



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:41 AM GMT

PDB ID : 2Y02
Title : TURKEY BETA1 ADRENERGIC RECEPTOR WITH STABILISING MUTATIONS AND BOUND AGONIST CARMOTEROL
Authors : Warne, A.; Moukhametzianov, R.; Baker, J.G.; Nehme, R.; Edwards, P.C.; Leslie, A.G.W.; Schertler, G.F.X.; Tate, C.G.
Deposited on : 2010-11-30
Resolution : 2.60 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

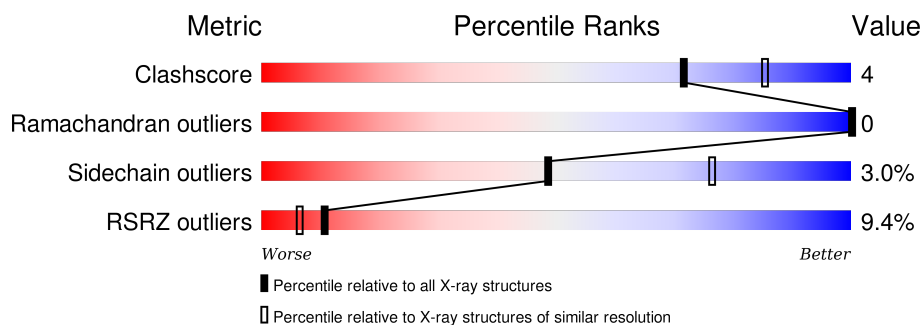
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	315	
1	B	315	

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	Y01	A	402	-	-	-	X
3	2CV	A	504	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2CV	A	505	-	-	-	X
3	2CV	B	502	-	-	-	X
3	2CV	B	504	-	-	-	X
3	2CV	B	505	-	-	-	X
5	NA	A	701	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5064 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-1 ADRENERGIC RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2269	1498	372	379	20			
1	B	298	Total	C	N	O	S	0	0	0
			2371	1560	396	395	20			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	EXPRESSION TAG	UNP P07700
A	32	GLY	-	EXPRESSION TAG	UNP P07700
A	68	SER	ARG	ENGINEERED MUTATION	UNP P07700
A	90	VAL	MET	ENGINEERED MUTATION	UNP P07700
A	116	LEU	CYS	ENGINEERED MUTATION	UNP P07700
A	227	ALA	TYR	ENGINEERED MUTATION	UNP P07700
A	.	-	CYS	DELETION	UNP P07700
A	.	-	GLU	DELETION	UNP P07700
A	.	-	GLY	DELETION	UNP P07700
A	.	-	ARG	DELETION	UNP P07700
A	.	-	PHE	DELETION	UNP P07700
A	.	-	TYR	DELETION	UNP P07700
A	.	-	GLY	DELETION	UNP P07700
A	.	-	SER	DELETION	UNP P07700
A	.	-	GLN	DELETION	UNP P07700
A	.	-	GLU	DELETION	UNP P07700
A	.	-	GLN	DELETION	UNP P07700
A	.	-	PRO	DELETION	UNP P07700
A	.	-	GLN	DELETION	UNP P07700
A	.	-	PRO	DELETION	UNP P07700
A	.	-	PRO	DELETION	UNP P07700
A	.	-	PRO	DELETION	UNP P07700
A	.	-	LEU	DELETION	UNP P07700
A	.	-	PRO	DELETION	UNP P07700
A	.	-	GLN	DELETION	UNP P07700

Continued on next page...

Continued from previous page...

