



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:47 am BST

PDB ID : 4EYU
Title : The free structure of the mouse C-terminal domain of KDM6B
Authors : Cheng, Z.J.; Patel, D.J.
Deposited on : 2012-05-01
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 ⓘ 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 : 2.11
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) : 2.11

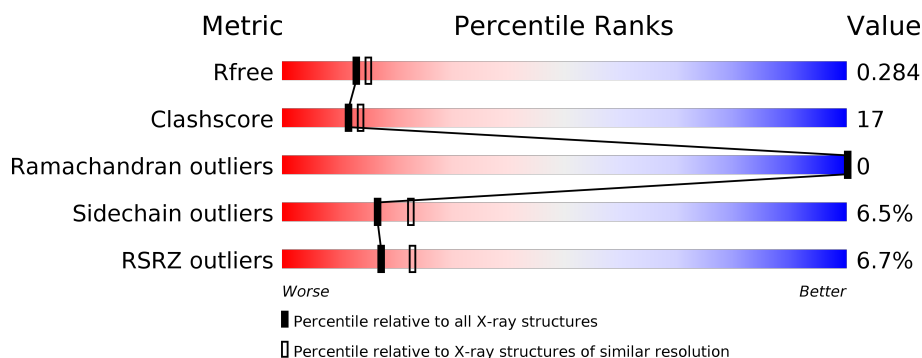
1 Overall quality at a glance

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 on 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 $\leq 5\%$. 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	486	<div> <div>7%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>• 6%</div> </div> </div>
1	B	486	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>26%</div> <div>• 7%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7525 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 Lysine-specific demethylase 6B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	1	0
			3676	2341	638	678	19			
1	B	453	Total	C	N	O	S	0	1	0
			3647	2325	634	669	19			

There are 52 discrepancies between the modelled and reference sequences:

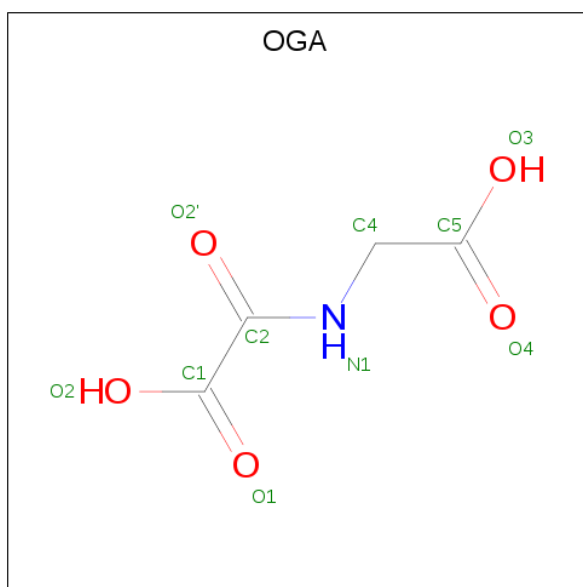
Chain	Residue	Modelled	Actual	Comment	Reference
A	1296	LEU	-	SEE REMARK 999	UNP Q5NCY0
A	1297	GLU	-	SEE REMARK 999	UNP Q5NCY0
A	1298	VAL	-	SEE REMARK 999	UNP Q5NCY0
A	1299	LEU	-	SEE REMARK 999	UNP Q5NCY0
A	1300	PHE	-	SEE REMARK 999	UNP Q5NCY0
A	1301	GLN	-	SEE REMARK 999	UNP Q5NCY0
A	1303	GLY	-	SEE REMARK 999	UNP Q5NCY0
A	1304	PRO	-	SEE REMARK 999	UNP Q5NCY0
A	1305	THR	-	SEE REMARK 999	UNP Q5NCY0
A	1306	LYS	-	SEE REMARK 999	UNP Q5NCY0
A	1307	ALA	-	SEE REMARK 999	UNP Q5NCY0
A	1308	ALA	-	SEE REMARK 999	UNP Q5NCY0
A	1309	ARG	-	SEE REMARK 999	UNP Q5NCY0
A	1310	LYS	-	SEE REMARK 999	UNP Q5NCY0
A	1311	SER	-	SEE REMARK 999	UNP Q5NCY0
A	1312	ALA	-	SEE REMARK 999	UNP Q5NCY0
A	1313	PRO	-	SEE REMARK 999	UNP Q5NCY0
A	1314	ALA	-	SEE REMARK 999	UNP Q5NCY0
A	1315	THR	-	SEE REMARK 999	UNP Q5NCY0
A	1316	GLY	-	SEE REMARK 999	UNP Q5NCY0
A	1317	GLY	-	SEE REMARK 999	UNP Q5NCY0
A	1318	GLY	-	SEE REMARK 999	UNP Q5NCY0
A	1319	SER	-	SEE REMARK 999	UNP Q5NCY0
A	1320	SER	-	SEE REMARK 999	UNP Q5NCY0
A	1321	GLY	-	SEE REMARK 999	UNP Q5NCY0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1322	SER	-	SEE REMARK 999	UNP Q5NCY0
B	1296	LEU	-	SEE REMARK 999	UNP Q5NCY0
B	1297	GLU	-	SEE REMARK 999	UNP Q5NCY0
B	1298	VAL	-	SEE REMARK 999	UNP Q5NCY0
B	1299	LEU	-	SEE REMARK 999	UNP Q5NCY0
B	1300	PHE	-	SEE REMARK 999	UNP Q5NCY0
B	1302	GLN	-	SEE REMARK 999	UNP Q5NCY0
B	1303	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1304	PRO	-	SEE REMARK 999	UNP Q5NCY0
B	1305	THR	-	SEE REMARK 999	UNP Q5NCY0
B	1306	LYS	-	SEE REMARK 999	UNP Q5NCY0
B	1307	ALA	-	SEE REMARK 999	UNP Q5NCY0
B	1308	ALA	-	SEE REMARK 999	UNP Q5NCY0
B	1309	ARG	-	SEE REMARK 999	UNP Q5NCY0
B	1310	LYS	-	SEE REMARK 999	UNP Q5NCY0
B	1311	SER	-	SEE REMARK 999	UNP Q5NCY0
B	1312	ALA	-	SEE REMARK 999	UNP Q5NCY0
B	1313	PRO	-	SEE REMARK 999	UNP Q5NCY0
B	1314	ALA	-	SEE REMARK 999	UNP Q5NCY0
B	1315	THR	-	SEE REMARK 999	UNP Q5NCY0
B	1316	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1317	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1318	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1319	SER	-	SEE REMARK 999	UNP Q5NCY0
B	1320	SER	-	SEE REMARK 999	UNP Q5NCY0
B	1321	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1322	SER	-	SEE REMARK 999	UNP Q5NCY0

