wwPDB X-ray Structure Validation Summary Report (i)

Jan 20, 2025 – 12:04 PM EST

PDB ID	:	8VQ8
Title	:	Immune receptor complex
Authors	:	Chaurasia, P.; Littler, D.R.; La Gruta, N.; Rossjohn, J.
Deposited on	:	2024-01-17
Resolution	:	2.01 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 (i) 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 (i)) were used in the production of this report:

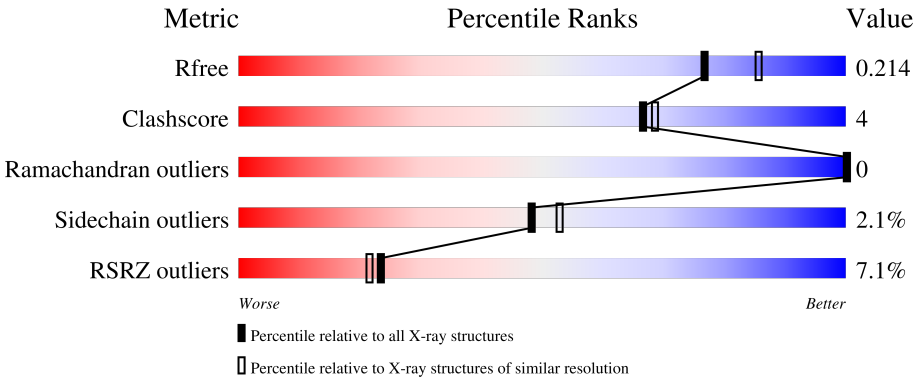
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.01 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	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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 <=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	207	2% 88% 10%
2	B	243	14% 87% 11%
3	C	188	3% 91% 7%
4	D	228	5% 55% 9% 35%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6625 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 T cell receptor - LCK1-1 TRAV6-5 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	3	0
			1560	983	249	320	8			

- Molecule 2 is a protein called T cell receptor - LCK1-1 TRBV1 Beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	4	0
			1914	1215	339	352	8			

- Molecule 3 is a protein called H-2 class II histocompatibility antigen, A-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	186	Total	C	N	O	S	0	5	0
			1503	972	238	290	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	181	THR	-	expression tag	UNP P14434
C	182	SER	-	expression tag	UNP P14434
C	183	GLY	-	expression tag	UNP P14434
C	184	LEU	-	expression tag	UNP P14434
C	185	GLU	-	expression tag	UNP P14434
C	186	VAL	-	expression tag	UNP P14434
C	187	LEU	-	expression tag	UNP P14434
C	188	PHE	-	expression tag	UNP P14434

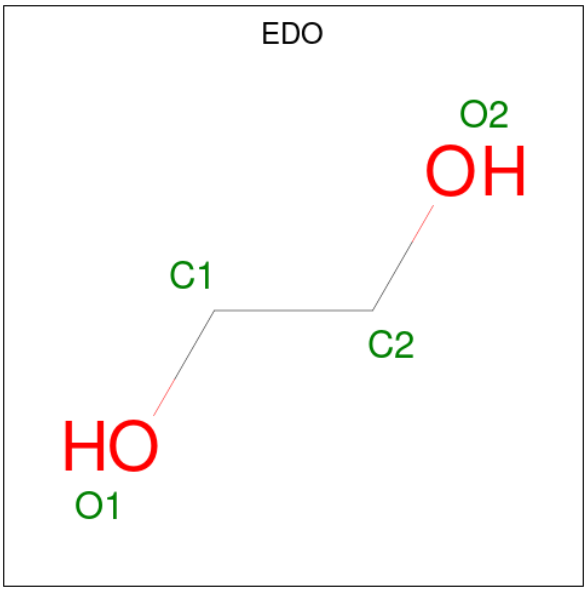
- Molecule 4 is a protein called Nucleoprotein,H-2 class II histocompatibility antigen, A beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	148	Total	C	N	O	S	0	1	0
			1215	759	218	234	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-13C	GLY	-	linker	UNP P69296
D	-13D	SER	-	linker	UNP P69296
D	-13E	GLY	-	linker	UNP P69296
D	-13F	GLY	-	linker	UNP P69296
D	-13G	SER	-	linker	UNP P69296
D	-13H	ILE	-	linker	UNP P69296
D	-13I	GLU	-	linker	UNP P69296
D	-13J	GLY	-	linker	UNP P69296
D	-13K	ARG	-	linker	UNP P69296
D	-13L	GLY	-	linker	UNP P69296
D	-13M	GLY	-	linker	UNP P69296
D	-13N	SER	-	linker	UNP P69296
D	-13O	GLY	-	linker	UNP P69296
D	-13P	ALA	-	linker	UNP P69296
D	-13Q	SER	-	linker	UNP P69296
D	187	THR	-	expression tag	UNP P14483
D	188	GLY	-	expression tag	UNP P14483
D	189	GLY	-	expression tag	UNP P14483
D	190	LEU	-	expression tag	UNP P14483
D	191	GLU	-	expression tag	UNP P14483
D	192	VAL	-	expression tag	UNP P14483
D	193	LEU	-	expression tag	UNP P14483
D	194	PHE	-	expression tag	UNP P14483
D	195	GLN	-	expression tag	UNP P14483

