Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 09:28 AM EDT

PDB ID	:	3BE8
Title	:	Crystal structure of the synaptic protein neuroligin 4
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Deposited on	:	2007-11-16
Resolution	:	2.20 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 (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:

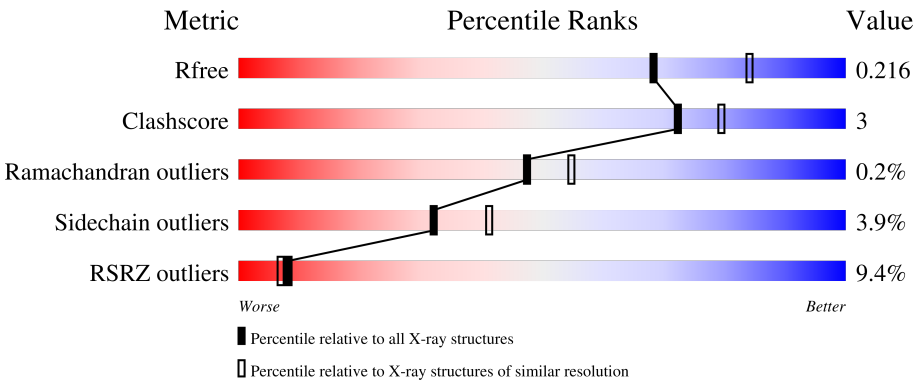
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	588	8% 82% 10% 8%
1	B	588	9% 83% 7% • 9%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	621	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9309 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 Neuroligin-4, X-linked.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	543	4345	2787	714	821	23	0	10	0
1	B	534	4261	2736	699	804	22	0	7	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ASP	-	expression tag	UNP Q8N0W4
A	-11	TYR	-	expression tag	UNP Q8N0W4
A	-10	LYS	-	expression tag	UNP Q8N0W4
A	-9	ASP	-	expression tag	UNP Q8N0W4
A	-8	ASP	-	expression tag	UNP Q8N0W4
A	-7	ASP	-	expression tag	UNP Q8N0W4
A	-6	ASP	-	expression tag	UNP Q8N0W4
A	-5	LYS	-	expression tag	UNP Q8N0W4
A	-4	LEU	-	expression tag	UNP Q8N0W4
A	-3	ALA	-	expression tag	UNP Q8N0W4
A	-2	ALA	-	expression tag	UNP Q8N0W4
A	-1	ALA	-	expression tag	UNP Q8N0W4
A	561	ARG	LYS	SEE REMARK 999	UNP Q8N0W4
B	-12	ASP	-	expression tag	UNP Q8N0W4
B	-11	TYR	-	expression tag	UNP Q8N0W4
B	-10	LYS	-	expression tag	UNP Q8N0W4
B	-9	ASP	-	expression tag	UNP Q8N0W4
B	-8	ASP	-	expression tag	UNP Q8N0W4
B	-7	ASP	-	expression tag	UNP Q8N0W4
B	-6	ASP	-	expression tag	UNP Q8N0W4
B	-5	LYS	-	expression tag	UNP Q8N0W4
B	-4	LEU	-	expression tag	UNP Q8N0W4
B	-3	ALA	-	expression tag	UNP Q8N0W4
B	-2	ALA	-	expression tag	UNP Q8N0W4
B	-1	ALA	-	expression tag	UNP Q8N0W4

