



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:20 PM UTC

PDB ID : 5O0O / pdb_00005o0o
Title : Deglycosylated Nogo Receptor with native disulfide structure 5
Authors : Pronker, M.F.; Janssen, B.J.C.
Deposited on : 2017-05-16
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 ⓘ 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:

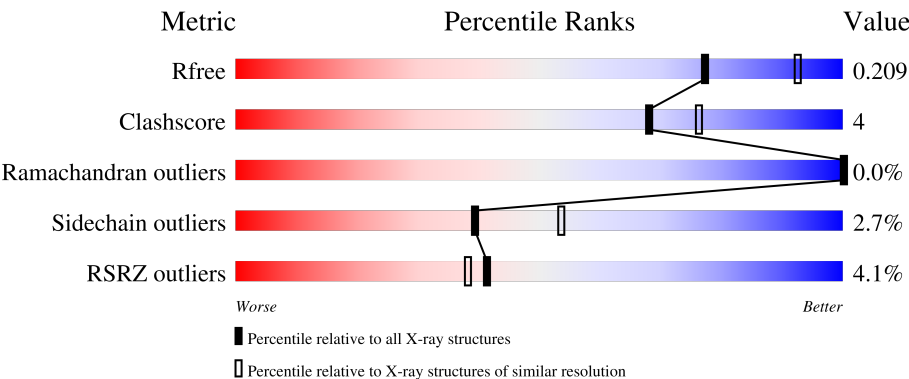
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	323	3% 88%10%..
1	B	323	3% 88%10%..
1	C	323	4% 85%10%..
1	D	323	6% 88%9%.
1	E	323	6% 88%10%.

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Mol	Chain	Length	Quality of chain
1	F	323	
1	G	323	
1	H	323	

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
4	CL	A	417	-	-	X	-
4	CL	C	407	-	-	X	-
4	CL	C	414	-	-	X	-
4	CL	D	406	-	-	X	-
4	CL	D	412	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21913 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 Reticulon-4 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2465	1553	459	438	15			
1	B	317	Total	C	N	O	S	0	1	0
			2491	1571	466	439	15			
1	C	313	Total	C	N	O	S	0	0	0
			2447	1542	456	434	15			
1	D	315	Total	C	N	O	S	0	1	0
			2470	1557	460	438	15			
1	E	315	Total	C	N	O	S	0	2	0
			2479	1560	465	439	15			
1	F	311	Total	C	N	O	S	0	2	0
			2453	1546	459	433	15			
1	G	312	Total	C	N	O	S	0	0	0
			2442	1540	455	432	15			
1	H	308	Total	C	N	O	S	0	2	0
			2429	1530	454	430	15			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP Q99PI8
A	25	SER	-	expression tag	UNP Q99PI8
A	26	PRO	-	expression tag	UNP Q99PI8
A	338	ALA	-	expression tag	UNP Q99PI8
A	339	ALA	-	expression tag	UNP Q99PI8
A	340	ALA	-	expression tag	UNP Q99PI8
A	341	HIS	-	expression tag	UNP Q99PI8
A	342	HIS	-	expression tag	UNP Q99PI8
A	343	HIS	-	expression tag	UNP Q99PI8
A	344	HIS	-	expression tag	UNP Q99PI8
A	345	HIS	-	expression tag	UNP Q99PI8
A	346	HIS	-	expression tag	UNP Q99PI8
B	24	GLY	-	expression tag	UNP Q99PI8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	25	SER	-	expression tag	UNP Q99PI8
B	26	PRO	-	expression tag	UNP Q99PI8
B	338	ALA	-	expression tag	UNP Q99PI8
B	339	ALA	-	expression tag	UNP Q99PI8
B	340	ALA	-	expression tag	UNP Q99PI8
B	341	HIS	-	expression tag	UNP Q99PI8
B	342	HIS	-	expression tag	UNP Q99PI8
B	343	HIS	-	expression tag	UNP Q99PI8
B	344	HIS	-	expression tag	UNP Q99PI8
B	345	HIS	-	expression tag	UNP Q99PI8
B	346	HIS	-	expression tag	UNP Q99PI8
C	24	GLY	-	expression tag	UNP Q99PI8
C	25	SER	-	expression tag	UNP Q99PI8
C	26	PRO	-	expression tag	UNP Q99PI8
C	338	ALA	-	expression tag	UNP Q99PI8
C	339	ALA	-	expression tag	UNP Q99PI8
C	340	ALA	-	expression tag	UNP Q99PI8
C	341	HIS	-	expression tag	UNP Q99PI8
C	342	HIS	-	expression tag	UNP Q99PI8
C	343	HIS	-	expression tag	UNP Q99PI8
C	344	HIS	-	expression tag	UNP Q99PI8
C	345	HIS	-	expression tag	UNP Q99PI8
C	346	HIS	-	expression tag	UNP Q99PI8
D	24	GLY	-	expression tag	UNP Q99PI8
D	25	SER	-	expression tag	UNP Q99PI8
D	26	PRO	-	expression tag	UNP Q99PI8
D	338	ALA	-	expression tag	UNP Q99PI8
D	339	ALA	-	expression tag	UNP Q99PI8
D	340	ALA	-	expression tag	UNP Q99PI8
D	341	HIS	-	expression tag	UNP Q99PI8
D	342	HIS	-	expression tag	UNP Q99PI8
D	343	HIS	-	expression tag	UNP Q99PI8
D	344	HIS	-	expression tag	UNP Q99PI8
D	345	HIS	-	expression tag	UNP Q99PI8
D	346	HIS	-	expression tag	UNP Q99PI8
E	24	GLY	-	expression tag	UNP Q99PI8
E	25	SER	-	expression tag	UNP Q99PI8
E	26	PRO	-	expression tag	UNP Q99PI8
E	338	ALA	-	expression tag	UNP Q99PI8
E	339	ALA	-	expression tag	UNP Q99PI8
E	340	ALA	-	expression tag	UNP Q99PI8
E	341	HIS	-	expression tag	UNP Q99PI8

