Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:38 AM GMT

PDB ID	:	2RJP
Title	:	Crystal structure of ADAMTS4 with inhibitor bound
Authors	:	Mosyak, L.; Stahl, M.; Somers, W.
Deposited on	:	2007-10-15
Resolution	:	2.80 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:

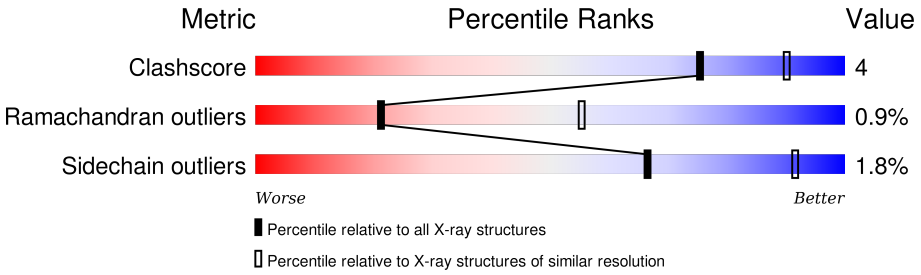
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	316	83% 9% • 8%
1	B	316	80% 10% 10%
1	C	316	82% 10% 8%
1	D	316	79% 9% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8872 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 ADAMTS-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2188	1368	390	406	24			
1	B	284	Total	C	N	O	S	0	0	0
			2128	1329	379	396	24			
1	C	290	Total	C	N	O	S	0	0	0
			2183	1365	389	405	24			
1	D	278	Total	C	N	O	S	0	0	0
			2093	1307	374	388	24			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	GLN	GLU	ENGINEERED	UNP O75173
A	521	ASP	-	EXPRESSION TAG	UNP O75173
A	522	TYR	-	EXPRESSION TAG	UNP O75173
A	523	LYS	-	EXPRESSION TAG	UNP O75173
A	524	ASP	-	EXPRESSION TAG	UNP O75173
A	525	ASP	-	EXPRESSION TAG	UNP O75173
A	526	ASP	-	EXPRESSION TAG	UNP O75173
A	527	ASP	-	EXPRESSION TAG	UNP O75173
A	528	LYS	-	EXPRESSION TAG	UNP O75173
B	362	GLN	GLU	ENGINEERED	UNP O75173
B	521	ASP	-	EXPRESSION TAG	UNP O75173
B	522	TYR	-	EXPRESSION TAG	UNP O75173
B	523	LYS	-	EXPRESSION TAG	UNP O75173
B	524	ASP	-	EXPRESSION TAG	UNP O75173
B	525	ASP	-	EXPRESSION TAG	UNP O75173
B	526	ASP	-	EXPRESSION TAG	UNP O75173
B	527	ASP	-	EXPRESSION TAG	UNP O75173
B	528	LYS	-	EXPRESSION TAG	UNP O75173
C	362	GLN	GLU	ENGINEERED	UNP O75173
C	521	ASP	-	EXPRESSION TAG	UNP O75173
C	522	TYR	-	EXPRESSION TAG	UNP O75173

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Chain	Residue	Modelled	Actual	Comment	Reference
C	523	LYS	-	EXPRESSION TAG	UNP O75173
C	524	ASP	-	EXPRESSION TAG	UNP O75173
C	525	ASP	-	EXPRESSION TAG	UNP O75173
C	526	ASP	-	EXPRESSION TAG	UNP O75173
C	527	ASP	-	EXPRESSION TAG	UNP O75173
C	528	LYS	-	EXPRESSION TAG	UNP O75173
D	362	GLN	GLU	ENGINEERED	UNP O75173
D	521	ASP	-	EXPRESSION TAG	UNP O75173
D	522	TYR	-	EXPRESSION TAG	UNP O75173
D	523	LYS	-	EXPRESSION TAG	UNP O75173
D	524	ASP	-	EXPRESSION TAG	UNP O75173
D	525	ASP	-	EXPRESSION TAG	UNP O75173
D	526	ASP	-	EXPRESSION TAG	UNP O75173
D	527	ASP	-	EXPRESSION TAG	UNP O75173
D	528	LYS	-	EXPRESSION TAG	UNP O75173

