Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 05:27 PM EST

PDB ID	:	6D0O
Title	:	rdpA dioxygenase holoenzyme
Authors	:	Rydel, T.J.; Sturman, E.J.; Zheng, M.; Evdokimov, A.
Deposited on	:	2018-04-10
Resolution	:	2.30 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 (i) 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 (1)) were used in the production of this report:

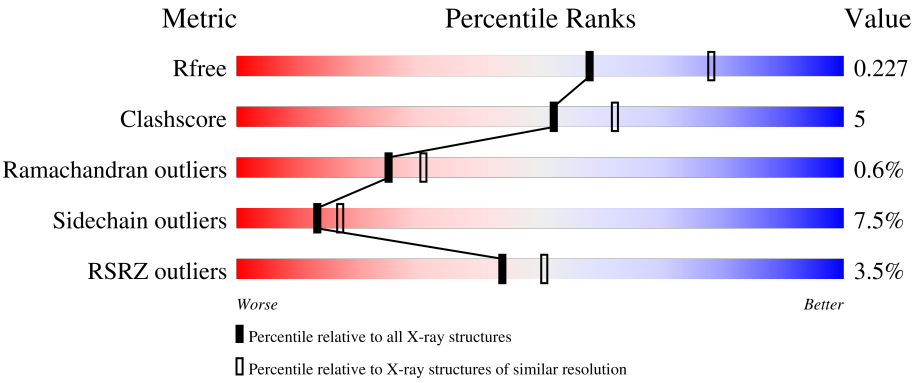
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	301	4% 72% 13% • • 9%
1	B	301	2% 75% 10% • 11%
1	C	301	% 82% 9% • 5%
1	D	301	6% 83% 10% • •

