Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 07:31 AM EST

PDB ID	:	5KTG
Title	:	Crystal structure of mouse Bak BH3-in-groove homodimer (GFP)
Authors	:	Mandal, T.; Choe, J.-Y.; Oh, K.J.
Deposited on	:	2016-07-11
Resolution	:	2.80 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:

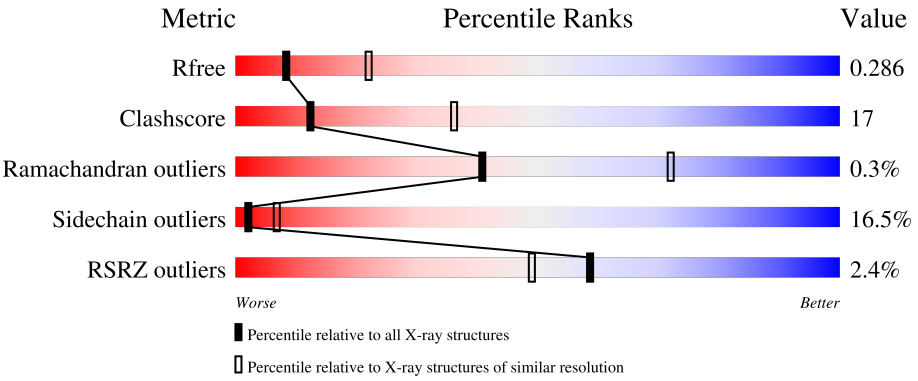
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	309	2% 59% 34% 7%
1	B	309	3% 56% 37% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4910 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 Green fluorescent protein, Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2455	1566	416	465	8			
1	B	309	Total	C	N	O	S	0	0	0
			2455	1566	416	465	8			

There are 16 discrepancies between the modelled and reference sequences:

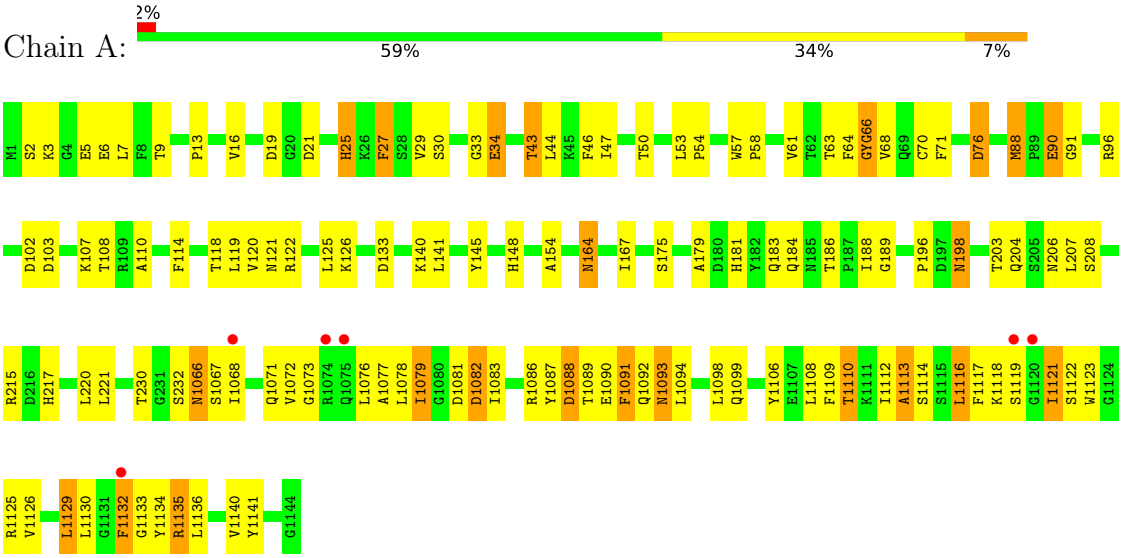
Chain	Residue	Modelled	Actual	Comment	Reference
A	66	CR2	SER	chromophore	UNP P42212
A	66	CR2	TYR	chromophore	UNP P42212
A	66	CR2	GLY	chromophore	UNP P42212
A	72	ALA	SER	conflict	UNP P42212
A	206	ASN	ALA	conflict	UNP P42212
A	231	GLY	-	linker	UNP P42212
A	232	SER	-	linker	UNP P42212
A	1084	CYS	ASN	conflict	UNP O08734
B	66	CR2	SER	chromophore	UNP P42212
B	66	CR2	TYR	chromophore	UNP P42212
B	66	CR2	GLY	chromophore	UNP P42212
B	72	ALA	SER	conflict	UNP P42212
B	206	ASN	ALA	conflict	UNP P42212
B	231	GLY	-	linker	UNP P42212
B	232	SER	-	linker	UNP P42212
B	1084	CYS	ASN	conflict	UNP O08734

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.

