



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2025 – 08:35 PM JST

PDB ID : 8HPY / pdb_00008hpy
Title : Crystal structure of human LGI1-ADAM22 complex
Authors : Liu, H.; Xu, F.
Deposited on : 2022-12-13
Resolution : 5.87 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

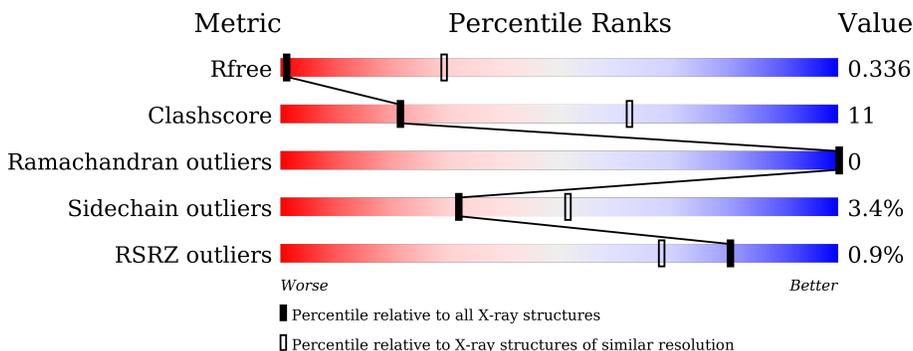
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.87 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}	164625	1071 (7.76-4.00)
Clashscore	180529	1112 (7.76-4.00)
Ramachandran outliers	177936	1003 (7.70-3.98)
Sidechain outliers	177891	1012 (7.80-3.96)
RSRZ outliers	164620	1066 (7.76-4.00)

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 $\leq 5\%$. 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	486	 75% 23%
1	B	486	 79% 19%
2	D	526	 71% 25%
2	E	526	 74% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15962 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 Disintegrin and metalloproteinase domain-containing protein 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	484	3710	2293	638	728	51	0	0	0
1	B	484	3710	2293	638	728	51	0	0	0

- Molecule 2 is a protein called Leucine-rich glioma-inactivated protein 1.

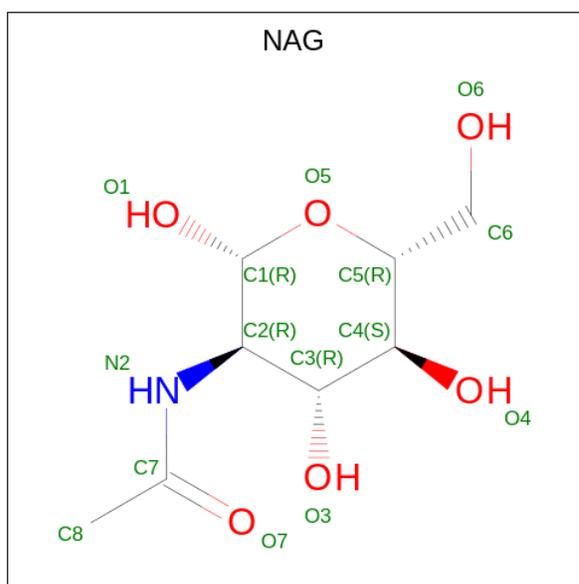
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	515	4183	2694	696	778	15	0	0	0
2	E	515	4183	2694	696	778	15	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	32	HIS	-	expression tag	UNP O95970
D	33	HIS	-	expression tag	UNP O95970
D	34	HIS	-	expression tag	UNP O95970
D	35	HIS	-	expression tag	UNP O95970
D	36	HIS	-	expression tag	UNP O95970
D	37	HIS	-	expression tag	UNP O95970
D	38	HIS	-	expression tag	UNP O95970
E	32	HIS	-	expression tag	UNP O95970
E	33	HIS	-	expression tag	UNP O95970
E	34	HIS	-	expression tag	UNP O95970
E	35	HIS	-	expression tag	UNP O95970
E	36	HIS	-	expression tag	UNP O95970
E	37	HIS	-	expression tag	UNP O95970
E	38	HIS	-	expression tag	UNP O95970