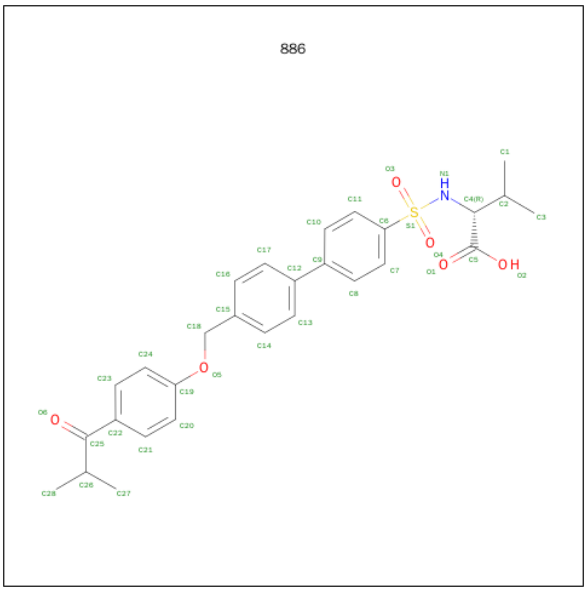
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total Ca 3 3	0	0
3	A	3	Total Ca 3 3	0	0
3	D	3	Total Ca 3 3	0	0
3	C	3	Total Ca 3 3	0	0

- Molecule 4 is N-({4'-[(4-ISOBUTYRYLPHENOXY)METHYL]BIPHENYL-4-YL}SULFONYL)-D-VALINE (three-letter code: 886) (formula: $C_{28}H_{31}NO_6S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O S 36 28 1 6 1	0	0
4	D	1	Total C N O S 36 28 1 6 1	0	0
4	C	1	Total C N O S 36 28 1 6 1	0	0
4	A	1	Total C N O S 36 28 1 6 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	33	Total O 33 33	0	0
5	B	45	Total O 45 45	0	0
5	C	29	Total O 29 29	0	0
5	D	13	Total O 13 13	0	0

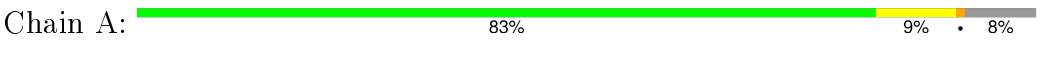
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: ADAMTS-4

Chain A:

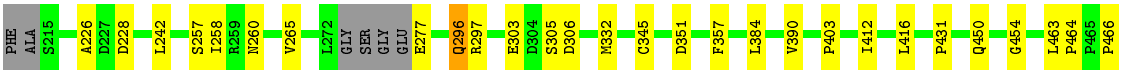


- Molecule 1: ADAMTS-4

Chain B:

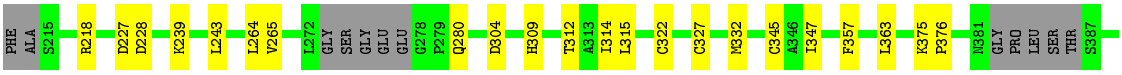
- Molecule 1: ADAMTS-4

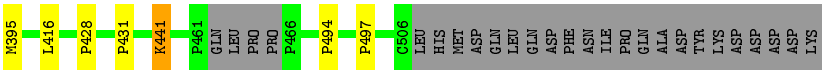
Chain C:



- Molecule 1: ADAMTS-4

Chain D:




M395
L416
P428
P431
K441
P461
GLN
LEU
PRO
PRO
P466
P494
P497
C506
LEU
HIS
MET
ASP
GLN
LEU
GLN
ASP
PHE
ASN
ILE
PRO
GLN
ALA
ASP
TYR
LYS
ASP
ASP
ASP
ASP
LYS

