Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:15 PM GMT

PDB ID	:	4L04
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	:	2.87 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:

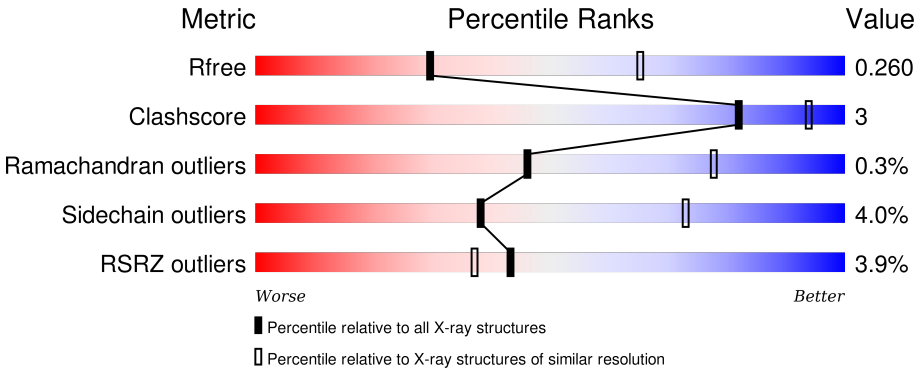
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.87 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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	2% 87% 9%
1	B	425	% 85% 12%
1	C	425	4% 84% 12%
1	D	425	5% 84% 13%
1	E	425	5% 84% 13%

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Mol	Chain	Length	Quality of chain
1	F	425	6% 88% 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
2	AKG	C	501	-	-	-	X
2	AKG	D	501	-	-	-	X
2	AKG	E	501	-	-	-	X
2	AKG	F	501	-	-	-	X
3	CA	A	502	-	-	-	X
3	CA	D	502	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19647 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	411	Total	C	N	O	S	0	0	0
			3221	2048	546	609	18			
1	B	412	Total	C	N	O	S	0	2	0
			3258	2071	553	616	18			
1	C	412	Total	C	N	O	S	0	0	0
			3206	2030	547	611	18			
1	D	412	Total	C	N	O	S	0	1	0
			3129	1982	535	596	16			
1	E	412	Total	C	N	O	S	0	1	0
			3226	2047	547	614	18			
1	F	412	Total	C	N	O	S	0	1	0
			3184	2025	543	598	18			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ASN	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	ASN	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

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

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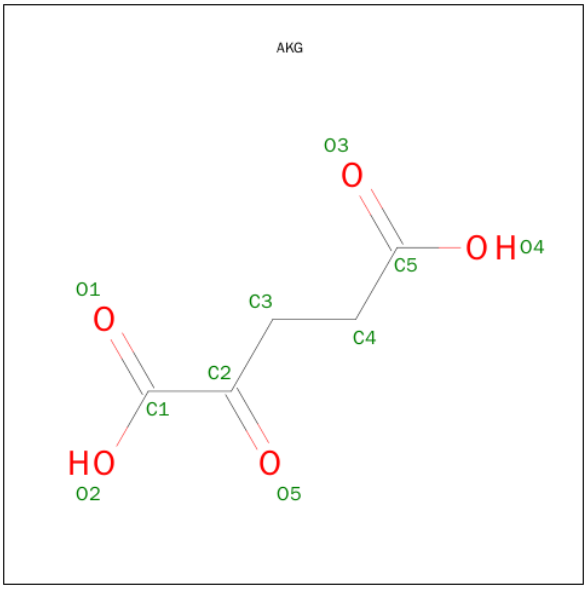
Chain	Residue	Modelled	Actual	Comment	Reference
E	425	HIS	-	EXPRESSION TAG	UNP O75874
F	97	ASN	GLY	CONFLICT	UNP O75874
F	415	SER	-	EXPRESSION TAG	UNP O75874
F	416	LEU	-	EXPRESSION TAG	UNP O75874
F	417	GLU	-	EXPRESSION TAG	UNP O75874
F	418	HIS	-	EXPRESSION TAG	UNP O75874
F	419	HIS	-	EXPRESSION TAG	UNP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

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



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

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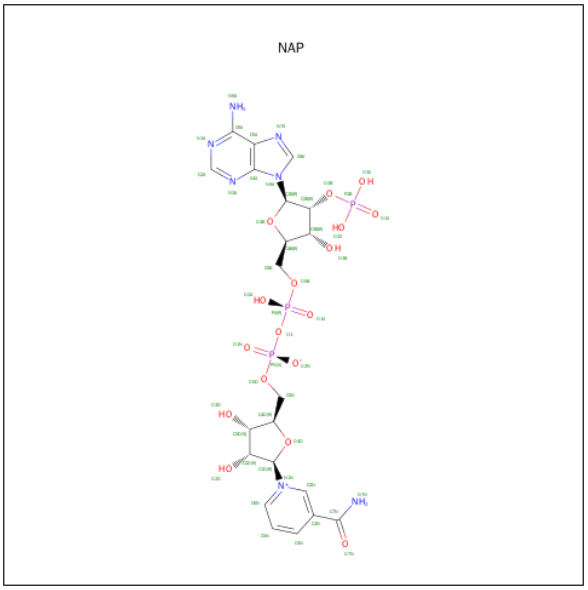
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O 10 5 5	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0
3	D	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0

- Molecule 4 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
4	A	1	Total C N O P 48 21 7 17 3	0	0
4	B	1	Total C N O P 48 21 7 17 3	0	0
4	C	1	Total C N O P 48 21 7 17 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is water.

