wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 06:58 AM EDT

PDB ID	:	1YM7
Title	:	G Protein-Coupled Receptor Kinase 2 (GRK2)
Authors	:	Lodowski, D.T.; Barnhill, J.F.; Pyskadlo, R.M.; Ghirlando, R.; Sterne-Marr, R.; Tesmer, J.J.G.
Deposited on	:	2005-01-20
Resolution	:	4.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

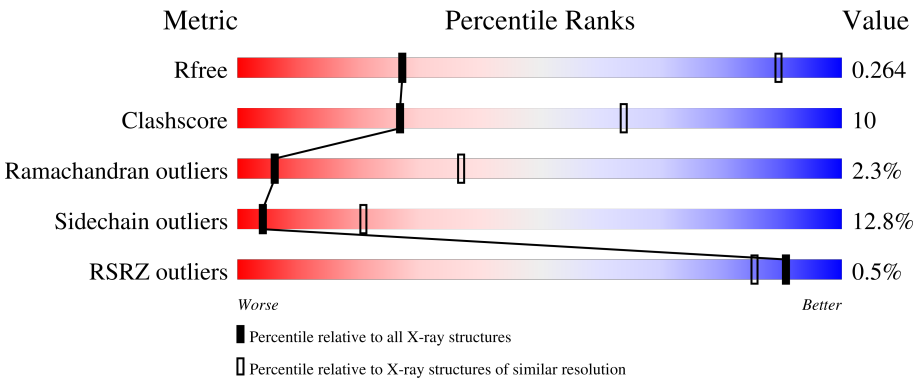
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 4.50 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	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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	689	.% 59% 24% 5% 12%
1	B	689	58% 25% • 12%
1	C	689	60% 24% • 12%
1	D	689	.% 61% 21% • 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 19846 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 Beta-adrenergic receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	608	4982	3177	865	905	35	0	0	0
1	B	608	4982	3177	865	905	35	0	0	0
1	C	607	4975	3173	864	903	35	0	0	0
1	D	599	4907	3132	850	890	35	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

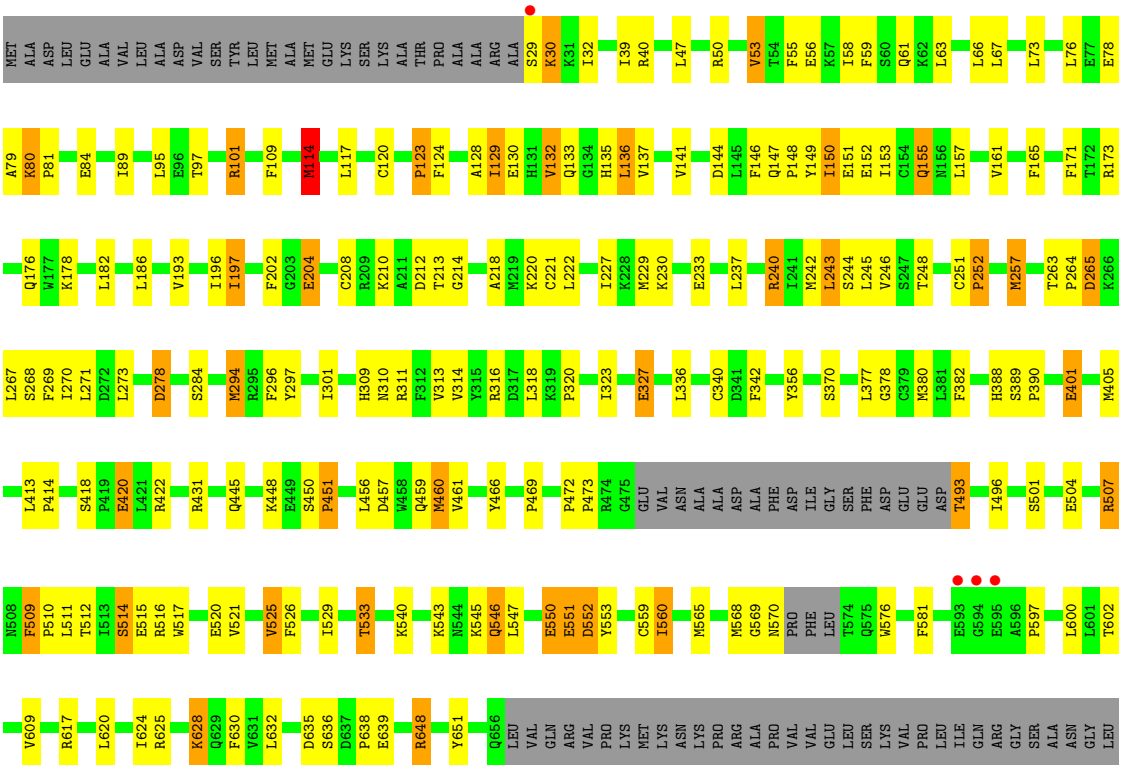
Chain	Residue	Modelled	Actual	Comment	Reference
A	670	ALA	SER	engineered mutation	UNP P21146
B	670	ALA	SER	engineered mutation	UNP P21146
C	670	ALA	SER	engineered mutation	UNP P21146
D	670	ALA	SER	engineered mutation	UNP P21146

