Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 02:13 AM EDT

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
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:

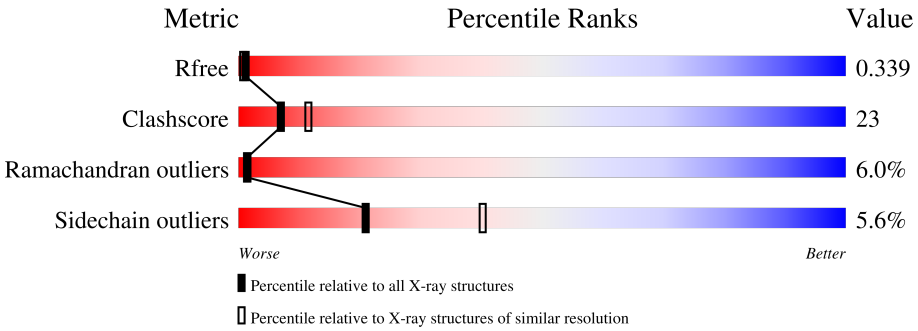
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 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%

Mol	Chain	Length	Quality of chain
1	A	334	61% 25% 5% 9%

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.

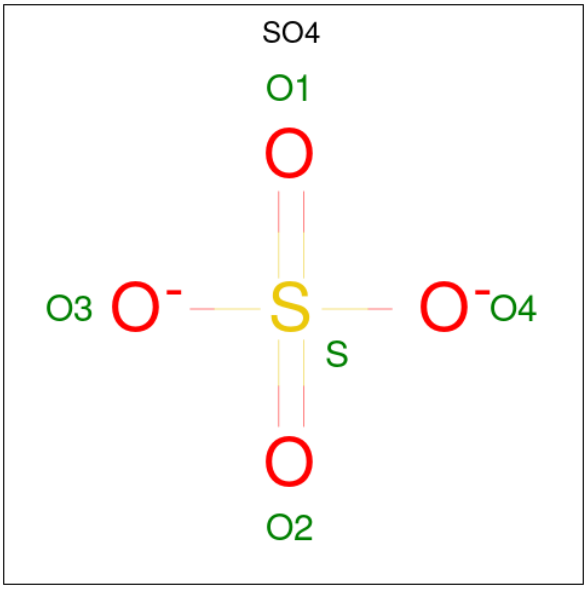
- Molecule 1 is a protein called Complement component C8 alpha chain.

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 mutation	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: O_4S).



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.

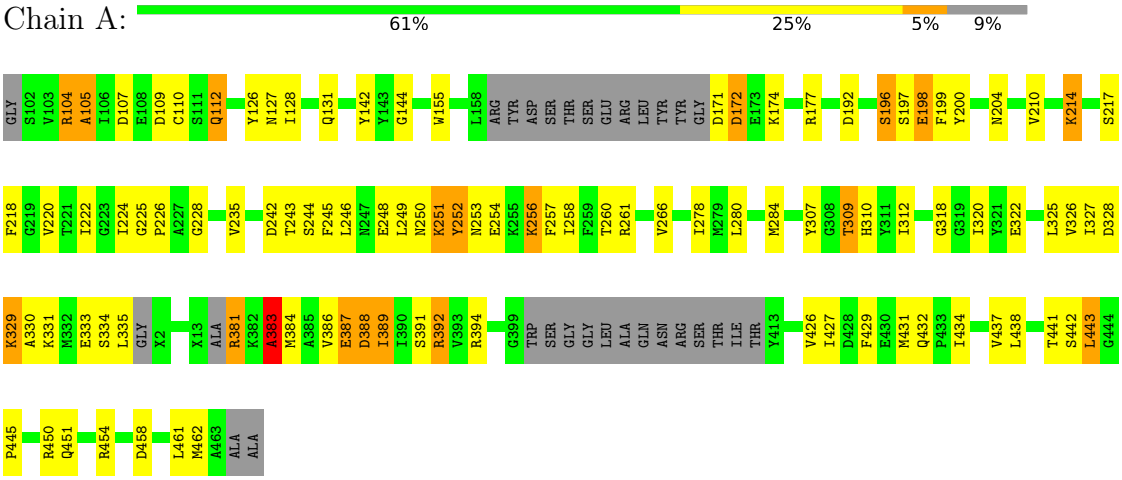
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	44	Total O 44 44	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, 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. 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. 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

Chain A:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.80 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.3.0008	Depositor
R, R_{free}	0.255 , 0.287 0.322 , 0.339	Depositor DCC
R_{free} test set	1089 reflections (5.10%)	wwPDB-VP
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
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	0.86	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.*

[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: 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

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

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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:196:SER:HA	1:A:218:PHE:HE2	1.51	0.74
1:A:325:LEU:CD2	1:A:389:ILE:HG13	2.17	0.74
1:A:245:PHE:O	1:A:249:LEU:HB2	1.91	0.71
1:A:104:ARG:O	1:A:105:ALA:CB	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:MET:HE3	1:A:434:ILE:HD11	1.73	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:242:ASP:O	1:A:246:LEU:HB2	2.07	0.55
1:A:330:ALA:HA	1:A:333:GLU:CD	2.27	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:309:THR:HG23	1:A:310:HIS:CE1	2.44	0.52
1:A:387:GLU:O	1:A:388:ASP:HB3	2.09	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:O	1:A:386:VAL:HG13	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

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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:381:ARG:O	1:A:381:ARG:HG2	2.15	0.46
1:A:442:SER:C	1:A:443:LEU:HG	2.34	0.46
1:A:225:GLY:HA2	1:A:432:GLN:NE2	2.29	0.46
1:A:284:MET:HE2	1:A:307:TYR:HB3	1.96	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:110:CYS:SG	1:A:177:ARG:CD	3.08	0.42
1:A:388:ASP:O	1:A:388:ASP:CG	2.57	0.42
1:A:249:LEU:O	1:A:250:ASN:C	2.58	0.42
1:A:386:VAL:O	1:A:387:GLU: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:110:CYS:SG	1:A:177:ARG:HD2	2.61	0.40
1:A:174:LYS:H	1:A:174:LYS:HG2	1.79	0.40
1:A:222:ILE:HG22	1:A:429:PHE:CZ	2.56	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%)	1 1

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%)	21 40

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

Sometimes 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 (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)

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	467	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	A	466	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	A	1	-	4,4,4	0.21	0	6,6,6	0.79	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 (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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.