- Molecule 2 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: C₄H₅NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	4	1	5		
2	B	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total	O	0	0
			88	88		

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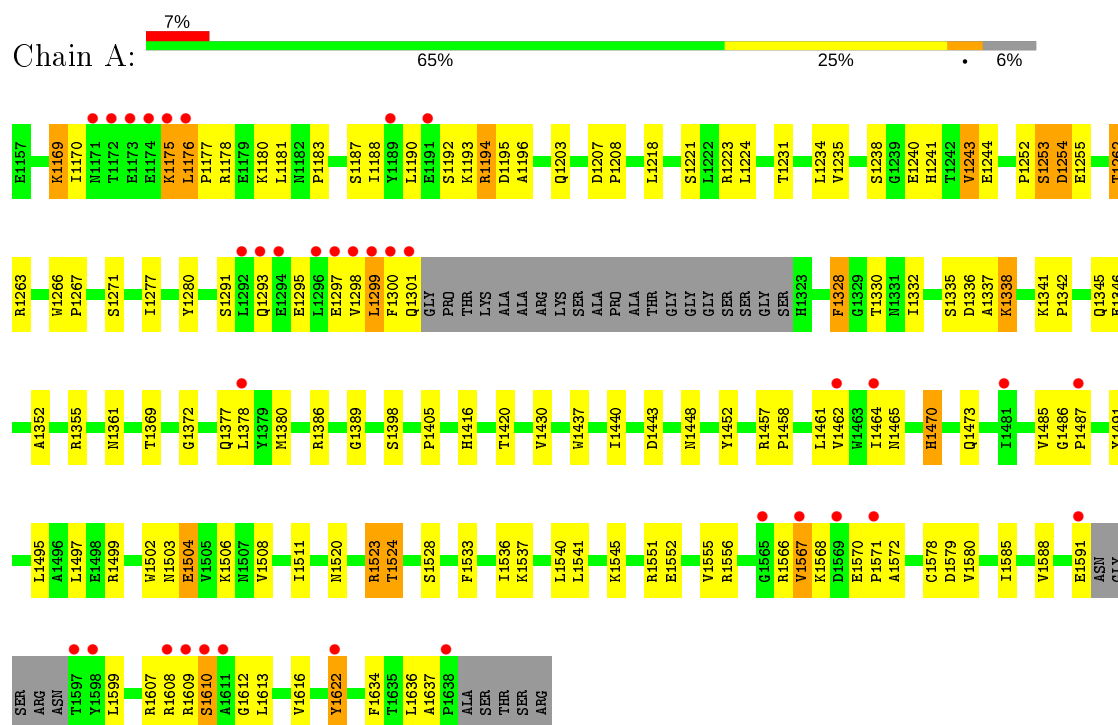
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	90	Total	O	0	0
			90	90		

