Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2022 – 12:31 am GMT

PDB ID	:	6XU2
Title	:	Human karyopherin RanBP5 (isoform-3)
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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:

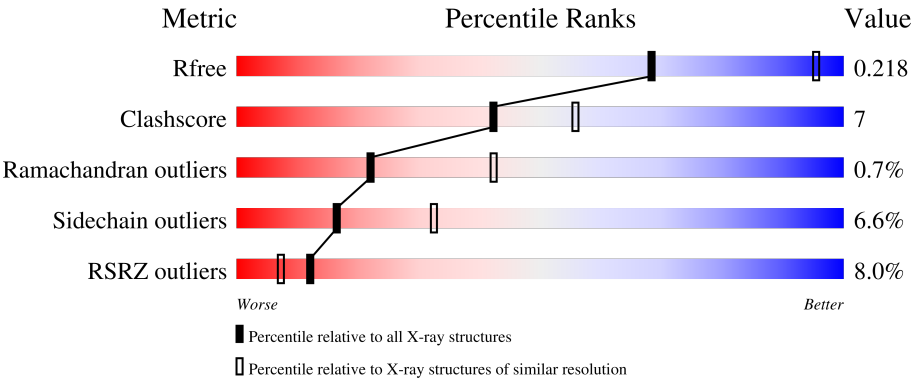
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.83 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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (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 <=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	8% 78% 19%
2	B	4	25% 25% 50% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FC0	B	1	-	-	-	X

2 Entry composition (i)

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 (three-letter code: NI) (formula: Ni).

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

- Molecule 4 is water.

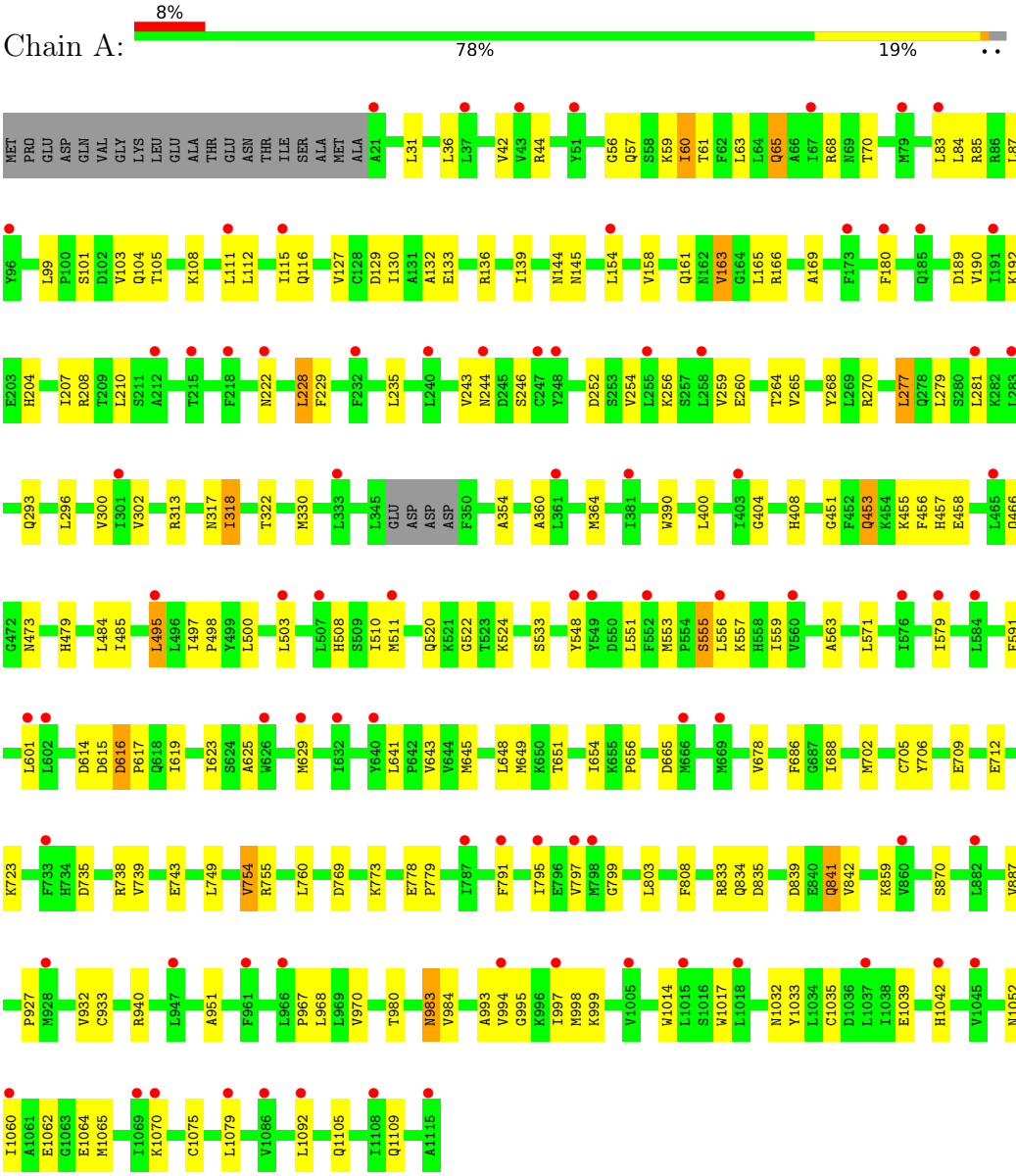
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		