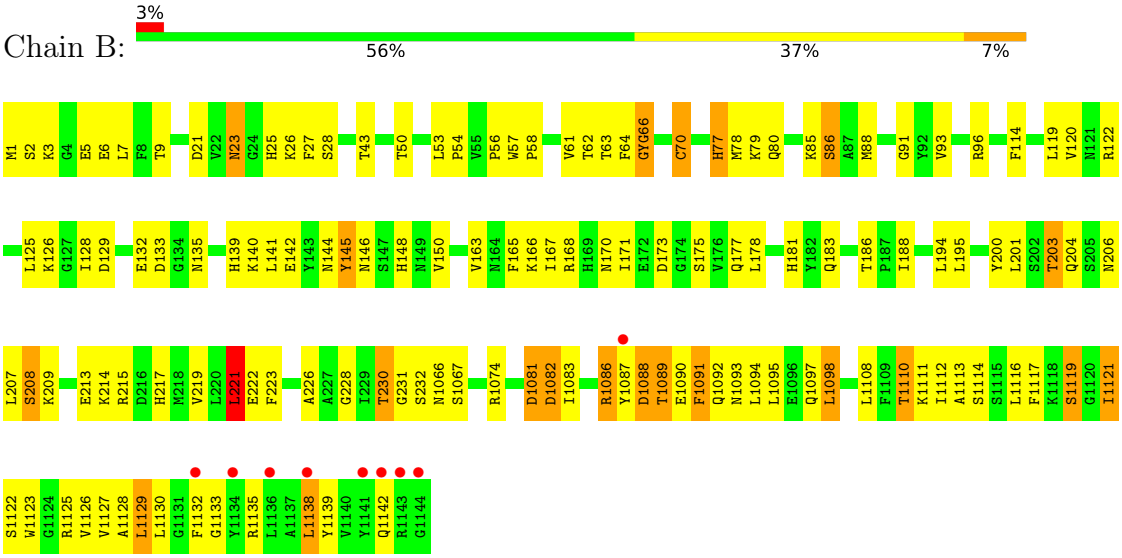
• Molecule 1: Green fluorescent protein, Bcl-2 homologous antagonist/killer

Chain A:



• Molecule 1: Green fluorescent protein, Bcl-2 homologous antagonist/killer

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	171.64Å 171.64Å 98.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.55 – 2.80 49.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.55-2.80) 94.8 (49.55-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.244 , 0.275 0.257 , 0.286	Depositor DCC
R_{free} test set	1949 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	62.9	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 17.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.057 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4910	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: CR2

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	0.90	5/2489 (0.2%)	1.04	2/3363 (0.1%)
1	B	0.88	0/2489	1.03	4/3363 (0.1%)
All	All	0.89	5/4978 (0.1%)	1.03	6/6726 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1134	TYR	CB-CG	6.10	1.60	1.51
1	A	1134	TYR	CD1-CE1	5.95	1.48	1.39
1	A	34	GLU	CG-CD	5.70	1.60	1.51
1	A	34	GLU	CB-CG	5.64	1.62	1.52
1	A	1134	TYR	CD2-CE2	5.62	1.47	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1122	SER	N-CA-C	-6.61	93.16	111.00
1	A	1066	ASN	N-CA-C	-6.37	93.80	111.00
1	A	1134	TYR	CA-CB-CG	5.79	124.40	113.40
1	B	221	LEU	CB-CG-CD1	5.74	120.76	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	122	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	1138	LEU	CA-CB-CG	5.17	127.20	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1066	ASN	Peptide
1	A	232	SER	Peptide
1	B	1098	LEU	Peptide
1	B	230	THR	Peptide
1	B	3	LYS	Peptide

