Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2021 – 10:03 AM GMT

PDB ID	:	6S2K
Title	:	Human Menin in complex with AJ21
Authors	:	Groves, M.R.; Gao, K.
Deposited on	:	2019-06-21
Resolution	:	3.10 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

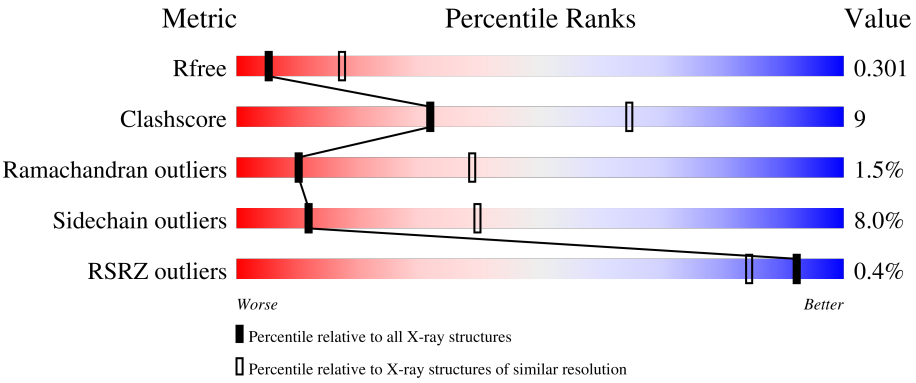
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 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	526	% 68% 18% · 11%
1	B	526	63% 23% · 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7284 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 Multiple endocrine neoplasia I, isoform CRA_b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3645	2343	616	672	14			
1	B	463	Total	C	N	O	S	0	0	0
			3610	2320	611	665	14			

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A024R5E3
A	2	ALA	-	expression tag	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	TRP	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	SER	deletion	UNP A0A024R5E3
A	?	-	LYS	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	GLU	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	LYS	deletion	UNP A0A024R5E3
A	?	-	LYS	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	LEU	deletion	UNP A0A024R5E3
A	?	-	ASP	deletion	UNP A0A024R5E3
A	?	-	LYS	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	LEU	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	THR	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	GLN	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	ALA	deletion	UNP A0A024R5E3
A	?	-	VAL	deletion	UNP A0A024R5E3
A	?	-	SER	deletion	UNP A0A024R5E3
A	?	-	GLY	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	ARG	deletion	UNP A0A024R5E3
A	?	-	LYS	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
A	?	-	PRO	deletion	UNP A0A024R5E3
B	1	GLY	-	expression tag	UNP A0A024R5E3
B	2	ALA	-	expression tag	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	ALA	deletion	UNP A0A024R5E3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	ALA	deletion	UNP A0A024R5E3
B	?	-	ALA	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	ALA	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	TRP	deletion	UNP A0A024R5E3
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	ALA	deletion	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	SER	deletion	UNP A0A024R5E3
B	?	-	LYS	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	GLU	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	LYS	deletion	UNP A0A024R5E3
B	?	-	LYS	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	ALA	deletion	UNP A0A024R5E3
B	?	-	LEU	deletion	UNP A0A024R5E3
B	?	-	ASP	deletion	UNP A0A024R5E3
B	?	-	LYS	deletion	UNP A0A024R5E3
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	LEU	deletion	UNP A0A024R5E3

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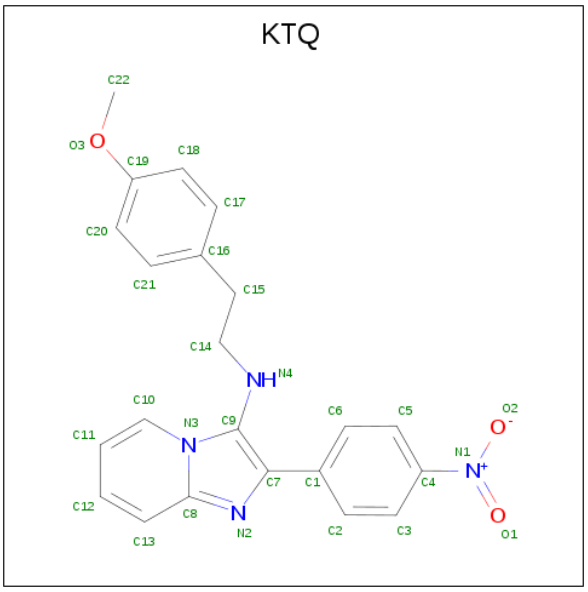
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	THR	deletion	UNP A0A024R5E3
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	GLN	deletion	UNP A0A024R5E3
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	ALA	deletion	UNP A0A024R5E3
B	?	-	VAL	deletion	UNP A0A024R5E3
B	?	-	SER	deletion	UNP A0A024R5E3
B	?	-	GLY	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	ARG	deletion	UNP A0A024R5E3
B	?	-	LYS	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3
B	?	-	PRO	deletion	UNP A0A024R5E3

