C:252:ASP:OD1	2.29	0.66
1:C:5:ILE:HD12	1:C:351:GLU:HB3	1.81	0.63
1:C:414:LEU:C	1:C:416:LEU:H	2.03	0.62
1:B:224:LYS:NZ	6:B:763:HOH:O	2.29	0.61
1:C:388:ARG:NH2	1:C:396:GLU:OE1	2.33	0.61
1:B:229:GLU:OE1	6:B:765:HOH:O	2.16	0.61
1:A:20:ARG:NH2	1:A:43:ASP:OD1	2.37	0.58
1:B:7:GLY:HA3	1:B:37:LEU:HD23	1.86	0.58
1:C:260:LYS:HE3	6:C:690:HOH:O	2.03	0.58
1:B:330:ILE:HD12	1:B:363:SER:HB3	1.87	0.56
1:B:229:GLU:OE2	1:B:233:LYS:NZ	2.34	0.56
1:A:107:VAL:HG23	1:A:134:ALA:HB2	1.91	0.52
1:A:362:VAL:HG23	1:A:408:LYS:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:THR:O	2:C:501:NAP:H2N	2.09	0.52
1:A:279:ASP:OD2	1:B:252:ASP:HB3	2.09	0.52
1:C:9:SER:OG	1:C:38:ASP:OD2	2.28	0.51
1:C:151:LYS:HG2	1:C:153:GLU:HG3	1.94	0.50
1:C:388:ARG:NH1	1:C:391:TYR:O	2.45	0.50
1:C:107:VAL:HG23	1:C:134:ALA:HB2	1.94	0.50
1:A:75:THR:O	2:A:501:NAP:H2N	2.12	0.49
1:C:359:LEU:O	1:C:363:SER:OG	2.30	0.49
1:C:359:LEU:HD13	1:C:405:LEU:HD22	1.95	0.49
1:C:365:GLU:OE1	1:C:408:LYS:NZ	2.46	0.48
1:C:397:PHE:CE2	1:C:401:LEU:HD11	2.48	0.48
1:C:109:ARG:HA	1:C:292:THR:O	2.14	0.48
1:A:140:ARG:NH2	6:A:815:HOH:O	2.46	0.48
1:C:403:GLU:HG2	6:C:709:HOH:O	2.14	0.48
1:A:158:PRO:HG2	1:A:163:GLN:HG2	1.96	0.48
2:C:501:NAP:O1X	2:C:501:NAP:O3B	2.32	0.47
1:B:247:GLU:OE1	6:B:673:HOH:O	2.20	0.47
1:A:301:LYS:O	1:A:342:HIS:NE2	2.34	0.47
1:A:247:GLU:OE2	6:A:852:HOH:O	2.21	0.47
1:C:127:PRO:HD2	1:C:205:TRP:CH2	2.49	0.46
2:B:501:NAP:O3B	2:B:501:NAP:O1X	2.30	0.46
1:B:75:THR:O	2:B:501:NAP:H2N	2.16	0.46
1:C:158:PRO:HD2	1:C:163:GLN:O	2.16	0.46
1:B:17:GLU:HB2	1:B:311:THR:HB	1.99	0.45
1:B:252:ASP:N	1:B:252:ASP:OD1	2.49	0.45
1:B:107:VAL:HG23	1:B:134:ALA:HB2	1.97	0.45
1:C:292:THR:HG22	1:C:334:PHE:HB3	1.99	0.45
1:C:210:SER:HA	1:C:249:ARG:O	2.17	0.45
6:B:756:HOH:O	1:C:4:LYS:HA	2.16	0.44
1:A:167:TYR:HB3	1:B:142:THR:HG21	1.99	0.44
1:A:330:ILE:HD12	1:A:363:SER:HB3	1.99	0.44
1:C:115:LYS:HG3	1:C:368:GLU:OE2	2.18	0.44
1:C:414:LEU:C	1:C:416:LEU:N	2.71	0.44
1:A:197:PHE:CZ	1:A:231:TYR:HB2	2.52	0.44
1:C:199:MET:HE1	1:C:203:LYS:HE2	1.98	0.43
1:B:334:PHE:HA	1:B:337:THR:OG1	2.18	0.43
1:C:109:ARG:NH1	6:C:602:HOH:O	2.51	0.43
1:C:4:LYS:HE3	1:C:4:LYS:HB3	1.75	0.43
1:A:229:GLU:HG3	1:A:233:LYS:NZ	2.33	0.43
1:A:382:GLY:O	1:A:386:VAL:HG23	2.18	0.42
1:A:212:LYS:HD2	1:A:212:LYS:HA	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PRO:HD2	1:A:163:GLN:O	2.20	0.42
1:A:17:GLU:HB2	1:A:311:THR:HB	2.00	0.42
1:B:109:ARG:HA	1:B:292:THR:O	2.19	0.42
1:C:9:SER:HA	1:C:38:ASP:O	2.20	0.41