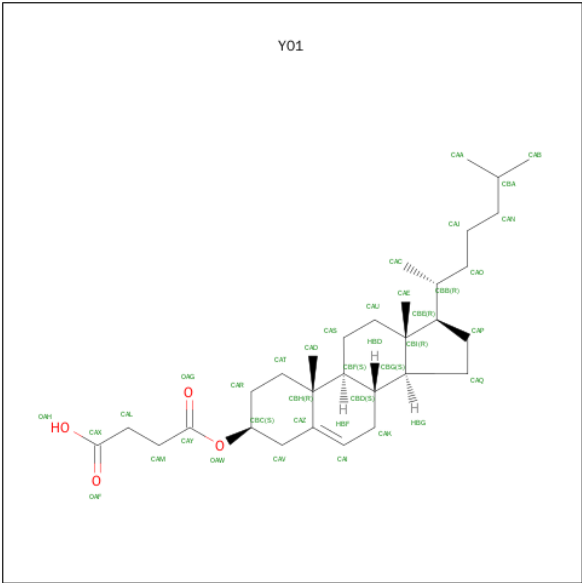
Chain	Residue	Modelled	Actual	Comment	Reference
A	.	-	HIS	DELETION	UNP P07700
A	.	-	GLN	DELETION	UNP P07700
A	.	-	PRO	DELETION	UNP P07700
A	.	-	ILE	DELETION	UNP P07700
A	.	-	LEU	DELETION	UNP P07700
A	.	-	GLY	DELETION	UNP P07700
A	.	-	ASN	DELETION	UNP P07700
A	.	-	GLY	DELETION	UNP P07700
A	.	-	ARG	DELETION	UNP P07700
A	282	LEU	ALA	ENGINEERED MUTATION	UNP P07700
A	327	ALA	PHE	ENGINEERED MUTATION	UNP P07700
A	338	MET	PHE	ENGINEERED MUTATION	UNP P07700
A	358	ALA	CYS	ENGINEERED MUTATION	UNP P07700
A	369	HIS	-	EXPRESSION TAG	UNP P07700
A	370	HIS	-	EXPRESSION TAG	UNP P07700
A	371	HIS	-	EXPRESSION TAG	UNP P07700
A	372	HIS	-	EXPRESSION TAG	UNP P07700
A	373	HIS	-	EXPRESSION TAG	UNP P07700
B	31	MET	-	EXPRESSION TAG	UNP P07700
B	32	GLY	-	EXPRESSION TAG	UNP P07700
B	68	SER	ARG	ENGINEERED MUTATION	UNP P07700
B	90	VAL	MET	ENGINEERED MUTATION	UNP P07700
B	116	LEU	CYS	ENGINEERED MUTATION	UNP P07700
B	227	ALA	TYR	ENGINEERED MUTATION	UNP P07700
B	.	-	CYS	DELETION	UNP P07700
B	.	-	GLU	DELETION	UNP P07700
B	.	-	GLY	DELETION	UNP P07700
B	.	-	ARG	DELETION	UNP P07700
B	.	-	PHE	DELETION	UNP P07700
B	.	-	TYR	DELETION	UNP P07700
B	.	-	GLY	DELETION	UNP P07700
B	.	-	SER	DELETION	UNP P07700
B	.	-	GLN	DELETION	UNP P07700
B	.	-	GLU	DELETION	UNP P07700
B	.	-	GLN	DELETION	UNP P07700
B	.	-	PRO	DELETION	UNP P07700
B	.	-	GLN	DELETION	UNP P07700
B	.	-	PRO	DELETION	UNP P07700
B	.	-	PRO	DELETION	UNP P07700
B	.	-	PRO	DELETION	UNP P07700
B	.	-	LEU	DELETION	UNP P07700
B	.	-	PRO	DELETION	UNP P07700

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	.	-	GLN	DELETION	UNP P07700
B	.	-	HIS	DELETION	UNP P07700
B	.	-	GLN	DELETION	UNP P07700
B	.	-	PRO	DELETION	UNP P07700
B	.	-	ILE	DELETION	UNP P07700
B	.	-	LEU	DELETION	UNP P07700
B	.	-	GLY	DELETION	UNP P07700
B	.	-	ASN	DELETION	UNP P07700
B	.	-	GLY	DELETION	UNP P07700
B	.	-	ARG	DELETION	UNP P07700
B	282	LEU	ALA	ENGINEERED MUTATION	UNP P07700
B	327	ALA	PHE	ENGINEERED MUTATION	UNP P07700
B	338	MET	PHE	ENGINEERED MUTATION	UNP P07700
B	358	ALA	CYS	ENGINEERED MUTATION	UNP P07700
B	369	HIS	-	EXPRESSION TAG	UNP P07700
B	370	HIS	-	EXPRESSION TAG	UNP P07700
B	371	HIS	-	EXPRESSION TAG	UNP P07700
B	372	HIS	-	EXPRESSION TAG	UNP P07700
B	373	HIS	-	EXPRESSION TAG	UNP P07700