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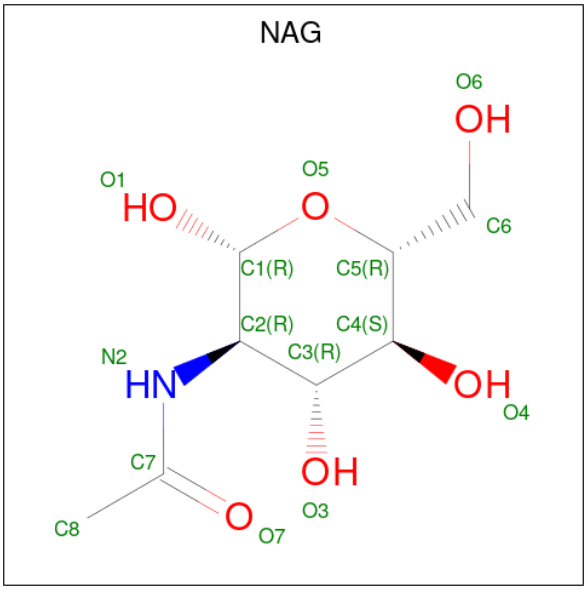
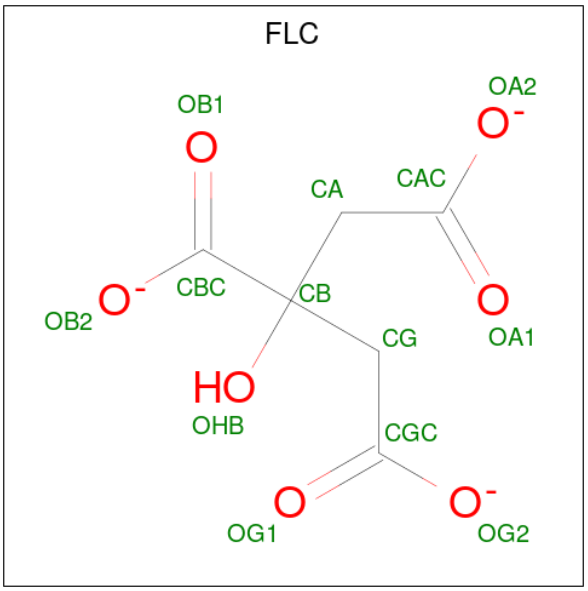
Chain	Residue	Modelled	Actual	Comment	Reference
B	561	ARG	LYS	SEE REMARK 999	UNP Q8N0W4

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



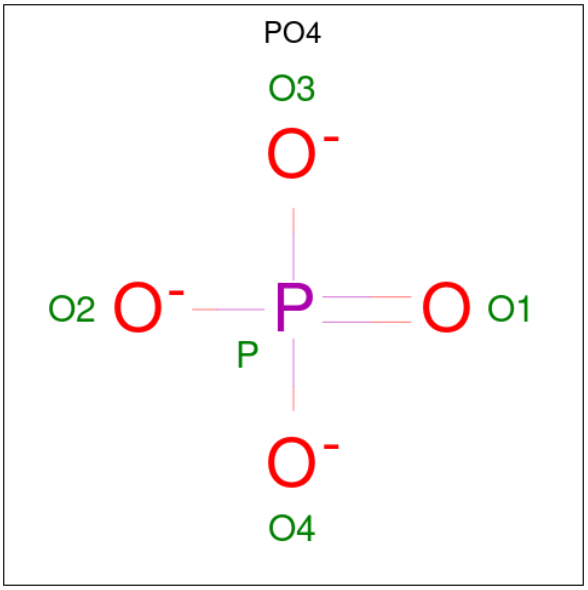
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	B	1	14	8	1	5	0	0
			Total	C	N	O		
2	B	1	14	8	1	5	0	0

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

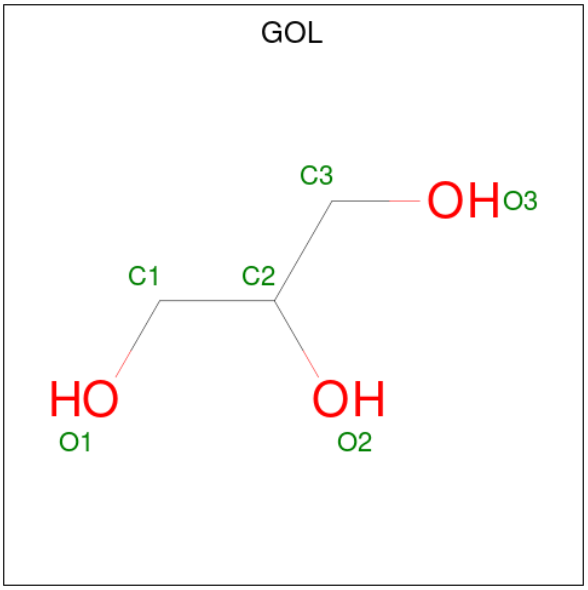
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Cl 3 3	0	0
5	B	3	Total Cl 3 3	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0

- Molecule 8 is water.

