Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2024 – 12:10 PM JST

PDB ID	:	8WK9
Title	:	Aldo-keto reductase KmAKR - Y28A/K29H/T63M/Q213A/Y296W/W297H
Authors	:	Xu, S.Y.; Zhou, L.; Xu, Y.; Wang, Y.J.; Zheng, Y.G.
Deposited on	:	2023-09-27
Resolution	:	2.39 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:

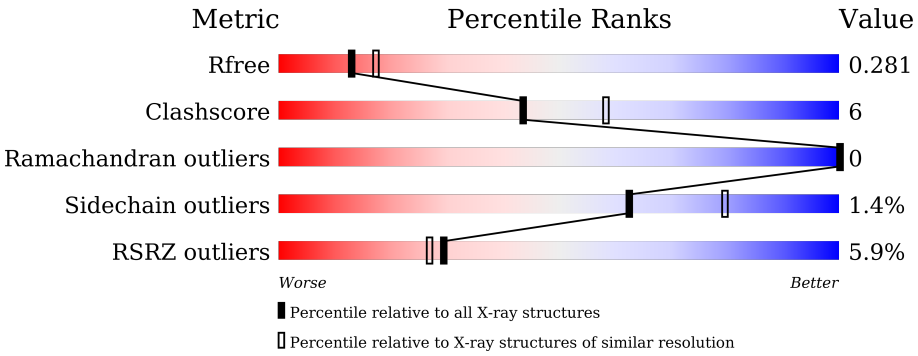
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 2.39 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	310	3% 82% 17%
1	B	310	5% 82% 16%
1	C	310	4% 83% 14%
1	D	310	10% 77% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9956 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 NADPH-dependent alpha-keto amide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2478	1602	397	478	1			
1	B	304	Total	C	N	O	S	0	0	0
			2447	1583	391	472	1			
1	C	302	Total	C	N	O	S	0	0	0
			2431	1575	390	465	1			
1	D	297	Total	C	N	O	S	0	0	0
			2389	1551	380	457	1			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ALA	TYR	engineered mutation	UNP W0TDP7
A	29	HIS	LYS	engineered mutation	UNP W0TDP7
A	63	MET	THR	engineered mutation	UNP W0TDP7
A	109	ASN	LYS	conflict	UNP W0TDP7
A	213	ALA	GLN	engineered mutation	UNP W0TDP7
A	296	TRP	TYR	engineered mutation	UNP W0TDP7
A	297	HIS	TRP	engineered mutation	UNP W0TDP7
B	28	ALA	TYR	engineered mutation	UNP W0TDP7
B	29	HIS	LYS	engineered mutation	UNP W0TDP7
B	63	MET	THR	engineered mutation	UNP W0TDP7
B	109	ASN	LYS	conflict	UNP W0TDP7
B	213	ALA	GLN	engineered mutation	UNP W0TDP7
B	296	TRP	TYR	engineered mutation	UNP W0TDP7
B	297	HIS	TRP	engineered mutation	UNP W0TDP7
C	28	ALA	TYR	engineered mutation	UNP W0TDP7
C	29	HIS	LYS	engineered mutation	UNP W0TDP7
C	63	MET	THR	engineered mutation	UNP W0TDP7
C	109	ASN	LYS	conflict	UNP W0TDP7
C	213	ALA	GLN	engineered mutation	UNP W0TDP7
C	296	TRP	TYR	engineered mutation	UNP W0TDP7
C	297	HIS	TRP	engineered mutation	UNP W0TDP7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	28	ALA	TYR	engineered mutation	UNP W0TDP7
D	29	HIS	LYS	engineered mutation	UNP W0TDP7
D	63	MET	THR	engineered mutation	UNP W0TDP7
D	109	ASN	LYS	conflict	UNP W0TDP7
D	213	ALA	GLN	engineered mutation	UNP W0TDP7
D	296	TRP	TYR	engineered mutation	UNP W0TDP7
D	297	HIS	TRP	engineered mutation	UNP W0TDP7

- Molecule 2 is water.