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	AKG	A	402	-	X	-	-
3	AKG	B	402	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9524 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 (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	2	0
			2199	1389	394	406	10			
1	B	267	Total	C	N	O	S	0	0	0
			2123	1343	377	394	9			
1	C	287	Total	C	N	O	S	8	2	0
			2295	1446	411	428	10			
1	D	289	Total	C	N	O	S	8	1	0
			2308	1454	417	427	10			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	GLY	ALA	conflict	UNP Q8KSC8
A	100	ASP	ASN	conflict	UNP Q8KSC8
A	229	SER	THR	conflict	UNP Q8KSC8
A	230	GLU	ASP	conflict	UNP Q8KSC8
A	231	LYS	ALA	conflict	UNP Q8KSC8
A	234	GLU	LYS	conflict	UNP Q8KSC8
A	238	SER	GLN	conflict	UNP Q8KSC8
A	241	PHE	TYR	conflict	UNP Q8KSC8
A	242	ALA	GLU	conflict	UNP Q8KSC8
A	246	LYS	ARG	conflict	UNP Q8KSC8
A	247	PRO	PHE	conflict	UNP Q8KSC8
A	248	GLU	ASP	conflict	UNP Q8KSC8
A	261	VAL	LEU	conflict	UNP Q8KSC8
A	271	TYR	ARG	conflict	UNP Q8KSC8
A	273	ILE	VAL	conflict	UNP Q8KSC8
A	274	ASN	PRO	conflict	UNP Q8KSC8
A	277	HIS	ALA	conflict	UNP Q8KSC8
A	279	GLN	LYS	conflict	UNP Q8KSC8
A	280	THR	PHE	conflict	UNP Q8KSC8
A	282	ILE	TYR	conflict	UNP Q8KSC8
A	284	HIS	THR	conflict	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	296	HIS	-	expression tag	UNP Q8KSC8
A	297	HIS	-	expression tag	UNP Q8KSC8
A	298	HIS	-	expression tag	UNP Q8KSC8
A	299	HIS	-	expression tag	UNP Q8KSC8
A	300	HIS	-	expression tag	UNP Q8KSC8
A	301	HIS	-	expression tag	UNP Q8KSC8
B	99	GLY	ALA	conflict	UNP Q8KSC8
B	100	ASP	ASN	conflict	UNP Q8KSC8
B	229	SER	THR	conflict	UNP Q8KSC8
B	230	GLU	ASP	conflict	UNP Q8KSC8
B	231	LYS	ALA	conflict	UNP Q8KSC8
B	234	GLU	LYS	conflict	UNP Q8KSC8
B	238	SER	GLN	conflict	UNP Q8KSC8
B	241	PHE	TYR	conflict	UNP Q8KSC8
B	242	ALA	GLU	conflict	UNP Q8KSC8
B	246	LYS	ARG	conflict	UNP Q8KSC8
B	247	PRO	PHE	conflict	UNP Q8KSC8
B	248	GLU	ASP	conflict	UNP Q8KSC8
B	261	VAL	LEU	conflict	UNP Q8KSC8
B	271	TYR	ARG	conflict	UNP Q8KSC8
B	273	ILE	VAL	conflict	UNP Q8KSC8
B	274	ASN	PRO	conflict	UNP Q8KSC8
B	277	HIS	ALA	conflict	UNP Q8KSC8
B	279	GLN	LYS	conflict	UNP Q8KSC8
B	280	THR	PHE	conflict	UNP Q8KSC8
B	282	ILE	TYR	conflict	UNP Q8KSC8
B	284	HIS	THR	conflict	UNP Q8KSC8
B	296	HIS	-	expression tag	UNP Q8KSC8
B	297	HIS	-	expression tag	UNP Q8KSC8
B	298	HIS	-	expression tag	UNP Q8KSC8
B	299	HIS	-	expression tag	UNP Q8KSC8
B	300	HIS	-	expression tag	UNP Q8KSC8
B	301	HIS	-	expression tag	UNP Q8KSC8
C	99	GLY	ALA	conflict	UNP Q8KSC8
C	100	ASP	ASN	conflict	UNP Q8KSC8
C	229	SER	THR	conflict	UNP Q8KSC8
C	230	GLU	ASP	conflict	UNP Q8KSC8
C	231	LYS	ALA	conflict	UNP Q8KSC8
C	234	GLU	LYS	conflict	UNP Q8KSC8
C	238	SER	GLN	conflict	UNP Q8KSC8
C	241	PHE	TYR	conflict	UNP Q8KSC8
C	242	ALA	GLU	conflict	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	246	LYS	ARG	conflict	UNP Q8KSC8
C	247	PRO	PHE	conflict	UNP Q8KSC8
C	248	GLU	ASP	conflict	UNP Q8KSC8
C	261	VAL	LEU	conflict	UNP Q8KSC8
C	271	TYR	ARG	conflict	UNP Q8KSC8
C	273	ILE	VAL	conflict	UNP Q8KSC8
C	274	ASN	PRO	conflict	UNP Q8KSC8
C	277	HIS	ALA	conflict	UNP Q8KSC8
C	279	GLN	LYS	conflict	UNP Q8KSC8
C	280	THR	PHE	conflict	UNP Q8KSC8
C	282	ILE	TYR	conflict	UNP Q8KSC8
C	284	HIS	THR	conflict	UNP Q8KSC8
C	296	HIS	-	expression tag	UNP Q8KSC8
C	297	HIS	-	expression tag	UNP Q8KSC8
C	298	HIS	-	expression tag	UNP Q8KSC8
C	299	HIS	-	expression tag	UNP Q8KSC8
C	300	HIS	-	expression tag	UNP Q8KSC8
C	301	HIS	-	expression tag	UNP Q8KSC8
D	99	GLY	ALA	conflict	UNP Q8KSC8
D	100	ASP	ASN	conflict	UNP Q8KSC8
D	229	SER	THR	conflict	UNP Q8KSC8
D	230	GLU	ASP	conflict	UNP Q8KSC8
D	231	LYS	ALA	conflict	UNP Q8KSC8
D	234	GLU	LYS	conflict	UNP Q8KSC8
D	238	SER	GLN	conflict	UNP Q8KSC8
D	241	PHE	TYR	conflict	UNP Q8KSC8
D	242	ALA	GLU	conflict	UNP Q8KSC8
D	246	LYS	ARG	conflict	UNP Q8KSC8
D	247	PRO	PHE	conflict	UNP Q8KSC8
D	248	GLU	ASP	conflict	UNP Q8KSC8
D	261	VAL	LEU	conflict	UNP Q8KSC8
D	271	TYR	ARG	conflict	UNP Q8KSC8
D	273	ILE	VAL	conflict	UNP Q8KSC8
D	274	ASN	PRO	conflict	UNP Q8KSC8
D	277	HIS	ALA	conflict	UNP Q8KSC8
D	279	GLN	LYS	conflict	UNP Q8KSC8
D	280	THR	PHE	conflict	UNP Q8KSC8
D	282	ILE	TYR	conflict	UNP Q8KSC8
D	284	HIS	THR	conflict	UNP Q8KSC8
D	296	HIS	-	expression tag	UNP Q8KSC8
D	297	HIS	-	expression tag	UNP Q8KSC8
D	298	HIS	-	expression tag	UNP Q8KSC8

