



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:25 PM UTC

PDB ID : 8TBQ / pdb_00008tbq
Title : The crystal structure of human VISTA extra cellular domain in complex with Fab fragment of pH-selective anti-VISTA antibody
Authors : van der Horst, E.H.; Mukherjee, A.; Thisted, T.
Deposited on : 2023-06-29
Resolution : 2.59 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 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

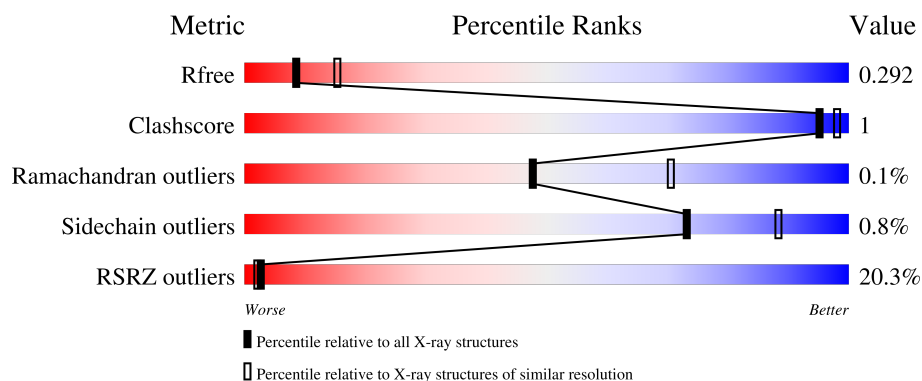
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	229	31% 91% 7%
1	H	229	7% 95% .
2	B	215	22% 79% 5% 16%
2	L	215	25% 95% .
3	P	159	12% 91% 5% .

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Mol	Chain	Length	Quality of chain
3	Q	159	13% 91% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8552 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 SNS-101 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	223	Total	C	N	O	S	0	1	0
			1639	1034	275	324	6			
1	A	213	Total	C	N	O	S	0	1	0
			1565	990	263	306	6			

- Molecule 2 is a protein called SNS-101 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1597	1009	263	321	4			
2	B	181	Total	C	N	O	S	0	1	0
			1328	830	221	273	4			

- Molecule 3 is a protein called V-type immunoglobulin domain-containing suppressor of T-cell activation.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	152	Total	C	N	O	S	0	0	0
			1170	724	219	219	8			
3	Q	152	Total	C	N	O	S	0	0	0
			1156	718	214	216	8			

There are 6 discrepancies between the modelled and reference sequences:

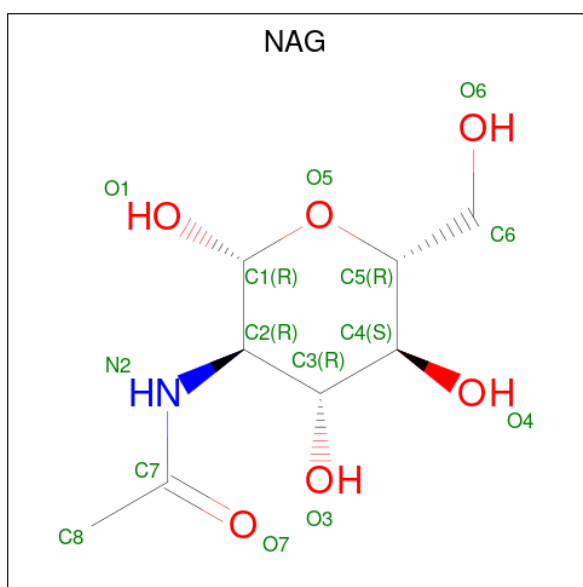
Chain	Residue	Modelled	Actual	Comment	Reference
P	91	GLN	ASN	conflict	UNP Q9H7M9
P	108	GLN	ASN	conflict	UNP Q9H7M9
P	190	GLN	ASN	conflict	UNP Q9H7M9
Q	91	GLN	ASN	conflict	UNP Q9H7M9
Q	108	GLN	ASN	conflict	UNP Q9H7M9
Q	190	GLN	ASN	conflict	UNP Q9H7M9