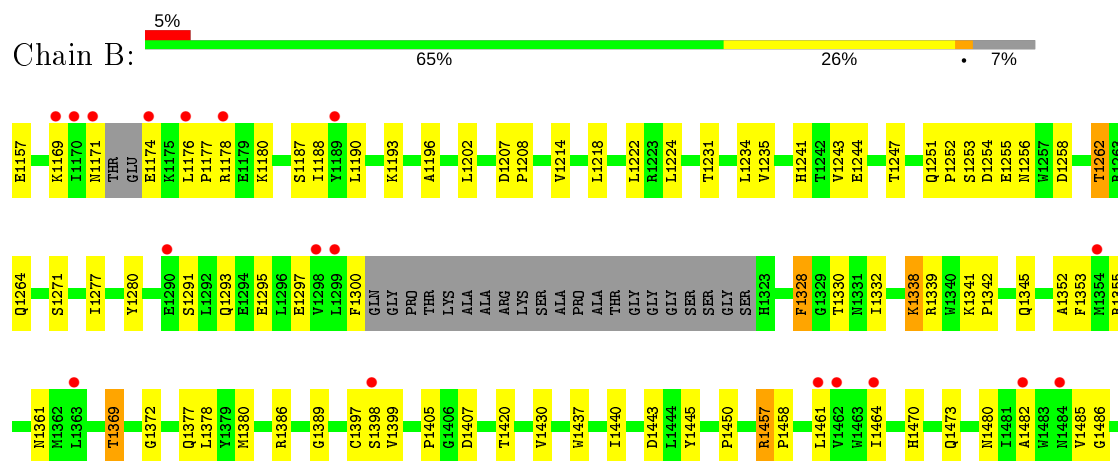
3 Residue-property plots

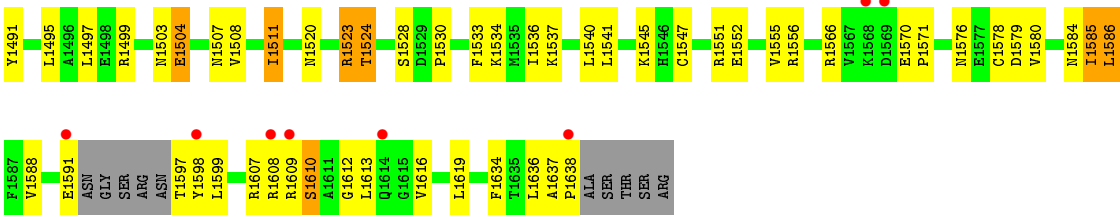
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Lysine-specific demethylase 6B



• Molecule 1: Lysine-specific demethylase 6B





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.98 Å 102.28 Å 145.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.45 – 2.30 38.45 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.45-2.30) 82.0 (38.45-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.08 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.230 , 0.268 0.257 , 0.284	Depositor DCC
R_{free} test set	2781 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	1.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7525	wwPDB-VP
Average B, all atoms (Å ²)	60.0	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 49.39 % 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 7.5095e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NI, ZN, OGA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/3775	0.49	0/5137
1	B	0.30	0/3745	0.50	0/5095
All	All	0.30	0/7520	0.50	0/10232

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	3676	0	3592	131	0
1	B	3647	0	3566	125	0
2	A	10	0	3	0	0
2	B	10	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	88	0	0	4	0
5	B	90	0	0	4	0
All	All	7525	0	7164	252	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 17.