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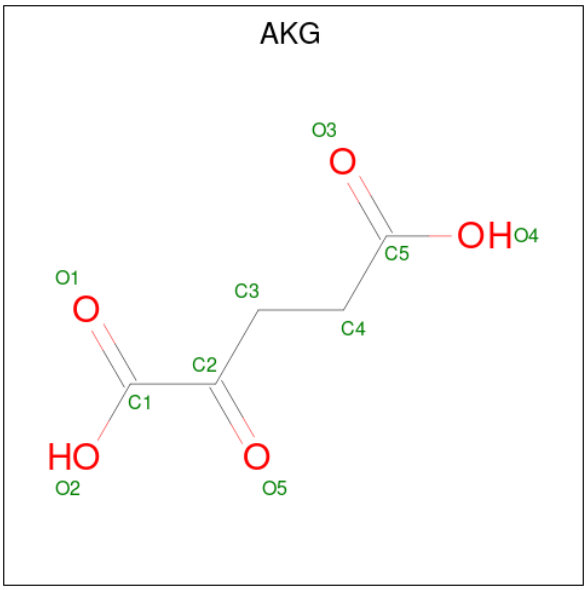
Chain	Residue	Modelled	Actual	Comment	Reference
D	299	HIS	-	expression tag	UNP Q8KSC8
D	300	HIS	-	expression tag	UNP Q8KSC8
D	301	HIS	-	expression tag	UNP Q8KSC8

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



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

- Molecule 4 is water.

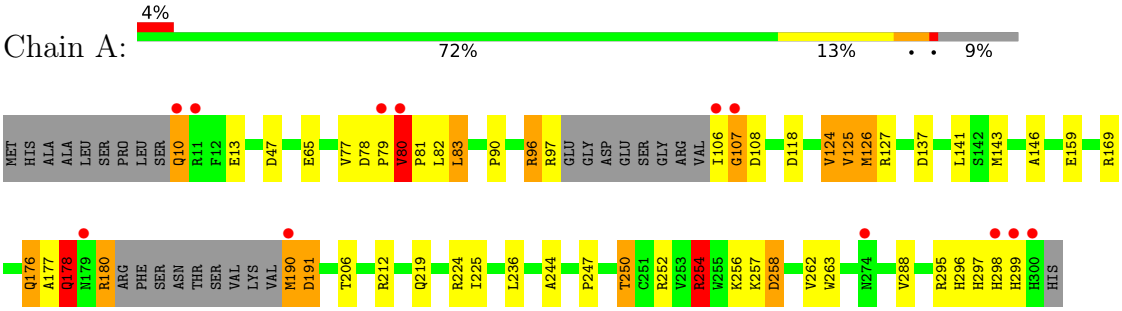
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	157	Total O 157 157	0	0
4	B	157	Total O 157 157	0	0
4	C	128	Total O 128 128	0	0
4	D	113	Total O 113 113	0	0

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.

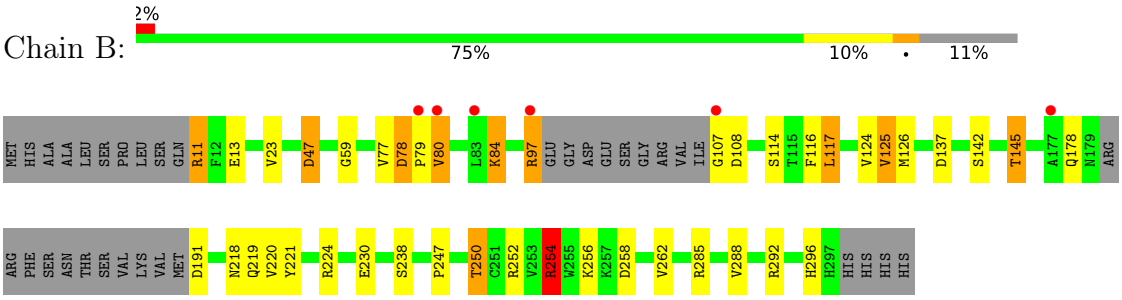
• Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

Chain A:



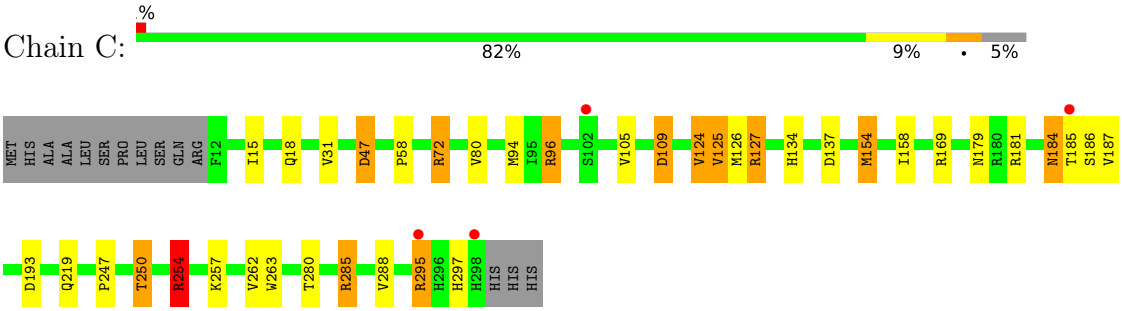
• Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