5.2 Too-close contacts (i)

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	2455	0	2395	78	2
1	B	2455	0	2395	94	1
All	All	4910	0	4790	164	2

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 (164) 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:133:ASP:O	1:B:140:LYS:NZ	2.03	0.91
1:B:64:PHE:O	1:B:66:CR2:HA31	1.71	0.90
1:B:1088:ASP:OD2	1:B:1135:ARG:NH1	2.18	0.77
1:B:1116:LEU:O	1:B:1119:SER:OG	2.02	0.76
1:B:66:CR2:HD1	1:B:222:GLU:OE2	1.89	0.73
1:B:208:SER:C	1:B:219:VAL:HG12	2.10	0.72
1:B:206:ASN:OD1	1:B:207:LEU:N	2.27	0.67
1:B:1130:LEU:HD12	1:B:1133:GLY:HA3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1122:SER:O	1:A:1126:VAL:HG23	1.97	0.65
1:B:1130:LEU:CD1	1:B:1133:GLY:HA3	2.27	0.65
1:B:209:LYS:NZ	1:B:217:HIS:O	2.30	0.65
1:B:96:ARG:NH2	1:B:183:GLN:OE1	2.31	0.62
1:A:1090:GLU:HA	1:A:1093:ASN:HB2	1.81	0.62
1:B:208:SER:O	1:B:219:VAL:HG12	1.99	0.62
1:A:58:PRO:HA	1:A:61:VAL:HG23	1.81	0.62
1:B:1123:TRP:O	1:B:1126:VAL:N	2.32	0.61
1:B:2:SER:O	1:B:5:GLU:N	2.30	0.60
1:A:1130:LEU:HD12	1:A:1133:GLY:HA3	1.84	0.59
1:B:171:ILE:HG22	1:B:173:ASP:H	1.67	0.59
1:B:1112:ILE:O	1:B:1116:LEU:HG	2.02	0.59
1:A:46:PHE:CE2	1:A:64:PHE:CG	2.92	0.58
1:B:232:SER:OG	1:B:1066:ASN:N	2.34	0.58
1:A:133:ASP:O	1:A:140:LYS:NZ	2.35	0.57
1:A:148:HIS:CD2	1:A:167:ILE:HD13	2.39	0.57
1:B:221:LEU:HD12	1:B:221:LEU:N	2.20	0.57
1:B:1087:TYR:O	1:B:1089:THR:N	2.38	0.56
1:B:27:PHE:HA	1:B:50:THR:HG21	1.86	0.56
1:B:64:PHE:C	1:B:66:CR2:HA31	2.26	0.56
1:A:76:ASP:N	1:A:76:ASP:OD1	2.39	0.55
1:B:66:CR2:CZ	1:B:203:THR:HG21	2.37	0.55
1:B:1123:TRP:HA	1:B:1126:VAL:HG23	1.88	0.55
1:B:1130:LEU:HD12	1:B:1133:GLY:CA	2.37	0.55
1:A:1088:ASP:OD2	1:A:1135:ARG:NH1	2.40	0.55
1:B:56:PRO:HG3	1:B:139:HIS:HA	1.89	0.55
1:B:66:CR2:HOH	1:B:145:TYR:HE2	1.54	0.54
1:A:1077:ALA:O	1:B:1125:ARG:NH1	2.40	0.54
1:A:90:GLU:HG3	1:A:189:GLY:HA3	1.90	0.53
1:A:64:PHE:C	1:A:66:CR2:HA31	2.28	0.53
1:A:1090:GLU:O	1:A:1094:LEU:HG	2.08	0.53
1:A:53:LEU:HD12	1:A:54:PRO:HD2	1.91	0.53
1:A:206:ASN:OD1	1:A:207:LEU:N	2.41	0.53
1:B:1117:PHE:CE1	1:B:1121:ILE:HG23	2.42	0.53
1:B:1:MET:HE1	1:B:79:LYS:HE2	1.91	0.53
1:A:7:LEU:HD12	1:A:114:PHE:CE2	2.44	0.52
1:A:1079:ILE:HG21	1:B:1128:ALA:CB	2.39	0.52
1:A:1092:GLN:N	1:A:1092:GLN:OE1	2.42	0.52
1:B:135:ASN:HA	1:B:140:LYS:HD2	1.91	0.52
1:A:1106:TYR:O	1:A:1110:THR:OG1	2.28	0.52
1:B:1088:ASP:HA	1:B:1091:PHE:CD2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:HIS:CD2	1:B:78:MET:HG3	2.45	0.52
1:A:1140:VAL:CG2	1:A:1141:TYR:N	2.71	0.51