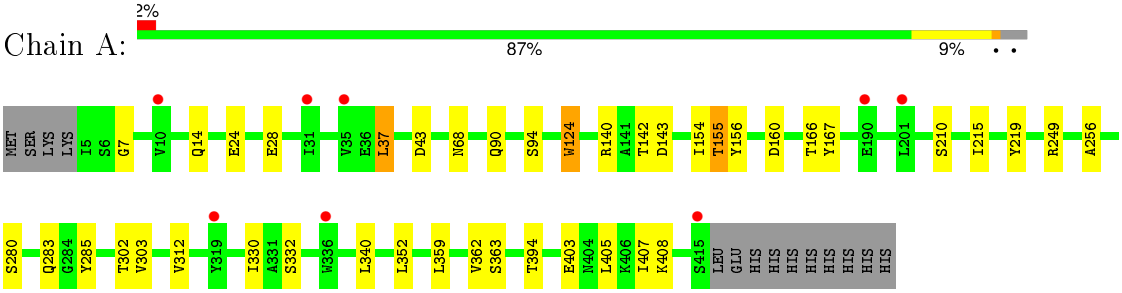
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		
5	B	13	Total	O	0	0
			13	13		
5	C	16	Total	O	0	0
			16	16		
5	D	8	Total	O	0	0
			8	8		
5	E	7	Total	O	0	0
			7	7		
5	F	7	Total	O	0	0
			7	7		

3 Residue-property plots

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.

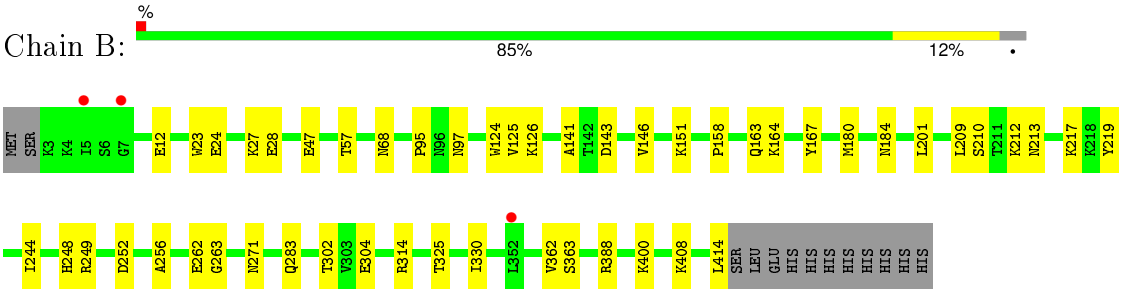
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain A:



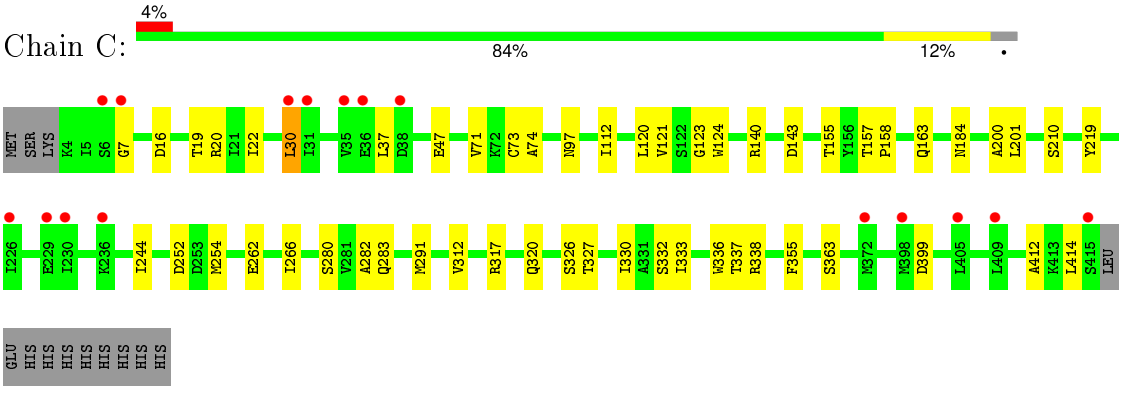
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain B:



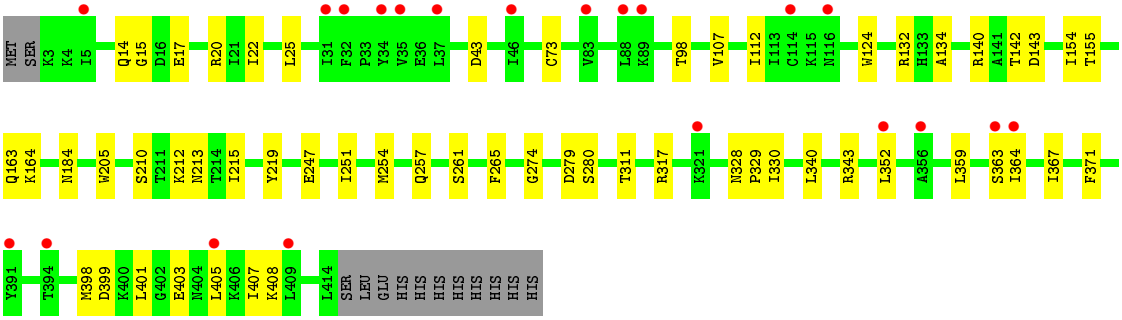
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain C:

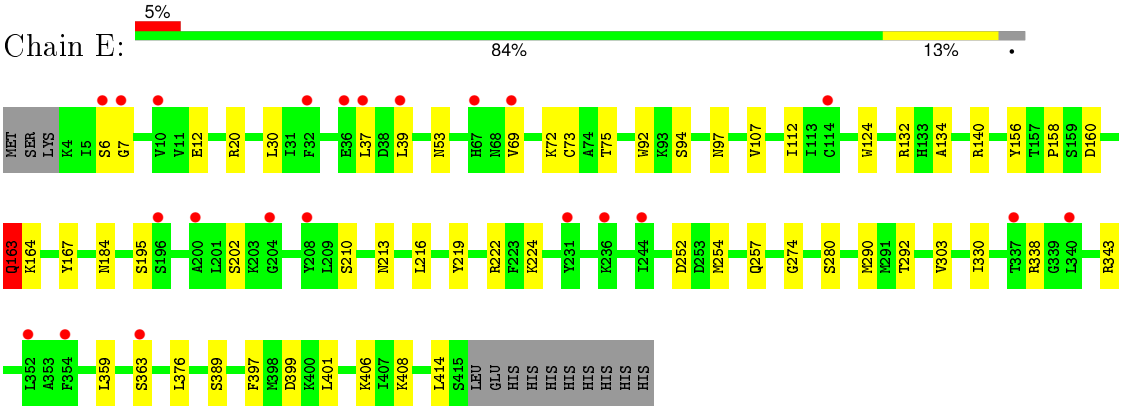


- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

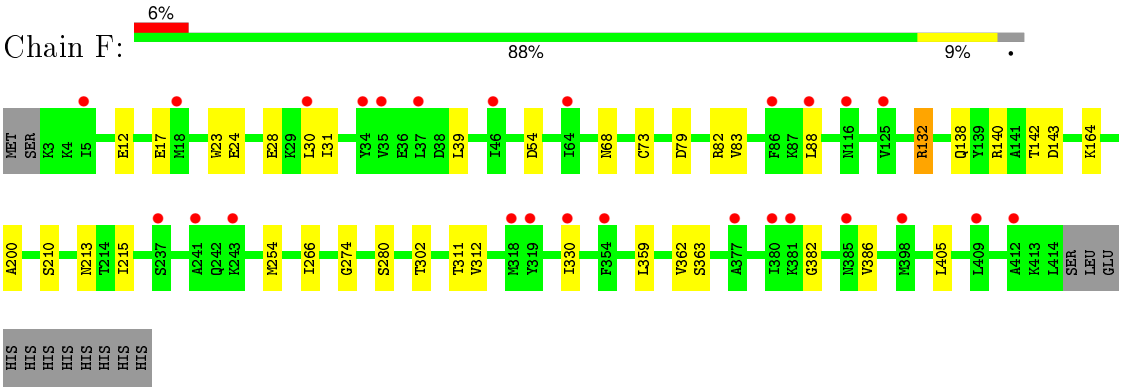
Chain D:



• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.41Å 116.62Å 275.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 2.87 49.24 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.24-2.87) 98.0 (49.24-2.87)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.200 , 0.259 0.201 , 0.260	Depositor DCC
R_{free} test set	3578 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 70754 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19647	wwPDB-VP
Average B, all atoms (Å^2)	72.0	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 59.99 % 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 1.6255e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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

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	0.47	0/3289	0.68	0/4446
1	B	0.47	0/3332	0.68	0/4499
1	C	0.47	0/3272	0.68	0/4422
1	D	0.45	0/3197	0.68	0/4336
1	E	0.47	0/3296	0.68	1/4456 (0.0%)
1	F	0.46	0/3255	0.69	0/4406
All	All	0.46	0/19641	0.68	1/26565 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	163	GLN	C-N-CA	5.21	134.72	121.70