- Molecule 2 is {N}-[2-(4-methoxyphenyl)ethyl]-2-(4-nitrophenyl)imidazo[1,2-a]pyridin-3-amine (three-letter code: KTQ) (formula: $C_{22}H_{20}N_4O_3$).

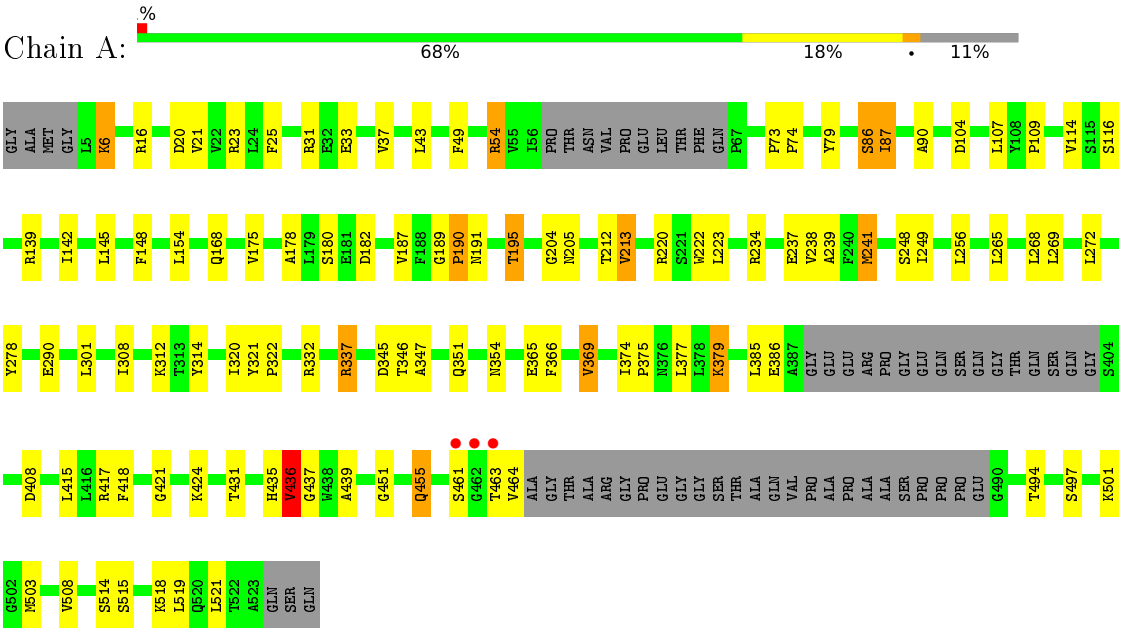


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			29	22	4	3		

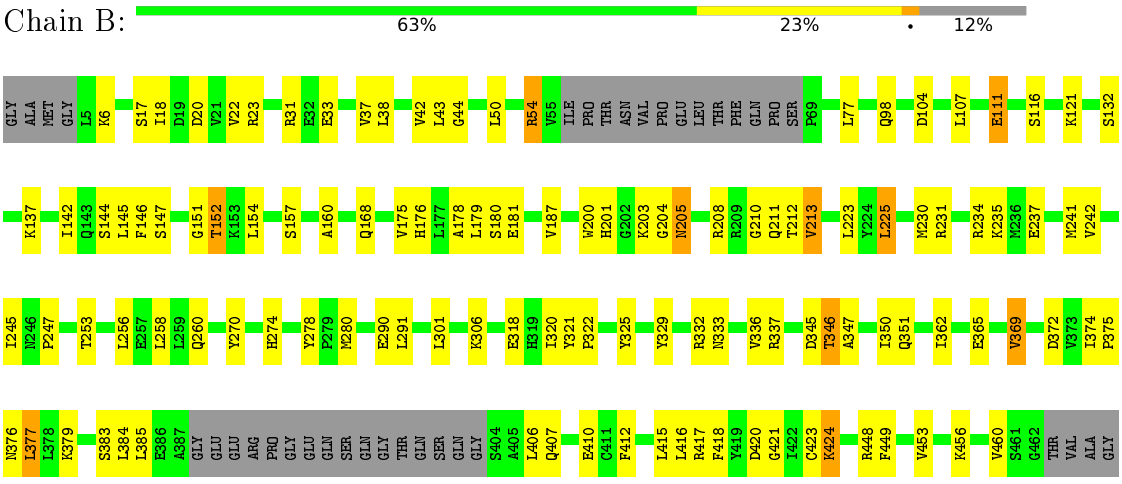
3 Residue-property plots (i)

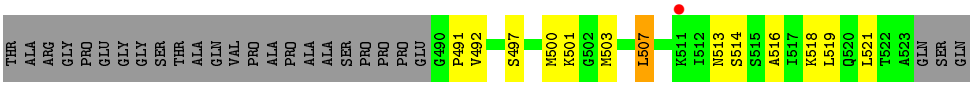
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Multiple endocrine neoplasia I, isoform CRA_b



- Molecule 1: Multiple endocrine neoplasia I, isoform CRA_b




THR
ALA
ARG
GLY
PRO
GLU
GLY
GLY
SER
THR
ALA
GLN
VAL
PRO
ALA
PRO
ALA
ALA
SER
PRO
PRO
PRO
GLU
G490
P491
V492
S497
M500
K501
G502
M503
L507
K511
I512
N513
S514
S515
A516
I517
K518
L519
Q520
L521
T522
A523
GLN
SER
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.40Å 101.31Å 126.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.04 – 3.10 47.04 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.2 (47.04-3.10) 95.2 (47.04-3.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.215 , 0.300 0.219 , 0.301	Depositor DCC
R_{free} test set	947 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	37.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 15.4	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	7284	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.69	0/3729	0.81	0/5069
1	B	0.69	0/3693	0.84	0/5018
All	All	0.69	0/7422	0.83	0/10087

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3645	0	3592	54	0
1	B	3610	0	3553	76	0
2	B	29	0	0	3	0
All	All	7284	0	7145	129	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 9.

