



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:26 AM GMT

PDB ID : 2QQH
Title : Structure of C8a-MACPF reveals mechanism of membrane attack in complement immune defense
Authors : Hadders, M.A.; Gros, P.
Deposited on : 2007-07-26
Resolution : 2.50 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

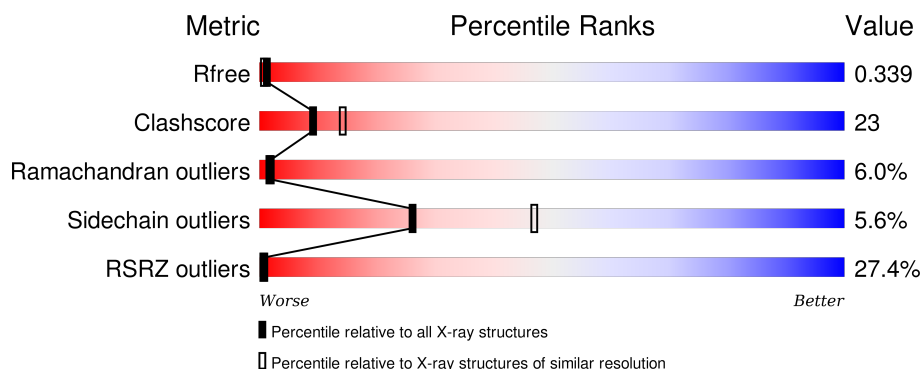
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	334	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2462 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 Complement component C8 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	2402	1522	404	464	12	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	GLY	-	EXPRESSION TAG	UNP P07357
A	102	SER	-	EXPRESSION TAG	UNP P07357
A	164	SER	CYS	ENGINEERED	UNP P07357
A	463	ALA	-	EXPRESSION TAG	UNP P07357
A	464	ALA	-	EXPRESSION TAG	UNP P07357
A	465	ALA	-	EXPRESSION TAG	UNP P07357

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0

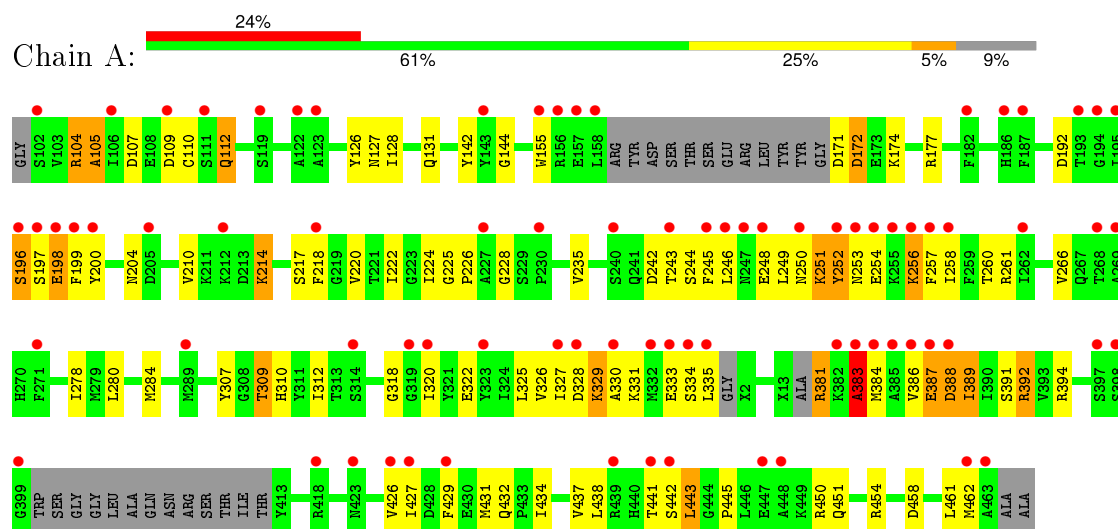
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	44	Total O 44 44	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 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: Complement component C8 alpha chain



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	178.92Å 178.92Å 75.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 37.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-2.50) 100.0 (37.56-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.3.0008	Depositor
R, R_{free}	0.255 , 0.287 0.320 , 0.339	Depositor DCC
R_{free} test set	1088 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 21345 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	2462	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 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	A	0.61	0/2391	0.69	0/3217

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	ARG	Peptide
1	A	383	ALA	Peptide

5.2 Too-close contacts [i](#)

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	2402	0	2286	108	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	15	0	0	0	0
3	A	1	0	0	0	0
4	A	44	0	0	2	0
All	All	2462	0	2286	108	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 23.