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

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



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

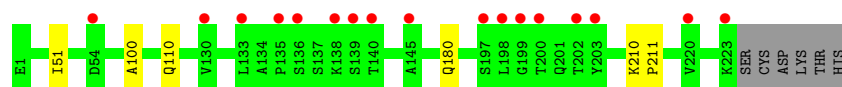
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	20	Total	O	0	0
			20	20		
6	L	16	Total	O	0	0
			16	16		
6	P	4	Total	O	0	0
			4	4		
6	A	4	Total	O	0	0
			4	4		
6	B	2	Total	O	0	0
			2	2		
6	Q	1	Total	O	0	0
			1	1		

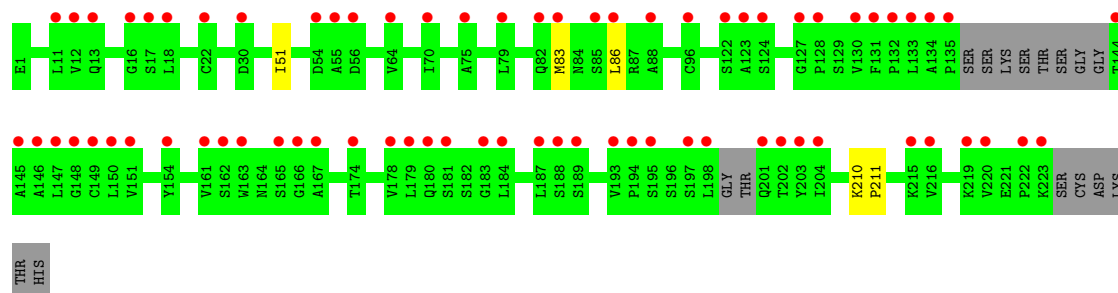
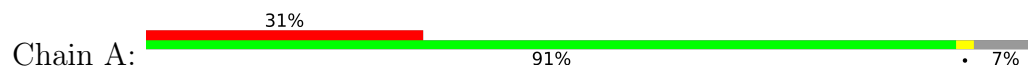
3 Residue-property plots [i](#)

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.

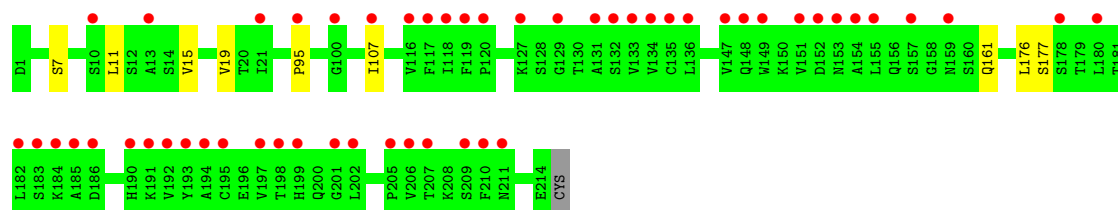
- Molecule 1: SNS-101 Fab heavy chain



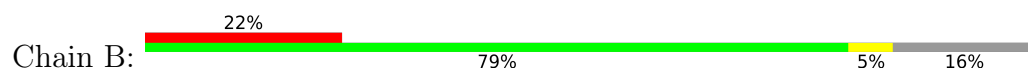
- Molecule 1: SNS-101 Fab heavy chain

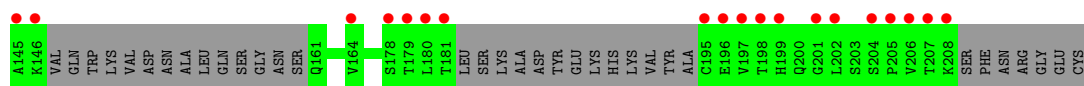


- Molecule 2: SNS-101 Fab light chain

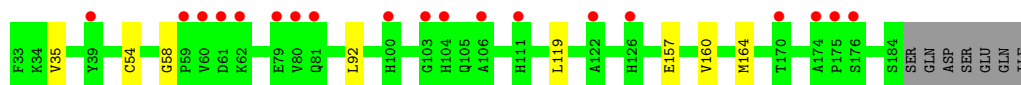
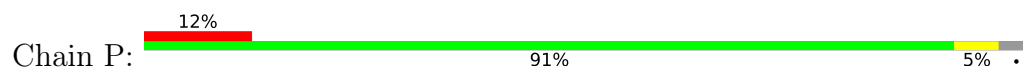


