Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:44 am BST

PDB ID	:	4XAS
Title	:	mGluR2 ECD ligand complex
Authors	:	Clawson, D.K.
Deposited on	:	2014-12-15
Resolution	:	2.35 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 following versions of software and data (see references ⓘ) were used in the production of this report:

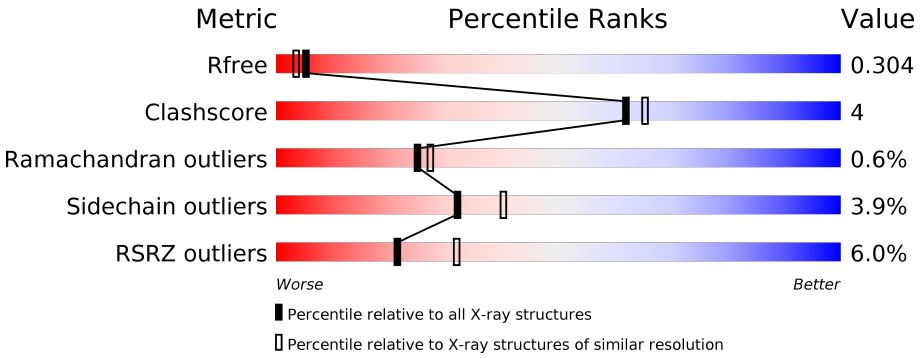
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 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	503	5% 74% 13% • 13%
1	B	503	6% 75% 12% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7067 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 Metabotropic glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3424	2179	601	631	13			
1	B	438	Total	C	N	O	S	0	0	0
			3406	2165	599	629	13			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q14416
A	0	ALA	-	expression tag	UNP Q14416
A	1	LEU	-	expression tag	UNP Q14416
A	234	SER	CYS	conflict	UNP Q14416
A	302	GLU	SER	conflict	UNP Q14416
A	494	GLU	-	expression tag	UNP Q14416
A	495	GLY	-	expression tag	UNP Q14416
A	496	HIS	-	expression tag	UNP Q14416
A	497	HIS	-	expression tag	UNP Q14416
A	498	HIS	-	expression tag	UNP Q14416
A	499	HIS	-	expression tag	UNP Q14416
A	500	HIS	-	expression tag	UNP Q14416
A	501	HIS	-	expression tag	UNP Q14416
B	-1	MET	-	initiating methionine	UNP Q14416
B	0	ALA	-	expression tag	UNP Q14416
B	1	LEU	-	expression tag	UNP Q14416
B	234	SER	CYS	conflict	UNP Q14416
B	302	GLU	SER	conflict	UNP Q14416
B	494	GLU	-	expression tag	UNP Q14416
B	495	GLY	-	expression tag	UNP Q14416
B	496	HIS	-	expression tag	UNP Q14416
B	497	HIS	-	expression tag	UNP Q14416
B	498	HIS	-	expression tag	UNP Q14416
B	499	HIS	-	expression tag	UNP Q14416
B	500	HIS	-	expression tag	UNP Q14416

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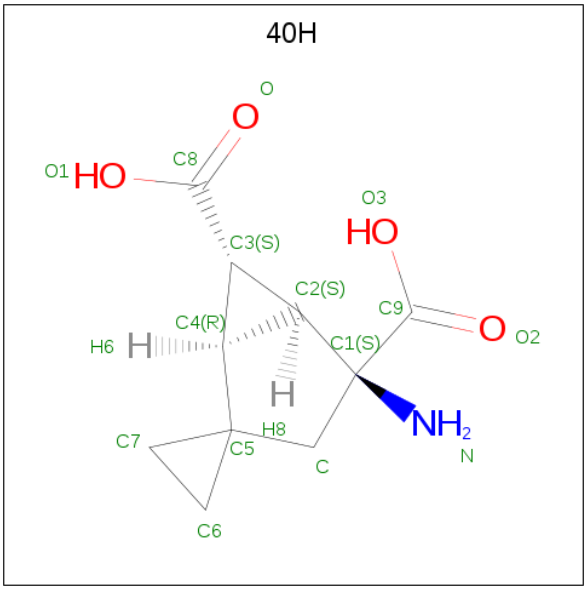
Chain	Residue	Modelled	Actual	Comment	Reference
B	501	HIS	-	expression tag	UNP Q14416