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

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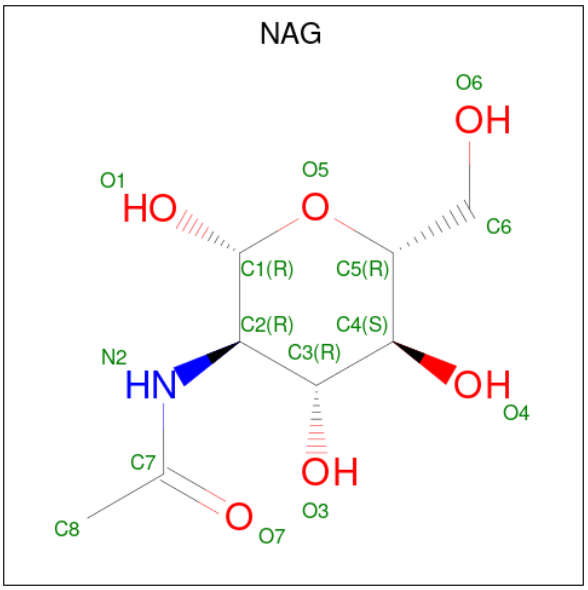
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is water.

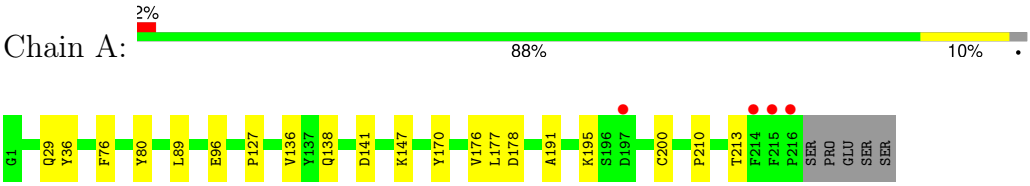
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	117	Total O 117 117	0	0
7	B	82	Total O 82 82	0	0
7	C	79	Total O 79 79	0	0
7	D	81	Total O 81 81	0	0

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.

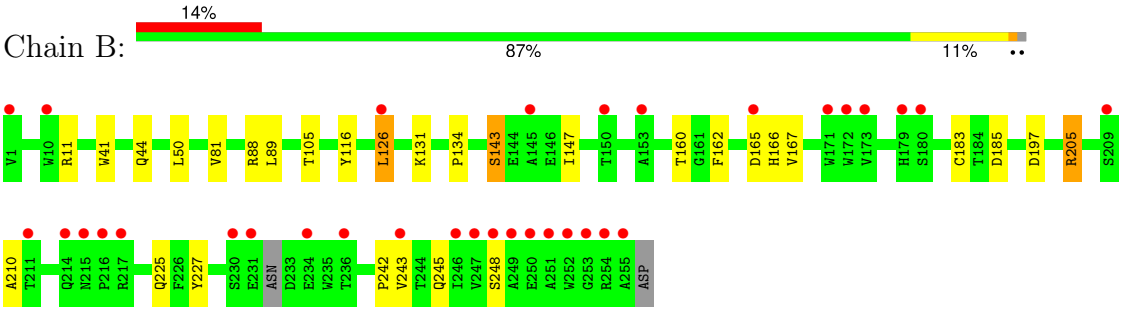
• Molecule 1: T cell receptor - LCK1-1 TRAV6-5 alpha chain

Chain A:



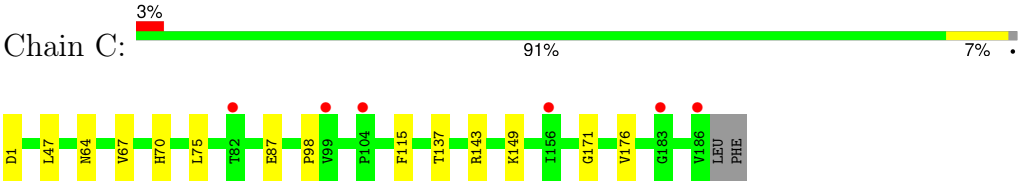
• Molecule 2: T cell receptor - LCK1-1 TRBV1 Beta chain

