wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2022 – 10:07 am BST

PDB ID	:	7QRE
Title	:	Structure of the hetero-tetramer complex between precursor membrane protein fragment (pr) and envelope protein (E) from tick-borne encephalitis virus
Authors	:	Vaney, M.C.; Dellarole, M.; Rey, F.A.
Deposited on	:	2022-01-11
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

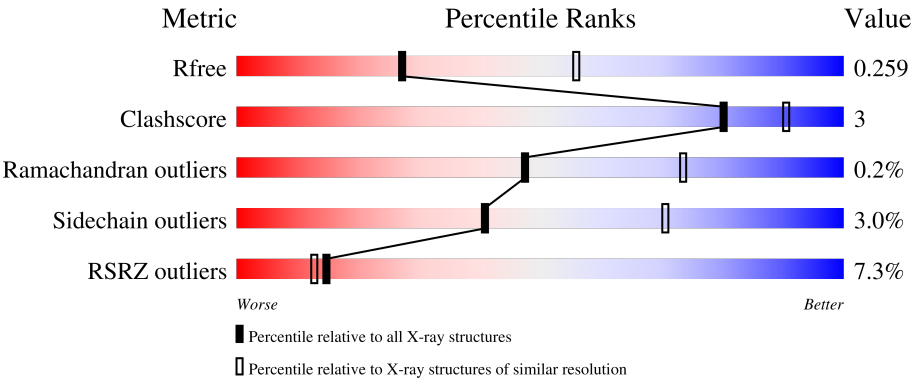
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	127	17%, 56%, 7%, 37%
2	A	439	3%, 83%, 8%, 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3739 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	80	Total	C	N	O	S	0	0	0
			606	365	105	129	7			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	89	GLY	-	expression tag	UNP P14336
D	90	PRO	-	expression tag	UNP P14336
D	91	PHE	-	expression tag	UNP P14336
D	92	GLU	-	expression tag	UNP P14336
D	93	ASP	-	expression tag	UNP P14336
D	94	ASP	-	expression tag	UNP P14336
D	95	ASP	-	expression tag	UNP P14336
D	96	ASP	-	expression tag	UNP P14336
D	97	LYS	-	expression tag	UNP P14336
D	98	ALA	-	expression tag	UNP P14336
D	99	GLY	-	expression tag	UNP P14336
D	100	TRP	-	expression tag	UNP P14336
D	101	SER	-	expression tag	UNP P14336
D	102	HIS	-	expression tag	UNP P14336
D	103	PRO	-	expression tag	UNP P14336
D	104	GLN	-	expression tag	UNP P14336
D	105	PHE	-	expression tag	UNP P14336
D	106	GLU	-	expression tag	UNP P14336
D	107	LYS	-	expression tag	UNP P14336
D	108	GLY	-	expression tag	UNP P14336
D	109	GLY	-	expression tag	UNP P14336
D	110	GLY	-	expression tag	UNP P14336
D	111	SER	-	expression tag	UNP P14336
D	112	GLY	-	expression tag	UNP P14336
D	113	GLY	-	expression tag	UNP P14336
D	114	GLY	-	expression tag	UNP P14336
D	115	SER	-	expression tag	UNP P14336

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Chain	Residue	Modelled	Actual	Comment	Reference
D	116	GLY	-	expression tag	UNP P14336
D	117	GLY	-	expression tag	UNP P14336
D	118	GLY	-	expression tag	UNP P14336
D	119	SER	-	expression tag	UNP P14336
D	120	TRP	-	expression tag	UNP P14336
D	121	SER	-	expression tag	UNP P14336
D	122	HIS	-	expression tag	UNP P14336
D	123	PRO	-	expression tag	UNP P14336
D	124	GLN	-	expression tag	UNP P14336
D	125	PHE	-	expression tag	UNP P14336
D	126	GLU	-	expression tag	UNP P14336
D	127	LYS	-	expression tag	UNP P14336