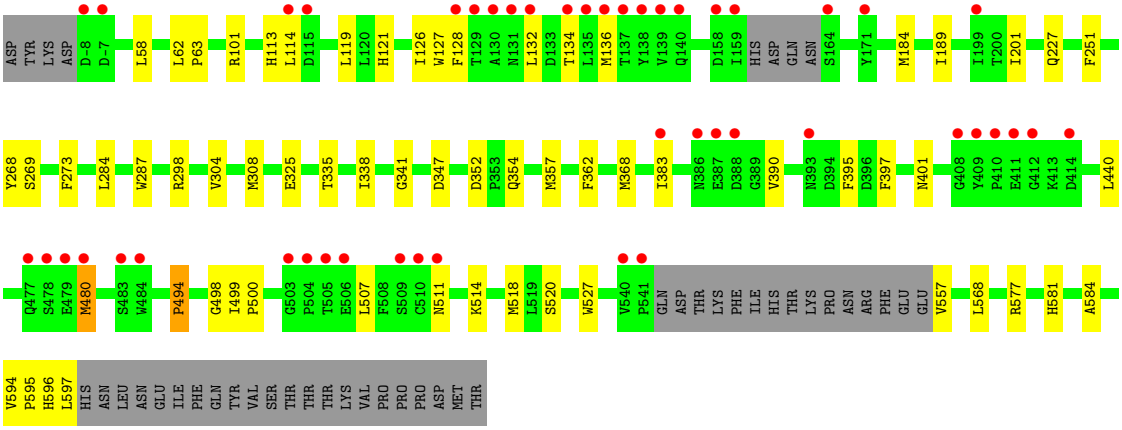
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	311	Total O 311 311	0	0
8	B	281	Total O 281 281	0	0

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.

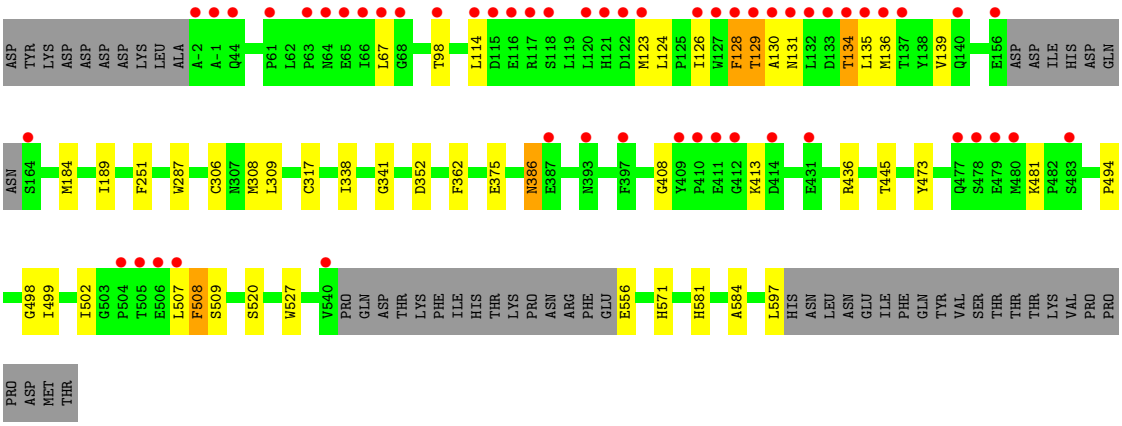
• Molecule 1: Neuroligin-4, X-linked

Chain A:



• Molecule 1: Neuroligin-4, X-linked

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	139.73Å 154.05Å 81.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.68 – 2.20 29.68 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.68-2.20) 99.9 (29.68-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.35 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.167 , 0.201 0.186 , 0.216	Depositor DCC
R_{free} test set	4474 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9309	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, NA, FLC, PO4, GOL

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	0.64	0/4493	0.71	1/6126 (0.0%)
1	B	0.59	0/4401	0.69	2/6002 (0.0%)
All	All	0.62	0/8894	0.70	3/12128 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	101	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	436	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	B	436	ARG	NE-CZ-NH2	5.27	122.93	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	508	PHE	Peptide

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	4345	0	4216	27	0
1	B	4261	0	4119	30	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
3	A	13	0	5	0	0
3	B	13	0	5	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	1	0	0	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	A	311	0	0	4	0
8	B	281	0	0	1	0
All	All	9309	0	8413	57	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 3.