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.

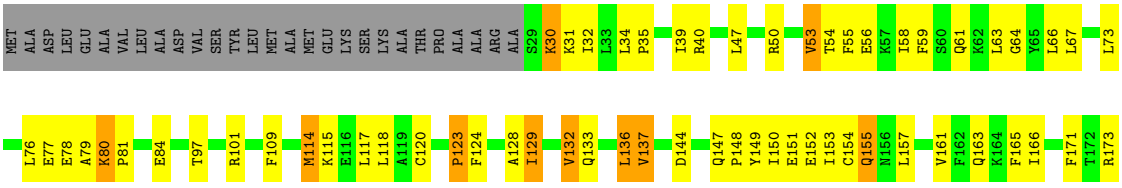
• Molecule 1: Beta-adrenergic receptor kinase 1

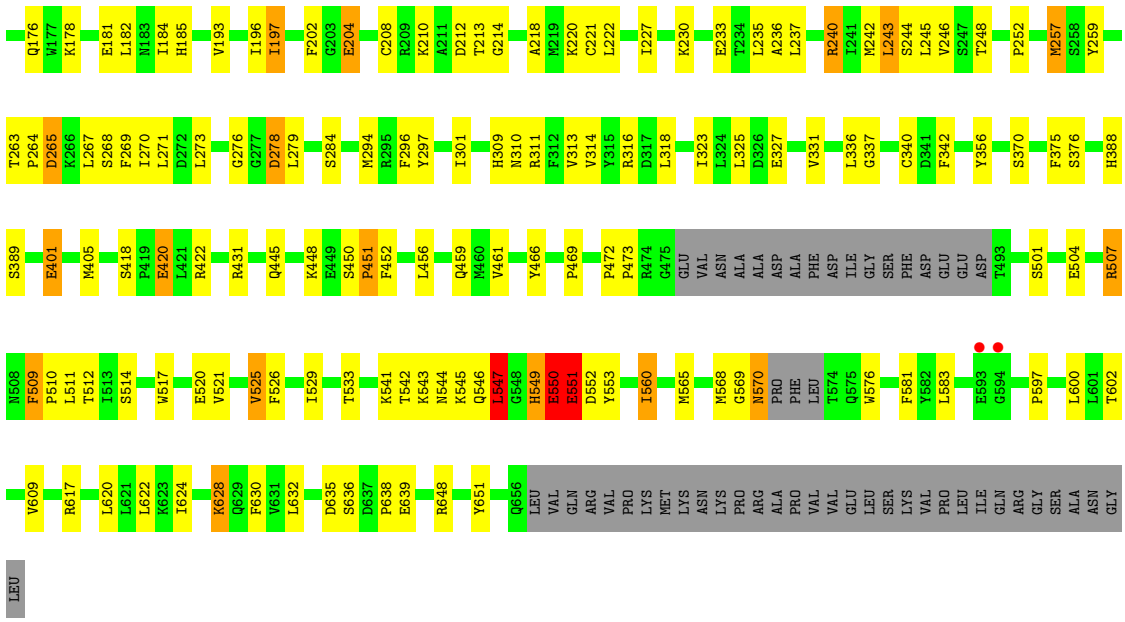
Chain A:



• Molecule 1: Beta-adrenergic receptor kinase 1

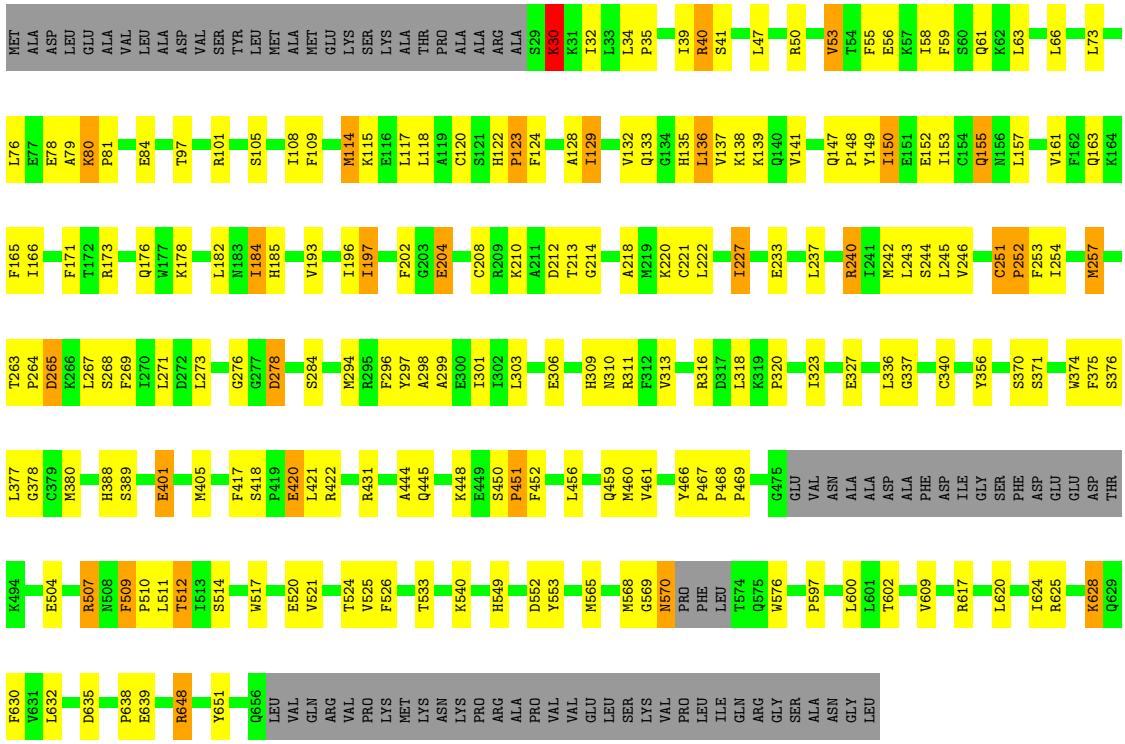
Chain B:





