



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 07:33 PM BST

PDB ID : 5XWD
Title : Crystal structure of the complex of 059-152-Fv and EGFR-ECD
Authors : Matsuda, T.; Ito, T.; Shirouzu, M.
Deposited on : 2017-06-29
Resolution : 2.89 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 : 2.13.1
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) : 2.13.1

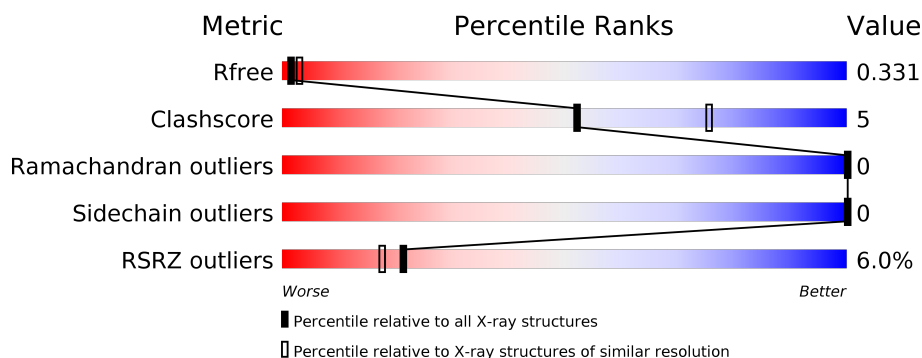
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 $\leq 5\%$. 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	651	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>
2	H	132	<div> <div>11%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>10%</div> </div> </div>
3	D	120	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>10%</div> </div> </div>
4	B	7	<div> <div></div> <div> <div>43%</div> <div>43%</div> <div>14%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	703	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6623 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4697	2898	838	901	60			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	620	GLY	-	expression tag	UNP P00533
A	621	SER	-	expression tag	UNP P00533
A	622	GLU	-	expression tag	UNP P00533
A	623	ASN	-	expression tag	UNP P00533
A	624	LEU	-	expression tag	UNP P00533
A	625	TYR	-	expression tag	UNP P00533
A	626	PHE	-	expression tag	UNP P00533
A	627	GLN	-	expression tag	UNP P00533

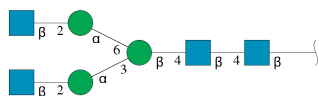
- Molecule 2 is a protein called VH chain of 059-152.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	119	Total	C	N	O	S	0	0	0
			909	581	144	180	4			

- Molecule 3 is a protein called VL chain of 059-152.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	108	Total	C	N	O	S	0	0	0
			810	506	139	163	2			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	7	Total	C	N	O	0	0	0
			89	50	4	35			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

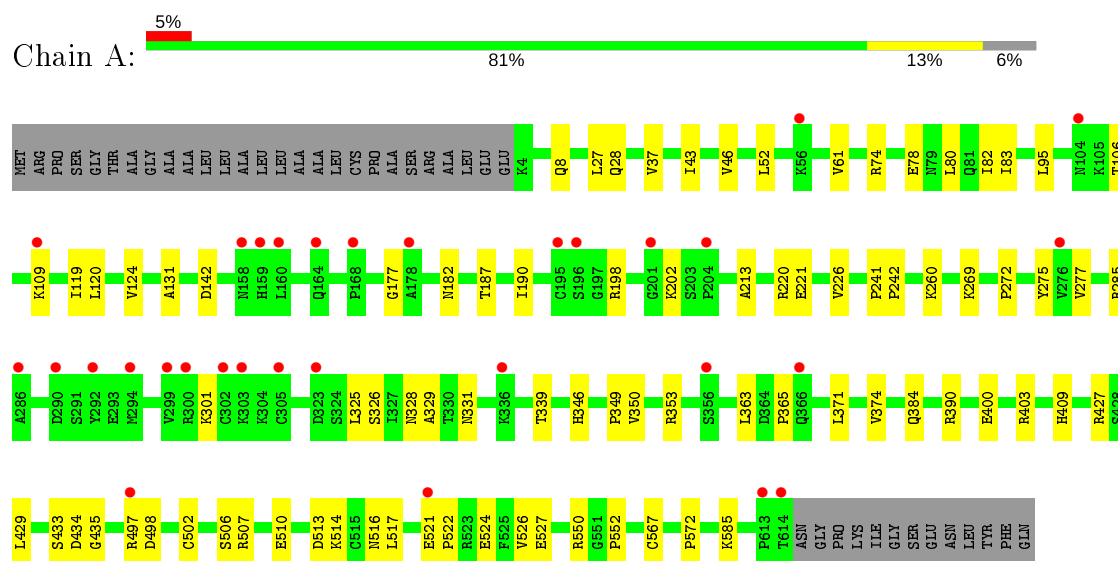
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	3	Total 3	Zn 3	0	0
6	A	15	Total 15	Zn 15	0	0
6	D	2	Total 2	Zn 2	0	0