All (57) 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:B:114:LEU:HD12	1:B:136:MET:SD	2.10	0.91
1:B:306:CYS:HG	1:B:317:CYS:HG	0.78	0.78
1:A:494:PRO:HA	1:A:499:ILE:HD12	1.71	0.73
1:B:386:ASN:HD22	1:B:386:ASN:N	1.85	0.72
1:B:386:ASN:N	1:B:386:ASN:ND2	2.40	0.69
1:A:113:HIS:ND1	8:A:930:HOH:O	2.28	0.65
1:B:508:PHE:HA	1:B:509:SER:CB	2.28	0.63
1:B:135:LEU:HD11	1:B:184[B]:MET:SD	2.39	0.63
1:B:508:PHE:HA	1:B:509:SER:HB3	1.81	0.61
1:A:132:LEU:HG	1:A:184[B]:MET:SD	2.41	0.61
1:A:581:HIS:HB3	1:A:584:ALA:HB2	1.83	0.59
1:B:114:LEU:CD1	1:B:136:MET:SD	2.89	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ILE:HD12	1:B:341:GLY:HA3	1.86	0.56
1:A:304:VAL:HG22	1:A:325:GLU:HG3	1.87	0.56
1:B:386:ASN:ND2	1:B:386:ASN:H	2.02	0.56
1:A:284:LEU:HD21	1:A:357:MET:HE1	1.88	0.56
1:A:113:HIS:HA	8:A:657:HOH:O	2.06	0.55
1:B:189:ILE:HD11	1:B:502:ILE:HG23	1.89	0.55
1:B:135:LEU:HD11	1:B:184[B]:MET:CE	2.37	0.54
1:B:499:ILE:HD13	1:B:508:PHE:CD2	2.43	0.53
1:B:473[A]:TYR:CE2	1:B:571:HIS:ND1	2.79	0.51
1:A:126:ILE:HD11	1:A:480:MET:HB2	1.93	0.50
1:B:135:LEU:HD11	1:B:184[B]:MET:HE1	1.92	0.50
1:B:124:LEU:CD1	1:B:129:THR:OG1	2.59	0.50
1:A:498:GLY:HA2	1:A:520:SER:OG	2.11	0.50
1:A:338:ILE:HD12	1:A:341:GLY:HA3	1.94	0.49
1:B:494:PRO:HA	1:B:499:ILE:HD12	1.95	0.48
1:B:556:GLU:HG2	8:B:709:HOH:O	2.13	0.48
1:B:131:ASN:HB3	1:B:134:THR:HG23	1.95	0.48
1:A:577[A]:ARG:NH1	8:A:755:HOH:O	2.47	0.48
1:A:284:LEU:HD11	1:A:357:MET:HE1	1.97	0.47
1:B:128:PHE:O	1:B:135:LEU:HD13	2.14	0.47
1:A:114:LEU:HD23	1:A:121:HIS:HB2	1.97	0.46
1:A:395:PHE:CD1	1:A:440:LEU:HD13	2.51	0.46
1:A:201:ILE:HD11	1:A:227:GLN:HG2	2.00	0.44
1:A:594:VAL:O	1:A:596:HIS:N	2.50	0.44
1:A:127:TRP:CE3	1:A:128:PHE:HA	2.53	0.44
1:A:268:TYR:OH	1:A:347:ASP:OD1	2.34	0.43
1:B:124:LEU:HD12	1:B:129:THR:OG1	2.18	0.43
1:A:284:LEU:HD11	1:A:357:MET:CE	2.49	0.42
1:A:284:LEU:HD22	1:A:354[B]:GLN:HG2	2.01	0.42
1:A:269:SER:HB3	1:A:273:PHE:HE1	1.84	0.42
1:B:581:HIS:HB3	1:B:584:ALA:HB2	2.00	0.42
1:A:397:PHE:CE2	1:A:401:ASN:ND2	2.88	0.42
1:B:124:LEU:HD13	1:B:129:THR:OG1	2.19	0.42
1:B:507:LEU:O	1:B:509:SER:HB2	2.20	0.42
1:A:499:ILE:N	1:A:500:PRO:CD	2.83	0.41
1:A:383:ILE:O	1:A:390:VAL:HG22	2.21	0.41
1:B:126:ILE:O	1:B:130:ALA:HB3	2.20	0.41
1:B:408:GLY:O	1:B:413:LYS:NZ	2.52	0.41
1:A:119:LEU:CD1	1:A:335:THR:HG23	2.50	0.41
1:B:139:VAL:CG1	1:B:139:VAL:O	2.68	0.41
1:B:189:ILE:HD11	1:B:502:ILE:CG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PRO:HD2	8:A:859:HOH:O	2.21	0.41
1:A:298:ARG:HD3	1:A:298:ARG:O	2.21	0.40
1:B:375:GLU:HB2	1:B:445:THR:HG23	2.02	0.40
1:B:498:GLY:HA2	1:B:520:SER:OG	2.22	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	547/588 (93%)	529 (97%)	17 (3%)	1 (0%)	47	55
1	B	535/588 (91%)	519 (97%)	15 (3%)	1 (0%)	47	55
All	All	1082/1176 (92%)	1048 (97%)	32 (3%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	595	PRO
1	B	128	PHE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	475/510 (93%)	452 (95%)	23 (5%)	25	32
1	B	464/510 (91%)	449 (97%)	15 (3%)	39	50
All	All	939/1020 (92%)	901 (96%)	38 (4%)	32	40