All (129) 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:33:GLU:HG3	1:B:168:GLN:HE21	1.38	0.87
1:B:201:HIS:O	1:B:205:ASN:CB	2.30	0.80
1:A:234:ARG:HA	1:A:237:GLU:OE1	1.90	0.72
1:B:372:ASP:O	1:B:376:ASN:ND2	2.26	0.68
1:B:178:ALA:HB2	1:B:187:VAL:HG13	1.77	0.67
1:B:374:ILE:HB	1:B:375:PRO:HD3	1.76	0.67
1:A:290:GLU:OE1	1:A:332:ARG:NH1	2.28	0.66
1:A:521:LEU:O	1:A:521:LEU:HG	1.97	0.65
1:B:369:VAL:HG12	2:B:601:KTQ:C22	2.27	0.65
1:A:43:LEU:HD12	1:A:241:MET:HG2	1.79	0.65
1:B:521:LEU:HG	1:B:521:LEU:O	1.97	0.64
1:B:235:LYS:HG2	1:B:274:HIS:CE1	2.32	0.64
1:B:290:GLU:OE1	1:B:332:ARG:NH1	2.31	0.63
1:A:435:HIS:O	1:A:437:GLY:N	2.31	0.63
1:A:314:TYR:OH	1:B:235:LYS:NZ	2.32	0.62
1:B:208:ARG:NH2	1:B:213:VAL:HA	2.14	0.61
1:B:180:SER:OG	1:B:181:GLU:N	2.31	0.61
1:B:320:ILE:HG21	1:B:362:ILE:HD11	1.83	0.61
1:A:175:VAL:O	1:A:234:ARG:NH2	2.34	0.60
1:B:208:ARG:HH22	1:B:213:VAL:HA	1.66	0.60
1:B:514:SER:O	1:B:518:LYS:HG3	2.02	0.59
1:B:320:ILE:HG23	1:B:346:THR:CG2	2.33	0.58
1:B:142:ILE:O	1:B:154:LEU:HA	2.03	0.58
1:B:50:LEU:O	1:B:54:ARG:NH1	2.37	0.58
1:A:148:PHE:HB2	1:A:154:LEU:HD21	1.86	0.57
1:A:20:ASP:HA	1:A:23:ARG:HH11	1.70	0.57
1:B:320:ILE:HG23	1:B:346:THR:HG23	1.87	0.56
1:A:497:SER:O	1:A:501:LYS:HG3	2.05	0.56
1:A:463:THR:HG22	1:A:501:LYS:HE3	1.87	0.56
1:B:20:ASP:OD1	1:B:23:ARG:NH1	2.39	0.55
1:B:456:LYS:O	1:B:491:PRO:HD2	2.07	0.55
1:A:182:ASP:HB2	1:A:222:TRP:CH2	2.41	0.55
1:A:234:ARG:O	1:A:237:GLU:HB2	2.08	0.54
1:A:54:ARG:HD2	1:A:249:ILE:HD13	1.90	0.54
1:B:180:SER:CB	1:B:223:LEU:O	2.56	0.54
1:B:104:ASP:HB3	1:B:107:LEU:HD12	1.90	0.54
1:A:21:VAL:O	1:A:25:PHE:HD1	1.91	0.53
1:B:415:LEU:O	1:B:418:PHE:HB3	2.08	0.53
1:B:43:LEU:HD12	1:B:241:MET:HG2	1.90	0.53
1:A:114:VAL:HG13	1:A:189:GLY:HA2	1.92	0.52
1:A:415:LEU:O	1:A:418:PHE:HB3	2.10	0.52
1:B:208:ARG:O	1:B:211:GLN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:VAL:O	1:A:241:MET:HB3	2.10	0.51
1:A:49:PHE:O	1:A:79:TYR:OH	2.20	0.50