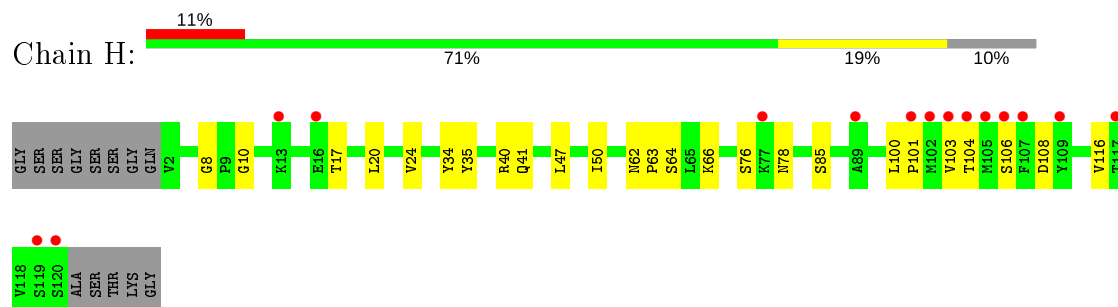
3 Residue-property plots [i](#)

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.

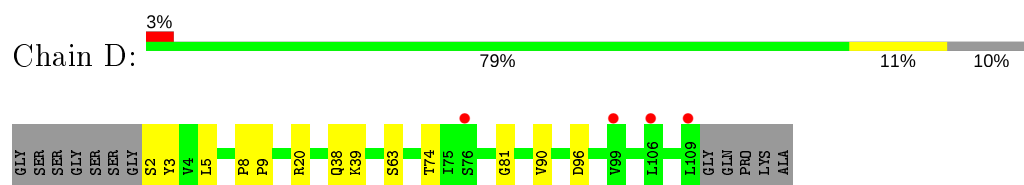
- Molecule 1: Epidermal growth factor receptor



- Molecule 2: VH chain of 059-152



- Molecule 3: VL chain of 059-152



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyra

nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 43% 43% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	203.43 Å 203.43 Å 113.82 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.49 – 2.89 32.49 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.4 (32.49-2.89) 97.4 (32.49-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.90 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.277 , 0.331 0.277 , 0.331	Depositor DCC
R_{free} test set	1533 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6623	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, BMA, NAG, MAN

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	0.24	0/4789	0.44	0/6479
2	H	0.24	0/933	0.44	0/1273
3	D	0.25	0/830	0.42	0/1133
All	All	0.24	0/6552	0.43	0/8885

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 [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	4697	0	4520	49	0
2	H	909	0	885	16	0
3	D	810	0	772	8	0
4	B	89	0	76	2	0
5	A	98	0	91	2	0
6	A	15	0	0	0	0
6	D	2	0	0	0	0
6	H	3	0	0	0	0
All	All	6623	0	6344	71	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 5.

