



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:33 PM UTC

PDB ID : 6XU2 / pdb_00006xu2
Title : Human karyopherin RanBP5 (isoform-3)
Authors : Swale, C.; McCarthy, A.A.; Berger, I.; Bieniossek, C.; Delmas, B.; Ruigrok, R.W.H.; Crepin, T.
Deposited on : 2020-01-17
Resolution : 2.83 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

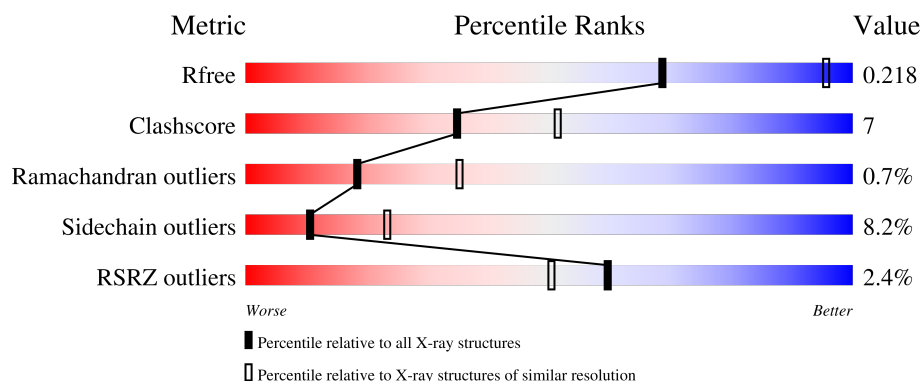
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

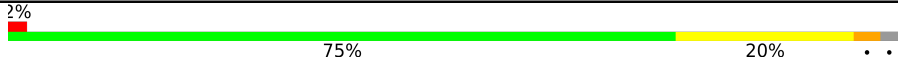
The reported resolution of this entry is 2.83 Å.

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}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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 $\leq 5\%$. 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	1115	 2% 75% 20% . .
2	B	4	 25% 50% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8533 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 Importin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1091	Total	C	N	O	S	0	0	0
			8476	5381	1427	1604	64			

- Molecule 2 is a protein called Antipain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	0	0	0
			42	27	10	5			

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

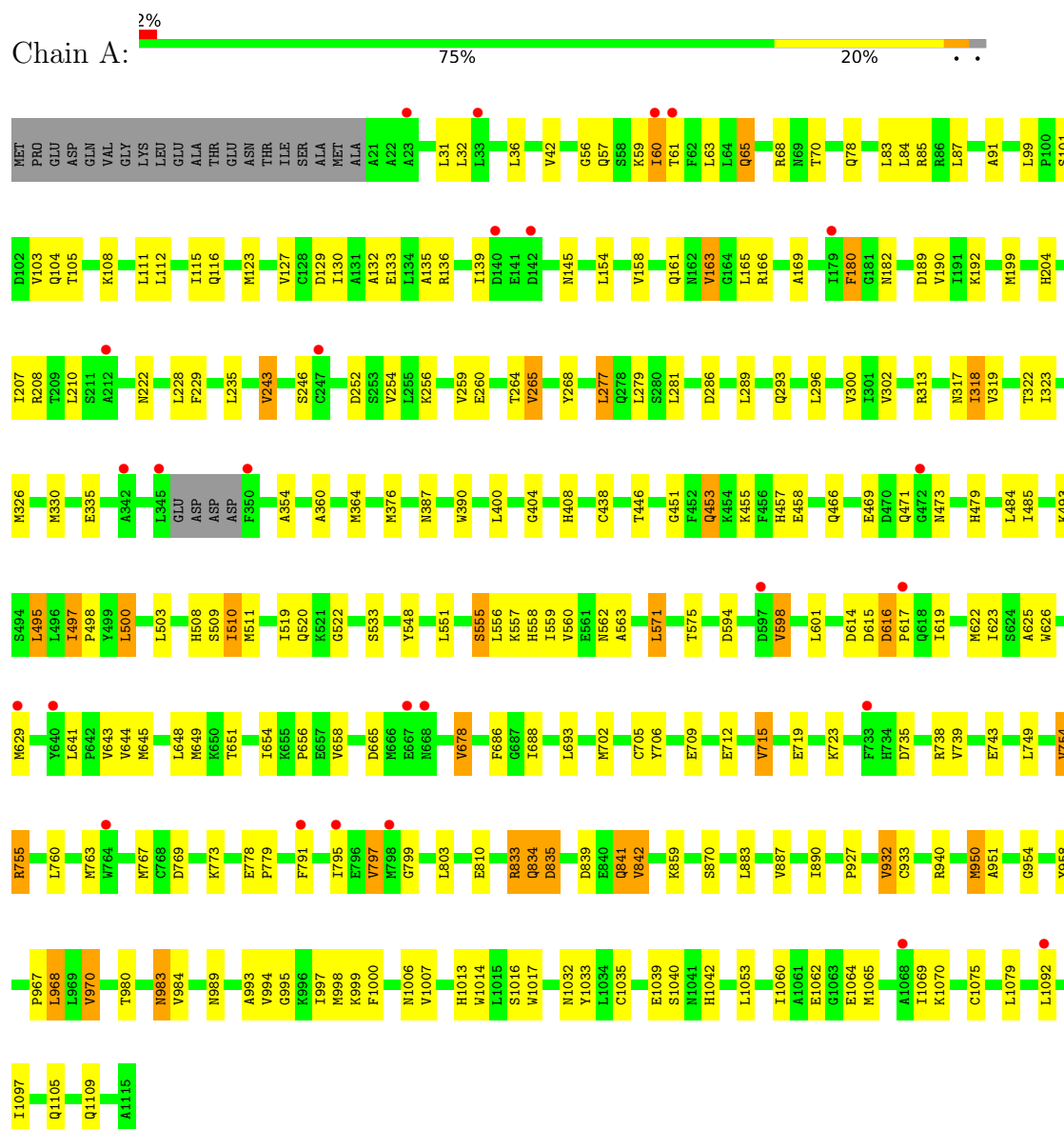
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		