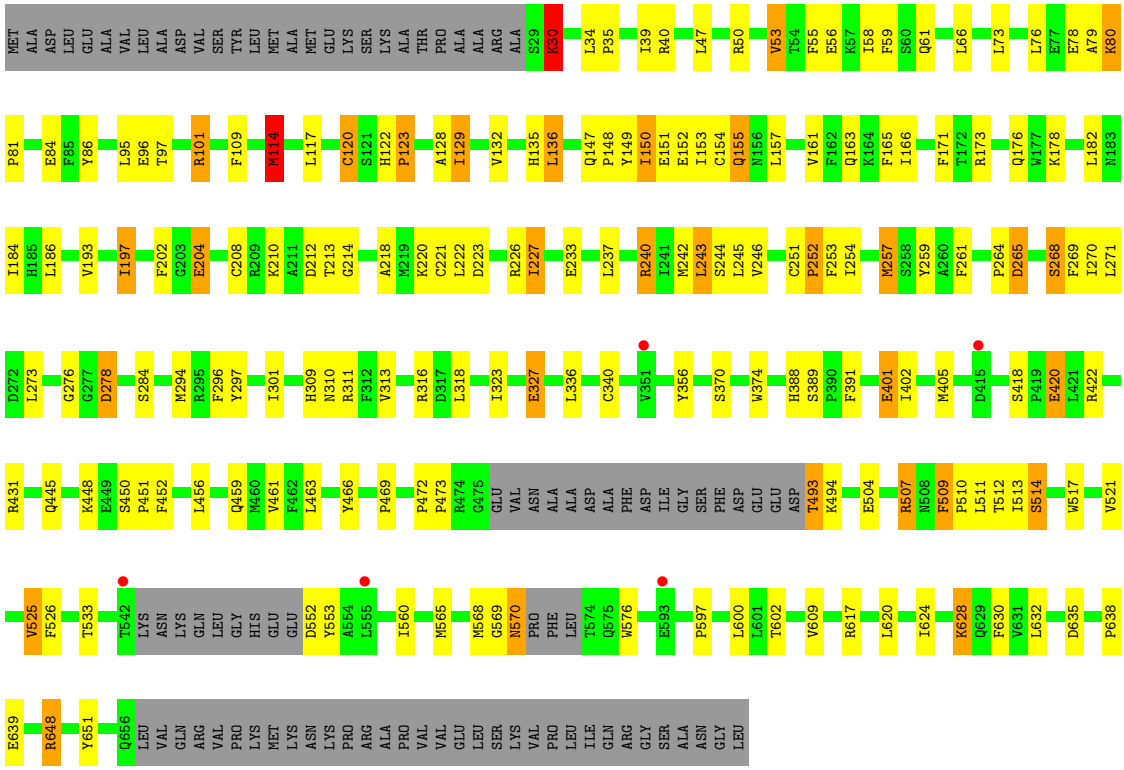
- Molecule 1: Beta-adrenergic receptor kinase 1

Chain C:



- Molecule 1: Beta-adrenergic receptor kinase 1

Chain D:


MET ALA ASP LEU GLU ALA VAL LEU ALA ASP VAL SER TYR LEU MET ALA MET GLU LYS SER LYS ALA THR PRO ALA ALA ARG ALA S29 K30 L34 P35 I39 R40 L47 R50 V53 T54 F55 E56 K57 I58 F59 S60 Q61 L66 L73 L76 E77 E78 A79 K80
P81 E84 F85 Y86 L95 E96 T97 R101 F109 M114 L117 C120 S121 H122 P123 A128 I129 V132 H135 L136 Q147 P148 Y149 I150 E151 E152 I153 C154 Q155 N156 L157 V161 F162 Q163 K164 F165 I166 F171 T172 R173 Q176 W177 K178 L182 N183
I184 H185 L186 V193 I197 F202 G203 E204 C208 R209 K210 A211 D212 T213 G214 A218 M219 K220 C221 L222 D223 R226 I227 E233 L237 R240 I241 M242 L243 S244 L245 V246 C251 P252 F253 I254 M257 S258 Y259 A260 F261 P264 D265 S268 F269 I270 L271
D272 L273 G276 G277 D278 S284 M294 R295 F296 Y297 I301 H309 N310 R311 F312 V313 R316 D317 L318 I323 E327 L336 C340 V351 Y356 S370 W374 H388 S389 P390 F391 E401 I402 M405 D415 S418 P419 E420 L421 R422
R431 Q445 K448 E449 S450 P451 F452 L456 Q459 M460 V461 F462 L463 Y466 P469 P472 P473 R474 G475 GLU VAL ASN ALA ALA ASP ALA PHE ASP ILE GLY SER PHE ASP GLU GLU ASP T493 K494 E504 R507 N508 F509 P510 L511 T512 I513 S514 W517 V521
V525 F526 T533 T542 LYS ASN LYS GLN LEU GLY HIS GLU GLU D552 Y553 A554 L555 I560 M565 M568 G569 N570 PRO PHE LEU T574 Q575 W576 E593 P597 L600 L601 T602 V609 R617 L620 I624 K628 Q629 F630 V631 L632 D635 P638
E639 R648 Y651 Q656 LEU VAL GLN ARG VAL PRO LYS MET LYS ASN LYS PRO ARG ALA PRO VAL VAL GLU LEU SER LYS VAL PRO LEU ILE GLN ARG GLY SER ALA ASN GLY LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	115.16Å 82.16Å 218.79Å 90.00° 95.57° 90.00°	Depositor
Resolution (Å)	14.98 – 4.50 19.99 – 3.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (14.98-4.50) 97.9 (19.99-3.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 3.94Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.224 , 0.279 0.258 , 0.264	Depositor DCC
R_{free} test set	1706 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	206.3	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 30.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19846	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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 (i)