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



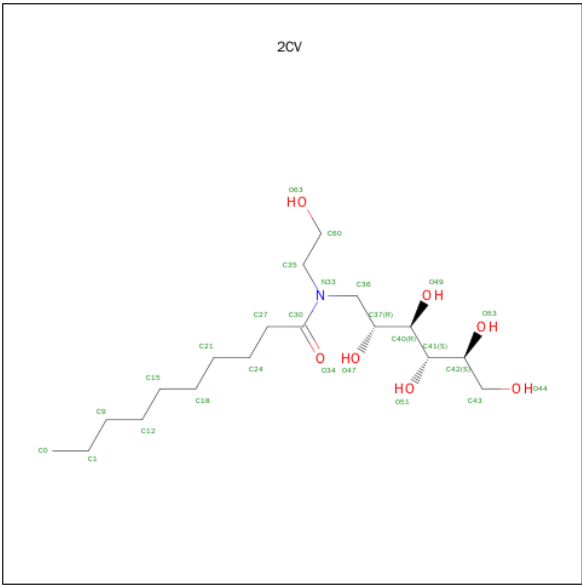
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	31	4		
2	A	1	Total	C	O	0	0
			35	31	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			35	31	4		
2	B	1	Total	C	O	0	0
			35	31	4		

- Molecule 3 is HEGA-10 (three-letter code: 2CV) (formula: C₁₈H₃₇NO₇).



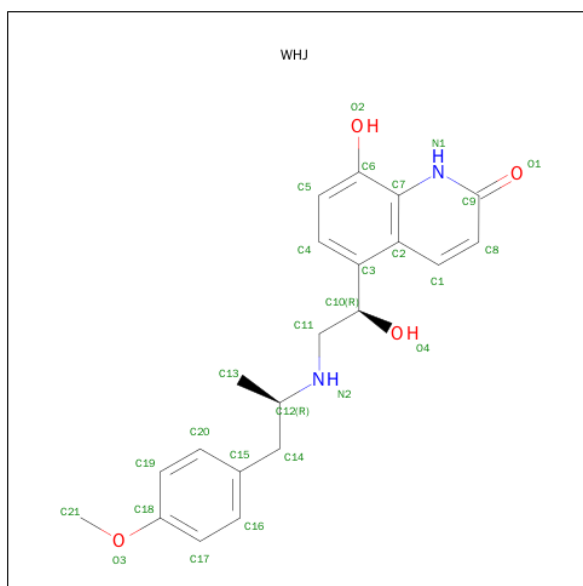
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	18	1	7		
3	A	1	Total	C			0	0
			5	5				
3	A	1	Total	C	N	O	0	0
			20	15	1	4		
3	A	1	Total	C	N	O	0	0
			26	18	1	7		
3	A	1	Total	C	N	O	0	0
			26	18	1	7		
3	B	1	Total	C	N	O	0	0
			20	15	1	4		
3	B	1	Total	C	N	O	0	0
			16	13	1	2		
3	B	1	Total	C	N	O	0	0
			16	13	1	2		
3	B	1	Total	C	N	O	0	0
			8	6	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			26	18	1	7		

- Molecule 4 is CARMOTEROL (three-letter code: WHJ) (formula: $C_{21}H_{24}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			27	21	2	4		
4	B	1	Total	C	N	O	0	0
			27	21	2	4		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