- Molecule 2 is (1R,4S,5S,6S)-4-aminospiro[bicyclo[3.1.0]hexane-2,1'-cyclopropane]-4,6-dicarboxylic acid (three-letter code: 40H) (formula: $C_{10}H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	1	4		
2	B	1	Total	C	N	O	0	0
			15	10	1	4		

- Molecule 3 is water.

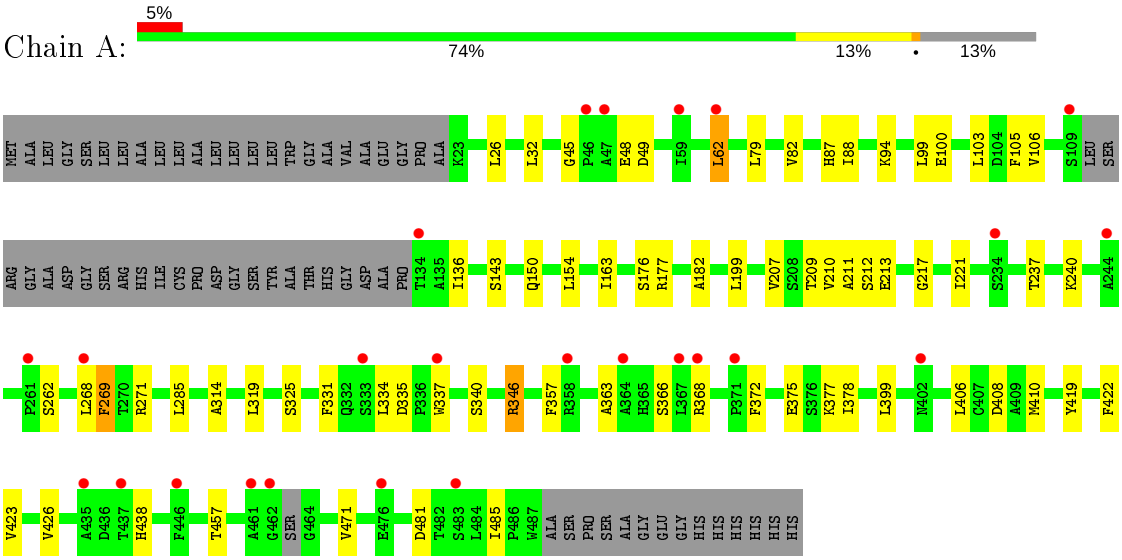
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total	O	0	0
			119	119		
3	B	88	Total	O	0	0
			88	88		

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 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.