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	62	LEU
1	A	134	THR
1	A	136	MET
1	A	189[A]	ILE
1	A	189[B]	ILE
1	A	251	PHE
1	A	287	TRP
1	A	308	MET
1	A	352	ASP
1	A	362	PHE
1	A	368[A]	MET
1	A	368[B]	MET
1	A	480	MET
1	A	494	PRO
1	A	507	LEU
1	A	511	ASN
1	A	514	LYS
1	A	518	MET
1	A	527	TRP
1	A	557	VAL
1	A	568	LEU
1	A	597	LEU
1	B	67	LEU
1	B	98	THR
1	B	123	MET
1	B	129	THR
1	B	134	THR
1	B	251	PHE
1	B	287	TRP
1	B	308	MET
1	B	309	LEU

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Mol	Chain	Res	Type
1	B	352	ASP
1	B	362	PHE
1	B	386	ASN
1	B	481	LYS
1	B	527	TRP
1	B	597	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	216	GLN
1	A	328	GLN
1	A	359	GLN
1	A	386	ASN
1	A	405	ASN
1	A	567	GLN
1	B	89	GLN
1	B	202	ASN
1	B	386	ASN
1	B	405	ASN
1	B	462	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
4	PO4	A	623	-	4,4,4	1.36	1 (25%)	6,6,6	1.58	2 (33%)
7	GOL	A	628	-	5,5,5	0.38	0	5,5,5	0.54	0
2	NAG	B	621	1	14,14,15	0.92	0	17,19,21	1.05	1 (5%)
4	PO4	B	624	-	4,4,4	0.90	0	6,6,6	0.86	0
2	NAG	A	620	1	14,14,15	1.06	1 (7%)	17,19,21	1.30	1 (5%)
7	GOL	B	627	-	5,5,5	0.38	0	5,5,5	0.55	0
2	NAG	B	620	1	14,14,15	0.82	0	17,19,21	1.73	4 (23%)
2	NAG	A	621	1	14,14,15	0.91	0	17,19,21	1.26	2 (11%)
3	FLC	A	622	-	12,12,12	1.01	0	17,17,17	1.54	5 (29%)
3	FLC	B	623	-	12,12,12	1.11	1 (8%)	17,17,17	1.00	1 (5%)