All (71) 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:516:ASN:HB2	1:A:524:GLU:HG3	1.66	0.76
1:A:427:ARG:NH1	1:A:498:ASP:OD1	2.27	0.68
1:A:331:ASN:HB3	4:B:1:NAG:H62	1.75	0.67
3:D:20:ARG:HG2	3:D:74:THR:HG22	1.77	0.66
1:A:213:ALA:HB3	1:A:226:VAL:HG23	1.76	0.66
1:A:527:GLU:OE2	1:A:550:ARG:NH2	2.30	0.64
1:A:349:PRO:HD3	1:A:384:GLN:HG3	1.78	0.64
1:A:82:ILE:HD11	1:A:120:LEU:HG	1.83	0.60
1:A:177:GLY:H	1:A:182:ASN:HB3	1.69	0.58
1:A:507:ARG:NH1	1:A:524:GLU:OE2	2.36	0.57
2:H:62:ASN:ND2	2:H:64:SER:OG	2.37	0.57
2:H:35:TYR:N	2:H:100:LEU:O	2.31	0.57
3:D:63:SER:OG	3:D:74:THR:OG1	2.23	0.57
1:A:142:ASP:O	1:A:198:ARG:NH1	2.37	0.56
1:A:187:THR:HG23	1:A:198:ARG:HE	1.72	0.55
1:A:326:SER:HA	1:A:346:HIS:HB2	1.88	0.54
2:H:101:PRO:HD2	2:H:106:SER:O	2.07	0.54
2:H:76:SER:HB3	4:B:5:NAG:H83	1.90	0.54
1:A:28:GLN:NE2	5:A:701:NAG:O7	2.38	0.54
1:A:37:VAL:HB	1:A:61:VAL:HG12	1.90	0.53
1:A:46:VAL:HG11	1:A:52:LEU:HD11	1.89	0.53
2:H:63:PRO:HA	2:H:66:LYS:HE3	1.91	0.53
1:A:353:ARG:NH2	3:D:96:ASP:HB2	2.24	0.53
2:H:103:VAL:HG23	2:H:104:THR:HG23	1.90	0.52
2:H:10:GLY:HA2	2:H:116:VAL:HG12	1.92	0.52
2:H:34:TYR:HA	2:H:101:PRO:HA	1.91	0.51
1:A:517:LEU:HD21	1:A:526:VAL:HG23	1.92	0.51
1:A:106:THR:HG23	1:A:109:LYS:HE3	1.92	0.51
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.91	0.51
1:A:220:ARG:NH1	1:A:221:GLU:OE2	2.45	0.50
2:H:24:VAL:O	2:H:78:ASN:ND2	2.45	0.50
1:A:83:ILE:HB	1:A:119:ILE:HG12	1.94	0.50
2:H:41:GLN:OE1	3:D:38:GLN:NE2	2.31	0.50
3:D:39:LYS:NZ	3:D:81:GLY:O	2.45	0.49
1:A:95:LEU:HB3	1:A:124:VAL:HG12	1.94	0.49
1:A:513:ASP:OD1	1:A:514:LYS:N	2.45	0.49
1:A:400:GLU:HA	1:A:429:LEU:HA	1.95	0.49
1:A:329:ALA:HB2	1:A:363:LEU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2:SER:OG	3:D:3:TYR:N	2.46	0.48
1:A:61:VAL:HG22	1:A:80:LEU:HD11	1.96	0.48
3:D:5:LEU:HD11	3:D:90:VAL:HG22	1.96	0.47
1:A:572:PRO:HD2	1:A:585:LYS:HD2	1.97	0.46
1:A:514:LYS:HB3	5:A:713:NAG:H2	1.98	0.46
2:H:35:TYR:HB2	2:H:100:LEU:HB3	1.98	0.46
1:A:409:HIS:O	1:A:409:HIS:ND1	2.47	0.45
1:A:339:THR:HA	1:A:374:VAL:HA	1.98	0.45
1:A:552:PRO:HB2	1:A:567:CYS:H	1.82	0.44
1:A:328:ASN:OD1	1:A:331:ASN:ND2	2.51	0.44
1:A:371:LEU:H	1:A:371:LEU:HD23	1.82	0.44
2:H:101:PRO:HG3	2:H:108:ASP:OD2	2.17	0.44
1:A:434:ASP:OD1	1:A:435:GLY:N	2.49	0.44
1:A:502:CYS:SG	1:A:506:SER:HB3	2.59	0.43
1:A:61:VAL:HG23	1:A:83:ILE:HA	2.00	0.43
1:A:277:VAL:HG13	1:A:301:LYS:HG3	2.00	0.43
2:H:17:THR:HA	2:H:85:SER:HA	2.01	0.43
1:A:272:PRO:HG2	1:A:275:TYR:CD1	2.54	0.42
2:H:41:GLN:HB3	2:H:47:LEU:HA	2.01	0.42
1:A:241:PRO:HA	1:A:242:PRO:HD3	1.94	0.42
1:A:403:ARG:O	1:A:433:SER:OG	2.37	0.42
1:A:8:GLN:HB2	1:A:285:ARG:NH2	2.34	0.42
1:A:109:LYS:HE2	1:A:131:ALA:HB1	2.02	0.42
1:A:74:ARG:NH2	1:A:78:GLU:OE2	2.52	0.42
1:A:497:ARG:HD3	1:A:510:GLU:HB2	2.02	0.42
1:A:521:GLU:HB3	1:A:522:PRO:HD3	2.01	0.42
1:A:325:LEU:HD23	1:A:350:VAL:HG11	2.01	0.41
3:D:8:PRO:HA	3:D:9:PRO:HD3	1.95	0.41
2:H:40:ARG:HB3	2:H:50:ILE:HD11	2.02	0.41
1:A:27:LEU:HD11	1:A:43:ILE:HA	2.02	0.41
1:A:260:LYS:HG2	1:A:269:LYS:HA	2.02	0.41
1:A:365:PRO:O	1:A:390:ARG:NH2	2.54	0.41
1:A:190:ILE:HD12	1:A:202:LYS:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	609/651 (94%)	565 (93%)	44 (7%)	0	100	100
2	H	117/132 (89%)	112 (96%)	5 (4%)	0	100	100
3	D	106/120 (88%)	103 (97%)	3 (3%)	0	100	100
All	All	832/903 (92%)	780 (94%)	52 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	533/561 (95%)	533 (100%)	0	100	100
2	H	104/112 (93%)	104 (100%)	0	100	100
3	D	90/97 (93%)	90 (100%)	0	100	100
All	All	727/770 (94%)	727 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	81	GLN
1	A	541	GLN