Chain B:



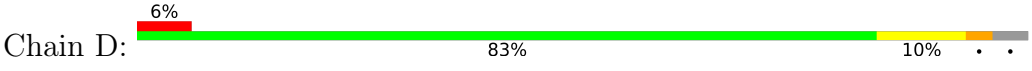
• Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

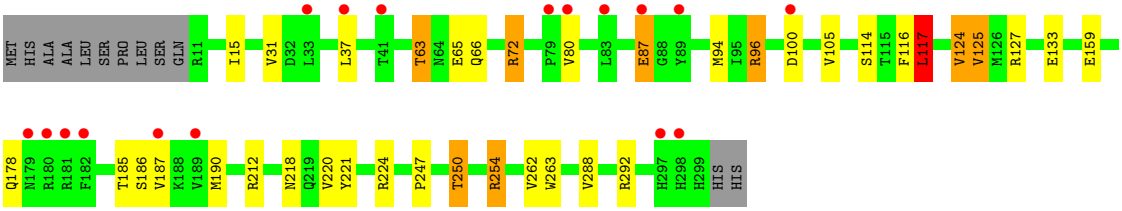
Chain C:



• Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

Chain D:




MET HIS ALA ALA LEU SER PRO LEU SER GLN R11 I15 V31 D32 L33 L37 T41 T63 N64 E65 Q66 R72 P79 V80 L83 E87 G88 Y89 M94 I95 R96 D100 V105 S114 T115 F116 L117 V124 V125 M126 R127 E133 E159
Q178 N179 R180 R181 F182 T185 S186 V187 K188 V189 M190 R212 N218 Q219 V220 Y221 R224 P247 T250 R254 V262 W263 V288 R292 H297 H298 H299 HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	153.01Å 153.01Å 156.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.30) 99.9 (49.47-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.186 , 0.228 0.191 , 0.227	Depositor DCC
R_{free} test set	3793 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	37.9	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.002 for l,-k,h 0.010 for -l,-k,-h 0.011 for -h,-l,-k 0.002 for -h,l,k 0.023 for -h,k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9524	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CO, AKG

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	0.92	2/2264 (0.1%)	1.10	15/3082 (0.5%)
1	B	0.98	3/2179 (0.1%)	1.05	10/2967 (0.3%)
1	C	0.96	6/2358 (0.3%)	1.06	11/3209 (0.3%)
1	D	0.82	2/2372 (0.1%)	1.00	7/3227 (0.2%)
All	All	0.92	13/9173 (0.1%)	1.05	43/12485 (0.3%)

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	A	0	4
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	8

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295[A]	ARG	CA-C	-10.95	1.24	1.52
1	C	295[B]	ARG	CA-C	-10.95	1.24	1.52
1	B	238	SER	CB-OG	-10.75	1.28	1.42
1	B	47	ASP	CB-CG	-8.86	1.33	1.51
1	C	295[A]	ARG	N-CA	7.83	1.62	1.46
1	C	295[B]	ARG	N-CA	7.83	1.62	1.46
1	D	159	GLU	CD-OE1	6.76	1.33	1.25
1	D	159	GLU	CD-OE2	6.33	1.32	1.25
1	A	65	GLU	CD-OE2	5.66	1.31	1.25
1	C	109[A]	ASP	CB-CG	5.56	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	109[B]	ASP	CB-CG	5.56	1.63	1.51
1	A	178	GLN	CA-C	5.08	1.66	1.52
1	B	59	GLY	N-CA	5.01	1.53	1.46