- Molecule 2: SNS-101 Fab light chain

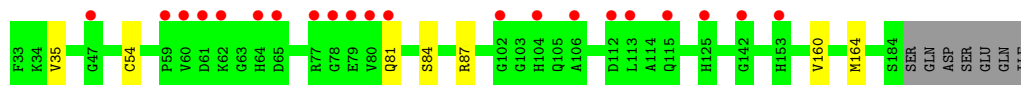
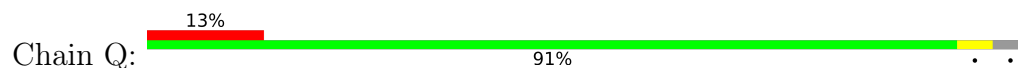




- Molecule 3: V-type immunoglobulin domain-containing suppressor of T-cell activation



- Molecule 3: V-type immunoglobulin domain-containing suppressor of T-cell activation



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.66Å 39.51Å 177.98Å 90.00° 117.12° 90.00°	Depositor
Resolution (Å)	158.41 – 2.59 158.41 – 2.59	Depositor EDS
% Data completeness (in resolution range)	63.9 (158.41-2.59) 63.9 (158.41-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.237 , 0.291 0.241 , 0.292	Depositor DCC
R_{free} test set	1291 reflections (1.26%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8552	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: NAG, EDO

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	0/1605	0.78	0/2191
1	H	0.50	0/1681	0.77	0/2295
2	B	0.51	0/1356	0.84	1/1851 (0.1%)
2	L	0.51	0/1634	0.82	1/2228 (0.0%)
3	P	0.51	0/1199	0.80	0/1630
3	Q	0.51	0/1184	0.79	0/1611
All	All	0.51	0/8659	0.80	2/11806 (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	L	95	PRO	N-CA-C	9.34	122.10	110.70
2	B	95	PRO	N-CA-C	8.82	121.45	110.70

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	1565	0	1453	2	0
1	H	1639	0	1549	3	0
2	B	1328	0	1202	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1597	0	1492	4	0
3	P	1170	0	1079	3	0
3	Q	1156	0	1069	3	0
4	H	8	0	12	0	0
5	P	14	0	13	0	0
5	Q	28	0	26	0	0
6	A	4	0	0	0	0
6	B	2	0	0	0	0
6	H	20	0	0	0	0
6	L	16	0	0	0	0
6	P	4	0	0	0	0
6	Q	1	0	0	0	0
All	All	8552	0	7895	20	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 1.