- Molecule 2 is a protein called Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	400	Total	C	N	O	S	0	1	0
			3063	1921	542	579	21			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	401	GLY	-	expression tag	UNP P14336
A	402	PRO	-	expression tag	UNP P14336
A	403	PHE	-	expression tag	UNP P14336
A	404	GLU	-	expression tag	UNP P14336
A	405	ASP	-	expression tag	UNP P14336
A	406	ASP	-	expression tag	UNP P14336
A	407	ASP	-	expression tag	UNP P14336
A	408	ASP	-	expression tag	UNP P14336
A	409	LYS	-	expression tag	UNP P14336
A	410	ALA	-	expression tag	UNP P14336
A	411	GLY	-	expression tag	UNP P14336
A	412	TRP	-	expression tag	UNP P14336
A	413	SER	-	expression tag	UNP P14336
A	414	HIS	-	expression tag	UNP P14336
A	415	PRO	-	expression tag	UNP P14336
A	416	GLN	-	expression tag	UNP P14336
A	417	PHE	-	expression tag	UNP P14336
A	418	GLU	-	expression tag	UNP P14336
A	419	LYS	-	expression tag	UNP P14336
A	420	GLY	-	expression tag	UNP P14336

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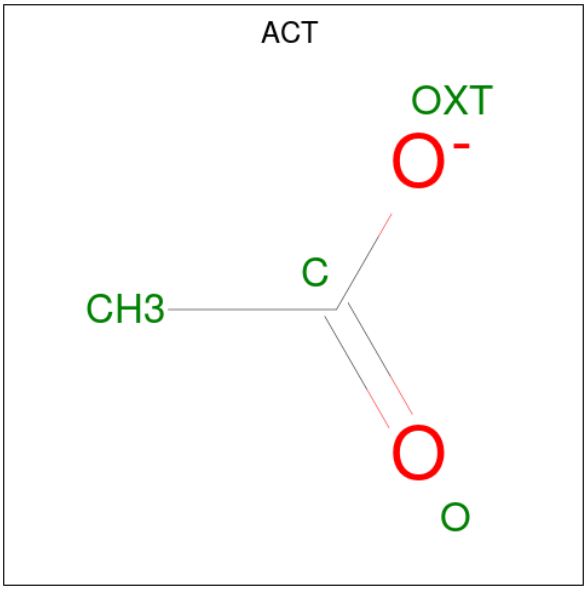
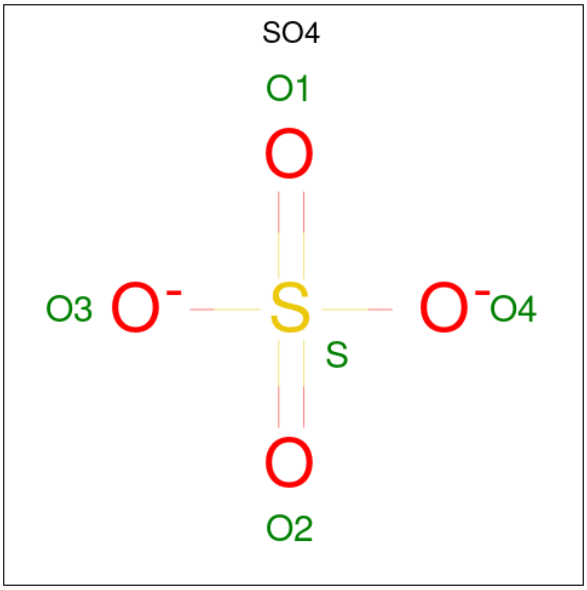
Chain	Residue	Modelled	Actual	Comment	Reference
A	421	GLY	-	expression tag	UNP P14336
A	422	GLY	-	expression tag	UNP P14336
A	423	SER	-	expression tag	UNP P14336
A	424	GLY	-	expression tag	UNP P14336
A	425	GLY	-	expression tag	UNP P14336
A	426	GLY	-	expression tag	UNP P14336
A	427	SER	-	expression tag	UNP P14336
A	428	GLY	-	expression tag	UNP P14336
A	429	GLY	-	expression tag	UNP P14336
A	430	GLY	-	expression tag	UNP P14336
A	431	SER	-	expression tag	UNP P14336
A	432	TRP	-	expression tag	UNP P14336
A	433	SER	-	expression tag	UNP P14336
A	434	HIS	-	expression tag	UNP P14336
A	435	PRO	-	expression tag	UNP P14336
A	436	GLN	-	expression tag	UNP P14336
A	437	PHE	-	expression tag	UNP P14336
A	438	GLU	-	expression tag	UNP P14336
A	439	LYS	-	expression tag	UNP P14336