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Mol	Chain	Res	Type
1	A	557	GLN
2	H	62	ASN

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 ⓘ

7 monosaccharides 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	NAG	B	1	1,4	14,14,15	0.53	0	17,19,21	1.16	1 (5%)
4	NAG	B	2	4	14,14,15	0.54	0	17,19,21	0.78	0
4	BMA	B	3	4	11,11,12	0.62	0	15,15,17	0.67	0
4	MAN	B	4	4	11,11,12	0.72	0	15,15,17	1.30	2 (13%)
4	NAG	B	5	4,6	14,14,15	0.57	0	17,19,21	0.79	0
4	MAN	B	6	4	11,11,12	0.61	0	15,15,17	0.72	0
4	NAG	B	7	4	14,14,15	0.55	0	17,19,21	1.30	2 (11%)

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	NAG	B	1	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	BMA	B	3	4	-	2/2/19/22	0/1/1/1
4	MAN	B	4	4	-	0/2/19/22	0/1/1/1
4	NAG	B	5	4,6	-	1/6/23/26	0/1/1/1
4	MAN	B	6	4	-	1/2/19/22	0/1/1/1
4	NAG	B	7	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	7	NAG	C1-O5-C5	3.67	117.16	112.19
4	B	4	MAN	C1-C2-C3	2.90	113.23	109.67
4	B	1	NAG	O5-C1-C2	-2.51	107.33	111.29
4	B	7	NAG	O5-C1-C2	2.18	114.73	111.29
4	B	4	MAN	C2-C3-C4	2.04	114.42	110.89

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3	BMA	O5-C5-C6-O6
4	B	3	BMA	C4-C5-C6-O6
4	B	5	NAG	O5-C5-C6-O6
4	B	6	MAN	O5-C5-C6-O6
4	B	7	NAG	O5-C5-C6-O6
4	B	7	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	NAG	1	0
4	B	5	NAG	1	0

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 20 are monoatomic - leaving 7 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
5	NAG	A	714	1	14,14,15	0.53	0	17,19,21	1.42	2 (11%)
5	NAG	A	701	1	14,14,15	0.54	0	17,19,21	0.71	0
5	NAG	A	703	1	14,14,15	0.55	0	17,19,21	0.73	0
5	NAG	A	711	1	14,14,15	0.52	0	17,19,21	0.69	0
5	NAG	A	713	1	14,14,15	0.52	0	17,19,21	0.95	0
5	NAG	A	712	1	14,14,15	0.52	0	17,19,21	0.69	0
5	NAG	A	702	1	14,14,15	0.55	0	17,19,21	0.64	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
5	NAG	A	714	1	-	2/6/23/26	0/1/1/1
5	NAG	A	701	1	-	0/6/23/26	0/1/1/1
5	NAG	A	703	1	-	0/6/23/26	0/1/1/1
5	NAG	A	711	1	-	0/6/23/26	0/1/1/1
5	NAG	A	713	1	-	1/6/23/26	0/1/1/1
5	NAG	A	712	1	-	0/6/23/26	0/1/1/1
5	NAG	A	702	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	714	NAG	C1-O5-C5	4.27	117.97	112.19
5	A	714	NAG	O5-C1-C2	2.37	115.03	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	714	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	702	NAG	O5-C5-C6-O6
5	A	713	NAG	C3-C2-N2-C7
5	A	714	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	NAG	1	0
5	A	713	NAG	1	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