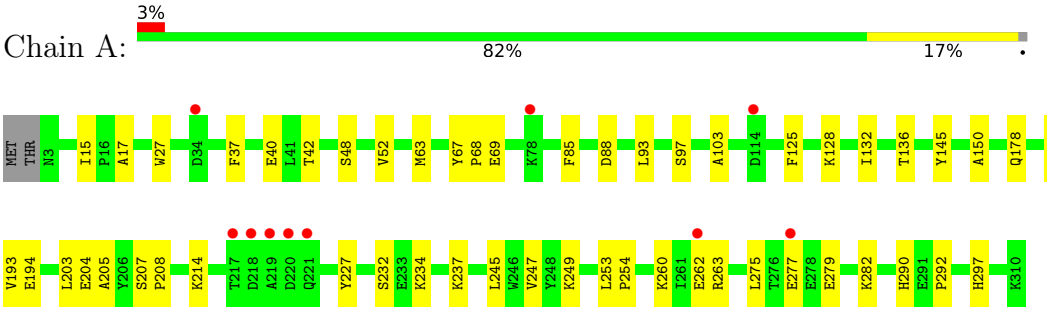
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	60	Total O 60 60	0	0
2	B	47	Total O 47 47	0	0
2	C	54	Total O 54 54	0	0
2	D	50	Total O 50 50	0	0

3 Residue-property plots

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.

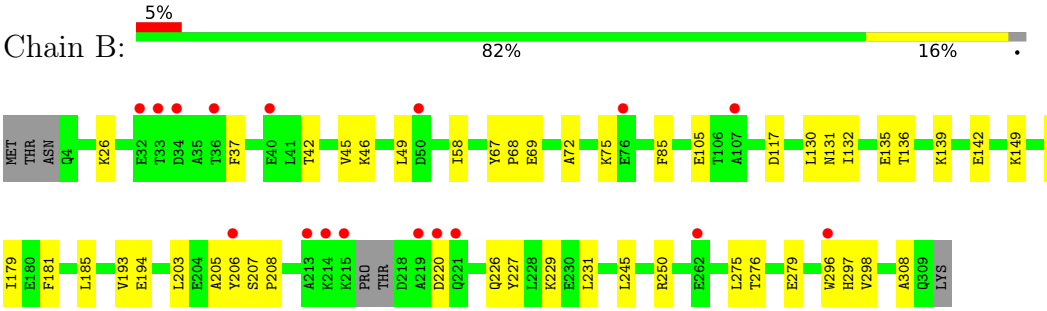
• Molecule 1: NADPH-dependent alpha-keto amide reductase

Chain A:



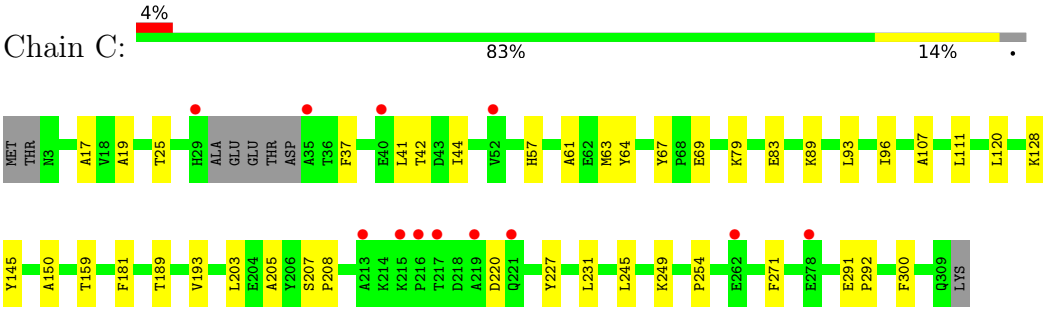
• Molecule 1: NADPH-dependent alpha-keto amide reductase

Chain B:



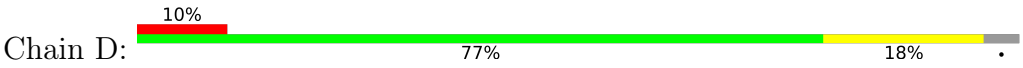
• Molecule 1: NADPH-dependent alpha-keto amide reductase