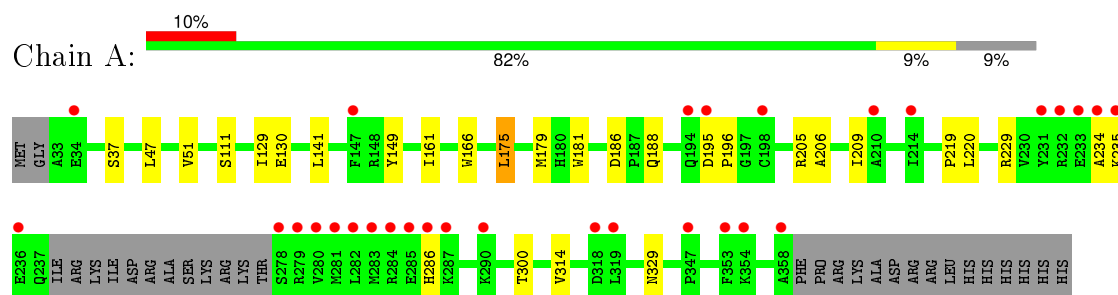
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	21	Total	O	0	0
			21	21		
6	B	19	Total	O	0	0
			19	19		

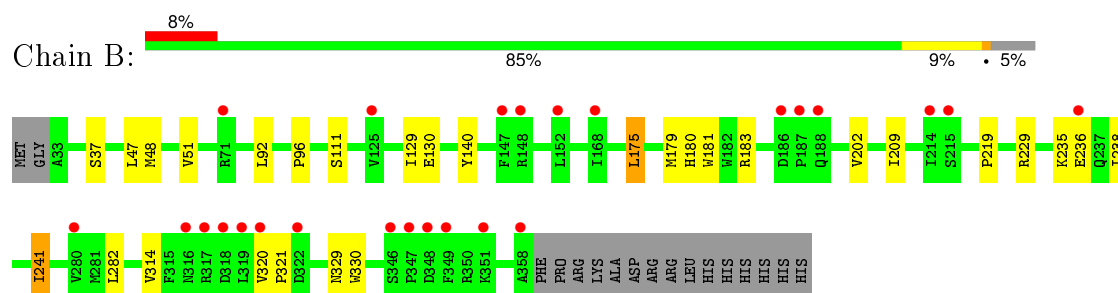
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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-1 ADRENERGIC RECEPTOR



• Molecule 1: BETA-1 ADRENERGIC RECEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.60 Å 61.70 Å 101.40 Å 90.00° 109.30° 90.00°	Depositor
Resolution (Å)	95.73 – 2.60 42.28 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.7 (95.73-2.60) 96.7 (42.28-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.61 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.229 , 0.268 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 31463 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5064	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, 2CV, Y01, WHJ

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	0.52	0/2323	0.58	0/3167
1	B	0.53	0/2426	0.59	0/3303
All	All	0.53	0/4749	0.58	0/6470

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	2269	0	2349	14	0
1	B	2371	0	2471	17	0
2	A	70	0	98	6	0
2	B	70	0	98	4	0
3	A	103	0	146	6	0
3	B	86	0	122	6	0
4	A	27	0	23	1	0
4	B	27	0	23	0	0
5	A	1	0	0	0	0
6	A	21	0	0	0	0
6	B	19	0	0	1	0
All	All	5064	0	5330	44	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 4.