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.57Å 82.62Å 99.33Å 90.00° 90.63° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80	Depositor
% Data completeness (in resolution range)	100.0 (50.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8872	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, 886

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	0.48	0/2249	0.56	0/3068
1	B	0.41	0/2184	0.53	0/2973
1	C	0.42	0/2244	0.54	0/3061
1	D	0.60	4/2148 (0.2%)	0.59	2/2923 (0.1%)
All	All	0.48	4/8825 (0.0%)	0.55	2/12025 (0.0%)

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	1
1	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	441	LYS	CD-CE	16.46	1.92	1.51
1	D	280	GLN	CD-OE1	8.17	1.42	1.24
1	D	441	LYS	CE-NZ	6.34	1.65	1.49
1	D	441	LYS	CG-CD	5.10	1.69	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	441	LYS	CD-CE-NZ	-7.90	93.52	111.70
1	D	441	LYS	CG-CD-CE	-7.57	89.18	111.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	464	PRO	Peptide
1	C	463	LEU	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	2188	0	2090	16	0
1	B	2128	0	2035	16	0
1	C	2183	0	2087	18	0
1	D	2093	0	1996	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	36	0	30	4	0
4	B	36	0	30	3	0
4	C	36	0	30	3	0
4	D	36	0	30	2	0
5	A	33	0	0	0	0
5	B	45	0	0	1	0
5	C	29	0	0	0	0
5	D	13	0	0	0	0
All	All	8872	0	8328	66	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 (66) 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:D:441:LYS:CD	1:D:441:LYS:CE	1.92	1.47
1:D:441:LYS:CG	1:D:441:LYS:CE	2.54	0.85
1:C:296:GLN:HG3	1:C:297:ARG:N	1.99	0.77
1:C:464:PRO:O	1:C:466:PRO:HD3	1.95	0.67
1:A:463:LEU:O	1:A:465:PRO:HD2	1.95	0.67
1:C:265:VAL:HG13	1:C:431:PRO:HB3	1.78	0.66
1:A:390:VAL:HA	4:A:510:886:H181	1.78	0.64
1:D:441:LYS:NZ	1:D:441:LYS:CD	2.60	0.64
1:D:314:ILE:HD11	1:D:363:LEU:HD21	1.78	0.64
1:B:293:CYS:HG	1:B:345:CYS:HG	1.43	0.62
1:A:296:GLN:HG3	1:A:313:ALA:CB	2.30	0.62
1:C:332:MET:HG3	4:C:510:886:H13	1.81	0.61
1:A:463:LEU:O	1:A:465:PRO:CD	2.48	0.61
1:A:296:GLN:HG3	1:A:313:ALA:HB2	1.83	0.61
1:C:357:PHE:HB3	4:C:510:886:C19	2.32	0.58
1:D:375:LYS:HB2	1:D:376:PRO:HD3	1.86	0.57
1:C:265:VAL:CG1	1:C:431:PRO:HB3	2.34	0.57
1:C:296:GLN:HG3	1:C:297:ARG:H	1.68	0.56
1:B:318:ARG:NH1	1:B:350:ASP:OD2	2.33	0.56
1:C:257:SER:OG	1:C:403:PRO:HD2	2.07	0.55
1:A:357:PHE:HB3	4:A:510:886:C19	2.35	0.55
1:B:427:LYS:HG2	1:B:428:PRO:HD2	1.90	0.53
1:C:476:LEU:HG	1:C:477:ASN:OD1	2.08	0.53
1:A:265:VAL:HG11	1:A:428:PRO:HG3	1.91	0.53
1:B:293:CYS:SG	1:B:345:CYS:SG	3.02	0.52
1:B:264:LEU:HD21	1:B:363:LEU:HD13	1.91	0.51