1:C:27:LYS:HB3	1:C:32:PHE:CE2	2.55	0.41
1:C:212:LYS:HD2	1:C:212:LYS:HA	1.78	0.41
1:C:400:LYS:HE3	6:C:708:HOH:O	2.20	0.41
1:B:18:MET:HB2	1:B:316:TYR:HB2	2.03	0.41
1:A:224:LYS:HE2	6:B:783:HOH:O	2.20	0.41
1:C:338:ARG:HA	1:C:338:ARG:HD3	1.88	0.41
1:A:408:LYS:HE2	6:A:855:HOH:O	2.19	0.41
1:C:321:LYS:HB2	1:C:323:GLN:HG3	2.03	0.41
1:C:151:LYS:HE3	1:C:151:LYS:HB2	1.66	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:690:HOH:O	6:C:711:HOH:O[4_556]	1.99	0.21
6:C:711:HOH:O	6:C:734:HOH:O[4_556]	1.99	0.21
6:C:640:HOH:O	6:C:697:HOH:O[4_556]	1.99	0.21
6:A:786:HOH:O	6:A:788:HOH:O[3_455]	2.08	0.12
6:C:625:HOH:O	6:C:682:HOH:O[4_556]	2.09	0.11
6:C:671:HOH:O	6:C:684:HOH:O[4_556]	2.11	0.09
6:A:787:HOH:O	6:A:787:HOH:O[3_455]	2.13	0.07
6:C:670:HOH:O	6:C:701:HOH:O[4_556]	2.13	0.07
6:A:785:HOH:O	6:A:787:HOH:O[3_455]	2.19	0.01

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	414/425 (97%)	405 (98%)	9 (2%)	0	100	100
1	B	410/425 (96%)	400 (98%)	10 (2%)	0	100	100
1	C	415/425 (98%)	406 (98%)	9 (2%)	0	100	100
All	All	1239/1275 (97%)	1211 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	349/362 (96%)	346 (99%)	3 (1%)	84	89
1	B	340/362 (94%)	334 (98%)	6 (2%)	66	72
1	C	345/362 (95%)	336 (97%)	9 (3%)	54	58
All	All	1034/1086 (95%)	1016 (98%)	18 (2%)	68	74

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ARG
1	A	202	SER
1	A	252	ASP
1	B	140	ARG
1	B	184	ASN
1	B	185	GLN
1	B	252	ASP
1	B	303	VAL
1	B	414	LEU
1	C	6	SER
1	C	19	THR
1	C	28	GLU
1	C	140	ARG
1	C	323	GLN
1	C	324	GLU

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Mol	Chain	Res	Type
1	C	363	SER
1	C	386	VAL
1	C	403	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	C	96	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 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	NAP	A	501	-	42,52,52	1.52	3 (7%)	54,80,80	1.77	4 (7%)
4	EDO	A	503	-	3,3,3	0.43	0	2,2,2	0.36	0
5	AKG	A	504	3	3,9,9	0.32	0	4,11,11	1.53	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAP	B	501	-	42,52,52	1.51	3 (7%)	54,80,80	1.78	2 (3%)
5	AKG	B	503	3	3,9,9	0.29	0	4,11,11	1.53	0
2	NAP	C	501	-	42,52,52	1.53	3 (7%)	54,80,80	1.80	3 (5%)
5	AKG	C	503	3	3,9,9	0.43	0	4,11,11	0.96	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
2	NAP	A	501	-	-	0/27/67/67	0/5/5/5
4	EDO	A	503	-	-	0/1/1/1	0/0/0/0
5	AKG	A	504	3	-	0/3/9/9	0/0/0/0
2	NAP	B	501	-	-	0/27/67/67	0/5/5/5
5	AKG	B	503	3	-	0/3/9/9	0/0/0/0
2	NAP	C	501	-	-	0/27/67/67	0/5/5/5