1:B:1082:ASP:OD1	1:B:1086:ARG:NH1	2.43	0.51
1:A:167:ILE:HB	1:A:179:ALA:HB3	1.93	0.51
1:A:88:MET:SD	1:A:91:GLY:HA2	2.49	0.51
1:A:1132:PHE:O	1:A:1136:LEU:N	2.43	0.51
1:A:13:PRO:HG2	1:A:118:THR:HA	1.93	0.51
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.75	0.50
1:B:2:SER:O	1:B:5:GLU:HB3	2.12	0.50
1:B:1091:PHE:CD2	1:B:1135:ARG:HG3	2.47	0.50
1:A:27:PHE:CD1	1:A:27:PHE:N	2.79	0.49
1:A:1079:ILE:HG21	1:B:1128:ALA:HB2	1.95	0.49
1:A:125:LEU:C	1:A:125:LEU:HD23	2.33	0.49
1:A:1076:LEU:HD23	1:B:1129:LEU:HD22	1.93	0.49
1:B:66:CR2:CE2	1:B:203:THR:HG21	2.42	0.49
1:A:46:PHE:O	1:A:217:HIS:HB2	2.13	0.48
1:B:88:MET:SD	1:B:91:GLY:HA2	2.53	0.48
1:B:146:ASN:ND2	1:B:168:ARG:O	2.46	0.48
1:A:1117:PHE:CE1	1:A:1121:ILE:HG23	2.48	0.48
1:B:1127:VAL:HG23	1:B:1128:ALA:H	1.78	0.48
1:A:1123:TRP:O	1:A:1126:VAL:N	2.46	0.48
1:B:1092:GLN:OE1	1:B:1092:GLN:N	2.26	0.48
1:A:29:VAL:HG13	1:A:47:ILE:O	2.14	0.48
1:A:1109:PHE:CZ	1:A:1129:LEU:HD22	2.48	0.48
1:A:27:PHE:HA	1:A:50:THR:HG21	1.96	0.48
1:A:96:ARG:NE	1:A:183:GLN:OE1	2.47	0.47
1:A:1110:THR:O	1:A:1113:ALA:HB3	2.14	0.47
1:B:1091:PHE:HD2	1:B:1135:ARG:HG3	1.78	0.47
1:B:208:SER:OG	1:B:219:VAL:HG13	2.15	0.47
1:B:213:GLU:OE2	1:B:215:ARG:NE	2.38	0.47
1:A:1125:ARG:HH12	1:B:1081:ASP:CG	2.17	0.47
1:B:62:THR:HB	1:B:96:ARG:NH1	2.30	0.47
1:B:63:THR:OG1	1:B:64:PHE:N	2.46	0.46
1:B:23:ASN:HD22	1:B:23:ASN:N	2.13	0.46
1:B:167:ILE:CG2	1:B:168:ARG:N	2.79	0.46
1:A:1140:VAL:HG23	1:A:1141:TYR:N	2.31	0.46
1:B:53:LEU:HD12	1:B:54:PRO:HD2	1.97	0.46
1:B:171:ILE:HD11	1:B:177:GLN:HB2	1.97	0.46
1:A:1094:LEU:O	1:A:1098:LEU:N	2.49	0.46
1:A:198:ASN:N	1:A:198:ASN:OD1	2.48	0.46
1:A:58:PRO:HA	1:A:61:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:SER:O	1:A:5:GLU:HB3	2.16	0.45
1:B:70:CYS:O	1:B:85:LYS:NZ	2.32	0.45
1:A:46:PHE:CE2	1:A:64:PHE:CD2	3.04	0.45
1:A:119:LEU:HG	1:A:120:VAL:N	2.31	0.45
1:B:171:ILE:HD11	1:B:177:GLN:CB	2.47	0.45
1:B:1095:LEU:HD13	1:B:1139:TYR:CB	2.47	0.44
1:A:43:THR:O	1:A:44:LEU:HD23	2.16	0.44
1:A:71:PHE:CE2	1:A:119:LEU:HD22	2.52	0.44
1:B:1:MET:N	1:B:1074:ARG:NH1	2.65	0.44
1:B:1123:TRP:HA	1:B:1126:VAL:CG2	2.47	0.44
1:A:25:HIS:N	1:A:25:HIS:ND1	2.65	0.44
1:A:1106:TYR:CD1	1:A:1106:TYR:C	2.90	0.44
1:B:58:PRO:HA	1:B:61:VAL:HG23	2.00	0.44
1:B:200:TYR:CE1	1:B:228:GLY:HA3	2.53	0.43
1:B:1098:LEU:HD13	1:B:1108:LEU:HD21	1.99	0.43
1:A:1068:ILE:O	1:A:1072:VAL:HG23	2.18	0.43
1:B:1094:LEU:HA	1:B:1097:GLN:HG2	1.99	0.43
1:A:29:VAL:HG12	1:A:30:SER:N	2.34	0.43
1:A:1068:ILE:HA	1:A:1071:GLN:HB2	2.00	0.43
