W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 26, 2024 – 12:12 AM EDT

PDB ID	:	7D85
Title	:	Crystal structure of anti-ErbB3 Fab ISU104 in complex with human ErbB3 extracellular domain 3
Authors	:	Yoo, Y.; Cho, H.S.
Deposited on	:	2020-10-07
Resolution	:	2.50 Å(reported)

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	:	2.37.1
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)	:	2.37.1

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 2.50 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.
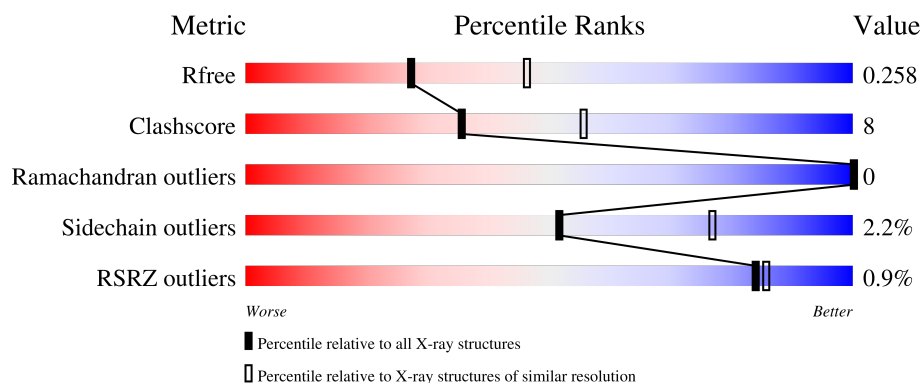
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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% 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	194	72% 27% ••
1	D	194	82% 16% ••
2	B	228	79% 17% •
2	E	228	79% 16% 5%
3	C	216	80% 19% •

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Mol	Chain	Length	Quality of chain
3	F	216	75% 23% •

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 9539 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 Receptor tyrosine-protein kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total 1503	C 945	N 275	O 273	S 10	0	0	0
1	D	193	Total 1503	C 945	N 275	O 273	S 10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	307	GLY	-	expression tag	UNP P21860
A	308	ILE	-	expression tag	UNP P21860
D	307	GLY	-	expression tag	UNP P21860
D	308	ILE	-	expression tag	UNP P21860

- Molecule 2 is a protein called Anti-ErbB3 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total 1629	C 1028	N 268	O 326	S 7	0	0	0
2	E	217	Total 1625	C 1026	N 267	O 325	S 7	0	0	0

- Molecule 3 is a protein called Anti-ErbB3 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total 1571	C 977	N 265	O 325	S 4	0	0	0
3	F	213	Total 1571	C 977	N 265	O 325	S 4	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	14	Total	O	0	0
			14	14		
5	C	7	Total	O	0	0
			7	7		
5	D	1	Total	O	0	0
			1	1		
5	E	7	Total	O	0	0
			7	7		

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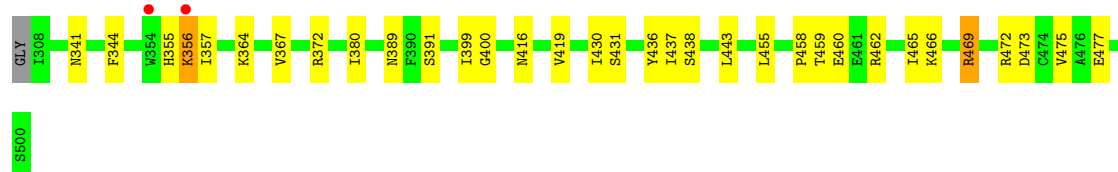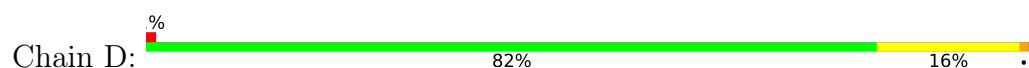| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	4	Total 4	O 4	0	0