All (108) 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:326:VAL:CG1	1:A:387:GLU:HG2	1.35	1.51
1:A:328:ASP:HB3	1:A:331:LYS:CG	1.71	1.18
1:A:326:VAL:CB	1:A:387:GLU:HG2	1.74	1.16
1:A:328:ASP:HB3	1:A:331:LYS:HG3	1.16	1.12
1:A:326:VAL:HG11	1:A:387:GLU:HG2	1.20	1.12
1:A:326:VAL:CG1	1:A:387:GLU:CG	2.31	1.07
1:A:326:VAL:HB	1:A:387:GLU:CG	1.84	1.05
1:A:309:THR:HG22	1:A:310:HIS:ND1	1.72	1.03
1:A:309:THR:CG2	1:A:310:HIS:ND1	2.22	1.02
1:A:328:ASP:OD2	1:A:331:LYS:HE3	1.58	1.01
1:A:326:VAL:HB	1:A:387:GLU:CB	1.94	0.98
1:A:198:GLU:O	1:A:260:THR:HG22	1.66	0.95
1:A:326:VAL:HB	1:A:387:GLU:HB3	1.48	0.94
1:A:199:PHE:O	1:A:200:TYR:CD2	2.23	0.92
1:A:326:VAL:HG12	1:A:387:GLU:HG2	1.50	0.92
1:A:326:VAL:CB	1:A:387:GLU:CG	2.44	0.89
1:A:326:VAL:O	1:A:387:GLU:HB2	1.74	0.87
1:A:328:ASP:CB	1:A:331:LYS:HG3	2.03	0.87
1:A:326:VAL:O	1:A:387:GLU:CB	2.24	0.85
1:A:438:LEU:HD11	1:A:450:ARG:HB2	1.57	0.84
1:A:328:ASP:OD2	1:A:331:LYS:CE	2.26	0.83
1:A:328:ASP:HB3	1:A:331:LYS:HG2	1.61	0.79
1:A:251:LYS:O	1:A:252:TYR:CD2	2.36	0.78
1:A:326:VAL:HG11	1:A:387:GLU:CG	2.04	0.78
1:A:128:ILE:HG22	1:A:309:THR:HG21	1.67	0.76
1:A:325:LEU:HD22	1:A:389:ILE:HG13	1.66	0.76
1:A:325:LEU:CD2	1:A:389:ILE:HG13	2.17	0.74
1:A:196:SER:HA	1:A:218:PHE:HE2	1.51	0.74
1:A:245:PHE:O	1:A:249:LEU:HB2	1.91	0.71
1:A:284:MET:HE3	1:A:434:ILE:HD11	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:O	1:A:105:ALA:CB	2.40	0.69
1:A:326:VAL:O	1:A:387:GLU:HB3	1.93	0.69
1:A:429:PHE:HE2	1:A:431:MET:CE	2.07	0.67
1:A:284:MET:CE	1:A:434:ILE:HD11	2.25	0.66
1:A:104:ARG:O	1:A:105:ALA:HB3	1.97	0.65
1:A:309:THR:HG23	1:A:310:HIS:ND1	2.11	0.64
1:A:245:PHE:CD2	1:A:392:ARG:HD3	2.33	0.64
1:A:220:VAL:HG12	4:A:507:HOH:O	1.97	0.63
1:A:429:PHE:HE2	1:A:431:MET:HE1	1.63	0.63
1:A:196:SER:HB2	1:A:261:ARG:O	2.02	0.60
1:A:258:ILE:HG22	1:A:327:ILE:HB	1.84	0.59
1:A:326:VAL:CB	1:A:387:GLU:CB	2.76	0.59
1:A:128:ILE:CG2	1:A:309:THR:HG21	2.32	0.58
1:A:192:ASP:HB3	1:A:217:SER:HB2	1.86	0.57
1:A:248:GLU:HA	1:A:251:LYS:HE2	1.86	0.57
1:A:328:ASP:OD2	1:A:331:LYS:NZ	2.39	0.56
1:A:110:CYS:SG	1:A:177:ARG:NE	2.78	0.56
1:A:171:ASP:O	1:A:172:ASP:HB3	2.05	0.55
1:A:330:ALA:HA	1:A:333:GLU:CD	2.27	0.55
1:A:242:ASP:O	1:A:246:LEU:HB2	2.07	0.55
1:A:328:ASP:O	1:A:329:LYS:C	2.46	0.55
1:A:309:THR:CG2	1:A:310:HIS:CE1	2.89	0.55
1:A:220:VAL:CG1	4:A:507:HOH:O	2.54	0.54
1:A:330:ALA:HA	1:A:333:GLU:OE1	2.08	0.54