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: Importin-5



• Molecule 2: Antipain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.10Å 126.25Å 149.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.43 – 2.83 96.43 – 2.83	Depositor EDS
% Data completeness (in resolution range)	81.0 (96.43-2.83) 81.0 (96.43-2.83)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.206 , 0.244 0.219 , 0.218	Depositor DCC
R_{free} test set	1867 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å ²)	117.7	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 92.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8533	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: RGL, FC0, NI

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	0.79	1/8641 (0.0%)	1.23	24/11730 (0.2%)
2	B	0.89	0/17	1.93	2/21 (9.5%)
All	All	0.79	1/8658 (0.0%)	1.23	26/11751 (0.2%)

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
2	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	ILE	CG1-CD1	5.15	1.71	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	PHE	CA-CB-CG	7.67	121.47	113.80
1	A	833	ARG	N-CA-C	-7.18	101.05	110.53
1	A	954	GLY	N-CA-C	6.47	120.47	112.64
1	A	387	ASN	CA-CB-CG	6.13	118.73	112.60
1	A	1006	ASN	CA-C-N	5.89	128.83	120.53
1	A	1006	ASN	C-N-CA	5.89	128.83	120.53
1	A	562	ASN	CA-CB-CG	5.86	118.46	112.60
2	B	2	ARG	CA-C-N	5.77	132.09	121.70
2	B	2	ARG	C-N-CA	5.77	132.09	121.70
1	A	797	VAL	CA-C-O	-5.75	115.29	121.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1000	PHE	CA-CB-CG	-5.56	108.24	113.80
1	A	715	VAL	N-CA-C	5.53	116.92	110.62
1	A	135	ALA	CA-C-N	5.51	127.60	120.44
1	A	135	ALA	C-N-CA	5.51	127.60	120.44
1	A	1069	ILE	CA-C-N	5.40	131.85	121.54
1	A	1069	ILE	C-N-CA	5.40	131.85	121.54
1	A	810	GLU	CA-C-N	5.24	127.30	120.28
1	A	810	GLU	C-N-CA	5.24	127.30	120.28
1	A	767	MET	N-CA-C	5.22	116.78	111.14
1	A	1040	SER	N-CA-C	5.18	117.39	110.35
1	A	835	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	493	LYS	CA-C-N	5.07	127.39	120.54
1	A	493	LYS	C-N-CA	5.07	127.39	120.54
1	A	438	CYS	CA-C-N	5.05	127.00	120.44
1	A	438	CYS	C-N-CA	5.05	127.00	120.44
1	A	182	ASN	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	3	VAL	Peptide,Mainchain

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	8476	0	8307	123	0
2	B	42	0	43	3	0
3	A	1	0	0	0	0
4	A	14	0	0	0	0
All	All	8533	0	8350	126	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 7.