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	254	ARG	NE-CZ-NH2	-10.33	115.13	120.30
1	D	212	ARG	NE-CZ-NH2	-8.79	115.90	120.30
1	A	254	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	212	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	B	47	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	C	109[A]	ASP	CB-CG-OD1	7.70	125.23	118.30
1	C	109[B]	ASP	CB-CG-OD1	7.70	125.23	118.30
1	B	224	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	A	126	MET	CG-SD-CE	-7.35	88.44	100.20
1	D	254	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	254	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	B	254	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	A	258	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	C	72	ARG	CA-CB-CG	6.68	128.10	113.40
1	D	117	LEU	CA-CB-CG	6.57	130.41	115.30
1	D	224	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	C	254	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	D	224	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	C	193	ASP	CB-CG-OD1	6.09	123.78	118.30
1	C	285	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	C	47	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	126	MET	CG-SD-CE	5.82	109.51	100.20
1	A	118	ASP	CB-CG-OD1	5.79	123.51	118.30
1	D	254	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	83	LEU	CB-CG-CD2	5.75	120.77	111.00
1	C	47	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	107	GLY	N-CA-C	5.70	127.34	113.10
1	A	96	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	B	219	GLN	CA-CB-CG	5.68	125.91	113.40
1	A	180	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	285	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	219	GLN	CA-CB-CG	5.47	125.44	113.40
1	C	154	MET	CG-SD-CE	-5.46	91.46	100.20
1	A	224	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	238	SER	N-CA-CB	5.44	118.67	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	127	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	87	GLU	N-CA-C	5.32	125.36	111.00
1	A	254	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	295	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	78	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	169	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	B	224	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	127	ARG	CB-CA-C	-5.02	100.36	110.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ASP	Peptide
1	A	177	ALA	Peptide
1	A	178	GLN	Peptide
1	A	80	VAL	Peptide
1	B	108	ASP	Peptide
1	C	297	HIS	Peptide
1	C	94	MET	Peptide
1	D	94	MET	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2199	0	2117	36	0
1	B	2123	0	2047	22	0
1	C	2295	0	2217	26	0
1	D	2308	0	2234	14	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	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	10	0	4	0	0
4	A	157	0	0	2	0
4	B	157	0	0	8	1
4	C	128	0	0	6	1
4	D	113	0	0	2	0
All	All	9524	0	8631	96	1

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 5.