1:A:126:TYR:OH	1:A:131:GLN:HG2	2.08	0.53
1:A:266:VAL:O	1:A:318:GLY:HA3	2.08	0.53
1:A:438:LEU:HD11	1:A:450:ARG:CB	2.34	0.53
1:A:438:LEU:CD1	1:A:450:ARG:HB2	2.35	0.53
1:A:387:GLU:O	1:A:388:ASP:HB3	2.09	0.52
1:A:309:THR:HG23	1:A:310:HIS:CE1	2.44	0.52
1:A:197:SER:O	1:A:198:GLU:HB2	2.08	0.52
1:A:224:ILE:O	1:A:228:GLY:HA3	2.08	0.52
1:A:383:ALA:HB3	1:A:384:MET:HG3	1.92	0.52
1:A:386:VAL:HG22	1:A:386:VAL:O	2.10	0.52
1:A:204:ASN:OD1	1:A:246:LEU:HD21	2.10	0.51
1:A:386:VAL:HG13	1:A:386:VAL:O	2.12	0.50
1:A:312:ILE:HD13	1:A:426:VAL:HG11	1.93	0.49
1:A:251:LYS:O	1:A:251:LYS:HG3	2.12	0.49
1:A:278:ILE:HD12	1:A:441:THR:HG21	1.94	0.49
1:A:112:GLN:HE21	1:A:172:ASP:HB2	1.77	0.49
1:A:220:VAL:HG13	1:A:427:ILE:HB	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASN:HA	1:A:309:THR:HB	1.95	0.49
1:A:199:PHE:O	1:A:200:TYR:CG	2.66	0.49
1:A:429:PHE:CE2	1:A:431:MET:HE3	2.47	0.49
1:A:235:VAL:HG22	1:A:320:ILE:HD13	1.95	0.48
1:A:322:GLU:O	1:A:391:SER:HA	2.13	0.48
1:A:458:ASP:O	1:A:462:MET:HG2	2.13	0.48
1:A:429:PHE:CE2	1:A:431:MET:CE	2.94	0.47
1:A:330:ALA:O	1:A:333:GLU:HB2	2.15	0.47
1:A:388:ASP:O	1:A:389:ILE:C	2.53	0.47
1:A:389:ILE:H	1:A:389:ILE:HD12	1.79	0.47
1:A:442:SER:C	1:A:443:LEU:HG	2.34	0.46
1:A:381:ARG:O	1:A:381:ARG:HG2	2.15	0.46
1:A:284:MET:HE2	1:A:307:TYR:HB3	1.96	0.46
1:A:225:GLY:HA2	1:A:432:GLN:NE2	2.29	0.46
1:A:155:TRP:CD1	1:A:174:LYS:HB3	2.51	0.46
1:A:328:ASP:O	1:A:331:LYS:HG2	2.16	0.46
1:A:326:VAL:CB	1:A:387:GLU:HB3	2.33	0.45
1:A:320:ILE:HG13	1:A:394:ARG:HB2	1.99	0.45
1:A:451:GLN:NE2	1:A:454:ARG:HH11	2.15	0.44
1:A:284:MET:HG3	1:A:307:TYR:CD1	2.52	0.44
1:A:326:VAL:HG12	1:A:387:GLU:CG	2.25	0.44
1:A:322:GLU:HB3	1:A:392:ARG:HB3	1.99	0.43
1:A:280:LEU:HD21	1:A:437:VAL:HG22	1.99	0.43
1:A:142:TYR:CZ	1:A:144:GLY:HA2	2.54	0.43
1:A:225:GLY:HA2	1:A:432:GLN:HE21	1.84	0.42
1:A:388:ASP:O	1:A:388:ASP:CG	2.57	0.42
1:A:110:CYS:SG	1:A:177:ARG:CD	3.08	0.42
1:A:386:VAL:O	1:A:387:GLU:C	2.58	0.42
1:A:249:LEU:O	1:A:250:ASN:C	2.58	0.42
1:A:200:TYR:OH	1:A:214:LYS:HE2	2.19	0.42
1:A:322:GLU:OE1	1:A:392:ARG:NH1	2.54	0.41
1:A:244:SER:O	1:A:248:GLU:HB2	2.20	0.41
1:A:441:THR:O	1:A:443:LEU:HG	2.20	0.41
1:A:222:ILE:HG22	1:A:429:PHE:CZ	2.56	0.40
1:A:110:CYS:SG	1:A:177:ARG:HD2	2.61	0.40
1:A:174:LYS:HG2	1:A:174:LYS:H	1.79	0.40
1:A:104:ARG:HA	1:A:104:ARG:HD3	1.81	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	284/334 (85%)	242 (85%)	25 (9%)	17 (6%)	2 2

