



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:58 PM GMT

PDB ID : 2Y04  
Title : TURKEY BETA1 ADRENERGIC RECEPTOR WITH STABILISING MUTATIONS AND BOUND PARTIAL AGONIST SALBUTAMOL  
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 : 3.05 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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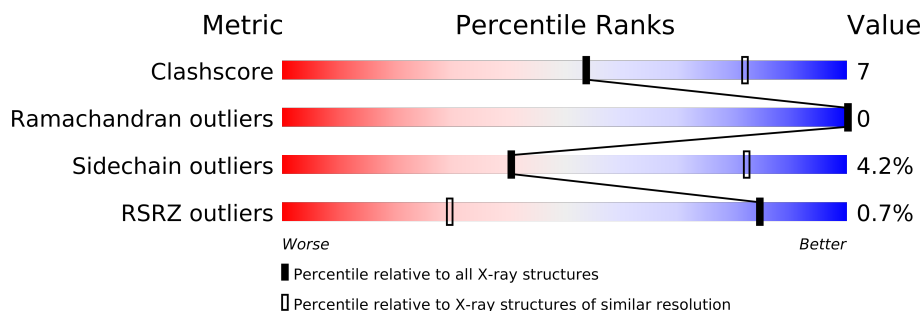
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.05 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	79885	2629 (3.12-3.00)
Ramachandran outliers	78287	2536 (3.12-3.00)
Sidechain outliers	78261	2539 (3.12-3.00)
RSRZ outliers	66119	2081 (3.12-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	Y01	B	402	-	X
3	2CV	A	503	-	X
3	2CV	A	504	-	X
3	2CV	A	505	-	X
3	2CV	B	504	-	X
3	2CV	B	505	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5019 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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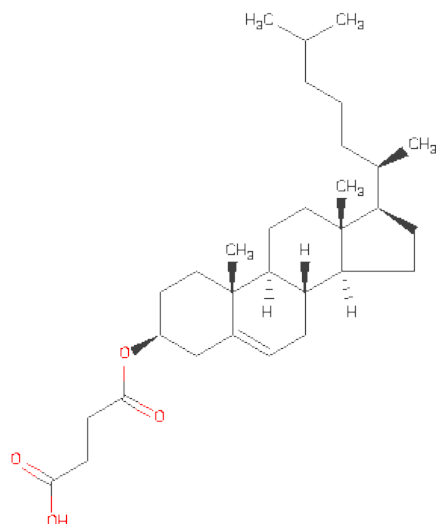
Chain	Residue	Modelled	Actual	Comment	Reference
A	.	-	HIS	DELETION	UNP P07700
A	.	-	GLN	DELETION	UNP P07700
A	.	-	PRO	DELETION	UNP P07700
A	.	-	ILE	DELETION	UNP P07700
A	.	-	LEU	DELETION	UNP P07700
A	.	-	GLY	DELETION	UNP P07700
A	.	-	ASN	DELETION	UNP P07700
A	.	-	GLY	DELETION	UNP P07700
A	.	-	ARG	DELETION	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

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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:  $C_{31}H_{50}O_4$ ).



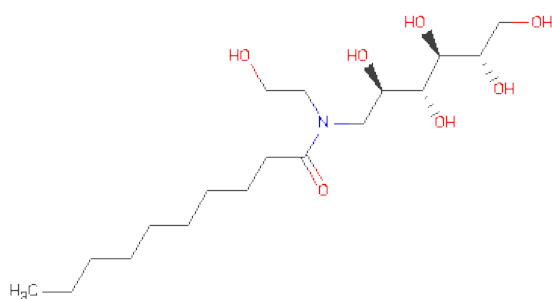
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	31	4		
2	A	1	Total	C	O	0	0
			35	31	4		

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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:  $C_{18}H_{37}NO_7$ ).