All (44) 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)
3:A:501:2CV:H271	3:B:505:2CV:H352	1.47	0.95
3:B:501:2CV:H601	3:B:501:2CV:H272	1.56	0.84
1:A:175:LEU:HD13	1:A:179:MET:HG3	1.65	0.78
3:B:501:2CV:C60	3:B:501:2CV:H272	2.17	0.75
1:B:175:LEU:HB2	6:B:2012:HOH:O	1.86	0.75
1:B:209:ILE:HD11	1:B:314:VAL:HG11	1.68	0.75
1:A:47:LEU:O	1:A:51:VAL:HG23	1.94	0.68
3:A:505:2CV:H37	3:A:505:2CV:H602	1.80	0.64
2:A:402:Y01:HAA1	3:A:505:2CV:H01C	1.80	0.63
1:A:209:ILE:HD11	1:A:314:VAL:HG11	1.79	0.63
1:B:235:LYS:O	1:B:238:ILE:HG13	2.01	0.60
1:A:161:ILE:HG12	2:A:401:Y01:HBC	1.86	0.57
1:B:241:ILE:HD12	1:B:282:LEU:HD23	1.88	0.55
1:B:47:LEU:O	1:B:51:VAL:HG23	2.07	0.55
1:A:181:TRP:HB3	3:A:501:2CV:H152	1.89	0.55
1:A:129:ILE:HG13	1:A:219:PRO:HB2	1.90	0.53
1:A:205:ARG:HG2	1:A:314:VAL:HG13	1.91	0.53
1:B:129:ILE:HG13	1:B:219:PRO:HB2	1.94	0.48
2:B:402:Y01:HAC1	2:B:402:Y01:HAE2	1.97	0.47
1:B:48:MET:HE2	1:B:330:TRP:CH2	2.49	0.47
3:A:505:2CV:H271	3:A:505:2CV:H352	1.73	0.46
1:A:234:ALA:O	1:A:286:HIS:HE1	2.00	0.45
1:B:181:TRP:HB3	3:B:501:2CV:H152	1.98	0.45
1:A:141:LEU:HD23	1:A:149:TYR:HD1	1.81	0.44
1:A:195:ASP:HA	1:A:196:PRO:HD3	1.84	0.44
2:A:402:Y01:HAC1	2:A:402:Y01:HAU2	1.99	0.44
1:A:130:GLU:HG2	2:A:401:Y01:HAC3	2.00	0.44
1:B:140:TYR:CE1	1:B:229:ARG:HB3	2.52	0.44
2:A:401:Y01:HAS2	2:A:401:Y01:HAD2	1.90	0.43
3:A:501:2CV:H271	3:B:505:2CV:H271	2.00	0.43
4:A:601:WHJ:H16	4:A:601:WHJ:H12	1.71	0.43
1:A:206:ALA:HA	2:B:401:Y01:OAG	2.18	0.43
1:B:179:MET:O	1:B:180:HIS:HB2	2.19	0.43
1:B:48:MET:CE	1:B:330:TRP:CH2	3.02	0.42
1:B:241:ILE:CD1	1:B:282:LEU:HD23	2.49	0.42
1:B:180:HIS:CE1	1:B:183:ARG:CZ	3.02	0.42
2:B:401:Y01:HAC3	2:B:401:Y01:HAJ2	1.86	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TRP:CE2	2:A:402:Y01:HAP1	2.55	0.42
3:B:505:2CV:H271	3:B:505:2CV:H352	1.75	0.41
1:A:220:LEU:HD11	1:A:300:THR:HG23	2.03	0.41
1:B:48:MET:HE2	1:B:330:TRP:HH2	1.86	0.41
1:B:130:GLU:HG2	2:B:401:Y01:HAC3	2.03	0.41
1:B:320:VAL:HA	1:B:321:PRO:HD2	1.93	0.41
1:B:92:LEU:O	1:B:96:PRO:HG2	2.21	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	282/315 (90%)	273 (97%)	9 (3%)	0	100	100
1	B	296/315 (94%)	289 (98%)	7 (2%)	0	100	100
All	All	578/630 (92%)	562 (97%)	16 (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	247/273 (90%)	239 (97%)	8 (3%)	46	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	258/273 (94%)	251 (97%)	7 (3%)	52 79
All	All	505/546 (92%)	490 (97%)	15 (3%)	48 76

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	SER
1	A	111	SER
1	A	175	LEU
1	A	186	ASP
1	A	188	GLN
1	A	229	ARG
1	A	235	LYS
1	A	329	ASN
1	B	37	SER
1	B	111	SER
1	B	175	LEU
1	B	202	VAL
1	B	236	GLU
1	B	241	ILE
1	B	329	ASN