1:B:168:GLN:HG3	1:B:234:ARG:NH1	2.26	0.50
1:A:6:LYS:N	1:A:6:LYS:HD2	2.27	0.50
1:B:347:ALA:HA	1:B:350:ILE:HG22	1.93	0.50
1:A:37:VAL:HA	1:A:145:LEU:HD12	1.94	0.50
1:B:321:TYR:N	1:B:322:PRO:CD	2.74	0.49
1:A:351:GLN:HB2	1:A:424:LYS:HB3	1.94	0.49
1:A:239:ALA:HA	1:A:269:LEU:HD13	1.95	0.49
1:B:180:SER:OG	1:B:223:LEU:O	2.25	0.49
1:B:38:LEU:O	1:B:42:VAL:HG23	2.13	0.49
1:A:321:TYR:N	1:A:322:PRO:CD	2.76	0.49
1:B:374:ILE:HB	1:B:375:PRO:CD	2.41	0.49
1:A:375:PRO:O	1:A:379:LYS:HB2	2.13	0.49
1:B:497:SER:O	1:B:501:LYS:HG3	2.12	0.48
1:B:321:TYR:CE1	2:B:601:KTQ:C11	2.96	0.48
1:B:242:VAL:O	1:B:245:ILE:HG13	2.13	0.48
1:B:178:ALA:HA	1:B:230:MET:O	2.14	0.48
1:B:351:GLN:HB2	1:B:424:LYS:HB3	1.96	0.48
1:A:514:SER:O	1:A:518:LYS:HG3	2.13	0.48
1:B:241:MET:HB2	1:B:241:MET:HE2	1.78	0.48
1:A:33:GLU:HG3	1:A:168:GLN:HE21	1.78	0.47
1:B:176:HIS:HD2	1:B:237:GLU:OE2	1.97	0.47
1:B:376:ASN:N	1:B:376:ASN:HD22	2.12	0.47
1:A:345:ASP:OD1	1:A:417:ARG:NH2	2.47	0.47
1:A:195:THR:OG1	1:A:213:VAL:HB	2.15	0.47
1:B:180:SER:HB2	1:B:223:LEU:O	2.14	0.47
1:B:329:TYR:O	1:B:333:ASN:ND2	2.48	0.47
1:A:337:ARG:NE	1:A:408:ASP:OD2	2.48	0.47
1:A:104:ASP:OD2	1:A:107:LEU:CD1	2.63	0.46
1:A:180:SER:CB	1:A:223:LEU:O	2.63	0.46
1:A:451:GLY:O	1:A:455:GLN:NE2	2.48	0.46
1:B:347:ALA:HB1	1:B:421:GLY:HA3	1.98	0.46
1:B:423:CYS:HB3	1:B:497:SER:HB2	1.97	0.46
1:B:345:ASP:OD1	1:B:417:ARG:NH2	2.49	0.46
1:A:439:ALA:HB1	1:A:518:LYS:HG2	1.98	0.46
1:B:203:LYS:C	1:B:205:ASN:H	2.18	0.46
1:B:132:SER:OG	1:B:152:THR:HG23	2.16	0.45
1:B:321:TYR:O	1:B:325:TYR:HD2	1.99	0.45
1:B:178:ALA:O	1:B:179:LEU:HD23	2.16	0.45
1:B:247:PRO:HA	1:B:258:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HA	1:A:145:LEU:CD1	2.47	0.45
1:B:420:ASP:HA	1:B:500:MET:HG3	1.98	0.45
1:A:347:ALA:HB1	1:A:421:GLY:HA3	1.98	0.45
1:B:175:VAL:O	1:B:234:ARG:NH2	2.49	0.45
1:A:515:SER:O	1:A:519:LEU:HD23	2.17	0.45
1:B:280:MET:SD	1:B:321:TYR:HD2	2.40	0.44