3 Residue-property plots ⓘ

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.
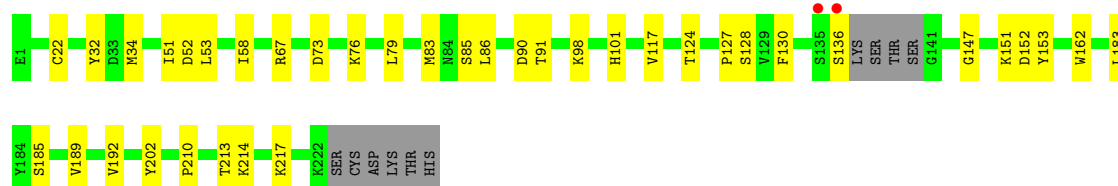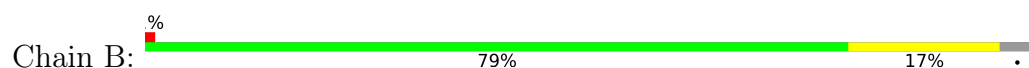
- Molecule 1: Receptor tyrosine-protein kinase erbB-3
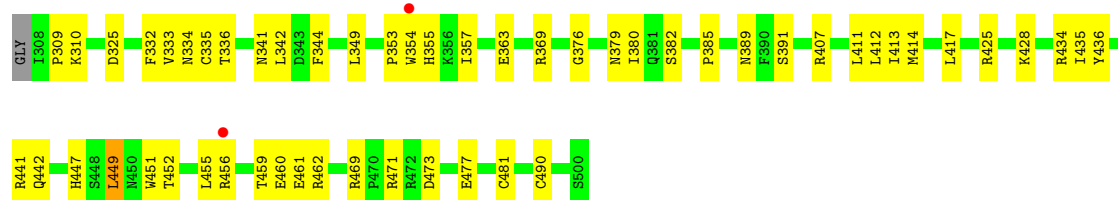
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

- Molecule 2: Anti-ErbB3 Fab heavy chain

- Molecule 2: Anti-ErbB3 Fab heavy chain

L167 Q179 L183 S187 V190 T191 V192 P193 S194 S195 S196 T199 Q200 T201 K222 SER CYS ASP LYS THR HIS

• Molecule 3: Anti-ErbB3 Fab light chain

Chain C:

GLN S2 V3 L4 S11 S25 S33 V34 S35 W36 S51 R55 F63 K67 S73 L74 E84 W92 V100 F101 G102 Q112 P113 P124 A134 T135 L136 L139 I140 S141 D142 F143 G146 K153 K170 Q171 Y176 L182 S183 L184

Q188 K193 S194 Y195 S196 C197 Q198 E207 E214 CYS SER

• Molecule 3: Anti-ErbB3 Fab light chain

Chain F:

GLN S2 P7 P8 P14 S26 S27 N28 S31 N32 S33 V34 Q38 L48 S51 D52 P56 V59 K67 E82 D83 E84 Q90 G91 W92 S95 V109 L110 G111 Q112 P113 P117 S118 V119 T120 L121 F122 P123 L136 F143 Y144 P145 G146

A147 V148 A154 P168 N173 Y181 L182 S183 L184 T185 Q188 S191 H192 K193 V199 T200 H201 S204 T205 K208 E214 CYS SER

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.29Å 77.78Å 93.94Å 90.00° 113.41° 90.00°	Depositor
Resolution (Å)	46.63 – 2.50 46.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.63-2.50) 99.2 (46.63-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.203 , 0.258 0.203 , 0.258	Depositor DCC
R_{free} test set	1247 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.4	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9539	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.52	0/1539	0.67	0/2084
1	D	0.46	0/1539	0.63	0/2084
2	B	0.51	0/1668	0.71	1/2272 (0.0%)
2	E	0.50	0/1664	0.69	0/2267
3	C	0.54	0/1610	0.66	0/2198
3	F	0.45	0/1610	0.64	0/2198
All	All	0.50	0/9630	0.67	1/13103 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	52	ASP	CB-CG-OD1	6.37	124.04	118.30

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	1503	0	1480	40	0
1	D	1503	0	1480	20	0
2	B	1629	0	1578	24	0
2	E	1625	0	1575	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1571	0	1516	24	0
3	F	1571	0	1516	31	0
4	A	56	0	52	8	0
4	D	42	0	39	1	0
5	A	6	0	0	0	0
5	B	14	0	0	0	0
5	C	7	0	0	0	0
5	D	1	0	0	0	0
5	E	7	0	0	0	0
5	F	4	0	0	0	0
All	All	9539	0	9236	151	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 8.