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	180	HIS

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 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	Y01	A	401	-	35,38,38	1.15	3 (8%)	54,57,57	1.86	12 (22%)
2	Y01	A	402	-	35,38,38	1.31	2 (5%)	54,57,57	1.18	6 (11%)
3	2CV	A	501	-	25,25,25	0.47	0	29,30,30	0.81	1 (3%)
3	2CV	A	502	-	4,4,25	0.46	0	3,3,30	0.36	0
3	2CV	A	503	-	19,19,25	0.57	0	19,21,30	0.59	0
3	2CV	A	504	-	25,25,25	0.86	1 (4%)	29,30,30	0.77	0
3	2CV	A	505	-	25,25,25	0.63	0	29,30,30	0.95	1 (3%)
4	WHJ	A	601	-	28,29,29	1.45	3 (10%)	35,40,40	1.50	6 (17%)
2	Y01	B	401	-	35,38,38	1.20	2 (5%)	54,57,57	1.72	9 (16%)
2	Y01	B	402	-	35,38,38	1.25	2 (5%)	54,57,57	1.43	8 (14%)
3	2CV	B	501	-	19,19,25	0.55	0	19,21,30	1.05	1 (5%)
3	2CV	B	502	-	15,15,25	0.77	0	15,16,30	0.60	0
3	2CV	B	503	-	15,15,25	0.71	0	15,16,30	0.54	0
3	2CV	B	504	-	7,7,25	0.46	0	7,7,30	0.38	0
3	2CV	B	505	-	25,25,25	0.70	0	29,30,30	0.87	1 (3%)
4	WHJ	B	601	-	28,29,29	1.47	4 (14%)	35,40,40	1.22	4 (11%)

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	Y01	A	401	-	-	0/17/77/77	0/4/4/4
2	Y01	A	402	-	-	1/17/77/77	0/4/4/4
3	2CV	A	501	-	-	0/34/34/34	0/0/0/0
3	2CV	A	502	-	-	0/2/2/34	0/0/0/0
3	2CV	A	503	-	-	0/22/22/34	0/0/0/0
3	2CV	A	504	-	-	0/34/34/34	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2CV	A	505	-	-	0/34/34/34	0/0/0/0
4	WHJ	A	601	-	-	0/15/15/15	0/3/3/3
2	Y01	B	401	-	-	0/17/77/77	0/4/4/4
2	Y01	B	402	-	-	0/17/77/77	0/4/4/4
3	2CV	B	501	-	-	0/22/22/34	0/0/0/0
3	2CV	B	502	-	-	0/16/16/34	0/0/0/0
3	2CV	B	503	-	-	0/16/16/34	0/0/0/0
3	2CV	B	504	-	-	0/5/5/34	0/0/0/0
3	2CV	B	505	-	-	0/34/34/34	0/0/0/0
4	WHJ	B	601	-	-	0/15/15/15	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	Y01	CAK-CAI	-5.08	1.39	1.50
2	A	402	Y01	CAK-CAI	-4.68	1.39	1.50
2	A	401	Y01	CAK-CAI	-4.64	1.40	1.50
2	B	401	Y01	CAK-CAI	-4.29	1.40	1.50
2	A	401	Y01	CBI-CBG	-2.20	1.50	1.55
3	A	504	2CV	C27-C30	2.06	1.56	1.51
4	B	601	WHJ	C4-C3	2.18	1.41	1.37
4	A	601	WHJ	C2-C7	2.45	1.48	1.42
2	B	402	Y01	CAI-CAZ	2.48	1.39	1.33
4	B	601	WHJ	C2-C7	2.61	1.49	1.42
2	A	401	Y01	CAI-CAZ	2.89	1.40	1.33
2	A	402	Y01	CAI-CAZ	2.96	1.40	1.33
2	B	401	Y01	CAI-CAZ	3.40	1.41	1.33
4	A	601	WHJ	C3-C2	3.90	1.49	1.43
4	B	601	WHJ	C6-C7	4.17	1.47	1.42
4	B	601	WHJ	C3-C2	4.26	1.50	1.43
4	A	601	WHJ	C6-C7	4.61	1.48	1.42