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



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

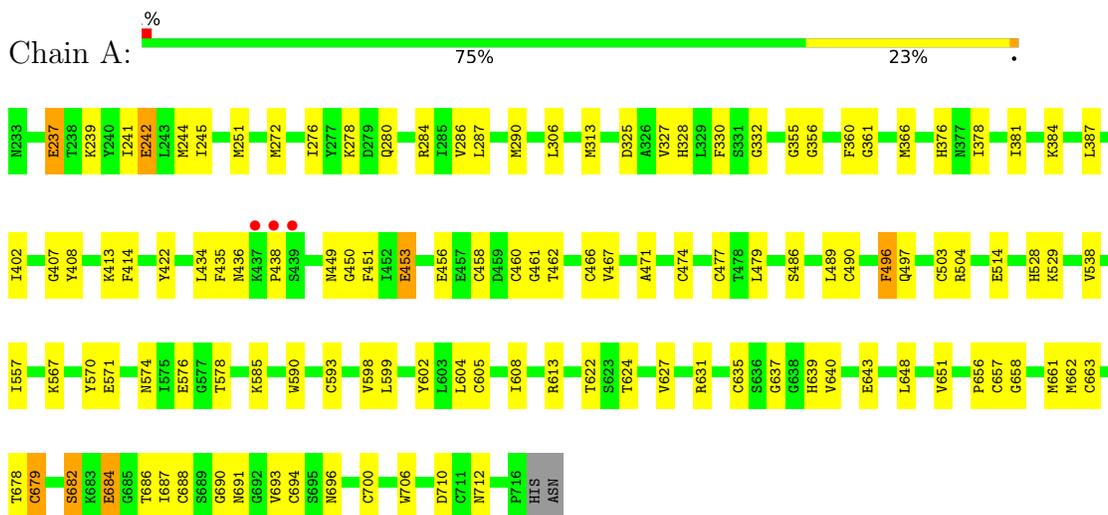
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	Ca 3	0	0
4	D	1	Total 1	Ca 1	0	0
4	B	3	Total 3	Ca 3	0	0
4	E	1	Total 1	Ca 1	0	0

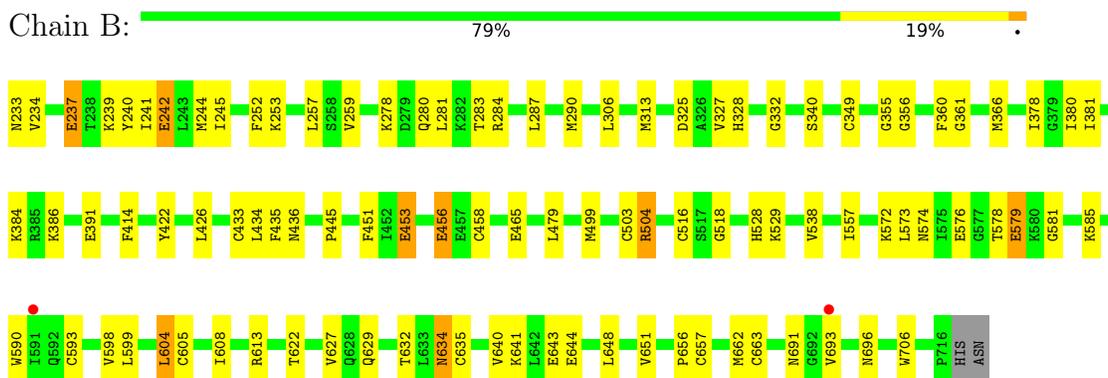
3 Residue-property plots [i](#)

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.