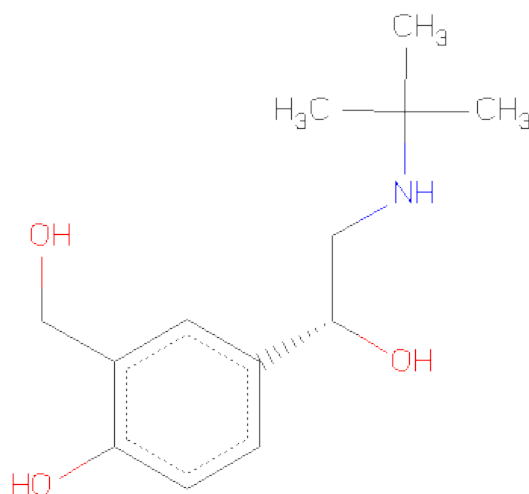
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	18	1	7		
3	A	1	Total	C			0	0
			5	5				
3	A	1	Total	C	N	O	0	0
			20	15	1	4		
3	A	1	Total	C	N	O	0	0
			26	18	1	7		
3	A	1	Total	C	N	O	0	0
			26	18	1	7		
3	B	1	Total	C	N	O	0	0
			20	15	1	4		
3	B	1	Total	C	N	O	0	0
			16	13	1	2		
3	B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

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

- Molecule 4 is SALBUTAMOL (three-letter code: 68H) (formula:  $C_{13}H_{21}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	13	1	3		
4	B	1	Total	C	N	O	0	0
			17	13	1	3		

- 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.

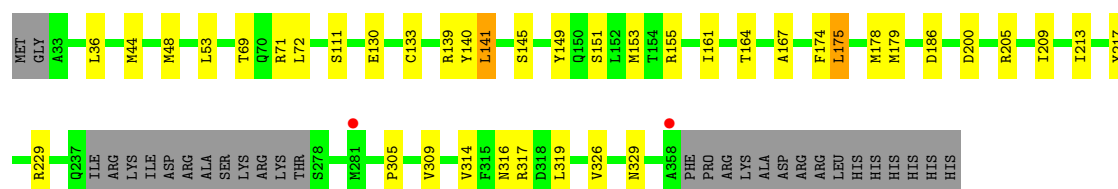
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	O	0	0
			10	10		
6	B	5	Total	O	0	0
			5	5		

### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

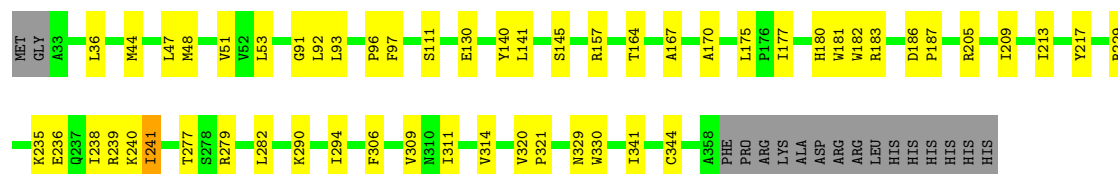
#### • Molecule 1: BETA-1 ADRENERGIC RECEPTOR

Chain A: 



#### • Molecule 1: BETA-1 ADRENERGIC RECEPTOR

Chain B: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.90Å 62.00Å 101.50Å 90.00° 109.90° 90.00°	Depositor
Resolution (Å)	95.40 – 3.05 38.62 – 3.05	Depositor EDS
% Data completeness (in resolution range)	95.0 (95.40-3.05) 95.0 (38.62-3.05)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.223 , 0.255 0.227 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	60.6	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 19354 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	5019	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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, 68H