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

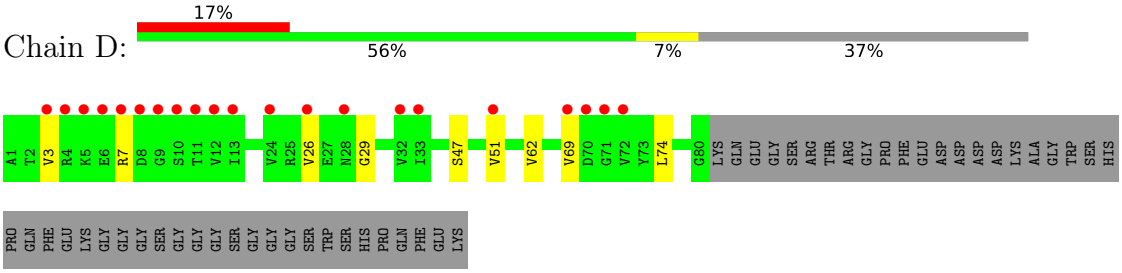
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	3	Total O 3 3	0	0
5	A	19	Total O 19 19	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

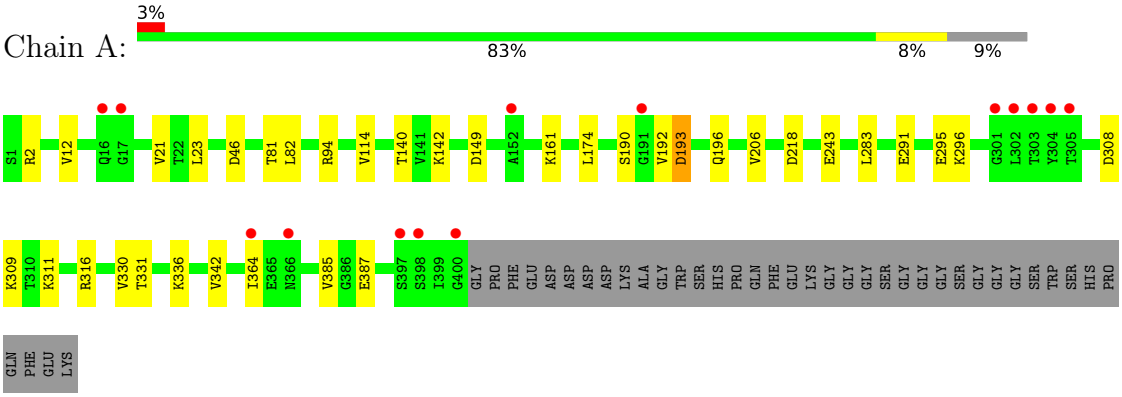
• Molecule 1: Genome polyprotein

Chain D:



• Molecule 2: Envelope protein E

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	164.32Å 164.32Å 164.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.54 – 2.70 49.54 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.54-2.70) 99.9 (49.54-2.70)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.188 , 0.249 0.199 , 0.259	Depositor DCC
R_{free} test set	1071 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	81.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3739	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: ACT, SO4

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	D	0.46	0/612	0.70	0/828
2	A	0.50	0/3131	0.76	0/4251
All	All	0.50	0/3743	0.75	0/5079

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	D	606	0	565	5	0
2	A	3063	0	3010	15	0
3	A	8	0	6	0	0
4	A	40	0	0	0	0
5	A	19	0	0	0	0
5	D	3	0	0	0	0
All	All	3739	0	3581	20	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.