All (252) 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:A:1336:ASP:OD1	1:A:1338:LYS:HE3	1.39	1.18
1:B:1338:LYS:HB2	1:B:1338:LYS:HZ2	1.03	1.07
1:A:1336:ASP:CG	1:A:1338:LYS:HE3	1.77	1.05
1:A:1238:SER:OG	1:A:1241:HIS:HB2	1.58	1.02
1:B:1585:ILE:HA	1:B:1619:LEU:O	1.62	1.00
1:A:1300:PHE:HB3	1:A:1301:GLN:OE1	1.62	0.99
1:B:1520:ASN:O	1:B:1524:THR:HG23	1.63	0.98
1:A:1520:ASN:O	1:A:1524:THR:HG23	1.65	0.97
1:B:1338:LYS:HB2	1:B:1338:LYS:NZ	1.62	0.97
1:B:1612:GLY:O	1:B:1613:LEU:HB2	1.66	0.95
1:A:1566:ARG:HG2	1:A:1570:GLU:OE1	1.70	0.92
1:B:1300:PHE:CD2	1:B:1300:PHE:O	2.30	0.85
1:A:1336:ASP:OD1	1:A:1338:LYS:CE	2.24	0.84
1:B:1585:ILE:HG22	1:B:1619:LEU:O	1.78	0.83
1:B:1280:TYR:CD2	1:B:1380:MET:HE2	2.13	0.82
1:A:1567:VAL:HG23	1:A:1570:GLU:CG	2.09	0.81
1:A:1280:TYR:HD2	1:A:1380:MET:CE	1.93	0.81
1:A:1194:ARG:NH1	1:B:1576:ASN:O	2.14	0.81
1:A:1280:TYR:HD2	1:A:1380:MET:HE1	1.46	0.80
1:A:1336:ASP:OD1	1:A:1338:LYS:HG2	1.81	0.80
1:A:1262:THR:HG22	1:A:1263:ARG:HB2	1.63	0.80
1:A:1295:GLU:HA	1:A:1295:GLU:OE1	1.81	0.80
1:B:1597:THR:HG22	1:B:1598:TYR:H	1.46	0.80
1:B:1280:TYR:HD2	1:B:1380:MET:HE2	1.47	0.80
1:A:1176:LEU:HB2	1:A:1448:ASN:OD1	1.83	0.79
1:B:1566:ARG:NH2	1:B:1570:GLU:O	2.16	0.78
1:B:1597:THR:HG22	1:B:1598:TYR:N	1.98	0.78
1:B:1607:ARG:HH11	1:B:1607:ARG:HG2	1.48	0.77
1:B:1300:PHE:HD2	1:B:1300:PHE:O	1.66	0.77
1:A:1280:TYR:CD2	1:A:1380:MET:HE1	2.21	0.76
1:A:1193:LYS:HD2	1:A:1221:SER:O	1.85	0.76
1:A:1607:ARG:HH21	1:A:1607:ARG:HG2	1.50	0.76
1:A:1612:GLY:O	1:A:1613:LEU:HB2	1.86	0.76
1:A:1218:LEU:HD22	1:A:1461:LEU:HD13	1.69	0.75
1:B:1218:LEU:CD2	1:B:1461:LEU:HD13	2.17	0.75
1:B:1585:ILE:CA	1:B:1619:LEU:O	2.36	0.74
1:B:1293:GLN:O	1:B:1297:GLU:HG2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1252:PRO:O	1:B:1386:ARG:NH2	2.20	0.73
1:B:1222:LEU:HB2	1:B:1224:LEU:CD1	2.18	0.73
1:A:1252:PRO:O	1:A:1386:ARG:NH2	2.21	0.73
1:A:1405:PRO:O	1:A:1458:PRO:HG3	1.89	0.72
1:B:1218:LEU:HD22	1:B:1461:LEU:HD13	1.68	0.72
1:A:1231:THR:O	1:A:1235:VAL:HG23	1.89	0.72
1:A:1613:LEU:O	1:A:1616:VAL:HB	1.90	0.71
1:A:1567:VAL:HG23	1:A:1570:GLU:HB2	1.73	0.71
1:A:1177:PRO:CG	1:A:1180:LYS:HE3	2.21	0.70
1:A:1567:VAL:HG23	1:A:1570:GLU:HG3	1.71	0.70
1:B:1613:LEU:O	1:B:1616:VAL:HB	1.90	0.70
1:A:1300:PHE:C	1:A:1301:GLN:OE1	2.30	0.69
1:B:1280:TYR:HD2	1:B:1380:MET:CE	2.04	0.69
1:A:1234:LEU:HD13	1:A:1378:LEU:HD21	1.75	0.68
1:B:1177:PRO:HD2	1:B:1180:LYS:HG3	1.76	0.68
1:B:1338:LYS:NZ	1:B:1338:LYS:CB	2.43	0.67
1:A:1352:ALA:HA	1:A:1355:ARG:HE	1.59	0.66
1:B:1352:ALA:HA	1:B:1355:ARG:HE	1.59	0.66
1:B:1570:GLU:HG2	1:B:1571:PRO:HD2	1.77	0.66
1:B:1591:GLU:CD	1:B:1599:LEU:HD21	2.16	0.65
1:A:1244:GLU:O	1:A:1330:THR:HG22	1.96	0.65
1:A:1254:ASP:N	1:A:1254:ASP:OD1	2.29	0.65
1:A:1567:VAL:HG23	1:A:1570:GLU:CB	2.26	0.65
1:B:1597:THR:CG2	1:B:1598:TYR:H	2.09	0.65
1:A:1398:SER:HB3	1:A:1464:ILE:HD13	1.79	0.65
1:B:1231:THR:O	1:B:1235:VAL:HG23	1.97	0.64
1:B:1407:ASP:OD1	1:B:1457:ARG:HG3	1.98	0.64
1:B:1511:ILE:HD12	5:B:1818:HOH:O	1.96	0.64
1:B:1171:ASN:ND2	1:B:1174:GLU:HB2	2.13	0.64
1:A:1556:ARG:HG3	1:A:1556:ARG:O	1.98	0.64
1:A:1457:ARG:HB3	1:A:1458:PRO:HD2	1.79	0.64
1:B:1218:LEU:CD2	1:B:1461:LEU:CD1	2.76	0.64
1:A:1280:TYR:CD2	1:A:1380:MET:CE	2.78	0.63
1:B:1607:ARG:NH1	1:B:1613:LEU:HG	2.13	0.63
1:B:1503:ASN:HB3	1:B:1508:VAL:O	1.98	0.63
1:B:1398:SER:HB3	1:B:1464:ILE:HD13	1.81	0.62
1:A:1218:LEU:CD2	1:A:1461:LEU:HD13	2.28	0.62
1:B:1637:ALA:HB1	1:B:1638:PRO:HD2	1.80	0.62
1:B:1504:GLU:HA	1:B:1504:GLU:OE2	1.99	0.61
1:B:1338:LYS:HD3	1:B:1338:LYS:C	2.19	0.61
1:A:1503:ASN:HB3	1:A:1508:VAL:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1591:GLU:CD	1:A:1599:LEU:HD11	2.21	0.60
1:A:1504:GLU:HA	1:A:1504:GLU:OE2	2.00	0.60
1:B:1338:LYS:HG3	1:B:1339:ARG:N	2.16	0.60
1:A:1175:LYS:HD2	1:A:1176:LEU:H	1.67	0.60
1:A:1335:SER:HA	5:A:1839:HOH:O	2.02	0.60
1:A:1567:VAL:CG2	1:A:1570:GLU:HG3	2.32	0.60
1:A:1607:ARG:O	1:A:1610:SER:O	2.20	0.59
