Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:29 am BST

PDB ID	:	4XAQ
Title	:	mGluR2 ECD and mGluR3 ECD with ligands
Authors	:	Clawson, D.K.
Deposited on	:	2014-12-15
Resolution	:	2.21 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:

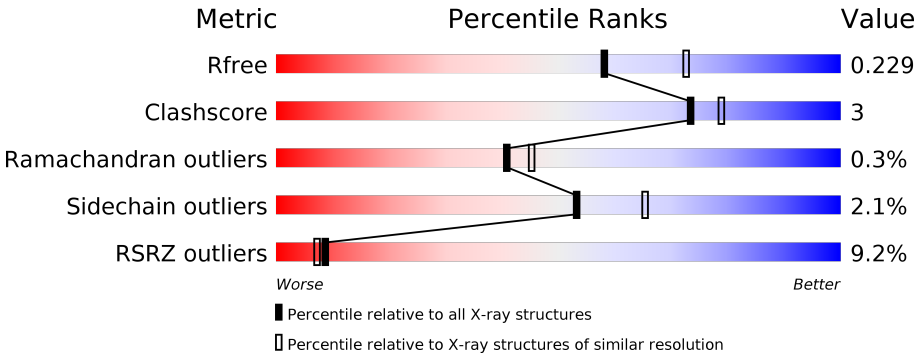
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	11% 80% 8% 12%
1	B	503	6% 78% 9% 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7532 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	443	Total	C	N	O	S	0	0	0
			3475	2206	623	633	13			
1	B	442	Total	C	N	O	S	0	4	0
			3491	2215	624	639	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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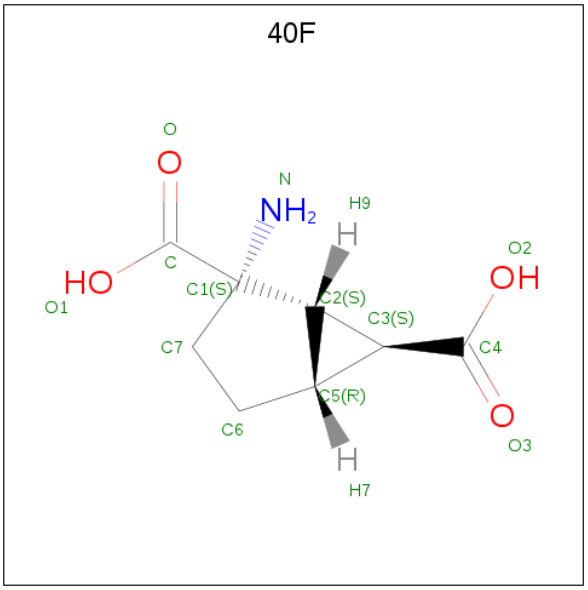
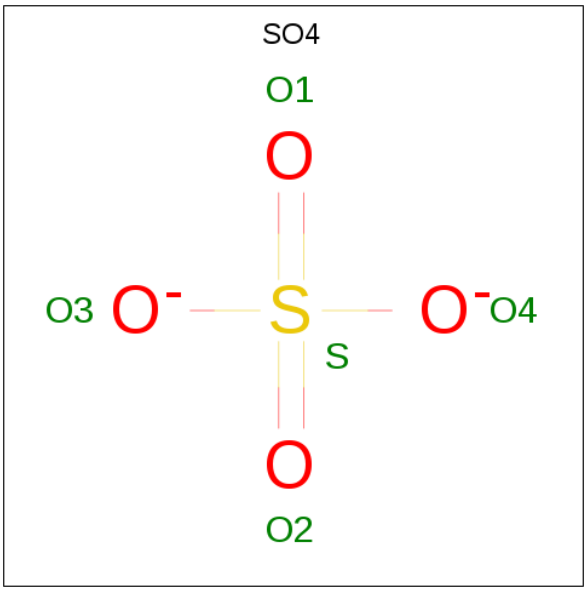
Chain	Residue	Modelled	Actual	Comment	Reference
B	501	HIS	-	expression tag	UNP Q14416

- Molecule 2 is (1S,2S,5R,6S)-2-aminobicyclo[3.1.0]hexane-2,6-dicarboxylic acid (three-letter code: 40F) (formula: $C_8H_{11}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	8	1	4		
2	B	1	Total	C	N	O	0	0
			13	8	1	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	2	Total Cl 2 2	0	0

- Molecule 5 is water.