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	WHJ	C15-C14-C12	-4.47	106.04	113.49
2	A	401	Y01	CBC-CAV-CAZ	-4.26	104.54	111.52
2	B	401	Y01	CBC-CAV-CAZ	-3.95	105.05	111.52
2	A	401	Y01	CBG-CBI-CBE	-3.80	95.62	100.09
2	A	401	Y01	CAR-CBC-CAV	-3.75	104.85	111.06
2	A	401	Y01	CAC-CBB-CBE	-3.62	106.93	112.96
4	B	601	WHJ	C15-C14-C12	-3.31	107.97	113.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	Y01	CAP-CAQ-CBG	-3.30	98.47	105.12
2	A	401	Y01	CBI-CBG-CBD	-2.98	109.71	114.37
2	B	402	Y01	CBG-CBI-CBE	-2.81	96.79	100.09
2	A	402	Y01	CBG-CBI-CBE	-2.79	96.81	100.09
3	B	501	2CV	C35-N33-C36	-2.72	112.81	115.45
2	A	401	Y01	CAU-CBI-CBE	-2.62	111.89	116.56
3	A	501	2CV	C35-N33-C36	-2.53	112.99	115.45
2	A	402	Y01	CBC-OAW-CAY	-2.52	111.84	117.89
2	B	401	Y01	CAR-CBC-CAV	-2.51	106.91	111.06
2	B	401	Y01	CBG-CBI-CBE	-2.50	97.15	100.09
4	A	601	WHJ	C2-C7-N1	-2.48	120.04	123.38
2	B	401	Y01	OAW-CAY-OAG	-2.45	117.10	123.67
2	B	401	Y01	CAT-CAR-CBC	-2.20	106.25	110.23
2	B	402	Y01	CAV-CAZ-CAI	-2.20	116.84	120.57
2	B	402	Y01	OAW-CBC-CAV	-2.17	103.41	107.98
2	B	401	Y01	CAC-CBB-CBE	-2.14	109.39	112.96
4	A	601	WHJ	C14-C15-C16	-2.14	116.42	120.90
4	A	601	WHJ	C19-C20-C15	-2.10	118.17	121.04
2	A	402	Y01	OAW-CAY-OAG	-2.07	118.10	123.67
2	B	402	Y01	OAW-CAY-OAG	-2.05	118.16	123.67
4	B	601	WHJ	C2-C7-N1	-2.01	120.67	123.38
2	A	402	Y01	CAV-CAZ-CBH	2.05	119.41	116.43
2	A	401	Y01	CAV-CAZ-CBH	2.29	119.76	116.43
2	A	401	Y01	OAW-CBC-CAR	2.40	114.25	108.34
2	A	402	Y01	CAK-CBD-CBF	2.47	113.09	109.71
2	A	401	Y01	CAP-CBE-CBB	2.50	116.50	112.05
2	A	401	Y01	CAO-CBB-CBE	2.69	115.89	110.24
2	A	401	Y01	OAW-CAY-CAM	2.69	117.38	111.53
4	B	601	WHJ	C9-N1-C7	2.83	120.02	116.76
2	B	402	Y01	CAV-CAZ-CBH	2.92	120.68	116.43
2	B	401	Y01	CAO-CBB-CBE	2.96	116.47	110.24
4	B	601	WHJ	C6-C7-N1	3.26	120.93	117.31
4	A	601	WHJ	C6-C7-N1	3.43	121.13	117.31
3	B	505	2CV	C35-N33-C36	3.47	118.82	115.45
4	A	601	WHJ	C9-N1-C7	3.69	121.01	116.76
2	B	402	Y01	OAW-CAY-CAM	3.80	119.78	111.53
2	B	402	Y01	OAW-CBC-CAR	3.82	117.75	108.34
3	A	505	2CV	C35-N33-C36	4.23	119.56	115.45
2	A	402	Y01	OAW-CAY-CAM	4.28	120.84	111.53
2	B	401	Y01	OAW-CAY-CAM	4.36	120.99	111.53
2	B	401	Y01	OAW-CBC-CAR	6.44	124.20	108.34
2	A	401	Y01	OAW-CBC-CAV	6.73	122.12	107.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	Y01	CBC-OAW-CAY-CAM