5.1 Standard geometry (i)

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	4/5093 (0.1%)	0.76	0/6842
1	B	0.88	8/5093 (0.2%)	0.79	1/6842 (0.0%)
1	C	0.68	0/5086	0.76	0/6832
1	D	0.57	0/5016	0.71	0/6739
All	All	0.74	12/20288 (0.1%)	0.75	1/27255 (0.0%)

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	1
1	B	0	1
All	All	0	2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	GLN	CD-OE1	25.76	1.80	1.24
1	B	550	GLU	CD-OE2	20.09	1.47	1.25
1	B	546	GLN	CD-OE1	13.80	1.54	1.24
1	B	547	LEU	C-N	10.28	1.51	1.33
1	B	551	GLU	CD-OE2	9.34	1.35	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	551	GLU	OE1-CD-OE2	5.76	130.21	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	493	THR	Peptide
1	B	547	LEU	Mainchain

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	4982	0	4968	106	0
1	B	4982	0	4968	106	0
1	C	4975	0	4961	108	0
1	D	4907	0	4894	89	0
All	All	19846	0	19791	404	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 10.

The worst 5 of 404 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:546:GLN:OE1	1:A:546:GLN:CD	1.80	1.18
1:D:493:THR:HG22	1:D:494:LYS:HG2	1.55	0.88
1:B:173:ARG:HA	1:B:176:GLN:OE1	1.82	0.79
1:C:297:TYR:O	1:C:301:ILE:HG12	1.81	0.79
1:A:130:GLU:OE2	1:C:115:LYS:HE2	1.82	0.78

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	602/689 (87%)	521 (86%)	68 (11%)	13 (2%)	6	38
1	B	602/689 (87%)	513 (85%)	75 (12%)	14 (2%)	6	37
1	C	601/689 (87%)	515 (86%)	72 (12%)	14 (2%)	6	37
1	D	591/689 (86%)	513 (87%)	64 (11%)	14 (2%)	6	36
All	All	2396/2756 (87%)	2062 (86%)	279 (12%)	55 (2%)	6	37

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	551	GLU
1	B	549	HIS
1	B	550	GLU
1	A	40	ARG
1	A	120	CYS

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	546/611 (89%)	468 (86%)	78 (14%)	3	18
1	B	546/611 (89%)	479 (88%)	67 (12%)	4	22
1	C	545/611 (89%)	476 (87%)	69 (13%)	4	21
1	D	538/611 (88%)	474 (88%)	64 (12%)	5	23
All	All	2175/2444 (89%)	1897 (87%)	278 (13%)	4	21

5 of 278 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	197	ILE
1	D	244	SER
1	D	493	THR
1	B	197	ILE
1	B	182	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	310	ASN
1	C	459	GLN
1	D	607	GLN
1	D	434	ASN
1	D	459	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	608/689 (88%)	-0.61	4 (0%) 87 82	40, 40, 40, 40	0
1	B	608/689 (88%)	-0.58	2 (0%) 94 90	40, 40, 40, 40	0
1	C	607/689 (88%)	-0.53	0 100 100	40, 40, 40, 40	0
1	D	599/689 (86%)	-0.44	5 (0%) 86 79	40, 40, 40, 40	0
All	All	2422/2756 (87%)	-0.54	11 (0%) 91 85	40, 40, 40, 40	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	593	GLU	6.5
1	A	593	GLU	3.6
1	D	351	VAL	3.2
1	A	595	GLU	3.1
1	D	593	GLU	3.1

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

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

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.