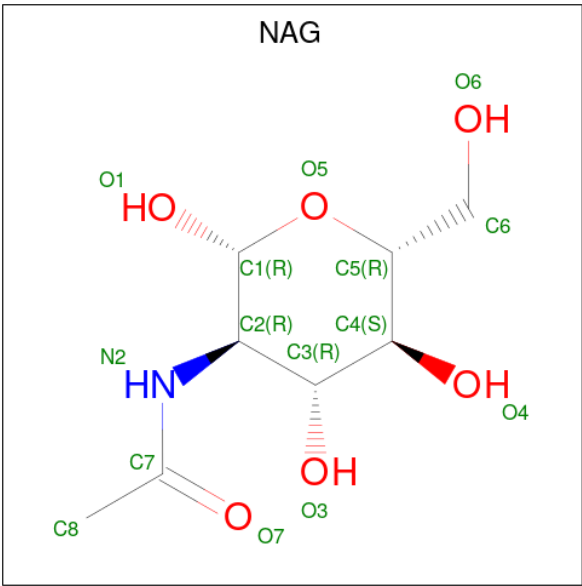
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Chain	Residue	Modelled	Actual	Comment	Reference
E	342	HIS	-	expression tag	UNP Q99PI8
E	343	HIS	-	expression tag	UNP Q99PI8
E	344	HIS	-	expression tag	UNP Q99PI8
E	345	HIS	-	expression tag	UNP Q99PI8
E	346	HIS	-	expression tag	UNP Q99PI8
F	24	GLY	-	expression tag	UNP Q99PI8
F	25	SER	-	expression tag	UNP Q99PI8
F	26	PRO	-	expression tag	UNP Q99PI8
F	338	ALA	-	expression tag	UNP Q99PI8
F	339	ALA	-	expression tag	UNP Q99PI8
F	340	ALA	-	expression tag	UNP Q99PI8
F	341	HIS	-	expression tag	UNP Q99PI8
F	342	HIS	-	expression tag	UNP Q99PI8
F	343	HIS	-	expression tag	UNP Q99PI8
F	344	HIS	-	expression tag	UNP Q99PI8
F	345	HIS	-	expression tag	UNP Q99PI8
F	346	HIS	-	expression tag	UNP Q99PI8
G	24	GLY	-	expression tag	UNP Q99PI8
G	25	SER	-	expression tag	UNP Q99PI8
G	26	PRO	-	expression tag	UNP Q99PI8
G	338	ALA	-	expression tag	UNP Q99PI8
G	339	ALA	-	expression tag	UNP Q99PI8
G	340	ALA	-	expression tag	UNP Q99PI8
G	341	HIS	-	expression tag	UNP Q99PI8
G	342	HIS	-	expression tag	UNP Q99PI8
G	343	HIS	-	expression tag	UNP Q99PI8
G	344	HIS	-	expression tag	UNP Q99PI8
G	345	HIS	-	expression tag	UNP Q99PI8
G	346	HIS	-	expression tag	UNP Q99PI8
H	24	GLY	-	expression tag	UNP Q99PI8
H	25	SER	-	expression tag	UNP Q99PI8
H	26	PRO	-	expression tag	UNP Q99PI8
H	338	ALA	-	expression tag	UNP Q99PI8
H	339	ALA	-	expression tag	UNP Q99PI8
H	340	ALA	-	expression tag	UNP Q99PI8
H	341	HIS	-	expression tag	UNP Q99PI8
H	342	HIS	-	expression tag	UNP Q99PI8
H	343	HIS	-	expression tag	UNP Q99PI8
H	344	HIS	-	expression tag	UNP Q99PI8
H	345	HIS	-	expression tag	UNP Q99PI8
H	346	HIS	-	expression tag	UNP Q99PI8