All (20) 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:L:15:VAL:HG22	2:L:107:ILE:HD11	1.81	0.62
2:B:109:ARG:HH21	2:B:112:ALA:HB2	1.67	0.59
2:B:20:THR:HG23	2:B:72:THR:HG23	1.83	0.59
3:P:92:LEU:HD12	3:P:119:LEU:HD12	1.85	0.58
3:P:54:CYS:SG	3:P:164:MET:HE1	2.50	0.51
1:H:180:GLN:HA	2:L:161:GLN:HE22	1.76	0.50
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.95	0.48
3:Q:54:CYS:SG	3:Q:164:MET:HE1	2.54	0.48
2:L:176:LEU:HD23	2:L:177:SER:N	2.29	0.48
2:L:11:LEU:HD11	2:L:19:VAL:HG13	1.97	0.46
2:B:31:ASN:N	2:B:31:ASN:HD22	2.15	0.44
2:B:6:GLN:HE21	2:B:100:GLY:HA3	1.83	0.43
3:Q:35:VAL:HG23	3:Q:160:VAL:HG23	2.01	0.42
3:Q:81:GLN:HB3	3:Q:84:SER:HB2	2.02	0.42
1:H:210:LYS:N	1:H:211:PRO:CD	2.83	0.41
1:H:100:ALA:HB2	1:H:110:GLN:HB3	2.02	0.41
2:B:4:LEU:HD23	2:B:25:ALA:HA	2.03	0.41
2:B:6:GLN:HE22	2:B:87:TYR:HA	1.85	0.41
1:A:210:LYS:N	1:A:211:PRO:CD	2.84	0.40
3:P:35:VAL:HG23	3:P:160:VAL:HG23	2.03	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	208/229 (91%)	202 (97%)	6 (3%)	0	100	100
1	H	222/229 (97%)	212 (96%)	10 (4%)	0	100	100
2	B	176/215 (82%)	166 (94%)	10 (6%)	0	100	100
2	L	212/215 (99%)	197 (93%)	15 (7%)	0	100	100
3	P	150/159 (94%)	139 (93%)	10 (7%)	1 (1%)	18	38
3	Q	150/159 (94%)	140 (93%)	10 (7%)	0	100	100
All	All	1118/1206 (93%)	1056 (94%)	61 (6%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	58	GLY

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	160/191 (84%)	159 (99%)	1 (1%)	78	91
1	H	173/191 (91%)	172 (99%)	1 (1%)	78	91
2	B	137/188 (73%)	135 (98%)	2 (2%)	57	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	168/188 (89%)	167 (99%)	1 (1%)	78	91
3	P	124/141 (88%)	123 (99%)	1 (1%)	73	88
3	Q	122/141 (86%)	121 (99%)	1 (1%)	73	88
All	All	884/1040 (85%)	877 (99%)	7 (1%)	73	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	51	ILE
2	L	7	SER
3	P	157	GLU
1	A	51	ILE
2	B	31	ASN
2	B	78	LEU
3	Q	87	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	110	GLN
1	H	111	HIS
2	L	161	GLN
3	P	169	GLN
1	A	39	GLN
2	B	6	GLN
2	B	24	GLN
2	B	31	ASN
2	B	38	GLN
2	B	138	ASN
3	Q	117	HIS
3	Q	128	ASN
3	Q	167	GLN

5.3.3 RNA ⓘ

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](#)

5 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	EDO	H	302	-	3,3,3	0.09	0	2,2,2	0.18	0
5	NAG	Q	202	3	14,14,15	0.41	0	17,19,21	0.68	0
5	NAG	Q	201	3	14,14,15	0.39	0	17,19,21	0.68	0
4	EDO	H	301	-	3,3,3	0.14	0	2,2,2	0.17	0
5	NAG	P	201	3	14,14,15	0.40	0	17,19,21	0.70	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
4	EDO	H	302	-	-	0/1/1/1	-
5	NAG	Q	202	3	-	0/6/23/26	0/1/1/1
5	NAG	Q	201	3	-	0/6/23/26	0/1/1/1
4	EDO	H	301	-	-	1/1/1/1	-
5	NAG	P	201	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	EDO	O1-C1-C2-O2

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

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	213/229 (93%)	1.60	72 (33%) 1 1	35, 69, 104, 111	1 (0%)
1	H	223/229 (97%)	0.54	17 (7%) 20 16	21, 39, 88, 134	1 (0%)
2	B	181/215 (84%)	1.24	48 (26%) 1 1	16, 45, 107, 121	1 (0%)
2	L	214/215 (99%)	1.19	53 (24%) 2 1	20, 46, 106, 124	0
3	P	152/159 (95%)	0.90	19 (12%) 8 6	26, 51, 96, 109	0
3	Q	152/159 (95%)	1.01	21 (13%) 6 5	34, 57, 90, 103	0
All	All	1135/1206 (94%)	1.08	230 (20%) 3 2	16, 53, 103, 134	3 (0%)