The worst 5 of 20 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)
2:A:12:VAL:HG21	2:A:23:LEU:HD21	1.44	0.99
2:A:193:ASP:HB3	2:A:196:GLN:HB2	1.70	0.72
2:A:336:LYS:HG2	2:A:364:ILE:HG22	1.73	0.70
2:A:46:ASP:HB3	2:A:140:THR:HG22	1.78	0.65
2:A:308:ASP:OD2	2:A:311:LYS:HG2	2.05	0.56

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	D	78/127 (61%)	71 (91%)	6 (8%)	1 (1%)	12 30
2	A	399/439 (91%)	378 (95%)	21 (5%)	0	100 100
All	All	477/566 (84%)	449 (94%)	27 (6%)	1 (0%)	47 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	7	ARG

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	D	67/101 (66%)	67 (100%)	0	100	100
2	A	329/357 (92%)	316 (96%)	13 (4%)	31	60
All	All	396/458 (86%)	383 (97%)	13 (3%)	41	67

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	243	GLU
2	A	283	LEU
2	A	331	THR
2	A	316[A]	ARG
2	A	316[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	196	GLN
2	A	366	ASN
2	A	391	GLN
1	D	68	ASN
1	D	55	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
4	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.13	0
3	ACT	A	502	-	1,3,3	5.93	1 (100%)	0,3,3	-	-
4	SO4	A	506	-	4,4,4	0.22	0	6,6,6	0.17	0
4	SO4	A	504	-	4,4,4	0.33	0	6,6,6	0.17	0
4	SO4	A	505	-	4,4,4	0.15	0	6,6,6	0.17	0
4	SO4	A	507	-	4,4,4	0.14	0	6,6,6	0.15	0
4	SO4	A	510	-	4,4,4	0.29	0	6,6,6	0.26	0
4	SO4	A	503	-	4,4,4	0.53	0	6,6,6	0.28	0
4	SO4	A	509	-	4,4,4	0.11	0	6,6,6	0.11	0
3	ACT	A	501	-	1,3,3	5.65	1 (100%)	0,3,3	-	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	ACT	CH3-C	5.93	1.56	1.48
3	A	501	ACT	CH3-C	5.65	1.55	1.48

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 (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, 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	D	80/127 (62%)	1.36	21 (26%) 0 0	71, 97, 133, 154	0
2	A	400/439 (91%)	0.32	14 (3%) 44 44	53, 76, 127, 151	0
All	All	480/566 (84%)	0.49	35 (7%) 15 13	53, 79, 128, 154	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	16	GLN	5.9
1	D	7	ARG	5.5
2	A	302	LEU	4.6
1	D	8	ASP	4.5
1	D	26	VAL	4.4

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 monosaccharides 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
3	ACT	A	502	4/4	0.63	0.32	116,118,118,119	0
4	SO4	A	510	5/5	0.76	0.29	152,152,153,153	0
3	ACT	A	501	4/4	0.77	0.26	97,98,99,101	0
4	SO4	A	505	5/5	0.80	0.34	171,171,171,172	0
4	SO4	A	509	5/5	0.88	0.18	158,159,159,159	0
4	SO4	A	507	5/5	0.92	0.28	145,146,147,147	0
4	SO4	A	508	5/5	0.93	0.40	148,149,150,150	0
4	SO4	A	506	5/5	0.96	0.16	132,133,133,133	0
4	SO4	A	503	5/5	0.98	0.14	93,94,95,97	0
4	SO4	A	504	5/5	0.98	0.14	105,106,106,110	0

6.5 Other polymers (i)

There are no such residues in this entry.