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	3221	0	3144	20	0
1	B	3258	0	3208	23	0
1	C	3206	0	3111	24	0
1	D	3129	0	2959	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3226	0	3147	25	0
1	F	3184	0	3075	19	0
2	A	10	0	4	1	0
2	B	10	0	4	0	0
2	C	10	0	4	0	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0
2	F	10	0	4	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	48	0	25	1	0
4	B	48	0	25	0	0
4	C	48	0	25	1	0
4	D	48	0	25	0	0
4	E	48	0	25	1	0
4	F	48	0	25	0	0
5	A	18	0	0	0	0
5	B	13	0	0	0	0
5	C	16	0	0	0	0
5	D	8	0	0	0	0
5	E	7	0	0	0	0
5	F	7	0	0	0	0
All	All	19647	0	18818	121	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 (121) 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:E:163:GLN:NE2	1:E:164:LYS:H	1.59	0.99
1:C:19:THR:HG21	1:C:74:ALA:HB3	1.64	0.79
1:E:163:GLN:HA	1:E:163:GLN:OE1	1.90	0.69
1:D:205:TRP:HB3	1:D:265:PHE:HA	1.75	0.68
1:A:142:THR:HG21	1:B:167:TYR:HB3	1.80	0.64
1:F:132:ARG:HB2	1:F:274:GLY:HA3	1.80	0.62
1:B:330:ILE:HD12	1:B:363:SER:HB3	1.82	0.62
1:E:69:VAL:HG11	1:E:343:ARG:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:ILE:HD13	1:E:330:ILE:HG22	1.83	0.61
1:A:362:VAL:HG23	1:A:408:LYS:HD2	1.82	0.61
1:D:17:GLU:HB2	1:D:311:THR:HB	1.82	0.61
1:E:158:PRO:HD2	1:E:163:GLN:O	2.00	0.61
1:A:155:THR:HB	1:A:166:THR:HA	1.82	0.61
1:B:68:ASN:HA	1:B:302:THR:HG23	1.83	0.60
1:E:107:VAL:HG23	1:E:134:ALA:HB2	1.85	0.58
1:A:219:TYR:HB2	1:B:143:ASP:HB2	1.85	0.57
1:D:155[A]:THR:HG21	1:D:164:LYS:HE3	1.86	0.56
1:D:398:MET:HA	1:D:401:LEU:HD12	1.87	0.56
1:D:107:VAL:HG23	1:D:134:ALA:HB2	1.87	0.56
1:C:16:ASP:O	1:C:19:THR:HG22	2.06	0.56
1:A:330:ILE:HD12	1:A:363:SER:HB3	1.87	0.56
1:A:340:LEU:HD22	1:A:352:LEU:HD11	1.88	0.55
1:C:22:ILE:HD11	1:C:327:THR:HB	1.88	0.55
1:C:158:PRO:HG2	1:C:163:GLN:HB2	1.88	0.54
1:E:163:GLN:CD	1:E:164:LYS:H	2.09	0.54
1:D:14:GLN:HB2	1:D:43:ASP:HA	1.89	0.54
1:D:340:LEU:HD22	1:D:352:LEU:HD11	1.90	0.53
1:E:216:LEU:HD21	1:F:138:GLN:HB3	1.90	0.53
1:C:19:THR:HG23	1:C:73:CYS:SG	2.48	0.53
1:E:132:ARG:HG3	1:E:274:GLY:HA3	1.91	0.53
1:C:333:ILE:O	1:C:337:THR:HG23	2.08	0.53
1:A:215:ILE:HG23	1:B:97:ASN:HD21	1.75	0.52
1:B:158:PRO:HD2	1:B:163:GLN:O	2.11	0.51
1:E:97:ASN:HD21	1:F:215:ILE:HD12	1.75	0.51
1:A:256:ALA:O	1:B:283:GLN:HG2	2.11	0.51
1:D:257:GLN:O	1:D:261:SER:HB3	2.11	0.51
1:F:17:GLU:HB2	1:F:311:THR:HB	1.93	0.51
1:E:290:MET:HG3	1:E:376:LEU:HD21	1.93	0.51
1:C:330:ILE:HD12	1:C:363:SER:HB3	1.93	0.50
1:F:24:GLU:O	1:F:28:GLU:HG2	2.12	0.50
1:A:14:GLN:HB2	1:A:43:ASP:HA	1.93	0.50
2:A:501:AKG:H42	4:A:504:NAP:C4N	2.41	0.50
1:D:112:ILE:HD13	1:D:330:ILE:HG22	1.93	0.50
1:D:22:ILE:HG21	1:D:329:PRO:HB3	1.93	0.49
1:B:209:LEU:HD23	1:B:248:HIS:HD2	1.77	0.49
1:D:403:GLU:O	1:D:407:ILE:HG12	2.12	0.49
1:C:112:ILE:HD13	1:C:330:ILE:HG22	1.94	0.49
1:E:7:GLY:HA3	1:E:37:LEU:HD23	1.94	0.49
1:B:141:ALA:HB1	1:B:180:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLY:HA3	1:A:37:LEU:HD23	1.95	0.48
1:E:210:SER:HB3	1:E:254:MET:HG2	1.95	0.48
1:B:362:VAL:HG23	1:B:408:LYS:HD2	1.94	0.47
1:E:53:ASN:HA	1:E:92:TRP:CH2	2.50	0.47
1:B:24:GLU:O	1:B:28:GLU:HG2	2.15	0.47
1:A:68:ASN:HA	1:A:302:THR:HG23	1.97	0.47
1:F:132:ARG:CB	1:F:274:GLY:HA3	2.45	0.47