Chain B:



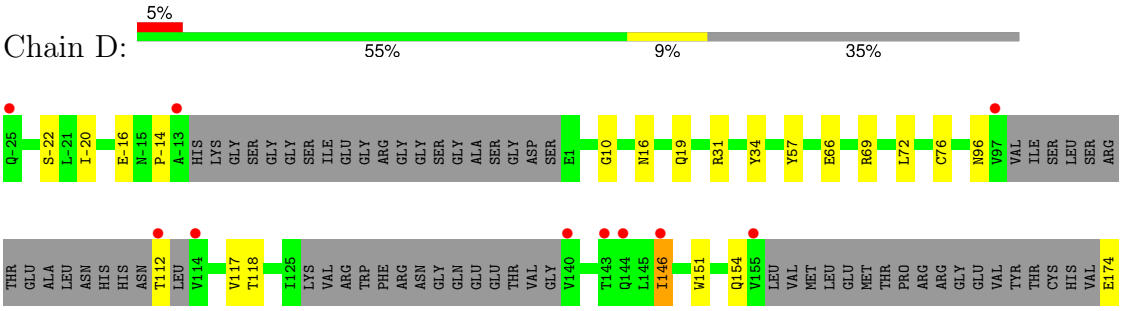
• Molecule 3: H-2 class II histocompatibility antigen, A-B alpha chain

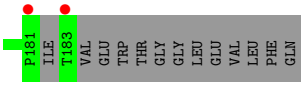
Chain C:



• Molecule 4: Nucleoprotein,H-2 class II histocompatibility antigen, A beta chain

Chain D:




P181
ILE
T183
VAL
GLU
TRP
THR
GLY
GLY
LEU
GLU
VAL
LEU
PHE
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	197.60Å 197.60Å 79.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.40 – 2.01 49.40 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.40-2.01) 100.0 (49.40-2.01)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.187 , 0.215 0.187 , 0.214	Depositor DCC
R_{free} test set	3839 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6625	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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	0.41	0/1597	0.59	0/2174
2	B	0.37	0/1964	0.59	0/2682
3	C	0.40	0/1547	0.55	0/2115
4	D	0.43	0/1242	0.61	0/1684
All	All	0.40	0/6350	0.59	0/8655

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

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	1560	0	1443	12	0
2	B	1914	0	1799	16	0
3	C	1503	0	1422	9	0
4	D	1215	0	1102	15	0
5	A	8	0	12	1	0
5	B	20	0	30	1	0
5	C	28	0	42	0	0
5	D	4	0	6	0	0
6	D	14	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	117	0	0	0	0
7	B	82	0	0	0	0
7	C	79	0	0	0	0
7	D	81	0	0	0	0
All	All	6625	0	5869	44	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.

The worst 5 of 44 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)
4:D:19:GLN:HE22	6:D:301:NAG:HN2	1.29	0.76
2:B:131:LYS:HE2	2:B:197:ASP:OD2	1.99	0.61
4:D:96:ASN:O	4:D:117:VAL:HA	2.00	0.60
4:D:-20:ILE:HD13	4:D:10:GLY:HA3	1.88	0.56
2:B:185:ASP:OD1	2:B:205:ARG:NH2	2.39	0.55

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	203/207 (98%)	198 (98%)	5 (2%)	0	100	100
2	B	241/243 (99%)	237 (98%)	4 (2%)	0	100	100
3	C	189/188 (100%)	186 (98%)	3 (2%)	0	100	100
4	D	137/228 (60%)	135 (98%)	2 (2%)	0	100	100
All	All	770/866 (89%)	756 (98%)	14 (2%)	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	174/185 (94%)	171 (98%)	3 (2%)	56	61
2	B	197/214 (92%)	192 (98%)	5 (2%)	42	45
3	C	167/168 (99%)	165 (99%)	2 (1%)	67	73
4	D	128/202 (63%)	124 (97%)	4 (3%)	35	36
All	All	666/769 (87%)	652 (98%)	14 (2%)	48	53