1:B:1251:GLN:OE1	1:B:1256:ASN:HA	2.02	0.59
1:B:1234:LEU:HD13	1:B:1378:LEU:HD21	1.84	0.59
1:A:1291:SER:O	1:A:1295:GLU:HG2	2.03	0.59
1:A:1300:PHE:CB	1:A:1301:GLN:OE1	2.46	0.59
1:B:1338:LYS:C	1:B:1338:LYS:CD	2.72	0.58
1:A:1541:LEU:HG	1:A:1545:LYS:HE3	1.85	0.58
1:A:1567:VAL:O	1:A:1570:GLU:HB2	2.02	0.58
1:B:1504:GLU:OE1	1:B:1580:VAL:HG23	2.02	0.58
1:B:1556:ARG:O	1:B:1556:ARG:HG3	2.04	0.58
1:B:1244:GLU:O	1:B:1330:THR:HG22	2.03	0.58
1:B:1541:LEU:HG	1:B:1545:LYS:HE3	1.85	0.58
1:A:1253:SER:HA	1:A:1473:GLN:OE1	2.04	0.58
1:B:1607:ARG:NH1	1:B:1607:ARG:HG2	2.17	0.58
1:A:1293:GLN:O	1:A:1297:GLU:HG2	2.04	0.58
1:A:1523:ARG:O	1:A:1523:ARG:HG3	2.03	0.58
1:A:1405:PRO:O	1:A:1458:PRO:CG	2.52	0.57
1:B:1291:SER:O	1:B:1295:GLU:HG2	2.04	0.57
1:B:1585:ILE:CG2	1:B:1619:LEU:O	2.49	0.57
1:B:1171:ASN:CG	1:B:1174:GLU:HB2	2.25	0.57
1:A:1193:LYS:HG3	1:B:1578:CYS:HA	1.86	0.57
1:B:1241:HIS:HB3	1:B:1277:ILE:HD12	1.87	0.56
1:A:1372:GLY:HA2	1:A:1377:GLN:CG	2.35	0.56
1:B:1372:GLY:HA2	1:B:1377:GLN:CG	2.35	0.56
1:A:1457:ARG:HB3	1:A:1458:PRO:CD	2.36	0.56
1:A:1607:ARG:NH2	1:A:1607:ARG:HG2	2.19	0.56
1:A:1218:LEU:CD2	1:A:1461:LEU:CD1	2.84	0.55
1:A:1336:ASP:C	1:A:1336:ASP:OD1	2.44	0.55
1:A:1461:LEU:C	1:A:1461:LEU:HD23	2.28	0.55
1:A:1241:HIS:HB3	1:A:1277:ILE:HD12	1.89	0.55
1:A:1190:LEU:HD13	1:A:1196:ALA:HB2	1.87	0.54
1:B:1361:ASN:HA	1:B:1486:GLY:O	2.07	0.54
1:B:1551:ARG:O	1:B:1555:VAL:HG23	2.08	0.54
1:B:1585:ILE:H	1:B:1585:ILE:HD13	1.73	0.54
1:A:1504:GLU:OE1	1:A:1580:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1170:ILE:HB	1:A:1416:HIS:CD2	2.42	0.54
1:B:1377:GLN:NE2	5:B:1833:HOH:O	2.31	0.53
1:B:1253:SER:HA	1:B:1473:GLN:OE1	2.08	0.53
1:A:1551:ARG:O	1:A:1555:VAL:HG23	2.08	0.53
1:A:1588:VAL:HA	1:A:1599:LEU:O	2.07	0.53
1:A:1567:VAL:CG2	1:A:1570:GLU:CG	2.84	0.53
1:A:1485:VAL:O	1:A:1487:PRO:HD3	2.08	0.53
1:A:1591:GLU:CD	1:A:1599:LEU:CD1	2.78	0.53
1:B:1338:LYS:CG	1:B:1339:ARG:N	2.72	0.53
1:B:1461:LEU:HD23	1:B:1461:LEU:C	2.30	0.53
1:B:1588:VAL:HA	1:B:1599:LEU:O	2.08	0.52
1:A:1499:ARG:NH1	5:A:1806:HOH:O	2.39	0.52
1:B:1591:GLU:HG3	1:B:1599:LEU:HD23	1.92	0.52
1:A:1254:ASP:O	1:A:1255:GLU:HG3	2.11	0.51
1:A:1223:ARG:NH1	1:B:1504:GLU:OE2	2.44	0.51
1:B:1405:PRO:O	1:B:1458:PRO:HG3	2.12	0.51
1:A:1240:GLU:HA	1:A:1240:GLU:OE1	2.11	0.50
1:A:1341:LYS:O	1:A:1345:GLN:HG3	2.10	0.50
1:B:1190:LEU:HD13	1:B:1196:ALA:HB2	1.92	0.50
1:B:1520:ASN:OD1	1:B:1523:ARG:NH1	2.42	0.50
1:B:1247:THR:HB	1:B:1271:SER:OG	2.11	0.50
1:B:1241:HIS:HB3	1:B:1277:ILE:CD1	2.42	0.50
1:A:1536:ILE:O	1:A:1540:LEU:HG	2.11	0.49
1:B:1591:GLU:OE2	1:B:1599:LEU:HD21	2.12	0.49
1:B:1389:GLY:HA3	1:B:1437:TRP:CZ3	2.48	0.49
1:A:1266:TRP:HB2	1:A:1267:PRO:HD3	1.95	0.49
1:B:1280:TYR:CD2	1:B:1380:MET:CE	2.87	0.49
1:B:1207:ASP:OD1	1:B:1208:PRO:HD2	2.13	0.49
1:B:1585:ILE:HG22	1:B:1619:LEU:C	2.32	0.49
1:B:1222:LEU:HB2	1:B:1224:LEU:HD13	1.92	0.48
1:A:1177:PRO:HG2	1:A:1180:LYS:HE3	1.94	0.48
1:B:1536:ILE:O	1:B:1540:LEU:HG	2.13	0.48
1:A:1361:ASN:HA	1:A:1486:GLY:O	2.12	0.48
1:B:1578:CYS:O	1:B:1579:ASP:HB2	2.13	0.48
1:B:1341:LYS:O	1:B:1345:GLN:HG3	2.13	0.48
1:B:1341:LYS:HB3	1:B:1342:PRO:HD3	1.95	0.48
1:B:1372:GLY:HA2	1:B:1377:GLN:HG3	1.94	0.48
1:A:1177:PRO:CD	1:A:1180:LYS:HE3	2.44	0.48
1:A:1346:GLU:OE2	5:A:1821:HOH:O	2.20	0.48
1:A:1440:ILE:O	1:A:1443:ASP:HB2	2.14	0.47
1:A:1607:ARG:NH2	1:A:1613:LEU:HG	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1372:GLY:HA2	1:A:1377:GLN:HG3	1.95	0.47
1:A:1533:PHE:CZ	1:A:1537:LYS:HD3	2.50	0.47
1:A:1578:CYS:O	1:A:1579:ASP:HB2	2.14	0.47
1:A:1169:LYS:HG2	1:A:1169:LYS:H	1.54	0.47
1:A:1389:GLY:HA3	1:A:1437:TRP:CZ3	2.50	0.47
1:B:1584:ASN:O	1:B:1586:LEU:CD2	2.63	0.47
1:B:1607:ARG:HA	1:B:1610:SER:O	2.14	0.47
1:A:1262:THR:HG22	1:A:1263:ARG:N	2.29	0.47
1:A:1341:LYS:HB3	1:A:1342:PRO:HD3	1.96	0.47
1:B:1533:PHE:CZ	1:B:1537:LYS:HD3	2.50	0.47
1:A:1178:ARG:O	1:A:1181:LEU:HB2	2.15	0.46
1:A:1566:ARG:CG	1:A:1570:GLU:OE1	2.54	0.46
1:B:1440:ILE:O	1:B:1443:ASP:HB2	2.15	0.46