1:C:219:TYR:HB2	1:D:143:ASP:HB2	1.97	0.47
1:A:403:GLU:O	1:A:407:ILE:HG12	2.15	0.47
1:F:68:ASN:O	1:F:302:THR:HA	2.15	0.47
1:A:359:LEU:HD13	1:A:405:LEU:HD22	1.97	0.46
1:F:210:SER:HB3	1:F:254:MET:HG2	1.96	0.46
1:D:210:SER:HB3	1:D:254:MET:HG2	1.97	0.46
1:F:83:VAL:HA	1:F:88:LEU:HD12	1.98	0.46
1:C:317:ARG:HH11	1:C:320:GLN:HE22	1.63	0.46
1:A:154:ILE:HG23	1:A:167:TYR:HB2	1.98	0.46
1:C:412:ALA:C	1:C:414:LEU:H	2.18	0.46
1:B:210:SER:HA	1:B:249:ARG:O	2.17	0.45
1:A:24:GLU:O	1:A:28:GLU:HB2	2.16	0.45
1:F:330:ILE:HD12	1:F:363:SER:HB3	1.97	0.45
1:E:330:ILE:HD12	1:E:363:SER:HB3	1.99	0.45
1:A:143:ASP:HB2	1:B:219:TYR:HB2	1.98	0.45
1:D:132:ARG:HG3	1:D:274:GLY:HA3	2.00	0.44
1:F:200:ALA:HA	1:F:266:ILE:HG13	1.99	0.44
1:E:338:ARG:HA	1:E:338:ARG:HD3	1.80	0.44
1:F:23:TRP:CE3	1:F:73:CYS:HB2	2.53	0.44
1:C:7:GLY:HA3	1:C:37:LEU:HD23	2.00	0.43
1:B:47:GLU:H	1:B:47:GLU:CD	2.22	0.43
1:B:141:ALA:HB1	1:B:180:MET:HE3	2.00	0.43
1:F:30:LEU:HD13	1:F:359:LEU:HD11	2.01	0.43
1:E:12:GLU:HB2	1:E:39:LEU:HD11	2.00	0.43
1:A:210:SER:HA	1:A:249:ARG:O	2.19	0.43
1:C:312:VAL:HG13	4:C:503:NAP:H3B	2.01	0.43
1:A:124:TRP:HB3	1:A:285:TYR:CE1	2.54	0.43
1:B:213:ASN:O	1:B:217:LYS:HA	2.19	0.43
1:D:212:LYS:HG2	1:D:251:ILE:HG22	2.01	0.43
1:D:22:ILE:HA	1:D:25:LEU:HD12	2.00	0.42
1:E:156:TYR:CE2	1:E:158:PRO:HD3	2.53	0.42
1:B:201:LEU:HD23	1:B:244:ILE:HD11	2.00	0.42
1:C:143:ASP:HB2	1:D:219:TYR:HB2	2.01	0.42
1:E:397:PHE:CE2	1:E:401:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:362:VAL:HG21	1:F:405:LEU:HA	2.01	0.42
1:D:367:ILE:HA	1:D:371:PHE:O	2.20	0.42
1:F:359:LEU:HD13	1:F:405:LEU:HD13	2.00	0.42
1:A:283:GLN:HG2	1:B:256:ALA:O	2.19	0.42
1:E:167:TYR:HB3	1:F:142:THR:HG21	2.02	0.42
1:C:123:GLY:O	1:C:262:GLU:HA	2.20	0.41
1:D:330:ILE:HD12	1:D:363:SER:HB3	2.01	0.41
1:B:57:THR:HG21	1:B:95:PRO:HA	2.02	0.41
1:C:97:ASN:HD21	1:D:215:ILE:HD12	1.85	0.41
1:C:120:LEU:HD12	1:C:283:GLN:O	2.20	0.41
1:C:71:VAL:HG11	1:C:336:TRP:HA	2.03	0.41
1:E:72:LYS:HG2	1:E:73:CYS:O	2.20	0.41
1:C:121:VAL:HG11	1:C:124:TRP:CE2	2.56	0.41
1:B:23:TRP:CD1	1:B:27:LYS:HE2	2.55	0.41
1:C:200:ALA:HA	1:C:266:ILE:HG13	2.03	0.41
1:C:30:LEU:O	1:C:355:PHE:HZ	2.03	0.41
1:E:75:THR:O	4:E:503:NAP:H2N	2.21	0.41
1:E:30:LEU:HD22	1:E:359:LEU:HD11	2.03	0.41
1:F:382:GLY:O	1:F:386:VAL:HG23	2.21	0.41
1:C:201:LEU:HD23	1:C:244:ILE:HD11	2.02	0.41
1:C:210:SER:HB3	1:C:254:MET:HG2	2.01	0.41
1:D:328:ASN:OD1	1:D:330:ILE:HG12	2.21	0.40
1:B:126:LYS:O	1:B:263:GLY:HA3	2.21	0.40
1:E:219:TYR:HB2	1:F:143:ASP:HB2	2.02	0.40
1:D:15:GLY:HA3	1:D:73:CYS:SG	2.60	0.40
1:A:156:TYR:CE1	1:B:146:VAL:HG13	2.56	0.40
1:B:125:VAL:HG22	1:B:262:GLU:HB2	2.03	0.40
1:F:79:ASP:H	1:F:82:ARG:HB2	1.87	0.40
1:C:282:ALA:HB2	1:C:291:MET:SD	2.61	0.40
1:D:359:LEU:HD13	1:D:405:LEU:HD22	2.02	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	409/425 (96%)	389 (95%)	19 (5%)	1 (0%)	52 83
1	B	412/425 (97%)	391 (95%)	19 (5%)	2 (0%)	34 69
1	C	410/425 (96%)	384 (94%)	26 (6%)	0	100 100
1	D	411/425 (97%)	386 (94%)	23 (6%)	2 (0%)	34 69
1	E	411/425 (97%)	389 (95%)	21 (5%)	1 (0%)	52 83
1	F	411/425 (97%)	387 (94%)	22 (5%)	2 (0%)	34 69
All	All	2464/2550 (97%)	2326 (94%)	130 (5%)	8 (0%)	46 78