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	248	SER
3	C	64	ASN
4	D	174	GLU
4	D	146	ILE
4	D	154	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
5	EDO	B	505	-	3,3,3	0.44	0	2,2,2	0.58	0
5	EDO	C	502	-	3,3,3	0.52	0	2,2,2	0.22	0
5	EDO	C	504	-	3,3,3	0.49	0	2,2,2	0.28	0
5	EDO	C	503	-	3,3,3	0.47	0	2,2,2	0.32	0
6	NAG	D	301	4	14,14,15	0.72	1 (7%)	17,19,21	0.98	2 (11%)
5	EDO	C	506	-	3,3,3	0.56	0	2,2,2	0.32	0
5	EDO	B	501	-	3,3,3	0.42	0	2,2,2	0.69	0
5	EDO	B	502	-	3,3,3	0.45	0	2,2,2	0.32	0
5	EDO	B	503	-	3,3,3	0.49	0	2,2,2	0.32	0
5	EDO	C	507	-	3,3,3	0.50	0	2,2,2	0.60	0
5	EDO	A	401	-	3,3,3	0.50	0	2,2,2	0.48	0
5	EDO	A	402	-	3,3,3	0.42	0	2,2,2	0.47	0
5	EDO	C	505	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	C	501	-	3,3,3	0.49	0	2,2,2	0.13	0
5	EDO	B	504	-	3,3,3	0.46	0	2,2,2	0.44	0
5	EDO	D	302	-	3,3,3	0.43	0	2,2,2	0.46	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	EDO	B	505	-	-	0/1/1/1	-
5	EDO	C	502	-	-	0/1/1/1	-
5	EDO	C	504	-	-	0/1/1/1	-
5	EDO	C	503	-	-	1/1/1/1	-
6	NAG	D	301	4	-	3/6/23/26	0/1/1/1
5	EDO	C	506	-	-	1/1/1/1	-
5	EDO	B	501	-	-	1/1/1/1	-
5	EDO	B	502	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	503	-	-	1/1/1/1	-
5	EDO	C	507	-	-	0/1/1/1	-
5	EDO	A	401	-	-	0/1/1/1	-
5	EDO	A	402	-	-	0/1/1/1	-
5	EDO	C	505	-	-	0/1/1/1	-
5	EDO	C	501	-	-	0/1/1/1	-
5	EDO	B	504	-	-	1/1/1/1	-
5	EDO	D	302	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	301	NAG	C1-C2	2.49	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	301	NAG	C2-N2-C7	2.55	126.32	122.90
6	D	301	NAG	C1-O5-C5	2.09	114.98	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	301	NAG	C3-C2-N2-C7
6	D	301	NAG	O5-C5-C6-O6
6	D	301	NAG	C4-C5-C6-O6
5	B	504	EDO	O1-C1-C2-O2
5	D	302	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	301	NAG	2	0
5	A	402	EDO	1	0
5	B	504	EDO	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, 95^{th} 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	202/207 (97%)	0.04	4 (1%) 64 63	16, 52, 86, 116	3 (1%)
2	B	241/243 (99%)	0.57	33 (13%) 8 6	19, 62, 115, 131	4 (1%)
3	C	186/188 (98%)	0.04	6 (3%) 50 48	17, 51, 89, 104	5 (2%)
4	D	148/228 (64%)	0.11	12 (8%) 19 18	17, 46, 103, 128	1 (0%)
All	All	777/866 (89%)	0.22	55 (7%) 23 21	16, 53, 104, 131	13 (1%)

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	114	VAL	5.0
2	B	217	ARG	4.7
2	B	255	ALA	4.6
3	C	186	VAL	4.3
4	D	155	VAL	4.2

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, 95^{th} 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
6	NAG	D	301	14/15	0.21	0.16	94,108,115,116	0
5	EDO	B	502	4/4	0.58	0.14	87,88,94,97	0
5	EDO	A	402	4/4	0.66	0.20	79,82,85,86	0
5	EDO	C	502	4/4	0.78	0.19	55,62,62,71	0
5	EDO	B	504	4/4	0.82	0.22	48,53,58,63	0
5	EDO	C	501	4/4	0.82	0.16	62,62,64,74	0
5	EDO	C	506	4/4	0.83	0.15	60,61,61,69	0
5	EDO	D	302	4/4	0.84	0.16	60,62,64,66	0
5	EDO	C	503	4/4	0.89	0.11	70,71,71,80	0
5	EDO	A	401	4/4	0.89	0.16	62,62,63,70	0
5	EDO	C	504	4/4	0.91	0.21	52,56,62,64	0
5	EDO	B	503	4/4	0.91	0.18	41,61,61,63	0
5	EDO	B	501	4/4	0.92	0.12	60,62,63,66	0
5	EDO	C	505	4/4	0.93	0.12	55,59,64,64	0
5	EDO	B	505	4/4	0.93	0.12	46,47,48,51	0
5	EDO	C	507	4/4	0.97	0.07	36,37,40,42	0

6.5 Other polymers (i)

There are no such residues in this entry.