1:A:220:LEU:HD12	1:A:221:LEU:N	2.34	0.43
1:A:1079:ILE:CG2	1:B:1128:ALA:HB2	2.48	0.43
1:A:1141:TYR:CD1	1:A:1141:TYR:C	2.91	0.43
1:B:1:MET:H1	1:B:1074:ARG:NH1	2.16	0.43
1:A:43:THR:HG23	1:A:221:LEU:HD23	1.99	0.43
1:A:141:LEU:HD12	1:A:141:LEU:N	2.33	0.43
1:A:1082:ASP:O	1:A:1086:ARG:HG2	2.19	0.43
1:B:1095:LEU:HB3	1:B:1139:TYR:CD2	2.54	0.43
1:A:1086:ARG:HB2	1:A:1087:TYR:CD2	2.54	0.43
1:B:1095:LEU:HD13	1:B:1139:TYR:HB2	2.01	0.43
1:A:1073:GLY:CA	1:B:1116:LEU:HD22	2.49	0.42
1:B:28:SER:H	1:B:50:THR:CG2	2.32	0.42
1:A:68:VAL:O	1:A:68:VAL:HG23	2.19	0.42
1:B:1094:LEU:C	1:B:1097:GLN:H	2.22	0.42
1:A:46:PHE:HE2	1:A:64:PHE:CG	2.35	0.42
1:B:1087:TYR:C	1:B:1089:THR:H	2.23	0.42
1:A:1088:ASP:HA	1:A:1091:PHE:HB2	2.00	0.42
1:A:1083:ILE:HA	1:A:1086:ARG:HG2	2.01	0.42
1:B:57:TRP:N	1:B:58:PRO:CD	2.83	0.42
1:B:148:HIS:CD2	1:B:167:ILE:HA	2.53	0.42
1:B:1111:LYS:O	1:B:1112:ILE:C	2.58	0.42
1:B:125:LEU:C	1:B:125:LEU:HD23	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HD21	1:B:114:PHE:CZ	2.55	0.42
1:B:27:PHE:CD1	1:B:27:PHE:C	2.93	0.42
1:B:119:LEU:HD23	1:B:120:VAL:N	2.35	0.42
1:B:213:GLU:OE2	1:B:215:ARG:HB2	2.19	0.42
1:A:33:GLY:HA3	1:A:44:LEU:HD23	2.02	0.42
1:B:206:ASN:OD1	1:B:206:ASN:C	2.57	0.42
1:B:230:THR:HG22	1:B:231:GLY:H	1.85	0.42
1:B:1110:THR:O	1:B:1113:ALA:HB3	2.20	0.42
1:A:63:THR:HG23	1:A:108:THR:HG21	2.02	0.41
1:B:201:LEU:CD2	1:B:226:ALA:HB2	2.50	0.41
1:A:1108:LEU:O	1:A:1112:ILE:HG12	2.20	0.41
1:B:200:TYR:CE1	1:B:228:GLY:CA	3.03	0.41
1:B:1090:GLU:O	1:B:1093:ASN:HB3	2.21	0.41
1:B:1138:LEU:O	1:B:1142:GLN:HB2	2.20	0.41
1:B:21:ASP:HB2	1:B:26:LYS:CD	2.49	0.41
1:A:125:LEU:HD23	1:A:126:LYS:N	2.35	0.41
1:A:154:ALA:HB2	1:A:196:PRO:HD2	2.03	0.41
1:A:1116:LEU:C	1:A:1116:LEU:HD23	2.41	0.41
1:A:1125:ARG:HH11	1:A:1125:ARG:HG2	1.84	0.41
1:B:150:VAL:N	1:B:201:LEU:O	2.46	0.41
1:B:77:HIS:CD2	1:B:77:HIS:H	2.39	0.41
1:A:53:LEU:HD22	1:A:57:TRP:CZ2	2.56	0.41
1:B:165:PHE:CE1	1:B:181:HIS:CG	3.09	0.41
1:B:173:ASP:HB3	1:B:175:SER:H	1.86	0.41
1:A:16:VAL:HG13	1:A:121:ASN:HB3	2.03	0.41
1:B:1:MET:HA	1:B:5:GLU:OE2	2.20	0.41
1:A:71:PHE:HE2	1:A:119:LEU:CD2	2.33	0.40
1:A:110:ALA:HA	1:A:122:ARG:O	2.22	0.40
1:A:154:ALA:HB2	1:A:196:PRO:O	2.21	0.40
1:B:148:HIS:HB2	1:B:203:THR:HG23	2.04	0.40
1:A:1109:PHE:CZ	1:A:1129:LEU:CD2	3.04	0.40
1:A:1118:LYS:HG2	1:B:195:LEU:O	2.20	0.40
1:B:86:SER:HB3	1:B:194:LEU:HG	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:GLN:NE2	1:B:214:LYS:O[3_664]	2.00	0.20
1:A:164:ASN:OD1	1:A:215:ARG:NH1[2_545]	2.13	0.07