All (96) 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:295[B]:ARG:HH11	1:C:295[B]:ARG:HB3	1.19	1.02
1:A:176:GLN:HE21	1:A:176:GLN:HA	1.22	1.00
1:A:143:MET:HE1	1:A:146:ALA:CB	2.07	0.84
1:C:280:THR:HB	4:C:509:HOH:O	1.78	0.82
1:A:143:MET:HE3	1:A:244:ALA:HB1	1.60	0.82
1:B:23:VAL:HG13	1:B:145:THR:HG21	1.65	0.79
1:D:63:THR:HG22	1:D:66:GLN:OE1	1.85	0.77
1:A:176:GLN:HA	1:A:176:GLN:NE2	1.98	0.76
1:A:10:GLN:OE1	1:A:47[B]:ASP:OD2	2.06	0.74
1:A:143:MET:HE1	1:A:146:ALA:HB2	1.70	0.73
1:C:134:HIS:ND1	4:C:503:HOH:O	2.22	0.72
1:C:154:MET:CE	1:C:158:ILE:HD13	2.22	0.69
1:A:107:GLY:HA2	4:A:502:HOH:O	1.92	0.68
1:A:143:MET:HA	1:A:143:MET:CE	2.23	0.68
1:C:154:MET:CE	1:C:158:ILE:HG21	2.25	0.67
1:C:154:MET:HE1	1:C:158:ILE:HG21	1.75	0.66
1:C:109[A]:ASP:OD2	1:C:219:GLN:NE2	2.29	0.65
1:B:258:ASP:OD2	4:B:503:HOH:O	2.14	0.65
1:D:72[B]:ARG:NH2	4:D:502:HOH:O	2.27	0.64
1:B:142:SER:HB3	1:B:145:THR:HG23	1.78	0.64
1:C:169:ARG:O	4:C:501:HOH:O	2.15	0.64
1:C:295[B]:ARG:HB3	1:C:295[B]:ARG:NH1	2.03	0.63
1:A:143:MET:HE1	1:A:146:ALA:HB3	1.80	0.61
1:B:114:SER:HB3	1:B:117:LEU:HD22	1.84	0.60
1:B:107:GLY:N	4:B:505:HOH:O	2.33	0.60
1:D:65:GLU:HG2	4:D:568:HOH:O	2.01	0.60
1:C:154:MET:HE1	1:C:158:ILE:CG2	2.32	0.59
1:A:296:HIS:CG	1:A:297:HIS:H	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LYS:HD3	1:B:84:LYS:H	1.71	0.56
1:C:58:PRO:O	4:C:502:HOH:O	2.17	0.56
1:C:154:MET:CE	1:C:158:ILE:CG2	2.82	0.56
1:D:218:ASN:ND2	1:D:221:TYR:H	2.04	0.55
1:A:141:LEU:HD13	1:A:143:MET:CE	2.36	0.55
1:A:206:THR:HG21	1:A:296:HIS:ND1	2.21	0.55
1:B:218:ASN:ND2	1:B:221:TYR:H	2.05	0.54
1:A:141:LEU:CD1	1:A:143:MET:CE	2.86	0.53
1:C:154:MET:HE3	1:C:158:ILE:HD13	1.90	0.53
1:B:218:ASN:HD21	1:B:221:TYR:H	1.55	0.53
1:A:141:LEU:CD1	1:A:143:MET:HE2	2.39	0.53
1:D:15:ILE:HG22	1:D:31:VAL:CG2	2.40	0.52
1:A:80:VAL:HB	1:A:82:LEU:HG	1.92	0.52
1:C:96:ARG:HG3	1:C:185:THR:HG22	1.92	0.52
1:C:154:MET:HE2	1:C:158:ILE:HD13	1.91	0.51
1:D:114:SER:HB3	1:D:117:LEU:HD22	1.93	0.51
1:B:218:ASN:HD22	1:B:220:VAL:H	1.59	0.50
1:A:141:LEU:HD13	1:A:143:MET:HE3	1.94	0.49
1:B:247:PRO:O	1:B:250:THR:HB	2.12	0.49
1:A:247:PRO:O	1:A:250:THR:HB	2.13	0.49
1:A:143:MET:HE1	1:A:143:MET:HA	1.95	0.49
1:D:247:PRO:O	1:D:250:THR:HB	2.13	0.48
1:A:96:ARG:O	1:A:97:ARG:NH1	2.46	0.48
1:C:184:ASN:HD22	1:C:185:THR:N	2.11	0.48
1:D:96:ARG:HG3	1:D:185:THR:HG22	1.95	0.48
1:D:218:ASN:HD21	1:D:221:TYR:H	1.60	0.48
1:A:80:VAL:HG23	1:A:90:PRO:O	2.14	0.47
1:B:11:ARG:HD3	4:B:647:HOH:O	2.15	0.47
1:C:247:PRO:O	1:C:250:THR:HB	2.14	0.47
1:C:125:VAL:HB	1:C:262:VAL:HG22	1.97	0.47
1:C:280:THR:HG22	4:C:611:HOH:O	2.15	0.47
1:A:143:MET:CE	1:A:244:ALA:HB1	2.39	0.47
1:D:116:PHE:CE1	1:D:117:LEU:HD13	2.51	0.46
1:B:252:ARG:NH1	1:C:250:THR:HG22	2.31	0.46
1:B:125:VAL:HB	1:B:262:VAL:HG22	1.98	0.46
1:A:125:VAL:HB	1:A:262:VAL:HG22	1.98	0.45
1:D:125:VAL:HB	1:D:262:VAL:HG22	1.98	0.45
1:B:84:LYS:H	1:B:84:LYS:CD	2.28	0.45
1:A:225:ILE:CD1	1:A:236:LEU:HD23	2.47	0.45
1:A:78[B]:ASP:OD1	1:A:80:VAL:HG13	2.17	0.45
1:A:178:GLN:N	1:A:178:GLN:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ASN:HD22	1:D:220:VAL:H	1.65	0.44
1:B:191:ASP:HA	4:B:593:HOH:O	2.16	0.44
1:B:11:ARG:CD	4:B:647:HOH:O	2.65	0.44
1:A:225:ILE:HD11	1:A:236:LEU:HD23	1.99	0.43
1:B:97:ARG:HA	4:B:637:HOH:O	2.17	0.43
1:B:116:PHE:CE1	1:B:117:LEU:HD13	2.53	0.43
1:B:145:THR:HB	4:B:649:HOH:O	2.19	0.43
1:A:141:LEU:HD13	1:A:143:MET:HE2	1.99	0.43
1:C:126:MET:CE	1:C:285:ARG:HD2	2.49	0.43
1:A:296:HIS:CG	1:A:297:HIS:N	2.87	0.43
1:C:15:ILE:HG22	1:C:31:VAL:CG2	2.49	0.43
1:C:134:HIS:HA	4:C:593:HOH:O	2.18	0.43
1:A:176:GLN:NE2	1:A:176:GLN:CA	2.72	0.42
1:C:179:ASN:O	1:C:181:ARG:HG2	2.19	0.42
1:A:143:MET:HA	1:A:143:MET:HE2	1.97	0.42
1:A:106:ILE:O	1:A:106:ILE:HG13	2.19	0.42
1:B:137:ASP:OD1	1:B:254:ARG:HG2	2.19	0.42
1:A:137:ASP:OD1	1:A:254:ARG:HG2	2.20	0.41
1:A:258:ASP:OD1	4:A:501:HOH:O	2.20	0.41
1:C:124:VAL:HG13	1:C:263:TRP:CE2	2.55	0.41
1:A:190:MET:O	1:A:191:ASP:HB3	2.20	0.41
1:B:254:ARG:HD3	4:B:638:HOH:O	2.20	0.41
1:D:124:VAL:HG13	1:D:263:TRP:CE2	2.56	0.41
1:C:137:ASP:OD1	1:C:254:ARG:HG2	2.21	0.41
1:A:124:VAL:HG13	1:A:263:TRP:CE2	2.57	0.40
1:B:78:ASP:C	1:B:80:VAL:H	2.25	0.40
1:A:252:ARG:NH1	1:D:250:THR:HG22	2.35	0.40