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	0.53	0/2323	0.60	0/3167
1	B	0.52	0/2426	0.61	0/3303
All	All	0.53	0/4749	0.61	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2269	0	2349	25	0
1	B	2371	0	2471	36	0
2	A	70	0	98	3	0
2	B	70	0	98	5	0
3	A	103	0	146	9	0
3	B	86	0	122	6	0
4	A	17	0	20	0	0
4	B	17	0	20	1	0
5	A	1	0	0	0	0
6	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	5	0	0	0	0
All	All	5019	0	5324	71	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (71) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:205:ARG:HG2	1:A:314:VAL:HG13	1.56	0.87
3:B:501:2CV:H272	3:B:501:2CV:H601	1.62	0.82
1:B:209:ILE:HD11	1:B:314:VAL:HG11	1.67	0.77
1:B:241:ILE:HD12	1:B:282:LEU:HD23	1.70	0.74
1:A:316:ASN:ND2	1:A:319:LEU:HD13	2.02	0.74
1:B:130:GLU:HG2	2:B:401:Y01:HAC3	1.78	0.65
1:A:316:ASN:HD22	1:A:319:LEU:HD13	1.62	0.64
1:B:170:ALA:HB2	3:B:505:2CV:H03C	1.83	0.61
1:B:241:ILE:CD1	1:B:282:LEU:HD23	2.31	0.59
3:A:501:2CV:H182	1:B:164:THR:HG23	1.86	0.57
3:A:503:2CV:H182	2:B:401:Y01:HAL2	1.86	0.56
1:B:140:TYR:CE1	1:B:229:ARG:HB3	2.41	0.55
1:A:141:LEU:HD23	1:A:149:TYR:HD1	1.71	0.55
1:A:205:ARG:CG	1:A:314:VAL:HG13	2.35	0.55
3:B:501:2CV:C60	3:B:501:2CV:H272	2.33	0.54
1:B:239:ARG:O	1:B:240:LYS:HB2	2.08	0.53
1:A:174:PHE:O	1:A:178:MET:HG2	2.09	0.52
1:B:309:VAL:HG22	1:B:320:VAL:HG21	1.92	0.52
1:B:180:HIS:CE1	1:B:183:ARG:HH21	2.28	0.52
1:A:175:LEU:HD13	1:A:179:MET:HG3	1.93	0.51
1:A:130:GLU:HG2	2:A:401:Y01:HAC3	1.94	0.50
1:B:167:ALA:HB2	3:B:505:2CV:H181	1.95	0.49
1:B:177:ILE:HA	1:B:182:TRP:CD1	2.47	0.48
1:B:306:PHE:CZ	4:B:601:68H:HA	2.48	0.48
1:B:180:HIS:CE1	1:B:183:ARG:NH2	2.81	0.48
1:A:44:MET:O	1:A:48:MET:HG2	2.13	0.48
1:B:44:MET:O	1:B:48:MET:HG2	2.12	0.48
1:B:140:TYR:HE1	1:B:229:ARG:HB3	1.76	0.48
1:A:205:ARG:NH1	1:A:314:VAL:O	2.46	0.48
1:B:290:LYS:O	1:B:294:ILE:HG13	2.13	0.48
1:A:205:ARG:NH1	3:A:503:2CV:O34	2.47	0.48
1:B:48:MET:HE1	1:B:330:TRP:CZ3	2.49	0.48
1:A:161:ILE:HG12	2:A:401:Y01:HBC	1.94	0.47
1:B:186:ASP:OD1	1:B:187:PRO:HD2	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:326:VAL:HG11	3:A:504:2CV:H02C	1.95	0.47
1:A:167:ALA:HB1	1:B:181:TRP:CZ3	2.50	0.46
1:B:93:LEU:O	1:B:97:PHE:HD2	1.99	0.46
1:A:317:ARG:HB2	1:A:317:ARG:HE	1.52	0.46
1:B:320:VAL:HA	1:B:321:PRO:HD2	1.82	0.45
2:B:401:Y01:HAC3	2:B:401:Y01:HAJ2	1.83	0.45
1:A:149:TYR:CE1	1:A:153:MET:HG3	2.52	0.45
1:B:92:LEU:O	1:B:96:PRO:HG2	2.17	0.45
3:A:503:2CV:H181	1:B:157:ARG:HD3	1.98	0.44
3:A:501:2CV:H271	3:B:505:2CV:H352	2.00	0.43
1:A:209:ILE:O	1:A:213:ILE:HG13	2.18	0.43
1:B:341:ILE:O	1:B:344:CYS:HB2	2.19	0.43
1:B:209:ILE:O	1:B:213:ILE:HG13	2.19	0.43
1:A:305:PRO:O	1:A:309:VAL:HG23	2.18	0.43
1:A:139:ARG:NE	1:A:139:ARG:HA	2.34	0.42
3:A:505:2CV:H37	3:A:505:2CV:H602	2.00	0.42
1:A:140:TYR:CE1	1:A:229:ARG:HB3	2.54	0.42
3:A:503:2CV:H271	3:A:503:2CV:H352	1.80	0.42
1:B:47:LEU:O	1:B:51:VAL:HG23	2.20	0.42
1:A:69:THR:HG22	1:A:72:LEU:H	1.84	0.42
2:B:401:Y01:CAR	2:B:401:Y01:OAG	2.67	0.42
1:B:91:GLY:O	1:B:96:PRO:HD3	2.20	0.42
3:A:505:2CV:H271	3:A:505:2CV:H352	1.82	0.42
1:B:205:ARG:NH1	1:B:314:VAL:O	2.53	0.41
1:B:277:THR:C	1:B:279:ARG:H	2.24	0.41
3:B:502:2CV:H272	3:B:502:2CV:H352	1.85	0.41
1:B:277:THR:O	1:B:279:ARG:N	2.53	0.41
1:A:164:THR:HG21	2:A:401:Y01:HAT2	2.01	0.41
1:A:69:THR:HG22	1:A:71:ARG:HB3	2.03	0.41
1:B:48:MET:HE3	1:B:48:MET:HB3	1.92	0.41
1:A:213:ILE:HA	1:A:217:TYR:HB2	2.03	0.41
1:A:71:ARG:HA	1:A:71:ARG:HE	1.86	0.41
1:B:180:HIS:C	1:B:182:TRP:H	2.24	0.40
1:B:213:ILE:HA	1:B:217:TYR:HB2	2.03	0.40
1:B:311:ILE:O	1:B:314:VAL:HB	2.21	0.40
1:B:235:LYS:O	1:B:238:ILE:HG13	2.22	0.40
2:B:401:Y01:HAS2	2:B:401:Y01:HAD2	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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%)	268 (95%)	14 (5%)	0	100	100
1	B	296/315 (94%)	281 (95%)	15 (5%)	0	100	100
All	All	578/630 (92%)	549 (95%)	29 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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%)	235 (95%)	12 (5%)	35	77
1	B	258/273 (94%)	249 (96%)	9 (4%)	48	87
All	All	505/546 (92%)	484 (96%)	21 (4%)	40	82