All (126) 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:101:SER:HA	1:A:104:GLN:HB2	1.50	0.93
1:A:950:MET:HE3	1:A:958:TYR:HB3	1.66	0.77
1:A:63:LEU:HD21	1:A:83:LEU:HB3	1.70	0.73
1:A:623:ILE:HG22	1:A:702:MET:HG3	1.70	0.73
1:A:166:ARG:HB3	1:A:207:ILE:HD11	1.70	0.72
1:A:105:THR:HA	1:A:108:LYS:HD2	1.71	0.72
1:A:453:GLN:HE21	1:A:453:GLN:H	1.35	0.72
1:A:139:ILE:HA	1:A:145:ASN:HA	1.76	0.65
1:A:115:ILE:HG12	1:A:127:VAL:HG23	1.79	0.64
1:A:980:THR:O	1:A:984:VAL:HG23	1.98	0.64
1:A:890:ILE:HD11	1:A:927:PRO:HB2	1.80	0.63
1:A:951:ALA:HB2	1:A:997:ILE:HD13	1.80	0.63
1:A:998:MET:HE1	1:A:1014:TRP:CG	2.35	0.61
1:A:277:LEU:HB3	1:A:318:ILE:HG12	1.81	0.61
1:A:715:VAL:HG21	1:A:754:VAL:CG1	2.31	0.60
1:A:1062:GLU:HA	1:A:1064:GLU:H	1.65	0.60
1:A:738:ARG:NH1	1:A:778:GLU:OE2	2.34	0.60
1:A:485:ILE:HG12	1:A:533:SER:HA	1.84	0.59
1:A:105:THR:HA	1:A:108:LYS:CD	2.32	0.59
1:A:56:GLY:HA2	1:A:59:LYS:HD2	1.85	0.59
1:A:1032:ASN:OD1	1:A:1075:CYS:HB3	2.04	0.58
1:A:833:ARG:O	1:A:834:GLN:HB2	2.03	0.57
1:A:313:ARG:CZ	1:A:841:GLN:HG3	2.35	0.56
2:B:3:VAL:HG22	2:B:4:RGL:HB2	1.85	0.56
1:A:453:GLN:H	1:A:453:GLN:NE2	2.04	0.56
1:A:799:GLY:HA3	1:A:870:SER:HB2	1.88	0.56
1:A:1062:GLU:HA	1:A:1064:GLU:N	2.21	0.55
1:A:84:LEU:HD23	1:A:130:ILE:HD13	1.88	0.55
1:A:154:LEU:HD22	1:A:169:ALA:HA	1.89	0.55
1:A:243:VAL:HG22	1:A:279:LEU:HD21	1.87	0.54
1:A:614:ASP:CG	1:A:615:ASP:H	2.15	0.54
1:A:940:ARG:HH22	1:A:983:ASN:HD22	1.55	0.54
1:A:471:GLN:HG3	1:A:473:ASN:HB3	1.89	0.54
1:A:994:VAL:HG11	1:A:1017:TRP:HZ3	1.72	0.54
1:A:132:ALA:O	1:A:133:GLU:HB2	2.08	0.54
1:A:932:VAL:O	1:A:940:ARG:HG2	2.07	0.54
1:A:404:GLY:O	1:A:408:HIS:HB3	2.08	0.53
1:A:330:MET:HA	1:A:354:ALA:HA	1.90	0.53
1:A:1035:CYS:O	1:A:1039:GLU:HG3	2.09	0.53
1:A:735:ASP:OD1	1:A:738:ARG:NH2	2.42	0.53
1:A:712:GLU:O	1:A:715:VAL:HG23	2.08	0.53
1:A:749:LEU:HB3	1:A:797:VAL:HG11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:VAL:HG11	1:A:204:HIS:CD2	2.45	0.52
1:A:246:SER:HB2	1:A:254:VAL:HG21	1.91	0.52
1:A:484:LEU:HD21	1:A:503:LEU:HD11	1.91	0.52
1:A:993:ALA:O	1:A:997:ILE:HG12	2.10	0.52
1:A:1014:TRP:HA	1:A:1017:TRP:CE3	2.45	0.51
1:A:192:LYS:HG3	1:A:235:LEU:HD11	1.92	0.51
1:A:319:VAL:HG23	1:A:376:MET:HE1	1.92	0.51
1:A:615:ASP:HA	1:A:619:ILE:HD12	1.92	0.51
1:A:705:CYS:O	1:A:709:GLU:HG2	2.11	0.51
1:A:967:PRO:HA	1:A:970:VAL:HG22	1.91	0.51
1:A:715:VAL:HG21	1:A:754:VAL:HG12	1.91	0.50
1:A:508:HIS:HD2	1:A:511:MET:CE	2.24	0.50
1:A:78:GLN:HG2	1:A:123:MET:HE1	1.92	0.50
1:A:995:GLY:HA2	1:A:998:MET:CE	2.42	0.50
1:A:57:GLN:HB3	1:A:99:LEU:HD21	1.93	0.49
1:A:715:VAL:HG11	1:A:755:ARG:HG3	1.94	0.49
1:A:623:ILE:CG2	1:A:702:MET:HG3	2.40	0.49
1:A:199:MET:HA	1:A:208:ARG:HG2	1.95	0.49
1:A:286:ASP:HB3	1:A:289:LEU:HD12	1.94	0.49
1:A:998:MET:HE1	1:A:1014:TRP:CD2	2.47	0.49
1:A:1062:GLU:HG3	1:A:1064:GLU:HB2	1.95	0.49
1:A:615:ASP:HA	1:A:619:ILE:CD1	2.42	0.48
1:A:555:SER:O	1:A:559:ILE:HG13	2.12	0.48
1:A:166:ARG:HB3	1:A:207:ILE:CD1	2.42	0.48
1:A:656:PRO:HB2	1:A:688:ILE:HD11	1.95	0.48
1:A:995:GLY:HA2	1:A:998:MET:HE2	1.96	0.48
1:A:940:ARG:HH12	1:A:983:ASN:HB3	1.77	0.47