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	611/651 (93%)	0.40	31 (5%) 28 24	65, 92, 126, 146	0
2	H	119/132 (90%)	0.78	15 (12%) 3 3	75, 95, 124, 132	0
3	D	108/120 (90%)	0.30	4 (3%) 41 37	62, 77, 91, 103	0
All	All	838/903 (92%)	0.44	50 (5%) 21 18	62, 90, 125, 146	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	SER	4.8
1	A	299	VAL	4.5
1	A	294	MET	4.0
1	A	178	ALA	3.9
2	H	120	SER	3.8
2	H	106	SER	3.8
2	H	104	THR	3.8
1	A	159	HIS	3.7
1	A	276	VAL	3.7
2	H	105	MET	3.6
1	A	104	ASN	3.5
2	H	89	ALA	3.4
1	A	196	SER	3.4
1	A	302	CYS	3.4
1	A	158	ASN	3.3
1	A	300	ARG	3.3
1	A	201	GLY	3.3
2	H	77	LYS	3.3
3	D	76	SER	3.3
1	A	109	LYS	3.2
1	A	286	ALA	3.2
2	H	16	GLU	2.9
3	D	109	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	521	GLU	2.8
3	D	106	LEU	2.7
1	A	290	ASP	2.6
1	A	323	ASP	2.6
1	A	195	CYS	2.6
1	A	168	PRO	2.6
2	H	102	MET	2.5
1	A	292	TYR	2.5
2	H	101	PRO	2.5
1	A	497	ARG	2.5
1	A	303	LYS	2.4
1	A	336	LYS	2.4
2	H	107	PHE	2.4
1	A	56	LYS	2.3
3	D	99	VAL	2.2
2	H	119	SER	2.2
1	A	613	PRO	2.2
2	H	103	VAL	2.1
1	A	305	CYS	2.1
1	A	366	GLN	2.1
2	H	109	TYR	2.1
2	H	13	LYS	2.1
1	A	614	THR	2.0
1	A	160	LEU	2.0
2	H	117	THR	2.0
1	A	204	PRO	2.0
1	A	164	GLN	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](#)

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, 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	B-factors(\AA^2)	Q<0.9
4	MAN	B	6	11/12	0.79	0.20	107,121,127,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	B	7	14/15	0.80	0.28	131,138,143,143	0
4	BMA	B	3	11/12	0.86	0.20	115,121,129,129	0
4	MAN	B	4	11/12	0.87	0.20	100,120,128,133	0
4	NAG	B	2	14/15	0.89	0.19	102,106,117,117	0
4	NAG	B	5	14/15	0.91	0.28	123,130,135,140	0
4	NAG	B	1	14/15	0.94	0.23	96,103,108,109	0

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, 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	B-factors(\AA^2)	Q<0.9
6	ZN	H	201	1/1	0.52	0.09	246,246,246,246	0
5	NAG	A	703	14/15	0.65	0.73	136,145,151,152	0
5	NAG	A	714	14/15	0.68	0.40	139,146,149,150	0
6	ZN	A	724	1/1	0.69	0.09	172,172,172,172	0
6	ZN	A	722	1/1	0.70	0.11	165,165,165,165	0
5	NAG	A	702	14/15	0.79	0.26	97,112,121,123	0
5	NAG	A	712	14/15	0.87	0.26	100,106,110,110	0
6	ZN	A	725	1/1	0.88	0.09	123,123,123,123	0
6	ZN	A	716	1/1	0.88	0.32	126,126,126,126	0
5	NAG	A	713	14/15	0.88	0.19	86,94,101,103	0
5	NAG	A	711	14/15	0.88	0.16	113,126,128,130	0
6	ZN	A	729	1/1	0.89	0.18	159,159,159,159	0
5	NAG	A	701	14/15	0.89	0.21	90,103,109,111	0
6	ZN	D	201	1/1	0.92	0.08	117,117,117,117	0
6	ZN	A	721	1/1	0.92	0.14	115,115,115,115	0
6	ZN	D	202	1/1	0.92	0.09	121,121,121,121	0
6	ZN	A	718	1/1	0.92	0.17	373,373,373,373	0
6	ZN	A	717	1/1	0.95	0.14	177,177,177,177	0
6	ZN	A	728	1/1	0.95	0.12	147,147,147,147	0
6	ZN	A	723	1/1	0.95	0.06	131,131,131,131	0
6	ZN	A	720	1/1	0.95	0.08	118,118,118,118	0
6	ZN	A	719	1/1	0.97	0.09	127,127,127,127	0
6	ZN	H	203	1/1	0.97	0.25	170,170,170,170	0
6	ZN	A	715	1/1	0.97	0.16	114,114,114,114	0
6	ZN	A	727	1/1	0.97	0.13	174,174,174,174	0
6	ZN	H	202	1/1	0.98	0.18	151,151,151,151	0
6	ZN	A	726	1/1	0.98	0.11	103,103,103,103	0

6.5 Other polymers

There are no such residues in this entry.