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	53	LEU
1	A	111	SER
1	A	133	CYS
1	A	141	LEU
1	A	145	SER
1	A	151	SER
1	A	155	ARG
1	A	175	LEU
1	A	186	ASP
1	A	200	ASP

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Mol	Chain	Res	Type
1	A	329	ASN
1	B	36	LEU
1	B	53	LEU
1	B	111	SER
1	B	141	LEU
1	B	145	SER
1	B	175	LEU
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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	335	ASN
1	B	286	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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	-	38,38,38	1.17	2 (5%)	57,57,57	1.83	12 (21%)
2	Y01	A	402	-	38,38,38	1.29	2 (5%)	57,57,57	1.24	5 (8%)
3	2CV	A	501	-	25,25,25	0.63	0	30,30,30	1.31	3 (10%)
3	2CV	A	502	-	4,4,25	0.63	0	3,3,30	0.63	0
3	2CV	A	503	-	18,19,25	4.02	1 (5%)	18,21,30	0.56	0
3	2CV	A	504	-	25,25,25	1.07	2 (8%)	30,30,30	0.71	0
3	2CV	A	505	-	25,25,25	0.87	0	30,30,30	0.95	2 (6%)
4	68H	A	601	-	17,17,17	1.74	2 (11%)	24,24,24	1.99	6 (25%)
2	Y01	B	401	-	38,38,38	1.26	3 (7%)	57,57,57	1.80	14 (24%)
2	Y01	B	402	-	38,38,38	1.27	2 (5%)	57,57,57	1.24	6 (10%)
3	2CV	B	501	-	18,19,25	4.20	1 (5%)	18,21,30	0.89	1 (5%)
3	2CV	B	502	-	14,15,25	0.82	0	14,16,30	0.53	0
3	2CV	B	503	-	14,15,25	0.84	1 (7%)	14,16,30	0.60	0
3	2CV	B	504	-	7,7,25	1.22	1 (14%)	7,7,30	0.74	0
3	2CV	B	505	-	25,25,25	0.75	0	30,30,30	0.87	2 (6%)
4	68H	B	601	-	17,17,17	1.65	1 (5%)	24,24,24	1.14	1 (4%)