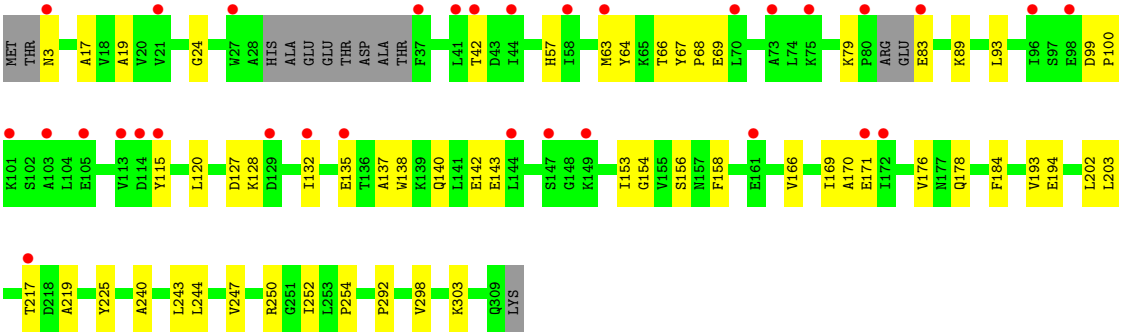
Chain C:



• Molecule 1: NADPH-dependent alpha-keto amide reductase

Chain D:




MET THR N3 A17 V18 A19 V20 V21 G24 W27 A28 HIS ALA GLU GLU THR ASP ALA THR F37 L41 T42 D43 I44 H57 I58 M63 Y64 K65 T66 Y67 P68 E69 L70 A73 L74 K75 K79 P80 ARG GLU E83 K89 L93 I96 S97 E98 D99 P100
K101 S102 A103 L104 E105 V113 D114 Y115 L120 D127 K128 D129 I132 E135 T136 A137 W138 K139 Q140 L141 E142 E143 L144 S147 G148 K149 I153 G154 V155 S156 N157 F158 E161 V166 I169 A170 E171 I172 V176 N177 Q178 F184 V193 E194 L202 L203
T217 D218 A219 Y225 A240 L243 L244 V247 R250 G251 I252 L253 P254 P292 V298 K303 Q309 LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.28Å 114.83Å 83.07Å 90.00° 101.32° 90.00°	Depositor
Resolution (Å)	81.46 – 2.39 81.46 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (81.46-2.39) 99.8 (81.46-2.39)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.220 , 0.283 0.221 , 0.281	Depositor DCC
R_{free} test set	2555 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	1.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 27.1	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	0.90	EDS
Total number of atoms	9956	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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

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	0.49	0/2533	0.54	0/3434
1	B	0.47	0/2500	0.52	0/3387
1	C	0.46	0/2485	0.51	0/3368
1	D	0.47	0/2441	0.52	0/3307
All	All	0.47	0/9959	0.52	0/13496

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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250	ARG	Sidechain
1	D	250	ARG	Sidechain

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	2478	0	2489	38	0
1	B	2447	0	2455	29	0
1	C	2431	0	2447	24	0
1	D	2389	0	2408	33	0
2	A	60	0	0	0	0
2	B	47	0	0	0	0
2	C	54	0	0	0	0
2	D	50	0	0	1	0
All	All	9956	0	9799	118	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 6.