All (1) 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)
4:B:592:HOH:O	4:C:624:HOH:O[4_454]	2.14	0.06

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	270/301 (90%)	258 (96%)	7 (3%)	5 (2%)	8 7
1	B	261/301 (87%)	255 (98%)	5 (2%)	1 (0%)	34 42
1	C	287/301 (95%)	281 (98%)	6 (2%)	0	100 100
1	D	288/301 (96%)	280 (97%)	7 (2%)	1 (0%)	41 50
All	All	1106/1204 (92%)	1074 (97%)	25 (2%)	7 (1%)	25 31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	D	87	GLU
1	A	298	HIS
1	A	191	ASP
1	A	299	HIS
1	B	79	PRO
1	A	79	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	238/259 (92%)	221 (93%)	17 (7%)	14 19
1	B	229/259 (88%)	210 (92%)	19 (8%)	11 14
1	C	249/259 (96%)	233 (94%)	16 (6%)	17 23
1	D	250/259 (96%)	229 (92%)	21 (8%)	11 13
All	All	966/1036 (93%)	893 (92%)	73 (8%)	13 16

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	13	GLU
1	A	77	VAL
1	A	80	VAL
1	A	83	LEU
1	A	124	VAL
1	A	125	VAL
1	A	126	MET
1	A	159	GLU
1	A	176	GLN
1	A	180	ARG
1	A	190	MET
1	A	250	THR
1	A	254	ARG
1	A	256	LYS
1	A	257	LYS
1	A	288	VAL
1	B	11	ARG
1	B	13	GLU
1	B	47	ASP
1	B	77	VAL
1	B	80	VAL
1	B	84	LYS
1	B	97	ARG
1	B	117	LEU
1	B	124	VAL
1	B	125	VAL
1	B	145	THR
1	B	178	GLN
1	B	230	GLU
1	B	250	THR
1	B	254	ARG
1	B	256	LYS
1	B	288	VAL
1	B	292	ARG
1	B	296	HIS
1	C	18	GLN
1	C	47	ASP
1	C	72	ARG
1	C	80	VAL
1	C	96	ARG
1	C	105	VAL
1	C	124	VAL

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Mol	Chain	Res	Type
1	C	125	VAL
1	C	127	ARG
1	C	184	ASN
1	C	186	SER
1	C	187	VAL
1	C	250	THR
1	C	254	ARG
1	C	257	LYS
1	C	288	VAL
1	D	37	LEU
1	D	63	THR
1	D	72[A]	ARG
1	D	72[B]	ARG
1	D	80	VAL
1	D	96	ARG
1	D	100	ASP
1	D	105	VAL
1	D	117	LEU
1	D	124	VAL
1	D	125	VAL
1	D	127	ARG
1	D	133	GLU
1	D	178	GLN
1	D	186	SER
1	D	187	VAL
1	D	190	MET
1	D	250	THR
1	D	254	ARG
1	D	288	VAL
1	D	292	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	176	GLN
1	B	18	GLN
1	B	178	GLN
1	B	218	ASN
1	C	184	ASN
1	C	219	GLN
1	D	176	GLN

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Mol	Chain	Res	Type
1	D	218	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 monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	AKG	D	402	2	9,9,9	2.72	1 (11%)	11,11,11	2.78	4 (36%)
3	AKG	B	402	2	9,9,9	2.73	4 (44%)	11,11,11	5.00	8 (72%)
3	AKG	A	402	2	9,9,9	1.29	1 (11%)	11,11,11	3.03	6 (54%)
3	AKG	C	402	2	9,9,9	1.86	3 (33%)	11,11,11	1.91	2 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AKG	D	402	2	-	1/9/9/9	-
3	AKG	B	402	2	-	7/9/9/9	-
3	AKG	A	402	2	-	5/9/9/9	-
3	AKG	C	402	2	-	1/9/9/9	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	AKG	C2-C1	-7.42	1.43	1.53
3	B	402	AKG	O1-C1	5.02	1.36	1.22
3	C	402	AKG	C2-C1	-3.83	1.48	1.53
3	B	402	AKG	O2-C1	3.83	1.41	1.30
3	B	402	AKG	C3-C2	3.72	1.55	1.51
3	B	402	AKG	O5-C2	-3.10	1.16	1.23
3	A	402	AKG	O3-C5	2.72	1.31	1.22
3	C	402	AKG	O1-C1	2.17	1.28	1.22
3	C	402	AKG	O3-C5	2.14	1.29	1.22