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	-	-	0/19/77/77	0/0/4/4
2	Y01	A	402	-	-	1/19/77/77	0/0/4/4
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	-	-	0/20/22/34	0/0/0/0
3	2CV	A	504	-	-	0/34/34/34	0/0/0/0
3	2CV	A	505	-	-	0/34/34/34	0/0/0/0
4	68H	A	601	-	-	0/12/12/12	0/1/1/1
2	Y01	B	401	-	-	1/19/77/77	0/0/4/4
2	Y01	B	402	-	-	0/19/77/77	0/0/4/4
3	2CV	B	501	-	-	0/20/22/34	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	68H	B	601	-	-	0/12/12/12	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	2CV	O49-C40	17.64	1.44	1.25
3	A	503	2CV	O49-C40	16.83	1.44	1.25
4	A	601	68H	C11-C12	6.11	1.49	1.39
4	B	601	68H	C11-C12	5.97	1.48	1.39
2	A	402	Y01	CAK-CAI	-5.03	1.39	1.50
2	B	401	Y01	CAK-CAI	-5.01	1.39	1.50
2	B	402	Y01	CAK-CAI	-4.71	1.39	1.50
2	A	401	Y01	CAK-CAI	-4.59	1.40	1.50
3	A	504	2CV	C36-C37	2.91	1.57	1.52
2	A	401	Y01	CAI-CAZ	2.86	1.40	1.33
3	B	504	2CV	C15-C18	-2.72	1.54	1.55
2	B	401	Y01	CAI-CAZ	2.69	1.40	1.33
2	B	402	Y01	CAI-CAZ	2.61	1.40	1.33
2	A	402	Y01	CAI-CAZ	2.39	1.39	1.33
4	A	601	68H	C4-N1	-2.24	1.45	1.48
2	B	401	Y01	CAR-CBC	2.15	1.56	1.51
3	A	504	2CV	C27-C30	2.13	1.56	1.51
3	B	503	2CV	C27-C30	2.10	1.56	1.51