All (118) 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:B:49:LEU:HD21	1:B:58:ILE:HD11	1.44	0.99
1:B:298:VAL:HG11	1:C:128:LYS:HD3	1.73	0.71
1:C:42:THR:HG22	1:C:69:GLU:O	1.91	0.69
1:A:132:ILE:CG1	1:A:136:THR:HB	2.22	0.68
1:B:132:ILE:HD11	1:B:136:THR:HG22	1.77	0.66
1:B:206:TYR:HE1	1:B:296:TRP:CD1	2.15	0.64
1:C:89:LYS:HG2	1:C:120:LEU:HB2	1.79	0.64
1:B:206:TYR:CE1	1:B:296:TRP:CD1	2.88	0.62
1:D:120:LEU:HA	1:D:154:GLY:O	2.02	0.60
1:A:132:ILE:HG12	1:A:136:THR:HB	1.85	0.59
1:B:42:THR:HG22	1:B:69:GLU:CA	2.33	0.59
1:D:135:GLU:HG3	1:D:169:ILE:HG12	1.84	0.59
1:A:125:PHE:CE1	1:D:303:LYS:HE2	2.37	0.58
1:A:260:LYS:HE3	1:A:263:ARG:NH2	2.19	0.58
1:A:42:THR:HG22	1:A:69:GLU:HA	1.86	0.57
1:A:42:THR:HG22	1:A:69:GLU:CA	2.34	0.57
1:D:132:ILE:HD11	1:D:137:ALA:HA	1.87	0.57
1:A:15:ILE:HG13	1:A:85:PHE:CZ	2.39	0.57
1:D:193:VAL:HA	1:D:203:LEU:HD11	1.86	0.57
1:D:67:TYR:N	1:D:68:PRO:CD	2.68	0.56
1:B:194:GLU:H	1:B:194:GLU:CD	2.09	0.56
1:C:227:TYR:CE2	1:C:231:LEU:HD11	2.41	0.56
1:B:37:PHE:CZ	1:B:42:THR:HG21	2.39	0.56
1:D:79:LYS:HD2	1:D:83:GLU:HB3	1.88	0.56
1:D:24:GLY:HA2	1:D:64:TYR:CG	2.41	0.55
1:D:194:GLU:HB3	2:D:436:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:O	1:A:249:LYS:HG2	2.07	0.55
1:C:193:VAL:HA	1:C:203:LEU:HD11	1.89	0.55
1:A:63:MET:HE3	1:A:93:LEU:HB3	1.89	0.54
1:B:220:ASP:O	1:B:226:GLN:NE2	2.27	0.54
1:B:42:THR:HG22	1:B:69:GLU:HA	1.90	0.54
1:B:245:LEU:HD23	1:B:275:LEU:HG	1.91	0.53
1:A:132:ILE:HG13	1:A:136:THR:HB	1.90	0.52
1:B:207:SER:N	1:B:208:PRO:CD	2.73	0.52
1:A:128:LYS:HB3	1:D:298:VAL:HG12	1.92	0.51
1:D:243:LEU:O	1:D:247:VAL:HG23	2.10	0.51
1:A:37:PHE:CZ	1:A:42:THR:HG21	2.46	0.51
1:B:67:TYR:N	1:B:68:PRO:CD	2.73	0.51
1:B:181:PHE:HB3	1:B:205:ALA:CB	2.41	0.51
1:D:89:LYS:HE2	1:D:178:GLN:OE1	2.11	0.51
1:D:138:TRP:CZ2	1:D:153:ILE:HD12	2.46	0.51
1:D:42:THR:HG22	1:D:69:GLU:HA	1.93	0.51
1:C:159:THR:HG22	1:C:189:THR:HG21	1.94	0.50
1:B:45:VAL:O	1:B:49:LEU:HG	2.13	0.49
1:D:184:PHE:O	1:D:292:PRO:HA	2.13	0.49
1:A:63:MET:CE	1:A:93:LEU:HB3	2.43	0.48
1:B:85:PHE:CE2	1:B:117:ASP:HB3	2.48	0.48
1:C:245:LEU:O	1:C:249:LYS:HG2	2.13	0.48
1:C:291:GLU:HG2	1:C:292:PRO:HD2	1.95	0.48
1:A:234:LYS:NZ	1:A:279:GLU:OE2	2.47	0.47
1:D:142:GLU:OE1	1:D:171:GLU:N	2.45	0.47
1:A:125:PHE:CE1	1:D:303:LYS:CE	2.98	0.47
1:A:27:TRP:CE2	1:C:25:THR:HG22	2.50	0.47
1:A:67:TYR:N	1:A:68:PRO:CD	2.78	0.46
1:A:145:TYR:HA	1:A:150:ALA:O	2.15	0.46
1:A:253:LEU:HD23	1:A:253:LEU:C	2.36	0.46
1:C:107:ALA:O	1:C:111:LEU:HG	2.16	0.46
1:D:93:LEU:O	1:D:127:ASP:HB2	2.16	0.46