1:A:1523:ARG:HG2	1:A:1524:THR:HG22	1.96	0.46
1:B:1338:LYS:HG3	1:B:1339:ARG:H	1.81	0.46
1:A:1566:ARG:HE	1:A:1622:TYR:HE1	1.64	0.46
1:B:1180:LYS:O	1:B:1450:PRO:HB3	2.16	0.46
1:B:1566:ARG:HD2	1:B:1570:GLU:OE1	2.16	0.46
1:A:1341:LYS:HB3	1:A:1342:PRO:CD	2.46	0.46
1:B:1341:LYS:HB3	1:B:1342:PRO:CD	2.46	0.46
1:B:1254:ASP:OD1	1:B:1254:ASP:N	2.33	0.46
1:B:1258:ASP:OD2	1:B:1262:THR:OG1	2.30	0.46
1:A:1591:GLU:OE2	1:A:1599:LEU:CD1	2.64	0.46
1:A:1243:VAL:HB	1:A:1332:ILE:HG12	1.98	0.46
1:A:1187:SER:O	1:A:1188:ILE:HD13	2.16	0.45
1:A:1528:SER:HA	1:A:1637:ALA:O	2.15	0.45
1:A:1572:ALA:HB1	5:A:1824:HOH:O	2.16	0.45
1:A:1299:LEU:HD22	1:A:1299:LEU:HA	1.78	0.45
1:B:1255:GLU:HG2	1:B:1264:GLN:HE21	1.82	0.45
1:B:1178:ARG:HH22	1:B:1445:TYR:HB3	1.82	0.44
1:B:1328:PHE:C	1:B:1328:PHE:CD1	2.90	0.44
1:A:1461:LEU:HD23	1:A:1462:VAL:N	2.32	0.44
1:B:1243:VAL:HB	1:B:1332:ILE:HG12	2.00	0.44
1:A:1280:TYR:CD2	1:A:1380:MET:HE2	2.52	0.44
1:B:1523:ARG:HG3	1:B:1524:THR:HG22	1.98	0.44
1:A:1298:VAL:O	1:A:1301:GLN:O	2.35	0.44
1:A:1328:PHE:C	1:A:1328:PHE:CD1	2.91	0.44
1:B:1497:LEU:HA	1:B:1497:LEU:HD12	1.75	0.44
1:B:1547:CYS:SG	1:B:1584:ASN:ND2	2.79	0.44
1:A:1591:GLU:HG3	1:A:1599:LEU:CD1	2.47	0.43
1:A:1491:TYR:CZ	1:A:1495:LEU:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:TYR:HD2	1:A:1380:MET:HE2	1.78	0.43
1:B:1338:LYS:HD3	1:B:1339:ARG:N	2.33	0.43
1:B:1591:GLU:CD	1:B:1599:LEU:CD2	2.86	0.43
1:A:1497:LEU:HA	1:A:1497:LEU:HD12	1.74	0.43
1:B:1171:ASN:OD1	1:B:1171:ASN:O	2.37	0.43
1:B:1528:SER:O	1:B:1636:LEU:HD11	2.18	0.43
1:B:1523:ARG:O	1:B:1523:ARG:HG3	2.18	0.43
1:A:1234:LEU:HD13	1:A:1378:LEU:CD2	2.47	0.43
1:A:1238:SER:OG	1:A:1241:HIS:CB	2.48	0.43
1:B:1218:LEU:HD23	1:B:1461:LEU:HD12	2.01	0.43
1:A:1338:LYS:H	1:A:1338:LYS:CE	2.31	0.43
1:A:1470:HIS:N	1:A:1470:HIS:ND1	2.67	0.43
1:A:1183:PRO:HB2	1:A:1452:TYR:CE2	2.54	0.42
1:B:1499:ARG:NH1	5:B:1809:HOH:O	2.47	0.42
1:B:1584:ASN:HB3	1:B:1585:ILE:H	1.63	0.42
1:B:1187:SER:O	1:B:1188:ILE:HD13	2.19	0.42
1:A:1176:LEU:HA	1:A:1176:LEU:HD12	1.80	0.42
1:A:1502:TRP:CZ2	1:A:1506:LYS:HE3	2.55	0.42
1:B:1397:CYS:HB2	1:B:1485:VAL:O	2.20	0.42
1:B:1511:ILE:CD1	5:B:1818:HOH:O	2.62	0.42
1:B:1234:LEU:CD1	1:B:1378:LEU:HD21	2.50	0.42
1:B:1504:GLU:CA	1:B:1504:GLU:OE2	2.65	0.42
1:B:1537:LYS:HD2	1:B:1634:PHE:HD2	1.85	0.42
1:A:1218:LEU:HD22	1:A:1461:LEU:CD1	2.44	0.42
1:A:1537:LYS:HD2	1:A:1634:PHE:HD2	1.85	0.42
1:B:1491:TYR:CZ	1:B:1495:LEU:HD11	2.55	0.41
1:B:1541:LEU:O	1:B:1545:LYS:HG3	2.20	0.41
1:B:1591:GLU:HG3	1:B:1599:LEU:CD2	2.51	0.41
1:B:1202:LEU:HD13	1:B:1353:PHE:CG	2.55	0.41
1:A:1175:LYS:HD2	1:A:1176:LEU:N	2.34	0.41
1:A:1607:ARG:NH2	1:A:1607:ARG:CG	2.80	0.41
1:A:1528:SER:O	1:A:1636:LEU:HD11	2.20	0.41
1:B:1188:ILE:HA	1:B:1188:ILE:HD13	1.83	0.41
1:A:1541:LEU:O	1:A:1545:LYS:HG3	2.21	0.41
1:A:1570:GLU:HG2	1:A:1571:PRO:HD2	2.01	0.41
1:B:1369:THR:O	1:B:1369:THR:HG22	2.19	0.41
1:A:1504:GLU:CA	1:A:1504:GLU:OE2	2.66	0.41
1:A:1537:LYS:HD2	1:A:1634:PHE:CD2	2.55	0.41
1:A:1193:LYS:HE3	1:B:1507:ASN:OD1	2.21	0.41
1:A:1192:SER:O	1:A:1195:ASP:HB2	2.20	0.41
1:A:1207:ASP:OD1	1:A:1208:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1337:ALA:O	1:A:1341:LYS:N	2.53	0.41
1:B:1378:LEU:HD12	1:B:1480:ASN:O	2.21	0.41
1:B:1537:LYS:HD2	1:B:1634:PHE:CD2	2.56	0.41
1:B:1218:LEU:HD23	1:B:1461:LEU:CD1	2.51	0.40
1:A:1591:GLU:HG3	1:A:1599:LEU:HD12	2.01	0.40
1:B:1157:GLU:HA	1:B:1157:GLU:OE2	2.22	0.40
1:A:1567:VAL:CG2	1:A:1570:GLU:CD	2.89	0.40
1:B:1530:PRO:O	1:B:1534:LYS:HG3	2.22	0.40
1:A:1207:ASP:O	1:A:1465:ASN:ND2	2.55	0.40
1:B:1399:VAL:O	1:B:1482:ALA:HA	2.20	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	451/486 (93%)	435 (96%)	16 (4%)	0	100	100
1	B	446/486 (92%)	434 (97%)	12 (3%)	0	100	100
All	All	897/972 (92%)	869 (97%)	28 (3%)	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	406/424 (96%)	376 (93%)	30 (7%)	13	17
1	B	402/424 (95%)	380 (94%)	22 (6%)	21	30
All	All	808/848 (95%)	756 (94%)	52 (6%)	17	23