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
7	GOL	A	628	-	-	4/4/4/4	-
2	NAG	B	621	1	-	2/6/23/26	0/1/1/1
2	NAG	A	620	1	-	2/6/23/26	0/1/1/1
7	GOL	B	627	-	-	4/4/4/4	-
2	NAG	B	620	1	-	2/6/23/26	0/1/1/1
2	NAG	A	621	1	1/1/5/7	0/6/23/26	0/1/1/1
3	FLC	A	622	-	-	2/16/16/16	-
3	FLC	B	623	-	-	2/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	623	PO4	P-O2	-2.43	1.47	1.54
2	A	620	NAG	O5-C5	2.18	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	623	FLC	OA2-CAC	-2.01	1.24	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	620	NAG	C8-C7-N2	4.30	123.39	116.10
2	B	620	NAG	O7-C7-C8	-3.47	115.62	122.06
2	A	620	NAG	O5-C1-C2	-3.28	106.11	111.29
3	A	622	FLC	OB2-CBC-CB	3.15	118.53	113.05
4	A	623	PO4	O3-P-O1	-2.72	100.95	110.89
2	B	620	NAG	O5-C1-C2	-2.65	107.10	111.29
2	A	621	NAG	O7-C7-C8	-2.54	117.33	122.06
2	A	621	NAG	O5-C1-C2	-2.44	107.43	111.29
3	A	622	FLC	CB-CA-CAC	-2.42	107.95	113.81
2	B	620	NAG	C2-N2-C7	2.40	126.32	122.90
2	B	621	NAG	O7-C7-C8	-2.21	117.95	122.06
3	A	622	FLC	OB1-CBC-CB	-2.17	119.17	122.25
4	A	623	PO4	O4-P-O2	2.17	114.94	107.97
3	B	623	FLC	OB2-CBC-CB	2.07	116.65	113.05
3	A	622	FLC	OA1-CAC-CA	-2.03	117.00	122.94
3	A	622	FLC	OG1-CGC-CG	-2.00	117.09	122.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	621	NAG	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	628	GOL	O1-C1-C2-C3
7	B	627	GOL	O1-C1-C2-C3
7	B	627	GOL	C1-C2-C3-O3
2	B	620	NAG	C8-C7-N2-C2
2	B	620	NAG	O7-C7-N2-C2
2	B	621	NAG	C4-C5-C6-O6
7	B	627	GOL	O2-C2-C3-O3
2	B	621	NAG	O5-C5-C6-O6
7	A	628	GOL	C1-C2-C3-O3
7	A	628	GOL	O1-C1-C2-O2
7	A	628	GOL	O2-C2-C3-O3
7	B	627	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	622	FLC	CB-CG-CGC-OG1
3	A	622	FLC	CB-CG-CGC-OG2
3	B	623	FLC	CB-CG-CGC-OG2
2	A	620	NAG	O5-C5-C6-O6
3	B	623	FLC	CB-CG-CGC-OG1
2	A	620	NAG	C4-C5-C6-O6