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	ALA
1	A	107	ASP
1	A	198	GLU
1	A	226	PRO
1	A	252	TYR
1	A	254	GLU
1	A	387	GLU
1	A	389	ILE
1	A	112	GLN
1	A	196	SER
1	A	256	LYS
1	A	172	ASP
1	A	383	ALA
1	A	388	ASP
1	A	251	LYS
1	A	329	LYS
1	A	445	PRO

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	252/273 (92%)	238 (94%)	14 (6%)	26	47

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ARG
1	A	109	ASP
1	A	210	VAL
1	A	214	LYS
1	A	243	THR
1	A	253	ASN
1	A	256	LYS
1	A	257	PHE
1	A	309	THR
1	A	334	SER
1	A	335	LEU
1	A	392	ARG
1	A	443	LEU
1	A	461	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	131	GLN
1	A	247	ASN
1	A	267	GLN
1	A	294	GLN
1	A	305	ASN
1	A	451	GLN
1	A	459	GLN

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	SO4	A	1	-	4,4,4	0.25	0	6,6,6	0.94	0
2	SO4	A	466	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	A	467	-	4,4,4	0.18	0	6,6,6	0.14	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	SO4	A	1	-	-	0/0/0/0	0/0/0/0
2	SO4	A	466	-	-	0/0/0/0	0/0/0/0
2	SO4	A	467	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

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, 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	292/334 (87%)	1.53	80 (27%) ⓘ ⓘ	25, 51, 68, 75	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	LEU	8.0
1	A	243	THR	7.8
1	A	199	PHE	7.2
1	A	197	SER	6.9
1	A	257	PHE	6.4
1	A	254	GLU	6.4
1	A	334	SER	6.3
1	A	256	LYS	5.7
1	A	252	TYR	5.6
1	A	332	MET	5.1
1	A	230	PRO	5.1
1	A	385	ALA	4.9
1	A	441	THR	4.9
1	A	245	PHE	4.9
1	A	158	LEU	4.9
1	A	330	ALA	4.8
1	A	398	SER	4.6
1	A	255	LYS	4.5
1	A	195	ILE	4.5
1	A	106	ILE	4.4
1	A	198	GLU	3.9
1	A	196	SER	3.9
1	A	384	MET	3.8
1	A	328	ASP	3.7
1	A	155	TRP	3.5
1	A	387	GLU	3.5
1	A	333	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	194	GLY	3.4
1	A	262	ILE	3.3
1	A	258	ILE	3.3
1	A	462	MET	3.2
1	A	250	ASN	3.1
1	A	246	LEU	3.1
1	A	323	TYR	3.1
1	A	388	ASP	3.1
1	A	418	ARG	3.0
1	A	327	ILE	3.0
1	A	218	PHE	2.9
1	A	397	SER	2.9
1	A	200	TYR	2.9
1	A	399	GLY	2.9
1	A	269	ALA	2.8
1	A	205	ASP	2.7
1	A	157	GLU	2.7
1	A	109	ASP	2.6
1	A	382	LYS	2.5
1	A	253	ASN	2.5
1	A	319	GLY	2.5
1	A	156	ARG	2.5
1	A	320	ILE	2.4
1	A	289	MET	2.4
1	A	314	SER	2.4
1	A	427	ILE	2.4
1	A	383	ALA	2.4
1	A	187	PHE	2.3
1	A	212	LYS	2.3
1	A	271	PHE	2.3
1	A	463	ALA	2.3
1	A	426	VAL	2.2
1	A	247	ASN	2.2
1	A	186	HIS	2.2
1	A	248	GLU	2.2
1	A	123	ALA	2.2
1	A	439	ARG	2.2
1	A	386	VAL	2.2
1	A	423	ASN	2.2
1	A	227	ALA	2.2
1	A	102	SER	2.1
1	A	119	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	122	ALA	2.1
1	A	182	PHE	2.1
1	A	429	PHE	2.1
1	A	143	TYR	2.1
1	A	448	ALA	2.1
1	A	442	SER	2.1
1	A	111	SER	2.0
1	A	193	THR	2.0
1	A	447	GLU	2.0
1	A	240	SER	2.0
1	A	268	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. 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
2	SO4	A	466	5/5	0.96	0.10	-2.21	86,86,87,87	0
2	SO4	A	1	5/5	0.98	0.12	-2.28	45,47,48,49	0
3	NI	A	500	1/1	0.96	0.27	-	36,36,36,36	0
2	SO4	A	467	5/5	0.59	0.20	-	174,174,175,175	0

6.5 Other polymers [i](#)

There are no such residues in this entry.