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	304/309 (98%)	288 (95%)	15 (5%)	1 (0%)	41 72
1	B	304/309 (98%)	284 (93%)	19 (6%)	1 (0%)	41 72
All	All	608/618 (98%)	572 (94%)	34 (6%)	2 (0%)	41 72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1088	ASP
1	A	1113	ALA

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	263/264 (100%)	218 (83%)	45 (17%)	2 6
1	B	263/264 (100%)	221 (84%)	42 (16%)	2 7
All	All	526/528 (100%)	439 (84%)	87 (16%)	2 7

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	6	GLU
1	A	9	THR
1	A	19	ASP

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Mol	Chain	Res	Type
1	A	21	ASP
1	A	25	HIS
1	A	27	PHE
1	A	34	GLU
1	A	43	THR
1	A	70	CYS
1	A	76	ASP
1	A	88	MET
1	A	90	GLU
1	A	102	ASP
1	A	103	ASP
1	A	107	LYS
1	A	145	TYR
1	A	164	ASN
1	A	175	SER
1	A	181	HIS
1	A	184	GLN
1	A	186	THR
1	A	188	ILE
1	A	198	ASN
1	A	203	THR
1	A	204	GLN
1	A	208	SER
1	A	230	THR
1	A	1067	SER
1	A	1078	LEU
1	A	1079	ILE
1	A	1081	ASP
1	A	1082	ASP
1	A	1088	ASP
1	A	1089	THR
1	A	1091	PHE
1	A	1093	ASN
1	A	1110	THR
1	A	1114	SER
1	A	1116	LEU
1	A	1119	SER
1	A	1121	ILE
1	A	1129	LEU
1	A	1132	PHE
1	A	1135	ARG
1	B	6	GLU