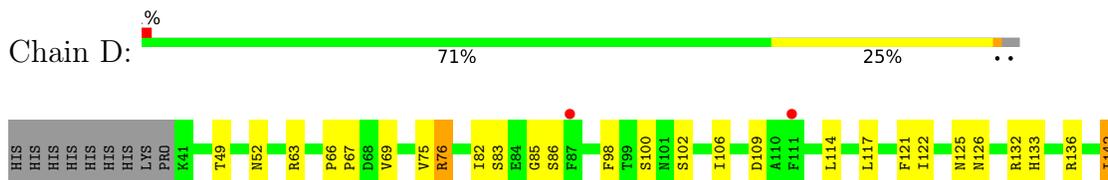
- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22



- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22



- Molecule 2: Leucine-rich glioma-inactivated protein 1



4 Data and refinement statistics i

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	280.34Å 280.34Å 280.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.08 – 5.87 48.08 – 5.87	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.08-5.87) 98.2 (48.08-5.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 5.73Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.303 , 0.343 0.304 , 0.336	Depositor DCC
R_{free} test set	497 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	283.5	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 566.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtrriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	15962	wwPDB-VP
Average B, all atoms (Å ²)	392.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: CA, 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	0.25	0/3773	0.47	0/5079
1	B	0.22	0/3773	0.48	1/5079 (0.0%)
2	D	0.16	0/4290	0.38	1/5821 (0.0%)
2	E	0.21	0/4290	0.41	0/5821
All	All	0.21	0/16126	0.43	2/21800 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	552	ILE	O-C-N	-5.27	117.57	123.26
1	B	518	GLY	N-CA-C	-5.08	109.03	115.08

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	3710	0	3566	80	0
1	B	3710	0	3566	81	0
2	D	4183	0	4100	100	0
2	E	4183	0	4099	88	0
3	A	42	0	39	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	42	0	39	5	0
3	D	42	0	39	0	0
3	E	42	0	39	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	15962	0	15487	336	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 11.

The worst 5 of 336 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)
2:D:223:ILE:HD11	2:D:555:LEU:CD1	1.68	1.20
2:D:223:ILE:HD11	2:D:555:LEU:HD11	1.19	1.09
2:D:223:ILE:CD1	2:D:555:LEU:HD11	1.98	0.92
1:B:237:GLU:HG2	1:B:435:PHE:HE1	1.32	0.92
1:B:237:GLU:HB2	1:B:504:ARG:HH22	1.34	0.92

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	482/486 (99%)	466 (97%)	16 (3%)	0	100 100
1	B	482/486 (99%)	471 (98%)	11 (2%)	0	100 100
2	D	513/526 (98%)	485 (94%)	28 (6%)	0	100 100
2	E	513/526 (98%)	488 (95%)	25 (5%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1990/2024 (98%)	1910 (96%)	80 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	418/420 (100%)	399 (96%)	19 (4%)	23	45
1	B	418/420 (100%)	404 (97%)	14 (3%)	33	52
2	D	473/483 (98%)	463 (98%)	10 (2%)	48	66
2	E	473/483 (98%)	456 (96%)	17 (4%)	30	50
All	All	1782/1806 (99%)	1722 (97%)	60 (3%)	32	51