1:D:322:CYS:SG	1:D:327:CYS:SG	3.06	0.51
1:B:390:VAL:HA	4:B:510:886:H181	1.92	0.51
1:B:296:GLN:HG3	1:B:313:ALA:CB	2.40	0.51
1:D:315:LEU:HB3	1:D:347:ILE:HG22	1.92	0.51
1:C:265:VAL:HG13	1:C:431:PRO:CB	2.42	0.49
1:B:450:GLN:HA	1:B:454:GLY:O	2.12	0.49
1:D:265:VAL:HG13	1:D:431:PRO:HB3	1.93	0.49
1:B:466:PRO:O	1:B:467:CYS:HB2	2.15	0.46
1:A:463:LEU:HG	1:A:464:PRO:HD3	1.97	0.46
1:A:427:LYS:HG2	1:A:428:PRO:HD2	1.96	0.46
1:C:412:ILE:O	1:C:416:LEU:HG	2.15	0.46
1:A:358:THR:O	1:A:362:GLN:HG2	2.16	0.46
1:C:258:ILE:HG23	1:C:260:ASN:H	1.80	0.45
1:D:332:MET:HG3	4:D:510:886:H13	1.97	0.45
1:D:239:LYS:O	1:D:243:LEU:HG	2.16	0.45
1:A:450:GLN:HA	1:A:454:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:ASP:HA	1:D:309:HIS:CG	2.52	0.44
1:C:466:PRO:C	1:C:468:ALA:H	2.21	0.44
1:C:303:GLU:C	1:C:305:SER:H	2.21	0.44
1:B:374:SER:O	1:B:378:ILE:HG12	2.18	0.43
1:C:450:GLN:HA	1:C:454:GLY:O	2.18	0.43
1:A:218:ARG:HD3	1:A:416:LEU:HD22	2.00	0.43
1:C:351:ASP:OD2	1:C:485:LYS:HE2	2.18	0.43
1:B:410:ARG:HD3	5:B:539:HOH:O	2.19	0.42
1:A:332:MET:HG3	4:A:510:886:H32	2.02	0.42
1:D:218:ARG:HD2	1:D:416:LEU:HD22	2.02	0.42
1:B:398:VAL:CG1	1:B:403:PRO:HA	2.50	0.42
4:B:510:886:H231	4:B:510:886:H282	2.02	0.42
1:B:304:ASP:HA	1:B:309:HIS:CG	2.55	0.41
1:B:357:PHE:HB3	4:B:510:886:C19	2.50	0.41
1:A:502:MET:HB2	1:A:507:LEU:HD12	2.01	0.41
1:A:306:ASP:HA	1:A:307:PRO:HD2	1.92	0.41
1:B:502:MET:HB2	1:B:507:LEU:HD12	2.01	0.41
1:B:255:HIS:CE1	1:B:257:SER:HG	2.37	0.41
1:C:226:ALA:HB2	1:C:242:LEU:HD11	2.03	0.41
1:C:390:VAL:HG13	4:C:510:886:H201	2.02	0.41
1:D:265:VAL:HG11	1:D:428:PRO:HG3	2.02	0.41
1:A:315:LEU:HB3	1:A:347:ILE:HG22	2.02	0.40
4:A:510:886:H282	4:A:510:886:H231	2.03	0.40
1:D:357:PHE:HB3	4:D:510:886:C19	2.52	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	287/316 (91%)	276 (96%)	8 (3%)	3 (1%)	19 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	276/316 (87%)	265 (96%)	10 (4%)	1 (0%)	39 74
1	C	286/316 (90%)	270 (94%)	14 (5%)	2 (1%)	26 62
1	D	270/316 (85%)	259 (96%)	7 (3%)	4 (2%)	13 40
All	All	1119/1264 (88%)	1070 (96%)	39 (4%)	10 (1%)	21 55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	PRO
1	D	395	MET
1	B	228	ASP
1	C	228	ASP
1	A	228	ASP
1	D	494	PRO
1	C	384	LEU
1	D	228	ASP
1	D	497	PRO
1	A	497	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	239/261 (92%)	233 (98%)	6 (2%)	55 86
1	B	232/261 (89%)	229 (99%)	3 (1%)	76 94
1	C	239/261 (92%)	235 (98%)	4 (2%)	68 92
1	D	228/261 (87%)	224 (98%)	4 (2%)	66 91
All	All	938/1044 (90%)	921 (98%)	17 (2%)	66 91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LEU