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	124	TRP
1	D	163	GLN
1	E	124	TRP
1	F	164	LYS
1	A	124	TRP
1	B	271	ASN
1	D	124	TRP
1	F	31	ILE

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	337/362 (93%)	326 (97%)	11 (3%)	45 79
1	B	345/362 (95%)	332 (96%)	13 (4%)	40 75
1	C	333/362 (92%)	320 (96%)	13 (4%)	39 74
1	D	312/362 (86%)	297 (95%)	15 (5%)	31 66
1	E	339/362 (94%)	318 (94%)	21 (6%)	23 53
1	F	326/362 (90%)	318 (98%)	8 (2%)	55 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1992/2172 (92%)	1911 (96%)	81 (4%)	38 72

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	90	GLN
1	A	94	SER
1	A	140	ARG
1	A	155	THR
1	A	160	ASP
1	A	280	SER
1	A	303	VAL
1	A	312	VAL
1	A	332	SER
1	A	394	THR
1	B	12	GLU
1	B	151	LYS
1	B	164	LYS
1	B	184	ASN
1	B	212	LYS
1	B	252	ASP
1	B	304	GLU
1	B	314[A]	ARG
1	B	314[B]	ARG
1	B	325	THR
1	B	388	ARG
1	B	400	LYS
1	B	414	LEU
1	C	20	ARG
1	C	30	LEU
1	C	47	GLU
1	C	140	ARG
1	C	155	THR
1	C	157	THR
1	C	184	ASN
1	C	252	ASP
1	C	280	SER
1	C	326	SER
1	C	332	SER
1	C	338	ARG
1	C	399	ASP

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Mol	Chain	Res	Type
1	D	20	ARG
1	D	98	THR
1	D	140	ARG
1	D	142	THR
1	D	154	ILE
1	D	184	ASN
1	D	213	ASN
1	D	247	GLU
1	D	279	ASP
1	D	280	SER
1	D	317	ARG
1	D	343	ARG
1	D	364	ILE
1	D	399	ASP
1	D	408	LYS
1	E	6	SER
1	E	20	ARG
1	E	94	SER
1	E	140	ARG
1	E	160	ASP
1	E	163	GLN
1	E	184	ASN
1	E	195	SER
1	E	202	SER
1	E	213	ASN
1	E	222	ARG
1	E	224	LYS
1	E	252	ASP
1	E	280	SER
1	E	292	THR
1	E	303	VAL
1	E	389	SER
1	E	399	ASP
1	E	406	LYS
1	E	408	LYS
1	E	414	LEU
1	F	12	GLU
1	F	39	LEU
1	F	54	ASP
1	F	132	ARG
1	F	140	ARG
1	F	213	ASN

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Mol	Chain	Res	Type
1	F	280	SER
1	F	312	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	B	97	ASN
1	B	228	GLN
1	C	96	ASN
1	C	320	GLN
1	E	97	ASN
1	E	163	GLN
1	E	309	HIS
1	F	68	ASN
1	F	96	ASN
1	F	393	ASN
1	F	404	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 18 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
2	AKG	A	501	3	3,9,9	0.47	0	4,11,11	0.49	0
4	NAP	A	504	-	42,52,52	1.65	3 (7%)	54,80,80	1.71	2 (3%)
2	AKG	B	501	3	3,9,9	0.34	0	4,11,11	1.29	0
4	NAP	B	502	-	42,52,52	1.54	3 (7%)	54,80,80	2.14	4 (7%)
2	AKG	C	501	3	3,9,9	0.55	0	4,11,11	1.08	0
4	NAP	C	503	-	42,52,52	1.70	3 (7%)	54,80,80	1.72	3 (5%)
2	AKG	D	501	3	3,9,9	0.43	0	4,11,11	0.56	0
4	NAP	D	503	-	42,52,52	1.65	3 (7%)	54,80,80	1.86	3 (5%)
2	AKG	E	501	3	3,9,9	0.32	0	4,11,11	1.19	0
4	NAP	E	503	-	42,52,52	1.61	3 (7%)	54,80,80	1.98	5 (9%)
2	AKG	F	501	3	3,9,9	0.22	0	4,11,11	1.41	1 (25%)
4	NAP	F	503	-	42,52,52	1.63	3 (7%)	54,80,80	2.08	5 (9%)