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1169	LYS
1	A	1175	LYS
1	A	1176	LEU
1	A	1194	ARG
1	A	1203	GLN
1	A	1224	LEU
1	A	1243	VAL
1	A	1253	SER
1	A	1254	ASP
1	A	1262	THR
1	A	1271	SER
1	A	1299	LEU
1	A	1328	PHE
1	A	1338	LYS
1	A	1369	THR
1	A	1420	THR
1	A	1430	VAL
1	A	1470	HIS
1	A	1504	GLU
1	A	1511	ILE
1	A	1523	ARG
1	A	1524	THR
1	A	1552	GLU
1	A	1567	VAL
1	A	1568	LYS
1	A	1585	ILE
1	A	1608	ARG
1	A	1609	ARG
1	A	1610	SER
1	A	1622	TYR
1	B	1169	LYS
1	B	1176	LEU
1	B	1193	LYS
1	B	1214	VAL
1	B	1262	THR

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Mol	Chain	Res	Type
1	B	1328	PHE
1	B	1338	LYS
1	B	1369	THR
1	B	1420	THR
1	B	1430	VAL
1	B	1457	ARG
1	B	1470	HIS
1	B	1504	GLU
1	B	1511	ILE
1	B	1523	ARG
1	B	1524	THR
1	B	1552	GLU
1	B	1585	ILE
1	B	1586	LEU
1	B	1608	ARG
1	B	1609	ARG
1	B	1610	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1264	GLN