1:A:322:THR:HG22	1:A:326:MET:HE2	1.97	0.47
1:A:1060:ILE:HG12	1:A:1079:LEU:HD22	1.95	0.47
1:A:85:ARG:HD3	1:A:129:ASP:HB3	1.97	0.47
1:A:246:SER:HB2	1:A:254:VAL:CG2	2.45	0.47
1:A:548:TYR:HA	1:A:551:LEU:HD23	1.97	0.47
1:A:890:ILE:HG12	1:A:890:ILE:O	2.15	0.47
1:A:229:PHE:CZ	1:A:265:VAL:HG21	2.51	0.46
1:A:252:ASP:HB3	1:A:293:GLN:HG2	1.98	0.46
1:A:508:HIS:HD2	1:A:511:MET:HE2	1.79	0.46
1:A:469:GLU:HG2	1:A:510:ILE:HD11	1.96	0.46
1:A:719:GLU:O	1:A:723:LYS:HG3	2.15	0.46
1:A:302:VAL:HG21	1:A:360:ALA:HB1	1.97	0.46
1:A:557:LYS:NZ	1:A:594:ASP:CB	2.79	0.46
1:A:933:CYS:SG	1:A:968:LEU:HD12	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LYS:O	1:A:260:GLU:HG3	2.15	0.46
1:A:139:ILE:CB	1:A:145:ASN:HB2	2.46	0.46
1:A:715:VAL:HG21	1:A:754:VAL:HG11	1.97	0.45
1:A:323:ILE:HA	1:A:326:MET:HE3	1.98	0.45
1:A:739:VAL:O	1:A:743:GLU:HG3	2.16	0.45
1:A:557:LYS:HZ1	1:A:594:ASP:CB	2.30	0.45
1:A:1053:LEU:HD23	1:A:1092:LEU:HD11	1.99	0.44
1:A:625:ALA:O	1:A:629:MET:HG2	2.17	0.44
1:A:259:VAL:HG22	1:A:300:VAL:HG22	1.99	0.44
1:A:556:LEU:HA	1:A:559:ILE:HD12	1.99	0.44
1:A:839:ASP:H	1:A:842:VAL:HG13	1.82	0.44
1:A:451:GLY:O	1:A:455:LYS:HG3	2.18	0.44
2:B:4:RGL:HA	2:B:4:RGL:HD1	1.79	0.44
2:B:2:ARG:O	2:B:3:VAL:O	2.36	0.44
1:A:769:ASP:O	1:A:773:LYS:HG2	2.18	0.43
1:A:457:HIS:CD2	1:A:495:LEU:CD1	3.01	0.43
1:A:622:MET:HE3	1:A:626:TRP:NE1	2.33	0.43
1:A:950:MET:HE2	1:A:950:MET:HB3	1.92	0.43
1:A:598:VAL:HG23	1:A:601:LEU:HD12	2.01	0.43
1:A:648:LEU:HD22	1:A:706:TYR:HE2	1.84	0.43
1:A:87:LEU:O	1:A:91:ALA:O	2.37	0.42
1:A:571:LEU:O	1:A:575:THR:OG1	2.33	0.42
1:A:678:VAL:HG13	1:A:686:PHE:HB3	2.00	0.42
1:A:719:GLU:HG3	1:A:763:MET:HE1	2.02	0.42
1:A:887:VAL:HA	1:A:890:ILE:HG22	2.01	0.42
1:A:645:MET:O	1:A:649:MET:HG2	2.19	0.42
1:A:940:ARG:HH22	1:A:983:ASN:ND2	2.16	0.42
1:A:133:GLU:HA	1:A:136:ARG:HB3	2.02	0.41
1:A:222:ASN:HD22	1:A:228:LEU:HD13	1.85	0.41
1:A:61:THR:O	1:A:65:GLN:OE1	2.38	0.41
1:A:127:VAL:HA	1:A:130:ILE:HD12	2.02	0.41
1:A:497:ILE:HA	1:A:500:LEU:HD13	2.01	0.41
1:A:615:ASP:O	1:A:616:ASP:HB2	2.20	0.41
1:A:116:GLN:HG2	1:A:165:LEU:HD21	2.03	0.41
1:A:229:PHE:HB3	1:A:268:TYR:HD1	1.85	0.41
1:A:277:LEU:HG	1:A:318:ILE:HG21	2.02	0.41
1:A:1105:GLN:O	1:A:1109:GLN:HG3	2.21	0.41
1:A:791:PHE:CZ	1:A:795:ILE:HD11	2.56	0.40
1:A:139:ILE:CB	1:A:145:ASN:CB	3.00	0.40
1:A:497:ILE:HG13	1:A:498:PRO:HD3	2.04	0.40
1:A:999:LYS:HD2	1:A:1033:TYR:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:HIS:O	1:A:1016:SER:OG	2.33	0.40
1:A:322:THR:HG21	1:A:364:MET:HE1	2.03	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	1087/1115 (98%)	1010 (93%)	70 (6%)	7 (1%)	21 39
2	B	1/4 (25%)	0	0	1 (100%)	0 0
All	All	1088/1119 (97%)	1010 (93%)	70 (6%)	8 (1%)	18 35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	616	ASP
1	A	617	PRO
2	B	3	VAL
1	A	563	ALA
1	A	1042	HIS
1	A	60	ILE
1	A	522	GLY
1	A	779	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	908/967 (94%)	834 (92%)	74 (8%)	11	24
2	B	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	910/969 (94%)	835 (92%)	75 (8%)	10	23