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	AKG	A	501	3	-	0/3/9/9	0/0/0/0
4	NAP	A	504	-	-	0/27/67/67	0/5/5/5
2	AKG	B	501	3	-	0/3/9/9	0/0/0/0
4	NAP	B	502	-	-	0/27/67/67	0/5/5/5
2	AKG	C	501	3	-	0/3/9/9	0/0/0/0
4	NAP	C	503	-	-	0/27/67/67	0/5/5/5
2	AKG	D	501	3	-	0/3/9/9	0/0/0/0
4	NAP	D	503	-	-	0/27/67/67	0/5/5/5
2	AKG	E	501	3	-	0/3/9/9	0/0/0/0
4	NAP	E	503	-	-	0/27/67/67	0/5/5/5
2	AKG	F	501	3	-	0/3/9/9	0/0/0/0
4	NAP	F	503	-	-	0/27/67/67	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	503	NAP	C2A-N1A	2.64	1.38	1.33
4	D	503	NAP	C2A-N1A	2.65	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	NAP	C2A-N1A	2.73	1.39	1.33
4	E	503	NAP	C2A-N1A	2.75	1.39	1.33
4	C	503	NAP	C2A-N1A	2.83	1.39	1.33
4	A	504	NAP	C2A-N1A	3.07	1.39	1.33
4	B	502	NAP	C2A-N3A	3.74	1.38	1.32
4	F	503	NAP	C2A-N3A	3.80	1.38	1.32
4	E	503	NAP	C2A-N3A	3.84	1.39	1.32
4	D	503	NAP	C2A-N3A	3.96	1.39	1.32
4	A	504	NAP	C2A-N3A	4.14	1.39	1.32
4	C	503	NAP	C2A-N3A	4.45	1.40	1.32
4	B	502	NAP	O7N-C7N	7.39	1.39	1.24
4	A	504	NAP	O7N-C7N	7.92	1.41	1.24
4	E	503	NAP	O7N-C7N	8.01	1.41	1.24
4	F	503	NAP	O7N-C7N	8.06	1.41	1.24
4	D	503	NAP	O7N-C7N	8.21	1.41	1.24
4	C	503	NAP	O7N-C7N	8.44	1.42	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	502	NAP	N3A-C2A-N1A	-13.51	118.55	128.89
4	E	503	NAP	N3A-C2A-N1A	-12.22	119.54	128.89
4	F	503	NAP	N3A-C2A-N1A	-12.18	119.57	128.89
4	D	503	NAP	N3A-C2A-N1A	-11.85	119.82	128.89
4	A	504	NAP	N3A-C2A-N1A	-10.83	120.60	128.89
4	C	503	NAP	N3A-C2A-N1A	-10.09	121.17	128.89
4	E	503	NAP	C4A-C5A-N7A	-2.35	107.32	109.48
4	B	502	NAP	C4A-C5A-N7A	-2.19	107.47	109.48
4	F	503	NAP	C4A-C5A-N7A	-2.12	107.53	109.48
4	E	503	NAP	O7N-C7N-N7N	-2.06	119.69	122.59
2	F	501	AKG	C3-C4-C5	-2.04	109.01	112.75
4	F	503	NAP	P2B-O2B-C2B	2.08	126.56	121.56
4	C	503	NAP	C3N-C7N-N7N	2.12	120.13	117.82
4	A	504	NAP	C3N-C7N-N7N	2.37	120.41	117.82
4	F	503	NAP	C3N-C7N-N7N	2.39	120.43	117.82
4	D	503	NAP	C3N-C7N-N7N	2.46	120.50	117.82
4	E	503	NAP	C3N-C7N-N7N	2.99	121.09	117.82
4	D	503	NAP	O4D-C1D-N1N	2.99	111.42	108.13
4	E	503	NAP	O4D-C1D-N1N	3.15	111.59	108.13
4	B	502	NAP	O4D-C1D-N1N	3.15	111.59	108.13
4	C	503	NAP	O4D-C1D-N1N	3.21	111.66	108.13
4	B	502	NAP	C3N-C7N-N7N	3.65	121.82	117.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	503	NAP	O4D-C1D-N1N	6.14	114.88	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	AKG	1	0
4	A	504	NAP	1	0
4	C	503	NAP	1	0
4	E	503	NAP	1	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	411/425 (96%)	-0.10	8 (1%)	70	67	39, 69, 98, 124	0
1	B	412/425 (96%)	-0.33	3 (0%)	89	88	38, 55, 79, 94	0
1	C	412/425 (96%)	0.03	16 (3%)	43	37	40, 69, 96, 130	0
1	D	412/425 (96%)	0.14	21 (5%)	32	26	40, 83, 116, 147	0
1	E	412/425 (96%)	0.10	22 (5%)	30	24	40, 71, 101, 121	0