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	OGA	B	1700	3	3,9,9	0.30	0	4,11,11	1.68	1 (25%)
2	OGA	A	1700	3	3,9,9	0.31	0	4,11,11	1.66	1 (25%)

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	OGA	B	1700	3	-	0/3/9/9	-
2	OGA	A	1700	3	-	0/3/9/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1700	OGA	C1-C2-N1	3.27	118.85	115.60
2	A	1700	OGA	C1-C2-N1	3.24	118.82	115.60

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 [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, 95th 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	456/486 (93%)	0.42	35 (7%) 13 17	26, 56, 90, 117	0
1	B	453/486 (93%)	0.43	26 (5%) 23 30	25, 58, 94, 125	0
All	All	909/972 (93%)	0.43	61 (6%) 17 23	25, 57, 91, 125	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1299	LEU	8.6
1	A	1299	LEU	7.8
1	A	1172	THR	6.8
1	B	1170	ILE	5.8
1	A	1171	ASN	5.3
1	A	1174	GLU	5.2
1	A	1567	VAL	5.1
1	B	1591	GLU	5.0
1	A	1591	GLU	4.9
1	B	1171	ASN	4.9
1	A	1173	GLU	4.8
1	B	1174	GLU	4.8
1	A	1300	PHE	4.8
1	A	1301	GLN	3.8
1	B	1482	ALA	3.7
1	A	1294	GLU	3.6
1	B	1178	ARG	3.5
1	A	1598	TYR	3.5
1	B	1176	LEU	3.4
1	B	1462	VAL	3.4
1	A	1569	ASP	3.4
1	A	1597	THR	3.2
1	B	1568	LYS	3.1
1	B	1169	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1610	SER	3.0
1	A	1611	ALA	2.9
1	A	1638	PRO	2.7
1	A	1298	VAL	2.7
1	A	1175	LYS	2.7
1	B	1598	TYR	2.7
1	A	1571	PRO	2.4
1	A	1292	LEU	2.4
1	A	1296	LEU	2.4
1	A	1608	ARG	2.3
1	A	1565	GLY	2.3
1	A	1189	TYR	2.3
1	A	1464	ILE	2.3
1	A	1481	ILE	2.3
1	A	1622	TYR	2.3
1	B	1464	ILE	2.3
1	B	1363	LEU	2.2
1	B	1608	ARG	2.2
1	B	1354	MET	2.2
1	B	1638	PRO	2.2
1	A	1297	GLU	2.2
1	A	1293	GLN	2.2
1	A	1487	PRO	2.2
1	B	1484	ASN	2.1
1	B	1614	GLN	2.2
1	A	1609	ARG	2.1
1	A	1191	GLU	2.1
1	A	1462	VAL	2.1
1	B	1290	GLU	2.1
1	B	1189	TYR	2.1
1	A	1176	LEU	2.1
1	B	1569	ASP	2.0
1	B	1609	ARG	2.0
1	B	1461	LEU	2.0
1	B	1298	VAL	2.0
1	A	1378	LEU	2.0
1	B	1398	SER	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 [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. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
2	OGA	A	1700	10/10	0.94	0.20	27,44,57,59	0
2	OGA	B	1700	10/10	0.96	0.19	31,44,54,57	0
4	ZN	A	1702	1/1	0.96	0.05	51,51,51,51	0
4	ZN	B	1702	1/1	0.97	0.04	49,49,49,49	0
3	NI	B	1701	1/1	0.97	0.14	36,36,36,36	0
3	NI	A	1701	1/1	0.98	0.11	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.