1:A:214:LYS:HD2	1:C:37:PHE:HB2	1.97	0.45
1:D:63:MET:CE	1:D:93:LEU:HB3	2.46	0.45
1:C:181:PHE:HB3	1:C:205:ALA:CB	2.47	0.45
1:D:17:ALA:O	1:D:254:PRO:HD2	2.16	0.45
1:B:227:TYR:CE2	1:B:231:LEU:HD11	2.51	0.45
1:D:169:ILE:HD12	1:D:169:ILE:O	2.17	0.45
1:C:19:ALA:HA	1:C:57:HIS:HB3	1.98	0.45
1:A:194:GLU:H	1:A:194:GLU:CD	2.20	0.44
1:C:67:TYR:CE2	1:C:107:ALA:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ASP:HB2	1:D:100:PRO:HD2	1.99	0.44
1:D:138:TRP:CH2	1:D:153:ILE:HD12	2.53	0.44
1:A:207:SER:N	1:A:208:PRO:CD	2.80	0.44
1:A:227:TYR:OH	1:A:279:GLU:HA	2.18	0.44
1:A:260:LYS:HD2	1:A:263:ARG:HG3	1.99	0.44
1:C:145:TYR:HA	1:C:150:ALA:O	2.17	0.44
1:A:48:SER:HA	1:A:52:VAL:HG23	1.99	0.44
1:C:61:ALA:HB3	1:C:64:TYR:CD2	2.53	0.44
1:D:156:SER:O	1:D:158:PHE:HD1	2.00	0.44
1:B:276:THR:OG1	1:B:279:GLU:HG3	2.18	0.44
1:B:72:ALA:HA	1:B:75:LYS:HE3	2.00	0.43
1:A:181:PHE:HB3	1:A:205:ALA:CB	2.48	0.43
1:C:79:LYS:HE3	1:C:83:GLU:HB3	2.00	0.43
1:B:42:THR:HG22	1:B:69:GLU:O	2.18	0.43
1:B:139:LYS:O	1:B:142:GLU:HB2	2.18	0.43
1:C:41:LEU:O	1:C:44:ILE:HG22	2.18	0.43
1:A:97:SER:HB3	1:A:103:ALA:HB2	2.01	0.43
1:B:135:GLU:HG3	1:B:169:ILE:HG12	2.00	0.43
1:D:138:TRP:CD1	1:D:166:VAL:HG13	2.54	0.43
1:A:15:ILE:HG13	1:A:85:PHE:CE1	2.54	0.42
1:A:247:VAL:HG11	1:A:254:PRO:HB3	2.00	0.42
1:A:178:GLN:HG3	1:A:204:GLU:HB2	1.99	0.42
1:C:17:ALA:HB3	1:C:271:PHE:CZ	2.54	0.42
1:C:17:ALA:O	1:C:254:PRO:HD2	2.19	0.42
1:D:176:VAL:HA	1:D:202:LEU:O	2.19	0.42
1:B:42:THR:CG2	1:B:69:GLU:HA	2.48	0.42
1:B:179:ILE:O	1:B:205:ALA:HA	2.20	0.42
1:C:63:MET:HA	1:C:96:ILE:CD1	2.48	0.42
1:D:203:LEU:HB2	1:D:252:ILE:HG12	2.01	0.42
1:B:169:ILE:HD12	1:B:169:ILE:C	2.40	0.42
1:D:240:ALA:O	1:D:244:LEU:HG	2.20	0.42
1:A:227:TYR:CZ	1:A:282:LYS:HD3	2.54	0.42
1:A:67:TYR:OH	1:A:88:ASP:OD1	2.27	0.42
1:C:93:LEU:HD11	1:C:300:PHE:CZ	2.55	0.42
1:C:207:SER:N	1:C:208:PRO:CD	2.82	0.42
1:D:64:TYR:O	1:D:66:THR:HG23	2.20	0.42
1:A:17:ALA:O	1:A:254:PRO:HD2	2.19	0.41
1:B:105:GLU:OE2	1:B:149:LYS:HD3	2.20	0.41
1:A:184:PHE:CZ	1:A:290:HIS:CD2	3.08	0.41
1:B:130:LEU:HD23	1:B:130:LEU:HA	1.91	0.41
1:B:185:LEU:HD12	1:B:308:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:GLN:O	1:D:143:GLU:HB2	2.21	0.41
1:D:166:VAL:O	1:D:170:ALA:HB2	2.20	0.41
1:A:232:SER:HB2	1:A:237:LYS:O	2.21	0.41
1:A:245:LEU:HD23	1:A:275:LEU:HG	2.03	0.41
1:B:193:VAL:HA	1:B:203:LEU:HD11	2.03	0.41
1:D:19:ALA:HA	1:D:57:HIS:HB3	2.02	0.40
1:D:219:ALA:HB1	1:D:225:TYR:CD2	2.56	0.40
1:A:184:PHE:O	1:A:292:PRO:HA	2.20	0.40
1:A:193:VAL:HA	1:A:203:LEU:HD11	2.02	0.40