The worst 5 of 151 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:460:GLU:HG3	2:E:85:SER:HB3	1.67	0.76
2:E:193:PRO:HG2	2:E:196:SER:HB2	1.72	0.72
2:B:85:SER:HB3	1:D:460:GLU:HG2	1.73	0.70
1:A:435:ILE:HD11	1:A:455:LEU:HD11	1.74	0.68
3:C:33:SER:HB2	3:C:51:SER:HA	1.77	0.66

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	191/194 (98%)	181 (95%)	10 (5%)	0	100	100
1	D	191/194 (98%)	179 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	214/228 (94%)	209 (98%)	5 (2%)	0	100	100
2	E	213/228 (93%)	209 (98%)	4 (2%)	0	100	100
3	C	211/216 (98%)	203 (96%)	8 (4%)	0	100	100
3	F	211/216 (98%)	207 (98%)	4 (2%)	0	100	100
All	All	1231/1276 (96%)	1188 (96%)	43 (4%)	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	168/168 (100%)	163 (97%)	5 (3%)	41	68
1	D	168/168 (100%)	165 (98%)	3 (2%)	59	81
2	B	183/193 (95%)	180 (98%)	3 (2%)	62	84
2	E	183/193 (95%)	181 (99%)	2 (1%)	73	89
3	C	179/182 (98%)	175 (98%)	4 (2%)	52	77
3	F	179/182 (98%)	173 (97%)	6 (3%)	37	63
All	All	1060/1086 (98%)	1037 (98%)	23 (2%)	52	77

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	469	ARG
3	F	90	GLN
2	E	194	SER
3	F	95	SER
2	B	214	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	NAG	D	602	1	14,14,15	1.39	1 (7%)	17,19,21	1.75	5 (29%)
4	NAG	A	601	1	14,14,15	0.56	0	17,19,21	0.86	1 (5%)
4	NAG	D	603	1	14,14,15	1.36	2 (14%)	17,19,21	2.15	8 (47%)
4	NAG	A	604	1	14,14,15	1.00	1 (7%)	17,19,21	1.96	5 (29%)
4	NAG	A	603	-	14,14,15	0.87	1 (7%)	17,19,21	1.19	1 (5%)
4	NAG	A	602	1	14,14,15	0.84	1 (7%)	17,19,21	0.68	0
4	NAG	D	601	1	14,14,15	1.55	3 (21%)	17,19,21	1.82	5 (29%)

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	D	602	1	-	1/6/23/26	0/1/1/1
4	NAG	A	601	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	603	1	-	2/6/23/26	0/1/1/1
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
4	NAG	A	603	-	-	5/6/23/26	0/1/1/1
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1
4	NAG	D	601	1	-	3/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	601	NAG	O5-C1	-3.42	1.38	1.43
4	D	603	NAG	C1-C2	-2.86	1.48	1.52
4	D	602	NAG	O5-C5	-2.82	1.37	1.43
4	A	602	NAG	C1-C2	2.72	1.56	1.52
4	D	601	NAG	O5-C5	-2.66	1.38	1.43

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	NAG	C1-O5-C5	-5.63	104.56	112.19
4	D	602	NAG	C4-C3-C2	-3.87	105.34	111.02
4	D	603	NAG	C2-N2-C7	-3.74	117.58	122.90
4	D	603	NAG	O5-C1-C2	-3.52	105.73	111.29
4	D	601	NAG	C1-O5-C5	-3.50	107.45	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	NAG	C1-C2-N2-C7
4	A	604	NAG	C4-C5-C6-O6
4	A	604	NAG	O5-C5-C6-O6
4	D	603	NAG	C8-C7-N2-C2
4	A	603	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	602	NAG	1	0
4	A	604	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	NAG	3	0
4	A	602	NAG	3	0

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(Å²)	Q<0.9
1	A	193/194 (99%)	-0.17	2 (1%)	82	84	27, 39, 53, 73	0
1	D	193/194 (99%)	-0.24	2 (1%)	82	84	28, 41, 60, 78	0
2	B	218/228 (95%)	-0.17	2 (0%)	84	86	22, 32, 61, 79	0
2	E	217/228 (95%)	-0.32	3 (1%)	75	77	23, 33, 53, 74	0
3	C	213/216 (98%)	-0.34	2 (0%)	84	86	27, 35, 47, 68	0
3	F	213/216 (98%)	-0.21	0	100	100	24, 38, 58, 68	0
All	All	1247/1276 (97%)	-0.24	11 (0%)	84	86	22, 36, 56, 79	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	354	TRP	4.8
2	B	136	SER	4.7
3	C	3	VAL	4.5
1	A	354	TRP	4.4
2	B	135	SER	4.0

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, 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(Å^2)	Q<0.9
4	NAG	A	603	14/15	0.77	0.27	51,72,78,81	0
4	NAG	A	604	14/15	0.79	0.17	45,60,67,69	0
4	NAG	D	603	14/15	0.82	0.18	54,63,70,72	0
4	NAG	D	602	14/15	0.90	0.17	53,59,65,70	0
4	NAG	D	601	14/15	0.90	0.16	45,49,54,54	0
4	NAG	A	602	14/15	0.91	0.18	49,57,64,69	0
4	NAG	A	601	14/15	0.93	0.12	39,43,48,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.