1	F	412/425 (96%)	0.22	26 (6%)	23	17	42, 81, 112, 151	0
All	All	2471/2550 (96%)	0.01	96 (3%)	43	37	38, 70, 105, 151	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	SER	9.2
1	D	35	VAL	6.6
1	F	35	VAL	6.1
1	D	363	SER	5.6
1	E	7	GLY	4.7
1	F	18	MET	4.5
1	D	409	LEU	4.1
1	E	37	LEU	4.1
1	F	34	TYR	4.0
1	C	409	LEU	4.0
1	F	380	ILE	3.8
1	E	196	SER	3.6
1	D	356	ALA	3.4
1	C	6	SER	3.4
1	D	114	CYS	3.4
1	F	381	LYS	3.3
1	D	352	LEU	3.3
1	F	37	LEU	3.3
1	C	236	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	231	TYR	3.2
1	E	10	VAL	3.2
1	F	241	ALA	3.1
1	F	318	MET	3.1
1	F	86	PHE	3.1
1	F	319	TYR	3.1
1	A	10	VAL	3.1
1	F	5	ILE	3.0
1	C	7	GLY	3.0
1	E	204	GLY	3.0
1	F	64	ILE	3.0
1	E	114	CYS	2.9
1	E	363	SER	2.9
1	D	5	ILE	2.9
1	D	321	LYS	2.9
1	E	200	ALA	2.9
1	D	37	LEU	2.9
1	E	337	THR	2.9
1	B	5	ILE	2.8
1	A	31	ILE	2.8
1	D	88	LEU	2.8
1	A	35	VAL	2.8
1	E	352	LEU	2.8
1	E	36	GLU	2.7
1	B	7	GLY	2.7
1	E	354	PHE	2.6
1	D	394	THR	2.6
1	F	385	ASN	2.6
1	C	372	MET	2.6
1	E	6	SER	2.6
1	F	330	ILE	2.6
1	C	30	LEU	2.6
1	D	34	TYR	2.6
1	F	46	ILE	2.6
1	F	377	ALA	2.5
1	C	398	MET	2.5
1	F	354	PHE	2.5
1	F	125	VAL	2.5
1	C	31	ILE	2.5
1	C	230	ILE	2.5
1	C	405	LEU	2.4
1	F	398	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	30	LEU	2.4
1	E	67	HIS	2.4
1	C	35	VAL	2.4
1	A	201	LEU	2.4
1	D	31	ILE	2.4
1	D	364	ILE	2.4
1	C	226	ILE	2.3
1	D	32	PHE	2.3
1	C	415	SER	2.3
1	F	237	SER	2.3
1	E	39	LEU	2.3
1	D	116	ASN	2.3
1	F	412	ALA	2.3
1	E	236	LYS	2.3
1	D	405	LEU	2.2
1	D	391	TYR	2.2
1	E	340	LEU	2.2
1	D	46	ILE	2.2
1	E	32	PHE	2.2
1	F	243	LYS	2.2
1	C	36	GLU	2.2
1	C	229	GLU	2.2
1	F	409	LEU	2.2
1	B	352	LEU	2.2
1	E	244	ILE	2.1
1	A	336	TRP	2.1
1	A	190	GLU	2.1
1	D	83	VAL	2.1
1	E	69	VAL	2.1
1	F	88	LEU	2.1
1	E	208	TYR	2.1
1	F	116	ASN	2.1
1	D	89	LYS	2.1
1	C	38	ASP	2.0
1	A	319	TYR	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, 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
2	AKG	C	501	10/10	0.88	0.30	4.10	79,85,88,88	0
2	AKG	E	501	10/10	0.90	0.35	3.71	91,96,98,98	0
2	AKG	F	501	10/10	0.90	0.29	3.37	86,90,99,99	0
3	CA	D	502	1/1	0.98	0.24	2.91	70,70,70,70	0
2	AKG	D	501	10/10	0.92	0.24	2.86	100,101,102,102	0
3	CA	A	502	1/1	0.97	0.24	2.46	70,70,70,70	0
3	CA	C	502	1/1	0.98	0.24	1.40	62,62,62,62	0
2	AKG	A	501	10/10	0.94	0.21	0.95	74,77,79,79	0
3	CA	A	503	1/1	0.99	0.18	0.92	53,53,53,53	0
3	CA	F	502	1/1	0.96	0.20	0.45	74,74,74,74	0
4	NAP	D	503	48/48	0.87	0.21	0.45	98,109,113,114	0
4	NAP	E	503	48/48	0.94	0.20	0.31	54,68,77,79	0
3	CA	E	502	1/1	0.98	0.23	0.17	72,72,72,72	0
4	NAP	F	503	48/48	0.91	0.20	0.10	84,99,103,105	0
4	NAP	C	503	48/48	0.96	0.18	0.05	50,61,74,75	0
4	NAP	B	502	48/48	0.98	0.17	-0.08	44,51,59,62	0
4	NAP	A	504	48/48	0.96	0.16	-0.49	43,59,68,71	0
2	AKG	B	501	10/10	0.95	0.15	-0.51	41,55,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.