5	AKG	C	503	3	-	0/3/9/9	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NAP	C2A-N1A	2.05	1.37	1.33
2	A	501	NAP	C2A-N1A	2.18	1.38	1.33
2	B	501	NAP	C2A-N1A	2.21	1.38	1.33
2	A	501	NAP	C2A-N3A	3.35	1.38	1.32
2	C	501	NAP	C2A-N3A	3.43	1.38	1.32
2	B	501	NAP	C2A-N3A	3.49	1.38	1.32
2	B	501	NAP	O7N-C7N	7.64	1.40	1.24
2	A	501	NAP	O7N-C7N	7.79	1.40	1.24
2	C	501	NAP	O7N-C7N	7.82	1.40	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	NAP	N3A-C2A-N1A	-11.09	120.41	128.89
2	B	501	NAP	N3A-C2A-N1A	-10.99	120.48	128.89
2	A	501	NAP	N3A-C2A-N1A	-10.83	120.60	128.89
5	A	504	AKG	C3-C4-C5	-2.52	108.13	112.75
2	A	501	NAP	O2B-C2B-C1B	-2.29	101.11	110.02
2	C	501	NAP	O7N-C7N-C3N	-2.25	117.13	119.59
2	A	501	NAP	C4A-C5A-N7A	-2.04	107.60	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	NAP	C3N-C7N-N7N	2.99	121.09	117.82
2	C	501	NAP	C3N-C7N-N7N	3.69	121.86	117.82
2	B	501	NAP	C3N-C7N-N7N	3.71	121.88	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAP	1	0
2	B	501	NAP	2	0
2	C	501	NAP	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, 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	416/425 (97%)	-0.06	2 (0%) 91 93	13, 22, 42, 79	0
1	B	412/425 (96%)	0.06	12 (2%) 55 63	14, 29, 51, 63	0
1	C	417/425 (98%)	0.20	13 (3%) 52 61	15, 30, 52, 83	0
All	All	1245/1275 (97%)	0.07	27 (2%) 65 71	13, 27, 48, 83	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	LYS	4.1
1	C	5	ILE	3.8
1	B	414	LEU	3.8
1	A	418	HIS	3.7
1	C	416	LEU	3.6
1	B	3	LYS	3.6
1	C	412	ALA	3.5
1	C	409	LEU	3.4
1	B	35	VAL	3.3
1	B	31	ILE	3.2
1	C	414	LEU	2.9
1	C	419	HIS	2.9
1	B	412	ALA	2.8
1	A	417	GLU	2.6
1	C	415	SER	2.6
1	B	241	ALA	2.6
1	C	113	ILE	2.5
1	C	354	PHE	2.3
1	C	352	LEU	2.3
1	B	405	LEU	2.3
1	B	5	ILE	2.2
1	B	409	LEU	2.2
1	B	32	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	410	ALA	2.1
1	C	84	GLU	2.1
1	C	37	LEU	2.1
1	B	38	ASP	2.1

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, 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	LLDF	B-factors(Å^2)	Q<0.9
5	AKG	B	503	10/10	0.95	0.14	0.38	31,33,46,51	0
2	NAP	A	501	48/48	0.98	0.14	0.29	9,16,21,26	0
2	NAP	C	501	48/48	0.96	0.13	0.27	13,24,39,55	0
5	AKG	C	503	10/10	0.93	0.13	0.14	24,28,41,43	0
2	NAP	B	501	48/48	0.97	0.11	0.01	19,26,32,34	0
3	CA	C	502	1/1	0.98	0.14	-0.06	29,29,29,29	0
5	AKG	A	504	10/10	0.97	0.12	-0.86	20,26,32,32	0
4	EDO	A	503	4/4	0.97	0.16	-1.17	14,17,19,23	0
3	CA	B	502	1/1	0.97	0.08	-1.92	33,33,33,33	0
3	CA	A	502	1/1	0.98	0.08	-3.38	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.