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 (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	543/588 (92%)	0.25	47 (8%)	10	8	19, 34, 68, 89	0
1	B	534/588 (90%)	0.34	54 (10%)	7	6	21, 37, 82, 115	0
All	All	1077/1176 (91%)	0.29	101 (9%)	8	7	19, 35, 72, 115	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	ALA	12.0
1	B	129	THR	9.9
1	B	66	ILE	9.0
1	B	410	PRO	8.6
1	B	409	TYR	7.8
1	A	-8	ASP	7.4
1	B	65	GLU	7.0
1	A	541	PRO	6.7
1	B	164	SER	6.5
1	A	409	TYR	6.3
1	A	136	MET	6.2
1	B	411	GLU	6.1
1	B	131	ASN	5.9
1	A	410	PRO	5.9
1	A	140	GLN	5.9
1	B	480	MET	5.7
1	A	505	THR	5.7
1	B	506	GLU	5.7
1	A	139	VAL	5.7
1	A	129	THR	5.6
1	B	540	VAL	5.5
1	A	480	MET	5.4
1	B	133	ASP	5.4
1	B	127	TRP	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	122	ASP	5.4
1	A	159	ILE	5.3
1	A	506	GLU	5.1
1	B	132	LEU	5.1
1	A	412	GLY	5.0
1	A	478	SER	4.9
1	B	479	GLU	4.9
1	A	479	GLU	4.9
1	A	483	SER	4.8
1	B	136	MET	4.8
1	A	-7	ASP	4.6
1	A	137	THR	4.6
1	B	128	PHE	4.5
1	A	386	ASN	4.5
1	B	121	HIS	4.5
1	A	387	GLU	4.4
1	B	505	THR	4.3
1	A	484	TRP	4.3
1	A	158	ASP	4.2
1	B	44	GLN	4.1
1	A	383	ILE	4.0
1	A	134	THR	4.0
1	A	411	GLU	3.9
1	A	131	ASN	3.9
1	B	116	GLU	3.9
1	A	540	VAL	3.8
1	B	414	ASP	3.8
1	B	64	ASN	3.8
1	A	164	SER	3.8
1	B	114	LEU	3.7
1	B	120	LEU	3.6
1	B	397	PHE	3.6
1	B	156	GLU	3.5
1	A	408	GLY	3.4
1	B	117	ARG	3.4
1	B	-1	ALA	3.3
1	A	388	ASP	3.3
1	A	138	TYR	3.3
1	B	115	ASP	3.3
1	B	98	THR	3.2
1	A	132	LEU	3.2
1	B	137	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	511	ASN	3.0
1	A	477	GLN	3.0
1	B	123	MET	3.0
1	B	504	PRO	2.9
1	A	128	PHE	2.9
1	A	114	LEU	2.8
1	B	134	THR	2.8
1	B	412	GLY	2.8
1	B	507	LEU	2.7
1	A	504	PRO	2.7
1	B	68	GLY	2.7
1	B	-2	ALA	2.6
1	A	130	ALA	2.6
1	B	387	GLU	2.6
1	A	510	CYS	2.5
1	B	61	PRO	2.5
1	B	63	PRO	2.5
1	A	115	ASP	2.5
1	A	135	LEU	2.4
1	B	135	LEU	2.4
1	B	477	GLN	2.3
1	B	393	ASN	2.3
1	A	503	GLY	2.3
1	A	414	ASP	2.3
1	B	126	ILE	2.3
1	A	509	SER	2.2
1	B	483	SER	2.2
1	B	431	GLU	2.2
1	B	140	GLN	2.2
1	B	478	SER	2.2
1	B	118	SER	2.2
1	A	171	TYR	2.1
1	B	67	LEU	2.1
1	A	199	ILE	2.1
1	A	393	ASN	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 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(Å^2)	Q<0.9
2	NAG	A	621	14/15	0.45	0.38	118,136,148,148	0
2	NAG	A	620	14/15	0.49	0.26	175,185,197,198	0
2	NAG	B	621	14/15	0.66	0.32	107,120,134,138	0
2	NAG	B	620	14/15	0.72	0.17	166,174,185,187	0
3	FLC	A	622	13/13	0.78	0.21	67,75,79,83	0
7	GOL	B	627	6/6	0.83	0.20	85,93,97,98	0
5	CL	A	624	1/1	0.86	0.56	113,113,113,113	0
7	GOL	A	628	6/6	0.91	0.22	82,90,93,96	0
5	CL	B	625	1/1	0.93	0.61	109,109,109,109	0
6	NA	A	626	1/1	0.93	0.29	43,43,43,43	0
5	CL	A	627	1/1	0.94	1.12	120,120,120,120	0
5	CL	B	622	1/1	0.95	1.13	120,120,120,120	0
4	PO4	A	623	5/5	0.96	0.13	38,45,53,53	0
3	FLC	B	623	13/13	0.96	0.12	49,54,58,62	0
5	CL	B	626	1/1	0.97	0.04	38,38,38,38	0
5	CL	A	625	1/1	0.99	0.05	38,38,38,38	0
4	PO4	B	624	5/5	0.99	0.10	44,45,52,53	0

6.5 Other polymers (i)

There are no such residues in this entry.