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	139	SER	6.5
2	L	210	PHE	5.8
2	L	182	LEU	5.4
2	B	198	THR	5.1
2	B	195	CYS	5.1
2	B	130	THR	5.0
2	B	197	VAL	4.6
2	L	211	ASN	4.6
1	A	12	VAL	4.5
2	L	192	VAL	4.5
2	L	193	TYR	4.4
2	L	195	CYS	4.3
1	A	133	LEU	4.1
1	A	161	VAL	4.1
2	L	194	ALA	4.0
1	A	195	SER	4.0
2	L	152	ASP	4.0
2	B	206	VAL	3.9
2	B	95	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	135	CYS	3.9
1	A	220	VAL	3.9
1	H	197	SER	3.8
2	B	205	PRO	3.8
2	L	100	GLY	3.8
3	Q	80	VAL	3.8
1	A	131	PHE	3.8
2	B	121	PRO	3.7
2	B	118	ILE	3.7
2	B	132	SER	3.7
2	L	10	SER	3.6
1	A	17	SER	3.5
2	B	96	PRO	3.5
1	A	179	LEU	3.5
3	Q	113	LEU	3.5
2	B	146	LYS	3.5
1	A	86	LEU	3.5
2	B	196	GLU	3.5
2	L	116	VAL	3.5
2	L	148	GLN	3.4
2	B	128	SER	3.4
2	B	117	PHE	3.4
1	A	163	TRP	3.4
2	B	124	GLU	3.4
1	A	215	LYS	3.4
2	B	119	PHE	3.4
1	A	201	GLN	3.3
2	B	180	LEU	3.3
2	L	206	VAL	3.3
2	B	116	VAL	3.3
1	A	130	VAL	3.3
1	A	135	PRO	3.2
1	A	16	GLY	3.2
2	B	131	ALA	3.2
1	A	150	LEU	3.2
2	B	179	THR	3.2
3	P	59	PRO	3.2
2	L	118	ILE	3.2
2	B	142	PRO	3.2
1	A	83	MET	3.2
1	A	123	ALA	3.1
2	B	136	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	181	THR	3.1
2	L	151	VAL	3.1
3	P	80	VAL	3.1
1	H	140	THR	3.1
1	A	166	GLY	3.1
2	B	134	VAL	3.1
2	L	180	LEU	3.0
1	A	188	SER	3.0
2	L	131	ALA	3.0
1	A	203	TYR	3.0
1	A	149	CYS	3.0
2	L	191	LYS	3.0
1	A	197	SER	3.0
2	L	135	CYS	3.0
2	L	201	GLY	3.0
2	B	208	LYS	2.9
1	A	134	ALA	2.9
1	A	79	LEU	2.9
1	A	198	LEU	2.9
2	L	197	VAL	2.9
2	L	185	ALA	2.9
2	B	114	PRO	2.9
1	A	30	ASP	2.9
1	A	148	GLY	2.8
1	H	135	PRO	2.8
1	A	189	SER	2.8
2	L	159	ASN	2.8
1	A	151	VAL	2.8
1	A	194	PRO	2.8
2	L	155	LEU	2.8
3	Q	61	ASP	2.8
2	B	111	VAL	2.8
1	A	146	ALA	2.8
1	H	223	LYS	2.8
2	L	154	ALA	2.7
1	A	180	GLN	2.7
1	A	56	ASP	2.7
2	B	100	GLY	2.7
1	A	222	PRO	2.7
2	L	132	SER	2.7
1	A	75	ALA	2.7
1	A	183	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	L	147	VAL	2.7
1	A	11	LEU	2.7
1	A	184	LEU	2.7
2	L	190	HIS	2.7
2	B	201	GLY	2.7
3	Q	142	GLY	2.7
2	L	198	THR	2.7
3	Q	79	GLU	2.7
3	Q	64	HIS	2.7
3	Q	59	PRO	2.6
1	A	187	LEU	2.6
2	B	133	VAL	2.6
2	B	120	PRO	2.6
2	L	134	VAL	2.6
3	P	104	HIS	2.6
2	L	95	PRO	2.6
3	P	79	GLU	2.6
2	L	184	LYS	2.6
2	B	207	THR	2.6
1	A	18	LEU	2.5
2	B	126	LEU	2.5