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.

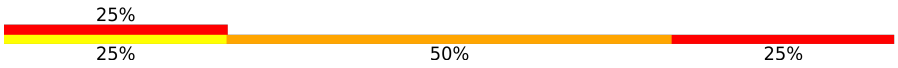
- Molecule 1: Importin-5

Chain A:



- Molecule 2: Antipain

Chain B:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.20%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[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: NI, FC0, RGL

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	0.44	0/8641	0.61	0/11730
2	B	0.64	0/17	1.10	0/21
All	All	0.44	0/8658	0.61	0/11751

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

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
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	113	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	116	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 (116) 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: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: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:995:GLY:HA2	1:A:998:MET:HE3	1.88	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:940:ARG:HH22	1:A:983:ASN:HD22	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:614:ASP:CG	1:A:615:ASP:H	2.15	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: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:508:HIS:HD2	1:A:511:MET:HE2	1.78	0.48
1:A:656:PRO:HB2	1:A:688:ILE:HD11	1.95	0.48
1:A:940:ARG:HH12	1:A:983:ASN:HB3	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASP:HB3	1:A:293:GLN:HG2	1.98	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
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:591:PHE:HZ	1:A:629:MET:HE1	1.82	0.45
1:A:739:VAL:O	1:A:743:GLU:HG3	2.16	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: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:553:MET:HE1	1:A:579:ILE:HG12	2.01	0.42
1:A:87:LEU:O	1:A:91:ALA:O	2.37	0.42
1:A:678:VAL:HG13	1:A:686:PHE:HB3	2.00	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:557:LYS:HZ3	1:A:594:ASP:CB	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:322:THR:HG21	1:A:364:MET:HE1	2.04	0.40
1:A:999:LYS:HD2	1:A:1033:TYR:CD1	2.56	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%)	25 46
2	B	1/4 (25%)	0	0	1 (100%)	0 0
All	All	1088/1119 (97%)	1010 (93%)	70 (6%)	8 (1%)	22 42

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%)	850 (94%)	58 (6%)	17 34
2	B	2/2 (100%)	0	2 (100%)	0 0
All	All	910/969 (94%)	850 (93%)	60 (7%)	16 32

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	36	LEU
1	A	42	VAL
1	A	44	ARG
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	144	ASN
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	202	GLN
1	A	210	LEU
1	A	228	LEU
1	A	244	ASN
1	A	264	THR
1	A	270	ARG
1	A	277	LEU
1	A	281	LEU
1	A	296	LEU
1	A	317	ASN
1	A	318	ILE
1	A	390	TRP
1	A	400	LEU
1	A	453	GLN
1	A	456	PHE

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Mol	Chain	Res	Type
1	A	458	GLU
1	A	466	GLN
1	A	479	HIS
1	A	495	LEU
1	A	520	GLN
1	A	524	LYS
1	A	555	SER
1	A	571	LEU
1	A	598	VAL
1	A	641	LEU
1	A	643	VAL
1	A	651	THR
1	A	654	ILE
1	A	665	ASP
1	A	754	VAL
1	A	760	LEU
1	A	803	LEU
1	A	808	PHE
1	A	835	ASP
1	A	841	GLN
1	A	859	LYS
1	A	983	ASN
1	A	1052	ASN
1	A	1065	MET
1	A	1070	LYS
2	B	2	ARG
2	B	3	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	116	GLN
1	A	144	ASN
1	A	202	GLN
1	A	272	HIS
1	A	439	ASN
1	A	453	GLN
1	A	508	HIS
1	A	638	GLN
1	A	983	ASN
1	A	989	ASN