1:A:346:THR:HG22	1:A:366:PHE:CZ	2.53	0.44
1:B:208:ARG:NH2	1:B:212:THR:O	2.51	0.44
1:A:73:PRO:HA	1:A:74:PRO:HD3	1.93	0.43
1:A:104:ASP:OD2	1:A:107:LEU:HD13	2.18	0.43
1:A:265:LEU:O	1:A:269:LEU:HD12	2.18	0.43
1:A:142:ILE:O	1:A:154:LEU:HA	2.18	0.43
1:B:18:ILE:O	1:B:22:VAL:HG23	2.18	0.43
1:A:321:TYR:N	1:A:322:PRO:HD2	2.33	0.43
1:A:365:GLU:O	1:A:369:VAL:HG13	2.19	0.43
1:B:168:GLN:HG3	1:B:234:ARG:HH11	1.84	0.43
1:B:270:TYR:OH	1:B:306:LYS:HE3	2.18	0.43
1:B:407:GLN:HA	1:B:453:VAL:HG21	2.01	0.43
1:A:178:ALA:HB2	1:A:187:VAL:HG13	2.00	0.43
1:A:374:ILE:HB	1:A:375:PRO:HD3	2.00	0.42
1:B:121:LYS:HD3	1:B:210:GLY:HA2	2.00	0.42
1:A:461:SER:HB3	1:A:501:LYS:HD2	2.01	0.42
1:B:151:GLY:O	1:B:152:THR:HG22	2.20	0.42
1:B:203:LYS:C	1:B:205:ASN:N	2.73	0.42
1:B:365:GLU:O	1:B:369:VAL:HG13	2.19	0.42
1:A:220:ARG:HB2	1:A:354:ASN:HD22	1.84	0.42
1:B:142:ILE:HA	1:B:147:SER:OG	2.20	0.42
1:B:513:ASN:O	1:B:516:ALA:N	2.47	0.42
1:B:406:LEU:HA	1:B:449:PHE:CE2	2.55	0.41
1:B:142:ILE:HA	1:B:147:SER:CB	2.51	0.41
1:B:176:HIS:CD2	1:B:237:GLU:OE2	2.73	0.41
1:A:308:ILE:HG22	1:A:312:LYS:HD2	2.03	0.41
1:A:455:GLN:HE21	1:A:455:GLN:CA	2.34	0.41
1:B:336:VAL:HG22	1:B:377:LEU:HD22	2.02	0.41
1:A:320:ILE:HG23	1:A:346:THR:HG23	2.03	0.41
1:B:412:PHE:CE2	1:B:416:LEU:HD11	2.56	0.41
1:A:268:LEU:HD11	1:A:272:LEU:HD11	2.02	0.41
1:B:137:LYS:HD2	1:B:200:TRP:CZ2	2.56	0.41
1:B:321:TYR:CZ	2:B:601:KTQ:C11	3.04	0.41
1:B:37:VAL:HA	1:B:145:LEU:HD12	2.01	0.41
1:A:87:ILE:O	1:A:90:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:SER:O	1:B:160:ALA:HB3	2.21	0.40
1:B:181:GLU:HG3	1:B:225:LEU:HD21	2.02	0.40
1:A:436:VAL:HG22	1:A:437:GLY:N	2.37	0.40
1:B:44:GLY:HA3	1:B:146:PHE:HB3	2.03	0.40
1:B:503:MET:O	1:B:507:LEU:HG	2.22	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	460/526 (88%)	403 (88%)	47 (10%)	10 (2%)	6 29
1	B	455/526 (86%)	412 (90%)	39 (9%)	4 (1%)	17 52
All	All	915/1052 (87%)	815 (89%)	86 (9%)	14 (2%)	10 39