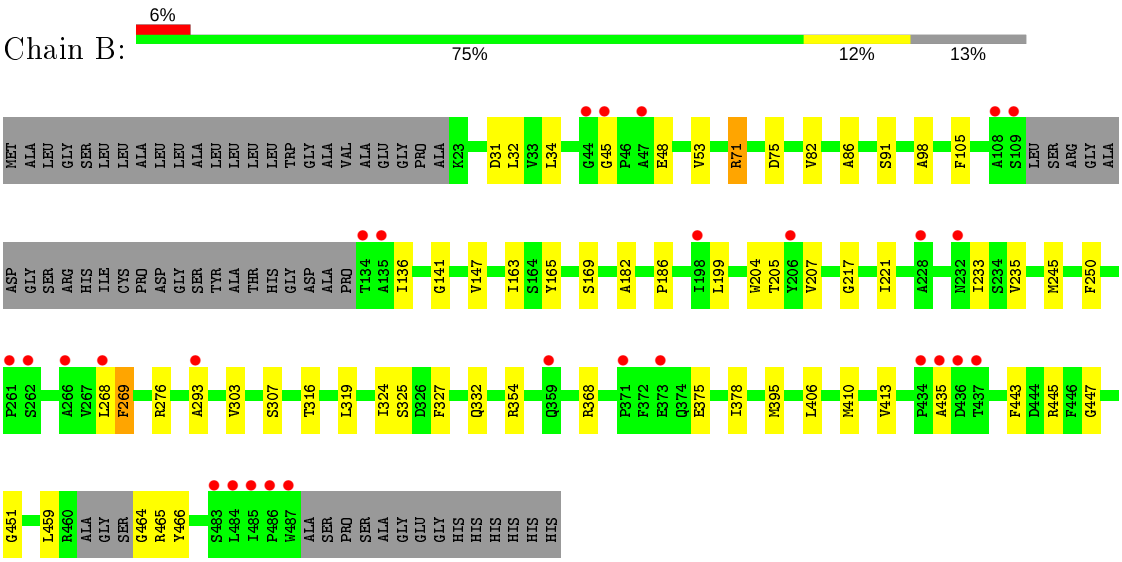
- Molecule 1: Metabotropic glutamate receptor 2

Chain A:



- Molecule 1: Metabotropic glutamate receptor 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	78.04Å 135.86Å 92.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.70 – 2.35 19.70 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.70-2.35) 97.5 (19.70-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.26Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.5	Depositor
R, R_{free}	0.212 , 0.280 0.229 , 0.304	Depositor DCC
R_{free} test set	1844 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7067	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: 40H

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	0.51	0/3507	0.72	0/4759
1	B	0.53	0/3489	0.71	0/4739
All	All	0.52	0/6996	0.71	0/9498