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Mol	Chain	Res	Type
1	B	9	THR
1	B	23	ASN
1	B	25	HIS
1	B	43	THR
1	B	70	CYS
1	B	77	HIS
1	B	80	GLN
1	B	86	SER
1	B	93	VAL
1	B	126	LYS
1	B	128	ILE
1	B	129	ASP
1	B	132	GLU
1	B	141	LEU
1	B	142	GLU
1	B	144	ASN
1	B	145	TYR
1	B	163	VAL
1	B	166	LYS
1	B	170	ASN
1	B	178	LEU
1	B	186	THR
1	B	188	ILE
1	B	203	THR
1	B	204	GLN
1	B	208	SER
1	B	221	LEU
1	B	223	PHE
1	B	1067	SER
1	B	1081	ASP
1	B	1082	ASP
1	B	1083	ILE
1	B	1086	ARG
1	B	1089	THR
1	B	1091	PHE
1	B	1110	THR
1	B	1114	SER
1	B	1119	SER
1	B	1121	ILE
1	B	1129	LEU
1	B	1132	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	177	GLN
1	A	185	ASN
1	A	1093	ASN
1	B	80	GLN
1	B	81	HIS
1	B	198	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
1	CR2	B	66	1	20,20,21	6.30	6 (30%)	25,27,29	4.36	8 (32%)
1	CR2	A	66	1	20,20,21	6.68	5 (25%)	25,27,29	3.41	6 (24%)

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
1	CR2	B	66	1	-	2/6/25/26	0/2/2/2
1	CR2	A	66	1	-	3/6/25/26	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CR2	CB2-CA2	26.01	1.56	1.35
1	B	66	CR2	CB2-CA2	24.38	1.55	1.35
1	A	66	CR2	O2-C2	11.90	1.48	1.23
1	B	66	CR2	O2-C2	10.53	1.45	1.23
1	B	66	CR2	CA2-C2	-7.92	1.40	1.48
1	A	66	CR2	CA2-C2	-5.67	1.43	1.48
1	A	66	CR2	CA1-C1	4.63	1.54	1.49
1	A	66	CR2	OH-CZ	3.30	1.44	1.37
1	B	66	CR2	OH-CZ	2.80	1.43	1.37
1	B	66	CR2	CA1-C1	2.44	1.52	1.49
1	B	66	CR2	C1-N3	-2.17	1.33	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	CR2	CA2-C2-N3	13.27	109.64	103.37
1	A	66	CR2	O2-C2-CA2	-11.11	124.72	130.96
1	B	66	CR2	O2-C2-CA2	-10.71	124.94	130.96
1	A	66	CR2	CA2-C2-N3	8.54	107.41	103.37
1	B	66	CR2	CG2-CB2-CA2	-6.83	121.58	129.94
1	A	66	CR2	CG2-CB2-CA2	-6.75	121.67	129.94
1	B	66	CR2	C1-CA1-N1	-6.41	98.68	112.85
1	B	66	CR2	C2-N3-C1	-5.39	105.36	107.99
1	B	66	CR2	C2-CA2-N2	-5.38	105.16	108.93
1	A	66	CR2	C2-CA2-N2	-4.60	105.71	108.93
1	B	66	CR2	CB2-CA2-N2	3.50	133.68	128.83
1	B	66	CR2	O3-C3-CA3	-3.47	115.93	126.39
1	A	66	CR2	O3-C3-CA3	-2.09	120.08	126.39
1	A	66	CR2	C2-N3-C1	-2.06	106.98	107.99

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CR2	N2-CA2-CB2-CG2
1	A	66	CR2	C2-CA2-CB2-CG2
1	B	66	CR2	C2-CA2-CB2-CG2
1	B	66	CR2	N2-CA2-CB2-CG2
1	A	66	CR2	C3-CA3-N3-C2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	66	CR2	6	0
1	A	66	CR2	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	308/309 (99%)	-0.29	6 (1%)	66	59	42, 66, 138, 174	0
1	B	308/309 (99%)	-0.09	9 (2%)	51	41	56, 104, 164, 190	0
All	All	616/618 (99%)	-0.19	15 (2%)	59	49	42, 84, 152, 190	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1144	GLY	6.1
1	B	1138	LEU	5.6
1	A	1120	GLY	3.8
1	A	1068	ILE	3.5
1	B	1142	GLN	3.5
1	B	1143	ARG	3.3
1	B	1134	TYR	3.2
1	A	1074	ARG	3.1
1	B	1136	LEU	3.0
1	B	1087	TYR	2.8
1	B	1141	TYR	2.7
1	A	1119	SER	2.5
1	A	1075	GLN	2.5
1	A	1132	PHE	2.2
1	B	1132	PHE	2.2

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

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
1	CR2	A	66	19/20	0.89	0.23	39,52,76,93	0
1	CR2	B	66	19/20	0.94	0.23	70,77,88,89	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.