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

C₈H₁₅NO₆).



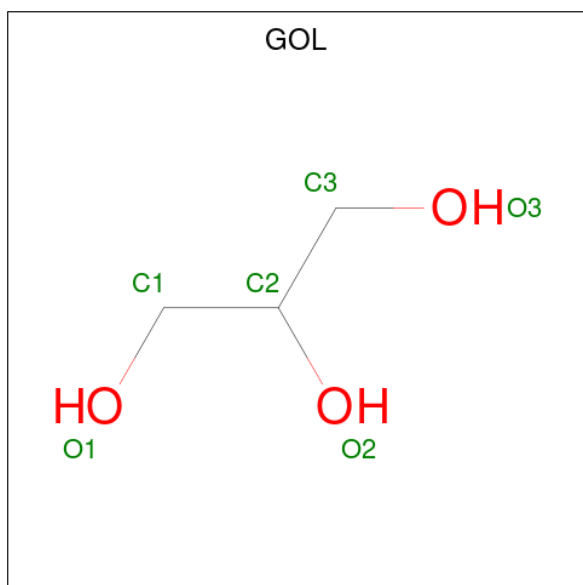
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total Cl 12 12	0	0
4	B	13	Total Cl 13 13	0	0
4	C	14	Total Cl 14 14	0	0
4	D	9	Total Cl 9 9	0	0
4	E	11	Total Cl 11 11	0	0
4	F	13	Total Cl 13 13	0	0
4	G	12	Total Cl 12 12	0	0
4	H	10	Total Cl 10 10	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	243	Total O 243 243	0	0
5	B	230	Total O 230 230	0	0
5	C	204	Total O 204 204	0	0