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	AKG	O1-C1-C2	-11.93	105.80	121.72
3	B	402	AKG	C3-C2-C1	8.15	131.10	115.97
3	D	402	AKG	O1-C1-C2	-7.26	112.02	121.72
3	A	402	AKG	O5-C2-C1	5.22	127.00	119.43
3	A	402	AKG	O1-C1-C2	-4.60	115.58	121.72
3	A	402	AKG	O2-C1-C2	4.55	126.41	113.97
3	A	402	AKG	C3-C4-C5	-4.41	104.11	113.60
3	B	402	AKG	O5-C2-C1	-4.36	113.11	119.43
3	B	402	AKG	O2-C1-O1	4.29	133.42	123.61
3	C	402	AKG	C3-C2-C1	4.18	123.74	115.97
3	D	402	AKG	O2-C1-C2	3.06	122.33	113.97
3	B	402	AKG	O3-C5-C4	-3.02	113.38	123.08
3	C	402	AKG	O1-C1-C2	-2.98	117.74	121.72
3	B	402	AKG	O4-C5-C4	2.77	122.93	114.03
3	D	402	AKG	O5-C2-C3	2.59	126.94	121.20
3	B	402	AKG	O5-C2-C3	-2.49	115.69	121.20
3	A	402	AKG	O2-C1-O1	-2.45	117.99	123.61
3	B	402	AKG	O2-C1-C2	2.30	120.27	113.97
3	D	402	AKG	O4-C5-C4	2.17	121.01	114.03
3	A	402	AKG	O5-C2-C3	-2.02	116.72	121.20

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	AKG	O2-C1-C2-C3
3	B	402	AKG	O2-C1-C2-C3
3	B	402	AKG	C1-C2-C3-C4
3	C	402	AKG	C1-C2-C3-C4
3	D	402	AKG	C1-C2-C3-C4
3	B	402	AKG	O1-C1-C2-O5
3	A	402	AKG	O1-C1-C2-C3
3	B	402	AKG	O1-C1-C2-C3
3	A	402	AKG	O2-C1-C2-O5
3	B	402	AKG	O5-C2-C3-C4
3	B	402	AKG	C3-C4-C5-O3
3	B	402	AKG	C3-C4-C5-O4
3	A	402	AKG	C1-C2-C3-C4
3	A	402	AKG	O1-C1-C2-O5

There are no ring outliers.

No monomer is involved in short contacts.

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	274/301 (91%)	-0.16	12 (4%)	34	41	23, 34, 94, 162	4 (1%)
1	B	267/301 (88%)	-0.35	6 (2%)	62	69	23, 34, 81, 122	5 (1%)
1	C	287/301 (95%)	-0.17	4 (1%)	75	80	27, 41, 76, 134	7 (2%)
1	D	289/301 (96%)	0.17	17 (5%)	22	28	26, 49, 91, 153	5 (1%)
All	All	1117/1204 (92%)	-0.12	39 (3%)	44	51	23, 39, 87, 162	21 (1%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	VAL	5.3
1	D	179	ASN	5.1
1	B	83	LEU	4.8
1	D	83	LEU	4.7
1	A	190	MET	4.1
1	D	189	VAL	4.0
1	A	79	PRO	3.8
1	A	274	ASN	3.8
1	C	298	HIS	3.7
1	A	11	ARG	3.7
1	A	298	HIS	3.6
1	A	300	HIS	3.6
1	A	106	ILE	3.6
1	B	79	PRO	3.6
1	D	298	HIS	3.3
1	D	80	VAL	3.2
1	A	299	HIS	3.2
1	C	295[A]	ARG	3.2
1	B	107	GLY	3.1
1	D	180	ARG	3.0
1	D	181	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	10	GLN	2.9
1	D	79	PRO	2.8
1	D	33	LEU	2.8
1	D	187	VAL	2.8
1	D	297	HIS	2.7
1	B	80	VAL	2.6
1	B	97	ARG	2.6
1	A	107	GLY	2.5
1	D	182	PHE	2.3
1	D	87	GLU	2.3
1	C	185	THR	2.2
1	B	177	ALA	2.2
1	D	89	TYR	2.2
1	D	41	THR	2.2
1	D	37	LEU	2.1
1	C	102	SER	2.1
1	A	179	ASN	2.1
1	D	100	ASP	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 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	AKG	A	402	10/10	0.85	0.20	39,73,81,88	0
3	AKG	B	402	10/10	0.91	0.19	36,59,72,82	0
3	AKG	D	402	10/10	0.98	0.10	37,47,53,61	0
2	CO	D	401	1/1	0.99	0.10	44,44,44,44	0
3	AKG	C	402	10/10	0.99	0.09	33,35,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CO	B	401	1/1	0.99	0.10	31,31,31,31	0
2	CO	C	401	1/1	1.00	0.14	33,33,33,33	0
2	CO	A	401	1/1	1.00	0.12	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.