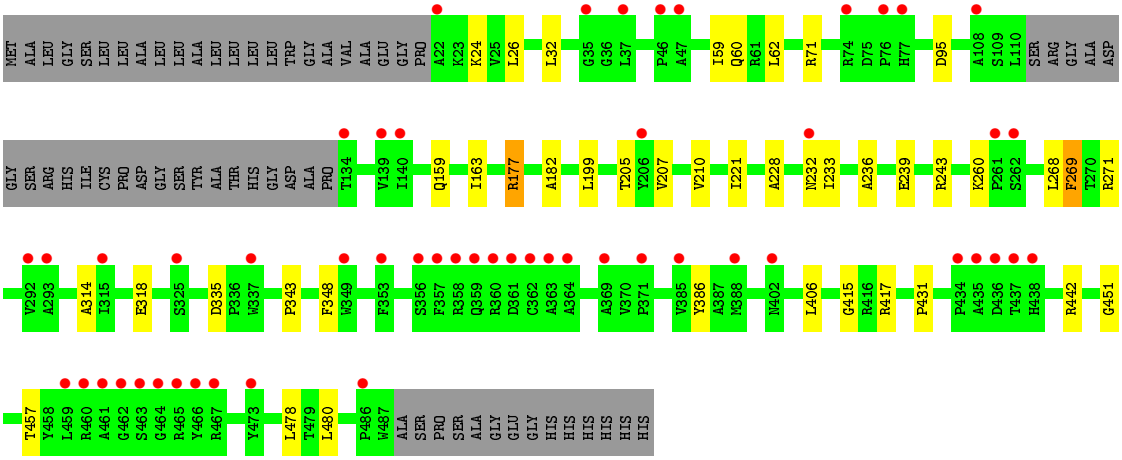
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	226	Total O 226 226	0	0
5	B	301	Total O 301 301	0	0

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.

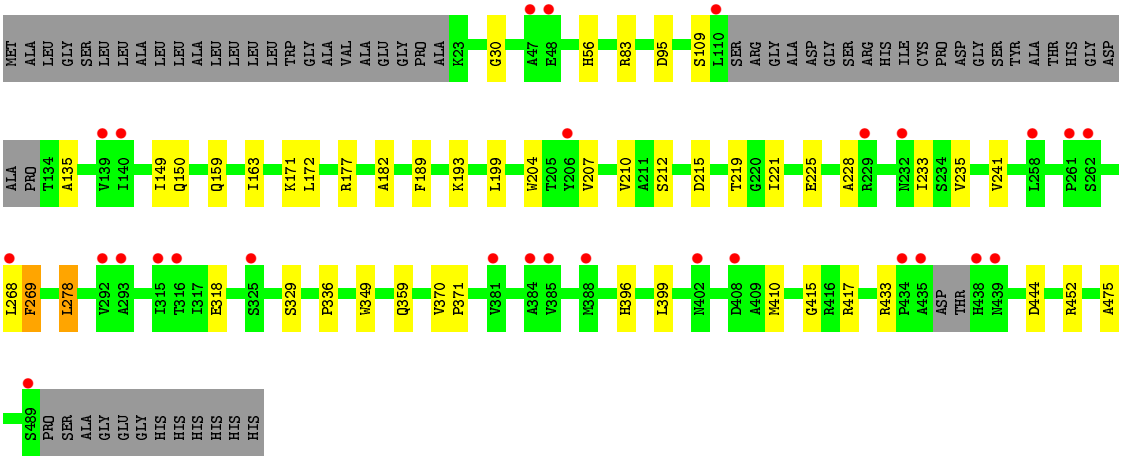
- Molecule 1: Metabotropic glutamate receptor 2

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	81.64Å 159.65Å 93.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.52 – 2.21 27.44 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.52-2.21) 99.6 (27.44-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.22Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.5	Depositor
R, R_{free}	0.186 , 0.225 0.193 , 0.229	Depositor DCC
R_{free} test set	1898 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7532	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 40F, SO4, CL

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	0.50	0/3559	0.64	0/4824
1	B	0.54	0/3573	0.68	1/4842 (0.0%)
All	All	0.52	0/7132	0.66	1/9666 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	444	ASP	CB-CG-OD1	5.54	123.29	118.30

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	3475	0	3362	20	0
1	B	3491	0	3368	26	0
2	A	13	0	8	0	0
2	B	13	0	8	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	2	0	0	1	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	226	0	0	1	0
5	B	301	0	0	2	0
All	All	7532	0	6746	45	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 3.