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	VAL
1	B	111	GLU
1	A	139	ARG
1	A	204	GLY
1	B	225	LEU
1	A	241	MET
1	A	385	LEU
1	B	204	GLY
1	B	205	ASN
1	A	86	SER
1	A	190	PRO
1	A	205	ASN
1	A	386	GLU

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Mol	Chain	Res	Type
1	A	109	PRO

5.3.2 Protein sidechains

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	383/435 (88%)	356 (93%)	27 (7%)	15 45
1	B	378/435 (87%)	344 (91%)	34 (9%)	9 34
All	All	761/870 (88%)	700 (92%)	61 (8%)	12 40

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	16	ARG
1	A	31	ARG
1	A	54	ARG
1	A	86	SER
1	A	87	ILE
1	A	116	SER
1	A	190	PRO
1	A	191	ASN
1	A	195	THR
1	A	212	THR
1	A	213	VAL
1	A	248	SER
1	A	256	LEU
1	A	278	TYR
1	A	301	LEU
1	A	337	ARG
1	A	369	VAL
1	A	377	LEU
1	A	379	LYS
1	A	431	THR
1	A	436	VAL

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Mol	Chain	Res	Type
1	A	455	GLN
1	A	464	VAL
1	A	494	THR
1	A	503	MET
1	A	508	VAL
1	B	6	LYS
1	B	17	SER
1	B	31	ARG
1	B	54	ARG
1	B	77	LEU
1	B	98	GLN
1	B	111	GLU
1	B	116	SER
1	B	144	SER
1	B	152	THR
1	B	213	VAL
1	B	231	ARG
1	B	253	THR
1	B	256	LEU
1	B	260	GLN
1	B	278	TYR
1	B	291	LEU
1	B	301	LEU
1	B	318	GLU
1	B	337	ARG
1	B	346	THR
1	B	369	VAL
1	B	377	LEU
1	B	379	LYS
1	B	383	SER
1	B	384	LEU
1	B	385	LEU
1	B	410	GLU
1	B	424	LYS
1	B	448	ARG
1	B	460	VAL
1	B	492	VAL
1	B	507	LEU
1	B	519	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	176	HIS
1	A	263	GLN
1	A	274	HIS
1	A	333	ASN
1	A	354	ASN
1	A	455	GLN
1	B	168	GLN
1	B	176	HIS
1	B	376	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

1 ligand is modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	468/526 (88%)	-0.41	3 (0%)	89	78	16, 31, 57, 93	0
1	B	463/526 (88%)	-0.37	1 (0%)	95	90	20, 31, 58, 79	0
All	All	931/1052 (88%)	-0.39	4 (0%)	92	84	16, 31, 58, 93	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	461	SER	4.3
1	A	462	GLY	2.5
1	B	511	LYS	2.3
1	A	463	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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
2	KTQ	B	601	29/29	0.81	0.41	77,100,120,123	0

6.5 Other polymers (i)

There are no such residues in this entry.