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	Y01	3	0
2	A	402	Y01	3	0
3	A	501	2CV	3	0
3	A	505	2CV	3	0
4	A	601	WHJ	1	0
2	B	401	Y01	3	0
2	B	402	Y01	1	0
3	B	501	2CV	3	0
3	B	505	2CV	3	0

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	286/315 (90%)	0.69	30 (10%) 8 5	11, 33, 75, 91	0
1	B	298/315 (94%)	0.56	25 (8%) 14 9	13, 32, 60, 80	0
All	All	584/630 (92%)	0.62	55 (9%) 11 6	11, 33, 67, 91	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	MET	8.0
1	A	280	VAL	6.5
1	A	281	MET	6.3
1	A	279	ARG	6.2
1	A	284	ARG	5.8
1	A	234	ALA	5.8
1	A	282	LEU	5.5
1	A	194	GLN	5.5
1	B	322	ASP	5.0
1	A	34	GLU	4.8
1	A	319	LEU	4.6
1	A	278	SER	4.4
1	A	231	TYR	4.4
1	A	287	LYS	4.1
1	B	188	GLN	4.1
1	B	148	ARG	4.1
1	A	286	HIS	4.1
1	B	187	PRO	3.6
1	A	236	GLU	3.5
1	B	349	PHE	3.3
1	B	351	LYS	3.3
1	B	346	SER	3.3
1	B	236	GLU	3.2
1	B	317	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	147	PHE	3.2
1	B	186	ASP	3.2
1	B	347	PRO	3.1
1	A	285	GLU	3.0
1	B	320	VAL	3.0
1	B	358	ALA	3.0
1	B	318	ASP	3.0
1	A	290	LYS	2.9
1	A	214	ILE	2.9
1	B	316	ASN	2.8
1	B	348	ASP	2.8
1	A	198	CYS	2.8
1	A	354	LYS	2.8
1	A	347	PRO	2.7
1	A	147	PHE	2.7
1	B	71	ARG	2.7
1	A	235	LYS	2.7
1	B	280	VAL	2.6
1	B	214	ILE	2.6
1	A	318	ASP	2.5
1	A	358	ALA	2.5
1	B	168	ILE	2.3
1	B	319	LEU	2.3
1	A	195	ASP	2.2
1	B	215	SER	2.2
1	A	232	ARG	2.2
1	A	210	ALA	2.2
1	A	353	PHE	2.1
1	B	125	VAL	2.1
1	A	233	GLU	2.0
1	B	152	LEU	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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	2CV	B	504	8/26	0.85	0.54	14.19	58,64,67,69	0
3	2CV	A	504	26/26	0.50	0.51	12.48	40,72,90,91	0
3	2CV	A	505	26/26	0.57	0.43	3.69	40,85,98,99	0
3	2CV	B	505	26/26	0.68	0.34	2.55	30,77,88,90	0
2	Y01	A	402	35/35	0.82	0.28	2.26	29,49,95,97	0
3	2CV	B	502	16/26	0.72	0.32	2.15	20,52,73,78	0
3	2CV	B	501	20/26	0.79	0.34	1.79	17,51,62,64	0
4	WHJ	A	601	27/27	0.91	0.26	1.53	21,24,67,70	0
5	NA	A	701	1/1	0.75	0.49	1.48	48,48,48,48	0
3	2CV	A	503	20/26	0.72	0.39	1.43	50,73,85,86	0
4	WHJ	B	601	27/27	0.92	0.26	1.09	16,25,49,54	0
3	2CV	A	501	26/26	0.73	0.29	0.92	16,50,62,63	0
2	Y01	A	401	35/35	0.85	0.29	0.89	15,27,47,52	0
3	2CV	B	503	16/26	0.75	0.33	0.66	48,66,89,90	0
2	Y01	B	402	35/35	0.88	0.21	0.54	35,41,74,75	0
2	Y01	B	401	35/35	0.91	0.26	0.22	13,22,47,50	0
3	2CV	A	502	5/26	0.81	0.28	0.14	34,37,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.