All (45) 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:399:LEU:HD21	1:B:417:ARG:HH22	1.49	0.75
1:B:396:HIS:HB2	1:B:410:MET:HE1	1.77	0.67
1:B:95:ASP:HB2	1:B:150:GLN:HG3	1.79	0.65
1:A:221:ILE:HG12	1:A:269:PHE:HB2	1.79	0.64
1:A:210:VAL:HB	1:A:268:LEU:HD22	1.83	0.59
1:B:199:LEU:HD13	1:B:207:VAL:HG11	1.85	0.58
1:A:236:ALA:HB1	1:A:260:LYS:HG2	1.85	0.58
1:B:56:HIS:HD2	5:B:828:HOH:O	1.87	0.58
1:A:24:LYS:HD3	1:A:343:PRO:HB2	1.87	0.57
1:B:210:VAL:HG11	1:B:278:LEU:HD11	1.89	0.55
1:A:199:LEU:HD13	1:A:207:VAL:HG11	1.89	0.54
1:B:370:VAL:HB	1:B:371:PRO:CD	2.36	0.54
1:A:478:LEU:HD11	1:A:480:LEU:HD23	1.91	0.53
1:B:210:VAL:HB	1:B:268:LEU:HD22	1.92	0.51
1:A:26:LEU:HD13	1:A:62:LEU:HD11	1.92	0.51
1:B:336:PRO:HG3	1:B:349:TRP:CD2	2.47	0.49
1:A:32:LEU:HG	1:A:406:LEU:HD11	1.94	0.49
1:B:56:HIS:CD2	5:B:828:HOH:O	2.64	0.48
1:A:271:ARG:HB3	4:A:604:CL:CL	2.50	0.48
1:B:225:GLU:HG2	1:B:235:VAL:HG21	1.95	0.47
1:A:386:TYR:CG	1:A:431:PRO:HG3	2.50	0.47
5:A:818:HOH:O	1:B:177:ARG:HD2	2.14	0.46
1:B:171:LYS:HE3	1:B:219:THR:HG21	1.98	0.46
1:B:199:LEU:HD22	1:B:204:TRP:HE3	1.81	0.45
1:B:396:HIS:CB	1:B:410:MET:HE1	2.43	0.45
1:A:177:ARG:HB3	1:A:177:ARG:HH11	1.80	0.45
1:B:370:VAL:HB	1:B:371:PRO:HD2	1.98	0.45
1:B:149:ILE:HG13	1:B:172:LEU:HD21	1.98	0.45
1:B:452:ARG:HH11	1:B:475:ALA:HB1	1.82	0.45
1:B:212:SER:HA	1:B:241:VAL:HG23	1.99	0.44
1:B:163:ILE:HA	1:B:182:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ARG:CZ	1:B:177:ARG:HD3	2.48	0.43
1:A:210:VAL:HG22	1:A:239:GLU:HB2	2.02	0.42
1:B:228:ALA:HB1	1:B:233:ILE:HB	2.02	0.42
1:A:205:THR:HG23	1:A:232:ASN:O	2.20	0.41
1:B:30:GLY:HA2	1:B:83:ARG:HG2	2.01	0.41
1:A:95:ASP:CG	1:A:243:ARG:HH22	2.24	0.41
1:B:189:PHE:CE2	1:B:193:LYS:HE2	2.56	0.41
1:A:163:ILE:HA	1:A:182:ALA:O	2.20	0.41
1:A:228:ALA:HB1	1:A:233:ILE:HB	2.03	0.41
1:A:59:ILE:HG13	1:A:348:PHE:HB2	2.02	0.41
1:A:159:GLN:O	1:A:415:GLY:HA3	2.21	0.41
1:A:314:ALA:O	1:A:457:THR:HA	2.21	0.41
1:B:221:ILE:HD13	1:B:269:PHE:HB2	2.03	0.41
1:B:159:GLN:O	1:B:415:GLY:HA3	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	439/503 (87%)	420 (96%)	18 (4%)	1 (0%)	47 54
1	B	440/503 (88%)	424 (96%)	14 (3%)	2 (0%)	29 30
All	All	879/1006 (87%)	844 (96%)	32 (4%)	3 (0%)	41 45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	135	ALA
1	B	109	SER
1	A	451	GLY

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	353/402 (88%)	345 (98%)	8 (2%)	50 62
1	B	355/402 (88%)	347 (98%)	8 (2%)	50 62
All	All	708/804 (88%)	692 (98%)	16 (2%)	53 62