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Mol	Chain	Res	Type
1	A	1050	ASN

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	FC0	B	1	2	12,13,15	0.98	1 (8%)	14,15,19	1.55	2 (14%)
2	RGL	B	4	2	9,10,10	2.67	2 (22%)	5,11,11	1.05	0

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	RGL	O-C	5.89	1.43	1.19
2	B	4	RGL	CZ-NE	5.15	1.43	1.33
2	B	1	FC0	O-C	3.16	1.32	1.19

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FC0	O-C-CA	-4.50	112.98	124.78
2	B	1	FC0	C-CA-N	2.55	114.33	109.73

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 monosaccharides 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, 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	1091/1115 (97%)	0.48	86 (7%) 12 8	89, 127, 215, 251	0
2	B	2/4 (50%)	1.33	1 (50%) 0 0	144, 144, 144, 162	0
All	All	1093/1119 (97%)	0.48	87 (7%) 12 7	89, 127, 215, 251	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	TYR	4.7
1	A	96	TYR	4.1
1	A	79	MET	4.0
1	A	552	PHE	4.0
1	A	602	LEU	3.7
1	A	185	GLN	3.7
1	A	247	CYS	3.5
1	A	1045	VAL	3.5
1	A	733	PHE	3.5
1	A	248	TYR	3.4
1	A	255	LEU	3.1
1	A	111	LEU	3.1
1	A	212	ALA	3.0
1	A	560	VAL	2.9
1	A	37	LEU	2.9
1	A	115	ILE	2.8
1	A	67	ILE	2.8
1	A	629	MET	2.8
1	A	632	ILE	2.8
1	A	1057	PHE	2.7
1	A	903	LEU	2.7
1	A	173	PHE	2.7
1	A	495	LEU	2.7
1	A	465	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	556	LEU	2.7
1	A	503	LEU	2.7
1	A	666	MET	2.7
1	A	1037	LEU	2.7
1	A	1115	ALA	2.6
1	A	549	TYR	2.6
1	A	381	ILE	2.6
1	A	576	ILE	2.6
1	A	966	LEU	2.6
1	A	584	LEU	2.6
1	A	1092	LEU	2.5
1	A	21	ALA	2.5
1	A	1079	LEU	2.5
1	A	333	LEU	2.5
1	A	215	THR	2.4
1	A	669	MET	2.4
1	A	994	VAL	2.4
1	A	301	ILE	2.4
1	A	218	PHE	2.4
1	A	507	LEU	2.4
1	A	797	VAL	2.3
1	A	795	ILE	2.3
1	A	180	PHE	2.3
1	A	1086	VAL	2.3
1	A	92	PHE	2.3
1	A	511	MET	2.3
1	A	947	LEU	2.3
1	A	640	TYR	2.3
1	A	798	MET	2.3
1	A	281	LEU	2.3
1	A	601	LEU	2.3
1	A	791	PHE	2.2
1	A	258	LEU	2.2
1	A	1069	ILE	2.2
1	A	860	VAL	2.2
1	A	43	VAL	2.2
1	A	1070	LYS	2.2
1	A	579	ILE	2.2
1	A	961	PHE	2.2
1	A	1018	LEU	2.2
1	A	232	PHE	2.2
1	A	928	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	598	VAL	2.1
1	A	240	LEU	2.1
1	A	244	ASN	2.1
1	A	283	LEU	2.1
1	A	1060	ILE	2.1
1	A	1005	VAL	2.1
1	A	1042	HIS	2.1
1	A	548	TYR	2.1
2	B	2	ARG	2.1
1	A	787	ILE	2.1
1	A	83	LEU	2.1
1	A	361	LEU	2.1
1	A	882	LEU	2.1
1	A	191	ILE	2.1
1	A	403	ILE	2.1
1	A	626	TRP	2.1
1	A	1108	ILE	2.0
1	A	222	ASN	2.0
1	A	1015	LEU	2.0
1	A	997	ILE	2.0
1	A	154	LEU	2.0

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, 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	FC0	B	1	13/15	0.57	0.41	158,163,164,164	0
2	RGL	B	4	11/11	0.80	0.33	130,131,137,139	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NI	A	1201	1/1	0.91	0.25	162,162,162,162	0

6.5 Other polymers (i)

There are no such residues in this entry.