1:C:140:GLN:O	1:C:144:LEU:HG	2.21	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	306/310 (99%)	301 (98%)	5 (2%)	0	100	100
1	B	300/310 (97%)	294 (98%)	6 (2%)	0	100	100
1	C	298/310 (96%)	293 (98%)	5 (2%)	0	100	100
1	D	291/310 (94%)	281 (97%)	10 (3%)	0	100	100
All	All	1195/1240 (96%)	1169 (98%)	26 (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	274/276 (99%)	270 (98%)	4 (2%)	60	77
1	B	270/276 (98%)	264 (98%)	6 (2%)	47	67
1	C	269/276 (98%)	268 (100%)	1 (0%)	89	95
1	D	265/276 (96%)	261 (98%)	4 (2%)	60	77
All	All	1078/1104 (98%)	1063 (99%)	15 (1%)	62	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	262	GLU
1	A	277	GLU
1	A	297	HIS
1	B	26	LYS
1	B	46	LYS
1	B	131	ASN
1	B	175	GLN
1	B	229	LYS
1	B	297	HIS
1	C	220	ASP
1	D	3	ASN
1	D	115	TYR
1	D	128	LYS
1	D	217	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	109	ASN
1	A	122	HIS
1	B	222	GLN
1	D	3	ASN
1	D	297	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	308/310 (99%)	0.28	10 (3%)	50	47	10, 23, 46, 82	0
1	B	304/310 (98%)	0.53	17 (5%)	31	28	11, 28, 52, 101	0
1	C	302/310 (97%)	0.38	12 (3%)	43	40	9, 25, 51, 85	0
1	D	297/310 (95%)	0.72	32 (10%)	12	10	10, 29, 53, 81	0
All	All	1211/1240 (97%)	0.48	71 (5%)	29	27	9, 26, 52, 101	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	THR	4.6
1	C	29	HIS	4.3
1	A	218	ASP	3.9
1	C	40	GLU	3.7
1	C	35	ALA	3.6
1	D	98	GLU	3.5
1	D	147	SER	3.4
1	D	70	LEU	3.4
1	C	215	LYS	3.3
1	D	21	VAL	3.3
1	D	132	ILE	3.3
1	D	75	LYS	3.3
1	D	3	ASN	3.2
1	D	172	ILE	3.2
1	C	217	THR	3.1
1	D	135	GLU	3.1
1	D	217	THR	3.1
1	B	107	ALA	3.0
1	B	33	THR	2.9
1	B	219	ALA	2.9
1	C	213	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	219	ALA	2.8
1	A	221	GLN	2.8
1	B	262	GLU	2.7
1	B	215	LYS	2.7
1	B	36	THR	2.7
1	C	262	GLU	2.6
1	D	44	ILE	2.6
1	B	214	LYS	2.6
1	B	221	GLN	2.6
1	A	219	ALA	2.5
1	D	80	PRO	2.5
1	B	50	ASP	2.5
1	A	277	GLU	2.5
1	B	206	TYR	2.5
1	D	115	TYR	2.5
1	D	83	GLU	2.5
1	A	78	LYS	2.5
1	A	34	ASP	2.4
1	D	41	LEU	2.4
1	D	105	GLU	2.4
1	A	114	ASP	2.4
1	D	171	GLU	2.4
1	B	34	ASP	2.4
1	D	129	ASP	2.4
1	D	144	LEU	2.4
1	C	216	PRO	2.4
1	B	76	GLU	2.3
1	D	149	LYS	2.3
1	D	58	ILE	2.3
1	D	96	ILE	2.3
1	D	103	ALA	2.3
1	B	220	ASP	2.3
1	D	63	MET	2.3
1	D	42	THR	2.3
1	B	213	ALA	2.2
1	D	73	ALA	2.2
1	D	114	ASP	2.2
1	B	32	GLU	2.2
1	D	101	LYS	2.2
1	D	27	TRP	2.2
1	A	262	GLU	2.1
1	D	161	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	113	VAL	2.1
1	C	278	GLU	2.1
1	A	220	ASP	2.1
1	C	52	VAL	2.0
1	B	40	GLU	2.0
1	B	296	TRP	2.0
1	D	37	PHE	2.0
1	C	221	GLN	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.