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	32	LEU
1	A	36	LEU
1	A	42	VAL
1	A	60	ILE
1	A	65	GLN
1	A	68	ARG
1	A	70	THR
1	A	103	VAL
1	A	111	LEU
1	A	112	LEU
1	A	158	VAL
1	A	161	GLN
1	A	163	VAL
1	A	180	PHE
1	A	189	ASP
1	A	190	VAL
1	A	210	LEU
1	A	243	VAL
1	A	264	THR
1	A	265	VAL
1	A	277	LEU
1	A	281	LEU
1	A	296	LEU
1	A	317	ASN
1	A	318	ILE
1	A	335	GLU
1	A	390	TRP
1	A	400	LEU
1	A	446	THR
1	A	453	GLN
1	A	458	GLU
1	A	466	GLN
1	A	479	HIS

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Mol	Chain	Res	Type
1	A	495	LEU
1	A	497	ILE
1	A	500	LEU
1	A	509	SER
1	A	519	ILE
1	A	520	GLN
1	A	555	SER
1	A	558	HIS
1	A	560	VAL
1	A	571	LEU
1	A	598	VAL
1	A	641	LEU
1	A	643	VAL
1	A	644	VAL
1	A	651	THR
1	A	654	ILE
1	A	658	VAL
1	A	665	ASP
1	A	678	VAL
1	A	693	LEU
1	A	754	VAL
1	A	755	ARG
1	A	760	LEU
1	A	803	LEU
1	A	834	GLN
1	A	835	ASP
1	A	841	GLN
1	A	842	VAL
1	A	859	LYS
1	A	883	LEU
1	A	932	VAL
1	A	950	MET
1	A	968	LEU
1	A	970	VAL
1	A	983	ASN
1	A	989	ASN
1	A	1007	VAL
1	A	1065	MET
1	A	1070	LYS
1	A	1097	ILE
2	B	3	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	146	GLN
1	A	184	GLN
1	A	202	GLN
1	A	224	HIS
1	A	272	HIS
1	A	317	ASN
1	A	453	GLN
1	A	502	ASN
1	A	508	HIS
1	A	516	GLN
1	A	529	GLN
1	A	762	GLN
1	A	983	ASN
1	A	989	ASN
1	A	1087	GLN
1	A	1099	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	RGL	B	4	2	9,10,10	2.79	2 (22%)	5,11,11	1.13	0
2	FC0	B	1	2	12,13,15	1.01	1 (8%)	15,15,19	1.52	2 (13%)