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	3424	0	3278	31	0
1	B	3406	0	3242	28	0
2	A	15	0	11	1	0
2	B	15	0	10	0	0
3	A	119	0	0	1	0
3	B	88	0	0	0	0
All	All	7067	0	6541	59	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 (59) 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:221:ILE:HG12	1:A:269:PHE:HB2	1.61	0.79
1:B:395:MET:HE1	1:B:413:VAL:HG13	1.71	0.71
1:A:99:LEU:HD22	1:A:150:GLN:HB3	1.74	0.68
1:A:45:GLY:H	1:A:48:GLU:HG3	1.59	0.67
1:A:211:ALA:HB2	1:A:221:ILE:HG13	1.77	0.67
1:B:163:ILE:HA	1:B:182:ALA:O	1.96	0.66
1:A:213:GLU:HG2	1:A:240:LYS:HD2	1.76	0.66
1:A:210:VAL:HB	1:A:268:LEU:HD22	1.82	0.62
1:B:199:LEU:HD23	1:B:204:TRP:HE3	1.63	0.61
1:B:221:ILE:HG12	1:B:269:PHE:HB2	1.87	0.56
1:A:471:VAL:HG11	1:A:485:ILE:HG23	1.87	0.56
1:B:141:GLY:HA2	1:B:165:TYR:CE2	2.41	0.55
1:B:32:LEU:HG	1:B:406:LEU:HD11	1.88	0.55
1:A:331:PHE:HA	1:A:334:LEU:HD12	1.89	0.54
1:A:319:LEU:HD22	1:A:377:LYS:HE3	1.91	0.53
1:B:186:PRO:HD2	1:B:319:LEU:HD23	1.90	0.53
1:A:199:LEU:HD13	1:A:207:VAL:HG11	1.93	0.51
1:B:443:PHE:HB3	1:B:447:GLY:HA2	1.93	0.50
1:B:105:PHE:HA	1:B:136:ILE:HG13	1.94	0.50
1:B:459:LEU:O	1:B:466:TYR:HA	2.12	0.50
1:A:423:VAL:O	1:A:426:VAL:HG22	2.12	0.49
1:B:245:MET:HB2	1:B:250:PHE:CE2	2.48	0.49
1:A:105:PHE:HA	1:A:136:ILE:HG13	1.95	0.48
1:B:276:ARG:HB2	1:B:303:VAL:HA	1.96	0.47
1:A:375:GLU:O	1:A:378:ILE:HG12	2.14	0.47
1:B:45:GLY:H	1:B:48:GLU:HG3	1.78	0.47
1:A:79:LEU:HD22	1:A:82:VAL:HB	1.97	0.46
1:B:34:LEU:O	1:B:86:ALA:HA	2.15	0.46
1:A:422:PHE:O	1:A:426:VAL:HG13	2.15	0.46
1:B:91:SER:HB2	1:B:98:ALA:HB2	1.98	0.45
1:A:26:LEU:HD13	1:A:62:LEU:HD11	1.98	0.45
1:A:212:SER:O	1:A:217:GLY:HA3	2.17	0.45
1:A:399:LEU:HD12	1:A:410:MET:HG3	1.99	0.45
1:B:98:ALA:CB	1:B:147:VAL:HG13	2.47	0.45
1:A:26:LEU:HB3	1:A:88:ILE:HB	1.99	0.45
1:B:395:MET:CE	1:B:413:VAL:HG13	2.42	0.44
1:A:106:VAL:HG21	1:A:154:LEU:HD11	1.99	0.44
1:A:209:THR:HB	1:A:221:ILE:HD12	1.99	0.44
1:A:32:LEU:HD21	1:A:406:LEU:HD21	1.99	0.44
1:A:419:TYR:HA	1:A:423:VAL:HB	1.99	0.44
1:B:207:VAL:O	1:B:235:VAL:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:GLU:HB3	1:B:378:ILE:HG12	1.99	0.44
1:B:293:ALA:HB3	1:B:316:THR:HG22	2.00	0.43
1:B:332:GLN:HB3	1:B:368:ARG:HG2	2.00	0.43
1:B:324:ILE:HG13	1:B:327:PHE:HB3	1.99	0.43
1:B:217:GLY:HA2	1:B:269:PHE:HB3	2.00	0.43
1:A:32:LEU:CD2	1:A:406:LEU:HD21	2.49	0.42
1:A:314:ALA:O	1:A:457:THR:HA	2.20	0.42
1:B:395:MET:HE2	1:B:410:MET:HG2	2.01	0.42
1:A:271:ARG:HA	2:A:601:40H:C6	2.49	0.42
1:B:205:THR:HA	1:B:233:ILE:HG23	2.01	0.42
1:B:31:ASP:HB2	1:B:82:VAL:HG13	2.02	0.42
1:B:71:ARG:HD2	1:B:71:ARG:HA	1.86	0.42
1:A:100:GLU:O	1:A:103:LEU:HB2	2.19	0.41
1:A:337:TRP:CH2	1:A:363:ALA:HA	2.55	0.41
1:A:94:LYS:HG3	3:A:813:HOH:O	2.19	0.41
1:A:163:ILE:HA	1:A:182:ALA:O	2.20	0.40
1:A:346:ARG:HG2	1:A:357:PHE:CE2	2.55	0.40
1:B:464:GLY:HA2	1:B:465:ARG:HA	1.82	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	434/503 (86%)	407 (94%)	24 (6%)	3 (1%)	22	23
1	B	432/503 (86%)	405 (94%)	25 (6%)	2 (0%)	29	32
All	All	866/1006 (86%)	812 (94%)	49 (6%)	5 (1%)	25	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	435	ALA
1	A	325	SER
1	A	368	ARG
1	B	451	GLY
1	A	372	PHE

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	346/402 (86%)	329 (95%)	17 (5%)	25	29
1	B	344/402 (86%)	334 (97%)	10 (3%)	42	52
All	All	690/804 (86%)	663 (96%)	27 (4%)	32	40