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	71	ARG
1	A	177	ARG
1	A	269	PHE
1	A	318	GLU
1	A	335	ASP
1	A	417	ARG
1	A	442	ARG
1	B	215	ASP
1	B	269	PHE
1	B	278	LEU
1	B	318[A]	GLU
1	B	318[B]	GLU
1	B	329	SER
1	B	359	GLN
1	B	433	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	40F	B	601	-	5,14,14	1.63	1 (20%)	5,23,23	1.00	0
3	SO4	B	602	-	4,4,4	0.22	0	6,6,6	0.17	0
3	SO4	A	602	-	4,4,4	0.14	0	6,6,6	0.25	0
2	40F	A	601	-	5,14,14	1.19	0	5,23,23	0.77	0

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	40F	B	601	-	-	0/0/31/31	0/2/2/2
2	40F	A	601	-	-	0/0/31/31	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	40F	C7-C1	3.34	1.58	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	443/503 (88%)	0.35	53 (11%) 4 3	23, 45, 76, 118	0
1	B	442/503 (87%)	-0.04	28 (6%) 20 18	22, 38, 65, 102	0
All	All	885/1006 (87%)	0.16	81 (9%) 9 7	22, 42, 73, 118	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	ALA	7.6
1	A	358	ARG	6.8
1	A	462	GLY	6.0
1	A	438	HIS	5.9
1	A	461	ALA	5.3
1	A	359	GLN	4.9
1	A	360	ARG	4.8
1	A	337	TRP	4.7
1	B	262	SER	4.6
1	B	402	ASN	4.4
1	A	140	ILE	4.4
1	A	464	GLY	4.4
1	A	437	THR	4.0
1	A	465	ARG	3.9
1	A	364	ALA	3.9
1	A	435	ALA	3.7
1	A	47	ALA	3.7
1	A	463	SER	3.6
1	B	434	PRO	3.6
1	A	460	ARG	3.5
1	A	46	PRO	3.4
1	B	439	ASN	3.4
1	A	434	PRO	3.4
1	B	261	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	262	SER	3.3
1	B	292	VAL	3.2
1	A	362	CYS	3.1
1	A	361	ASP	3.1
1	A	363	ALA	3.1
1	B	140	ILE	3.0
1	A	369	ALA	3.0
1	A	325	SER	3.0
1	A	385	VAL	3.0
1	A	232	ASN	2.9
1	A	402	ASN	2.8
1	A	74	ARG	2.8
1	B	139	VAL	2.8
1	A	459	LEU	2.7
1	A	467	ARG	2.7
1	B	268	LEU	2.7
1	A	77	HIS	2.6
1	B	489	SER	2.6
1	B	293	ALA	2.6
1	B	435	ALA	2.6
1	A	134	THR	2.6
1	B	47	ALA	2.6
1	A	357	PHE	2.5
1	A	371	PRO	2.5
1	A	353	PHE	2.5
1	A	356	SER	2.5
1	B	408	ASP	2.5
1	A	108	ALA	2.4
1	A	206	TYR	2.4
1	B	229	ARG	2.4
1	A	261	PRO	2.4
1	A	139	VAL	2.4
1	A	436	ASP	2.3
1	A	466	TYR	2.3
1	A	486	PRO	2.3
1	B	388	MET	2.3
1	A	76	PRO	2.3
1	B	48	GLU	2.2
1	B	315	ILE	2.2
1	A	292	VAL	2.2
1	A	35	GLY	2.2
1	A	388	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	325	SER	2.2
1	A	349	TRP	2.2
1	A	473	TYR	2.1
1	B	381	VAL	2.1
1	B	438	HIS	2.1
1	A	37	LEU	2.1
1	B	385	VAL	2.1
1	A	315	ILE	2.1
1	B	232	ASN	2.1
1	B	258	LEU	2.1
1	B	206	TYR	2.1
1	A	293	ALA	2.1
1	B	384	ALA	2.1
1	B	110	LEU	2.0
1	B	316	THR	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 (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. 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
3	SO4	B	602	5/5	0.95	0.10	60,61,65,69	0
4	CL	A	604	1/1	0.97	0.08	68,68,68,68	0
3	SO4	A	602	5/5	0.97	0.08	67,69,71,73	0
4	CL	A	603	1/1	0.98	0.14	35,35,35,35	0
2	40F	B	601	13/13	0.98	0.13	20,23,26,27	0
2	40F	A	601	13/13	0.98	0.12	25,29,33,34	0
4	CL	B	603	1/1	0.99	0.10	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.