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Mol	Chain	Res	Type
1	A	293	CYS
1	A	312	THR
1	A	479	HIS
1	A	481	MET
1	A	502	MET
1	B	289	LEU
1	B	306	ASP
1	B	481	MET
1	C	277	GLU
1	C	296	GLN
1	C	306	ASP
1	C	345	CYS
1	D	227	ASP
1	D	264	LEU
1	D	312	THR
1	D	345	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	234	HIS

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 20 ligands modelled in this entry, 16 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	$\#\|Z\| > 2$
4	886	A	510	2	35,38,38	1.36	4 (11%)	49,54,54	1.17	5 (10%)
4	886	B	510	2	35,38,38	1.26	2 (5%)	49,54,54	1.49	6 (12%)
4	886	C	510	2	35,38,38	1.22	3 (8%)	49,54,54	1.64	6 (12%)
4	886	D	510	2	35,38,38	1.36	2 (5%)	49,54,54	1.12	4 (8%)

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
4	886	A	510	2	-	0/32/36/36	0/3/3/3
4	886	B	510	2	-	0/32/36/36	0/3/3/3
4	886	C	510	2	-	0/32/36/36	0/3/3/3
4	886	D	510	2	-	0/32/36/36	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	510	886	C26-C25	2.04	1.54	1.51
4	A	510	886	O3-S1	2.20	1.45	1.43
4	C	510	886	C26-C25	2.34	1.54	1.51
4	C	510	886	C4-N1	2.58	1.51	1.48
4	B	510	886	C4-N1	2.86	1.52	1.48
4	A	510	886	C4-N1	3.01	1.52	1.48
4	C	510	886	S1-N1	3.43	1.67	1.61
4	D	510	886	C4-N1	3.59	1.53	1.48
4	B	510	886	S1-N1	3.86	1.68	1.61
4	A	510	886	S1-N1	3.91	1.68	1.61
4	D	510	886	S1-N1	4.42	1.69	1.61

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	510	886	O6-C25-C22	-3.89	115.23	120.58
4	C	510	886	O6-C25-C22	-3.73	115.44	120.58
4	C	510	886	C2-C4-N1	-3.61	103.97	110.49
4	B	510	886	O6-C25-C22	-3.60	115.63	120.58
4	C	510	886	C4-N1-S1	-3.10	115.47	121.47
4	B	510	886	C1-C2-C4	-3.06	108.50	111.30
4	B	510	886	C2-C4-N1	-2.53	105.93	110.49
4	C	510	886	C6-S1-N1	-2.43	104.21	107.71
4	D	510	886	O6-C25-C22	-2.40	117.27	120.58
4	C	510	886	C7-C6-S1	-2.27	117.16	119.78
4	A	510	886	C2-C4-N1	-2.27	106.40	110.49
4	A	510	886	C6-S1-N1	-2.17	104.59	107.71
4	D	510	886	C4-N1-S1	-2.16	117.28	121.47
4	B	510	886	C7-C6-S1	-2.07	117.39	119.78
4	B	510	886	C22-C25-C26	2.03	125.61	120.14
4	A	510	886	C3-C2-C4	2.13	113.24	111.30
4	D	510	886	C18-O5-C19	2.23	123.69	117.70
4	A	510	886	C18-O5-C19	2.43	124.21	117.70
4	B	510	886	C3-C2-C4	5.17	116.03	111.30
4	D	510	886	C3-C2-C4	5.49	116.32	111.30
4	C	510	886	C3-C2-C4	7.19	117.88	111.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	510	886	4	0
4	B	510	886	3	0
4	C	510	886	3	0
4	D	510	886	2	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.