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	62	LEU
1	A	87	HIS
1	A	143	SER
1	A	176	SER
1	A	177	ARG
1	A	237	THR
1	A	262	SER
1	A	269	PHE
1	A	285	LEU
1	A	335	ASP
1	A	340	SER
1	A	346	ARG
1	A	366	SER
1	A	408	ASP
1	A	438	HIS
1	A	481	ASP
1	B	53	VAL
1	B	71	ARG

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Mol	Chain	Res	Type
1	B	75	ASP
1	B	169	SER
1	B	268	LEU
1	B	269	PHE
1	B	307	SER
1	B	325	SER
1	B	354	ARG
1	B	445	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	332	GLN
1	A	469	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	40H	B	601	-	6,17,17	2.00	3 (50%)	11,30,30	1.26	1 (9%)
2	40H	A	601	-	6,17,17	1.65	1 (16%)	11,30,30	1.63	1 (9%)

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	40H	B	601	-	-	0/0/41/41	0/3/3/3
2	40H	A	601	-	-	0/0/41/41	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	40H	C-C5	-3.44	1.49	1.54
2	B	601	40H	C-C5	-3.22	1.49	1.54
2	B	601	40H	C5-C4	-2.59	1.51	1.54
2	B	601	40H	C7-C5	2.04	1.53	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	40H	C8-C3-C2	-4.56	111.64	122.71
2	B	601	40H	C8-C3-C4	-2.42	116.84	122.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	40H	1	0

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^{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	440/503 (87%)	0.27	25 (5%)	23	34	27, 47, 73, 104	0
1	B	438/503 (87%)	0.32	28 (6%)	19	28	24, 47, 79, 130	0
All	All	878/1006 (87%)	0.30	53 (6%)	21	32	24, 47, 77, 130	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	437	THR	9.2
1	A	435	ALA	8.6
1	B	435	ALA	8.5
1	B	134	THR	8.2
1	B	261	PRO	6.1
1	A	402	ASN	5.3
1	A	371	PRO	4.8
1	B	108	ALA	4.6
1	A	337	TRP	4.5
1	A	47	ALA	4.5
1	B	109	SER	4.3
1	B	487	TRP	4.0
1	A	364	ALA	3.9
1	A	46	PRO	3.9
1	B	262	SER	3.9
1	B	486	PRO	3.6
1	A	358	ARG	3.6
1	A	134	THR	3.5
1	B	47	ALA	3.3
1	B	436	ASP	3.3
1	B	228	ALA	3.2
1	B	371	PRO	3.1
1	A	462	GLY	3.0
1	B	434	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	483	SER	2.8
1	B	135	ALA	2.8
1	A	476	GLU	2.8
1	A	446	PHE	2.7
1	B	268	LEU	2.7
1	B	198	ILE	2.6
1	A	234	SER	2.5
1	B	45	GLY	2.5
1	B	206	TYR	2.4
1	B	359	GLN	2.4
1	A	59	ILE	2.4
1	B	485	ILE	2.3
1	A	261	PRO	2.3
1	A	367	LEU	2.3
1	B	266	ALA	2.3
1	B	373	GLU	2.3
1	B	293	ALA	2.3
1	A	437	THR	2.3
1	B	483	SER	2.3
1	A	333	SER	2.2
1	A	461	ALA	2.2
1	A	368	ARG	2.2
1	A	62	LEU	2.2
1	A	109	SER	2.2
1	B	44	GLY	2.2
1	B	484	LEU	2.1
1	B	232	ASN	2.1
1	A	268	LEU	2.1
1	A	244	ALA	2.0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	40H	B	601	15/15	0.95	0.14	25,33,39,40	0
2	40H	A	601	15/15	0.97	0.11	27,31,40,40	0

6.5 Other polymers

There are no such residues in this entry.