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	RGL	B	4	2	-	4/8/9/9	-
2	FC0	B	1	2	-	5/7/9/12	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	RGL	O-C	6.18	1.43	1.20
2	B	4	RGL	CZ-NE	5.28	1.43	1.33
2	B	1	FC0	O-C	3.30	1.32	1.20

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FC0	O-C-CA	-4.58	112.98	124.77
2	B	1	FC0	C-CA-N	2.50	114.33	109.50

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	FC0	N-CA-CB-CG
2	B	4	RGL	O-C-CA-CB
2	B	4	RGL	N-CA-CB-CG
2	B	4	RGL	C-CA-CB-CG
2	B	4	RGL	CA-CB-CG-CD
2	B	1	FC0	CA-CB-CG-CD1
2	B	1	FC0	CA-CB-CG-CD2
2	B	1	FC0	O1-C1-N-CA
2	B	1	FC0	CB-CA-N-C1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	RGL	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 [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	1091/1115 (97%)	0.14	26 (2%) 59 50	89, 127, 215, 251	0
2	B	2/4 (50%)	1.21	0 100 100	144, 144, 144, 162	0
All	All	1093/1119 (97%)	0.14	26 (2%) 59 50	89, 127, 215, 251	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	597	ASP	4.3
1	A	345	LEU	4.3
1	A	617	PRO	4.0
1	A	1068	ALA	3.6
1	A	791	PHE	3.5
1	A	142	ASP	3.5
1	A	733	PHE	3.3
1	A	629	MET	2.8
1	A	668	ASN	2.8
1	A	212	ALA	2.6
1	A	61	THR	2.5
1	A	350	PHE	2.5
1	A	640	TYR	2.5
1	A	23	ALA	2.4
1	A	342	ALA	2.4
1	A	179	ILE	2.3
1	A	798	MET	2.3
1	A	472	GLY	2.3
1	A	60	ILE	2.2
1	A	795	ILE	2.2
1	A	764	TRP	2.1
1	A	1092	LEU	2.1
1	A	247	CYS	2.1
1	A	33	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	140	ASP	2.1
1	A	667	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	FC0	B	1	13/15	0.68	0.16	158,163,164,164	0
2	RGL	B	4	11/11	0.81	0.19	130,131,137,139	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
3	NI	A	1201	1/1	0.91	0.11	162,162,162,162	0

6.5 Other polymers [i](#)

There are no such residues in this entry.