2	L	133	VAL	2.5
3	P	60	VAL	2.5
1	A	181	SER	2.5
2	L	209	SER	2.5
2	B	204	SER	2.5
3	P	106	ALA	2.5
3	P	126	HIS	2.5
3	Q	104	HIS	2.5
1	A	174	THR	2.5
2	B	202	LEU	2.5
1	A	216	VAL	2.5
3	P	174	ALA	2.5
2	B	12	SER	2.5
2	L	205	PRO	2.4
3	P	103	GLY	2.4
1	A	145	ALA	2.4
1	A	127	GLY	2.4
3	Q	62	LYS	2.4
1	A	144	THR	2.4
1	A	165	SER	2.4
1	H	138	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	54	ASP	2.4
3	Q	81	GLN	2.4
2	L	199	HIS	2.4
3	Q	77	ARG	2.4
2	L	157	SER	2.4
2	L	136	LEU	2.4
2	B	123	ASP	2.4
1	A	96	CYS	2.4
1	A	162	SER	2.3
3	Q	115	GLN	2.3
2	B	141	TYR	2.3
1	H	130	VAL	2.3
2	L	127	LYS	2.3
1	A	55	ALA	2.3
2	B	113	ALA	2.3
3	Q	125	HIS	2.3
1	A	132	PRO	2.3
3	Q	60	VAL	2.3
2	L	120	PRO	2.3
1	A	202	THR	2.3
2	L	178	SER	2.3
3	P	61	ASP	2.3
2	B	145	ALA	2.2
1	H	199	GLY	2.2
1	A	82	GLN	2.2
2	L	129	GLY	2.2
2	B	199	HIS	2.2
1	A	128	PRO	2.2
3	P	39	TYR	2.2
3	P	62	LYS	2.2
3	Q	47	GLY	2.2
3	Q	102	GLY	2.2
1	A	147	LEU	2.2
2	L	107	ILE	2.2
2	B	178	SER	2.2
1	H	220	VAL	2.2
1	A	178	VAL	2.2
3	P	170	THR	2.2
1	H	133	LEU	2.2
1	H	198	LEU	2.2
2	L	202	LEU	2.2
3	Q	78	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	P	100	HIS	2.2
2	B	137	LEU	2.2
2	B	164	VAL	2.1
1	H	200	THR	2.1
1	A	154	TYR	2.1
1	A	204	ILE	2.1
2	L	21	ILE	2.1
1	A	122	SER	2.1
3	Q	65	ASP	2.1
3	Q	112	ASP	2.1
1	A	88	ALA	2.1
1	A	167	ALA	2.1
2	L	186	ASP	2.1
3	P	175	PRO	2.1
3	P	111	HIS	2.1
2	L	149	TRP	2.1
1	H	136	SER	2.1
1	A	22	CYS	2.1
2	L	183	SER	2.1
3	P	176	SER	2.1
1	A	13	GLN	2.1
1	A	64	VAL	2.1
2	L	117	PHE	2.1
3	Q	153	HIS	2.1
2	B	125	GLN	2.0
3	P	81	GLN	2.0
2	L	13	ALA	2.0
3	P	122	ALA	2.0
3	Q	106	ALA	2.0
1	H	202	THR	2.0
1	A	219	LYS	2.0
2	L	207	THR	2.0
1	H	54	ASP	2.0
1	H	203	TYR	2.0
1	A	85	SER	2.0
1	A	193	VAL	2.0
2	L	119	PHE	2.0
1	H	145	ALA	2.0
1	A	223	LYS	2.0
2	L	153	ASN	2.0
1	A	70	ILE	2.0
2	B	28	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	124	SER	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](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	EDO	H	302	4/4	0.73	0.21	51,53,54,55	0
5	NAG	Q	202	14/15	0.73	0.17	73,77,86,86	0
5	NAG	P	201	14/15	0.78	0.13	52,54,57,60	0
4	EDO	H	301	4/4	0.81	0.14	29,29,29,30	0
5	NAG	Q	201	14/15	0.85	0.11	66,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.