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	68H	C3-N1-C4	7.74	124.80	116.50
2	B	401	Y01	OAW-CBC-CAR	6.77	125.14	108.36
2	A	401	Y01	CAR-CBC-CAV	-5.07	102.53	111.10
2	A	401	Y01	OAW-CBC-CAR	5.01	120.77	108.36
2	B	401	Y01	OAW-CAY-CAM	4.96	122.43	111.56
2	A	402	Y01	OAW-CAY-CAM	4.68	121.80	111.56
4	B	601	68H	C3-N1-C4	4.43	121.25	116.50
3	A	501	2CV	C37-C36-N33	4.31	119.54	113.35
2	B	402	Y01	OAW-CAY-CAM	4.25	120.87	111.56
2	A	401	Y01	OAW-CBC-CAV	4.05	117.48	108.03
2	A	401	Y01	CAC-CBB-CBE	-4.01	105.93	112.96
2	A	401	Y01	CBC-CAV-CAZ	-3.82	105.19	111.51
3	A	505	2CV	C35-N33-C36	3.26	120.22	116.29
2	B	402	Y01	OAW-CBC-CAR	3.26	116.44	108.36
2	B	401	Y01	CAC-CBB-CBE	-3.15	107.44	112.96
2	A	401	Y01	CBG-CBI-CBE	-3.11	95.95	100.07
2	B	401	Y01	CAR-CBC-CAV	-3.01	106.01	111.10
2	A	401	Y01	OAW-CAY-CAM	2.95	118.03	111.56
2	A	402	Y01	CAV-CAZ-CBH	2.84	120.80	116.42
2	A	401	Y01	CAQ-CBG-CBD	-2.84	114.51	119.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	Y01	CAO-CBB-CBE	2.72	116.36	110.25
2	A	402	Y01	CAR-CBC-CAV	2.67	115.61	111.10
2	A	401	Y01	CBF-CBD-CBG	2.57	112.45	109.04
2	B	401	Y01	CBC-CAV-CAZ	-2.54	107.32	111.51
4	A	601	68H	C13-C8-C1	2.51	123.38	120.10
2	B	401	Y01	OAW-CAY-OAG	-2.50	116.94	123.65
4	A	601	68H	C2-C12-C11	-2.49	116.40	119.84
2	B	401	Y01	CAU-CBI-CBE	-2.45	111.94	116.53
3	A	505	2CV	C42-C41-C40	2.44	116.41	112.43
3	B	505	2CV	C37-C36-N33	2.43	116.84	113.35
3	A	501	2CV	C35-N33-C36	-2.41	113.38	116.29
3	A	501	2CV	C37-C40-C41	2.40	116.34	112.43
3	B	505	2CV	C42-C41-C40	2.40	116.34	112.43
4	A	601	68H	C1-C3-N1	-2.35	107.64	110.79
2	B	402	Y01	CAV-CAZ-CBH	2.29	119.94	116.42
2	B	401	Y01	CBG-CBI-CBE	-2.25	97.08	100.07
2	B	402	Y01	CAP-CAQ-CBG	-2.24	100.60	105.14
2	A	402	Y01	CAK-CBD-CBF	2.21	112.72	109.68
2	A	401	Y01	CAS-CAU-CBI	-2.17	108.89	112.83
2	B	402	Y01	CAU-CBI-CBE	-2.15	112.49	116.53
2	B	401	Y01	CAQ-CBG-CBD	-2.14	115.62	119.03
2	B	401	Y01	CAV-CAZ-CBH	2.14	119.71	116.42
4	A	601	68H	C9-C8-C1	-2.14	116.55	120.75
2	B	401	Y01	CAQ-CBG-CBI	-2.13	100.82	103.82
2	B	402	Y01	CBG-CBI-CBE	-2.13	97.25	100.07
2	B	401	Y01	CAS-CBF-CBH	-2.10	110.17	113.08
3	B	501	2CV	C60-C35-N33	2.09	117.91	112.30
2	B	401	Y01	CAT-CBH-CBF	2.06	111.34	108.60
2	A	401	Y01	CBI-CBE-CBB	-2.02	115.71	119.45
2	B	401	Y01	CBI-CBE-CBB	-2.02	115.72	119.45
4	A	601	68H	C2-C12-C13	2.02	125.21	120.49
2	A	402	Y01	OAW-CAY-OAG	-2.01	118.27	123.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	Y01	CAY-OAW-CBC-CAR
2	A	402	Y01	CBC-OAW-CAY-CAM

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	286/315 (90%)	-0.21	2 (0%) 84 30	17, 42, 86, 99	0
1	B	298/315 (94%)	-0.32	0 100 100	18, 41, 82, 90	0
All	All	584/630 (92%)	-0.27	2 (0%) 84 50	17, 42, 84, 99	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	MET	3.2
1	A	358	ALA	2.1

### 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 ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	2CV	B	504	8/26	0.74	27.22	52,65,69,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	2CV	A	504	26/26	0.62	24.48	62,90,113,115	0
3	2CV	A	505	26/26	0.37	3.82	75,119,128,129	0
2	Y01	B	402	35/35	0.33	3.43	50,59,90,91	0
3	2CV	B	505	26/26	0.41	3.25	77,109,114,117	0
3	2CV	A	503	20/26	0.33	2.35	58,81,92,93	0
2	Y01	A	402	35/35	0.23	1.88	66,70,114,116	0
3	2CV	B	502	16/26	0.30	1.86	24,64,84,86	0
3	2CV	B	503	16/26	0.46	1.56	59,86,106,107	0
3	2CV	A	501	26/26	0.23	0.77	13,57,76,78	0
3	2CV	A	502	5/26	0.23	0.74	36,39,41,42	0
4	68H	B	601	17/17	0.17	0.62	25,33,38,40	0
3	2CV	B	501	20/26	0.17	0.46	24,58,69,71	0
2	Y01	A	401	35/35	0.18	0.31	13,23,66,71	0
2	Y01	B	401	35/35	0.19	0.26	13,20,50,54	0
5	NA	A	701	1/1	0.21	-0.18	59,59,59,59	0
4	68H	A	601	17/17	0.14	-0.39	13,24,30,34	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.