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	552	ILE
2	E	483	GLN
1	B	503	CYS
2	E	476	SER
2	E	539	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	52	ASN
2	E	370	HIS
2	E	488	GLN
2	E	412	GLN
2	E	254	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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
3	NAG	D	603	2	14,14,15	1.02	1 (7%)	17,19,21	0.79	1 (5%)
3	NAG	A	802	1	14,14,15	0.55	0	17,19,21	0.53	0
3	NAG	E	603	2	14,14,15	0.41	0	17,19,21	0.51	0
3	NAG	B	802	1	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
3	NAG	A	801	1	14,14,15	0.33	0	17,19,21	0.50	0
3	NAG	B	801	1	14,14,15	0.54	0	17,19,21	0.45	0
3	NAG	E	602	2	14,14,15	0.90	1 (7%)	17,19,21	0.74	1 (5%)
3	NAG	D	601	2	14,14,15	0.34	0	17,19,21	0.34	0
3	NAG	A	803	1	14,14,15	0.70	1 (7%)	17,19,21	0.43	0
3	NAG	B	803	1	14,14,15	0.41	0	17,19,21	0.57	0
3	NAG	E	601	2	14,14,15	0.35	0	17,19,21	0.37	0
3	NAG	D	602	2	14,14,15	0.37	0	17,19,21	0.43	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
3	NAG	D	603	2	-	2/6/23/26	0/1/1/1
3	NAG	A	802	1	-	0/6/23/26	0/1/1/1
3	NAG	E	603	2	-	0/6/23/26	0/1/1/1
3	NAG	B	802	1	-	2/6/23/26	0/1/1/1
3	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	NAG	B	801	1	-	1/6/23/26	0/1/1/1
3	NAG	E	602	2	-	1/6/23/26	0/1/1/1
3	NAG	D	601	2	-	0/6/23/26	0/1/1/1
3	NAG	A	803	1	-	1/6/23/26	0/1/1/1
3	NAG	B	803	1	-	0/6/23/26	0/1/1/1
3	NAG	E	601	2	-	0/6/23/26	0/1/1/1
3	NAG	D	602	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	603	NAG	O5-C1	-3.64	1.37	1.43
3	E	602	NAG	O5-C1	3.22	1.48	1.43
3	A	803	NAG	O5-C1	-2.22	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	NAG	C1-O5-C5	2.63	115.76	112.19
3	E	602	NAG	C1-O5-C5	2.38	115.41	112.19
3	D	603	NAG	C1-O5-C5	-2.22	109.19	112.19

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	NAG	O5-C5-C6-O6
3	B	802	NAG	C4-C5-C6-O6
3	D	603	NAG	O5-C5-C6-O6
3	E	602	NAG	O5-C5-C6-O6
3	B	801	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	NAG	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	484/486 (99%)	-0.30	3 (0%) 85 74	349, 444, 521, 625	0
1	B	484/486 (99%)	-0.26	2 (0%) 89 79	312, 390, 497, 523	0
2	D	515/526 (97%)	-0.27	7 (1%) 73 61	276, 343, 396, 472	0
2	E	515/526 (97%)	-0.23	5 (0%) 79 66	295, 381, 436, 479	0
All	All	1998/2024 (98%)	-0.27	17 (0%) 81 68	276, 387, 498, 625	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	438	PRO	5.4
1	B	591	ILE	2.8
2	D	87	PHE	2.8
2	D	518	ASN	2.7
2	D	111	PHE	2.6

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 monosaccharides 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. 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
3	NAG	A	803	14/15	0.29	0.10	598,613,624,630	0
3	NAG	D	601	14/15	0.40	0.12	366,389,413,419	0
4	CA	B	804	1/1	0.40	0.18	404,404,404,404	0
3	NAG	A	801	14/15	0.42	0.13	509,522,532,532	0
3	NAG	D	603	14/15	0.46	0.12	375,391,421,421	0
3	NAG	B	803	14/15	0.47	0.09	508,523,543,560	0
3	NAG	E	601	14/15	0.69	0.11	349,374,386,390	0
3	NAG	B	802	14/15	0.69	0.09	342,369,386,398	0
3	NAG	A	802	14/15	0.74	0.07	425,447,472,473	0
3	NAG	B	801	14/15	0.74	0.07	471,500,505,512	0
3	NAG	E	603	14/15	0.75	0.09	396,426,446,448	0
4	CA	E	604	1/1	0.77	0.08	363,363,363,363	0
3	NAG	D	602	14/15	0.78	0.08	326,341,360,370	0
4	CA	A	804	1/1	0.82	0.07	472,472,472,472	0
4	CA	D	604	1/1	0.85	0.07	368,368,368,368	0
4	CA	B	806	1/1	0.90	0.08	419,419,419,419	0
3	NAG	E	602	14/15	0.91	0.04	347,357,368,376	0
4	CA	A	806	1/1	0.91	0.08	464,464,464,464	0
4	CA	A	805	1/1	0.93	0.07	461,461,461,461	0
4	CA	B	805	1/1	0.94	0.05	524,524,524,524	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.