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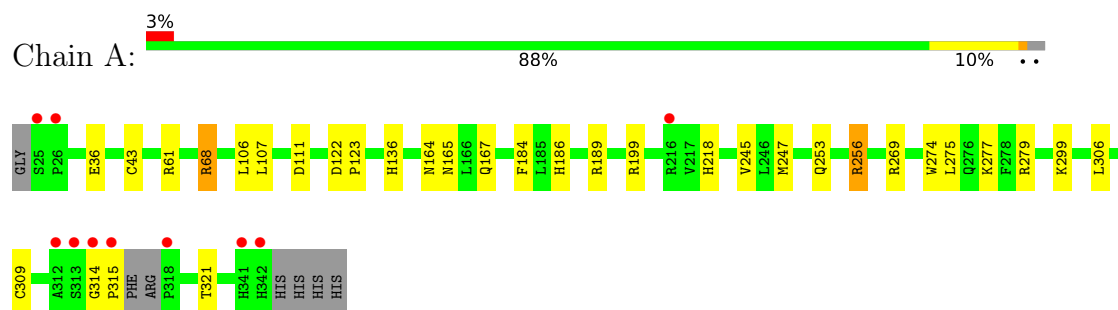
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	249	Total 249	O 249	0	0
5	E	200	Total 200	O 200	0	0
5	F	258	Total 258	O 258	0	0
5	G	194	Total 194	O 194	0	0
5	H	187	Total 187	O 187	0	0

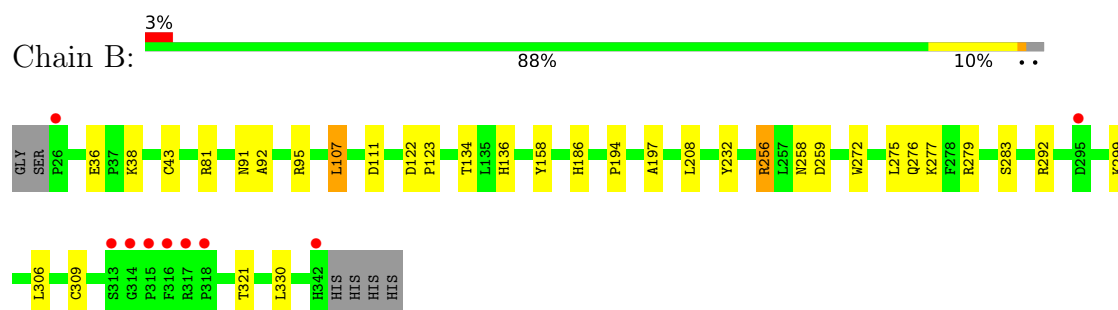
3 Residue-property plots [i](#)

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.

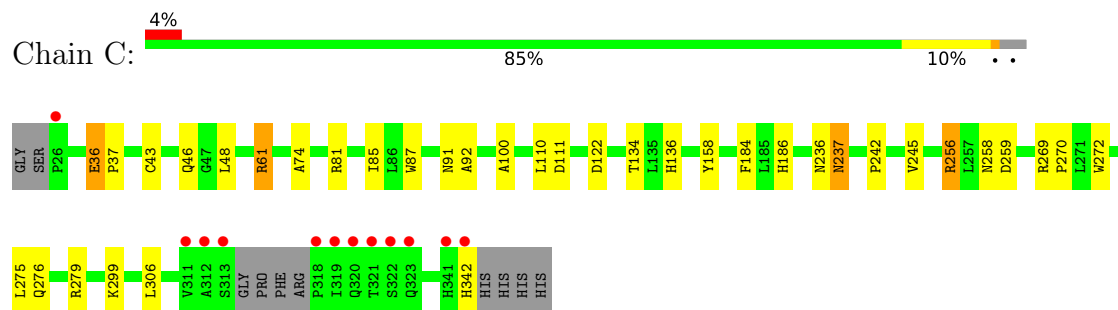
• Molecule 1: Reticulon-4 receptor



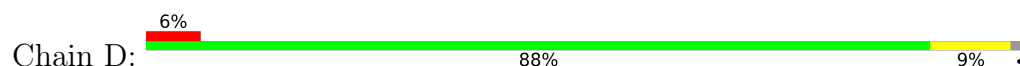
• Molecule 1: Reticulon-4 receptor



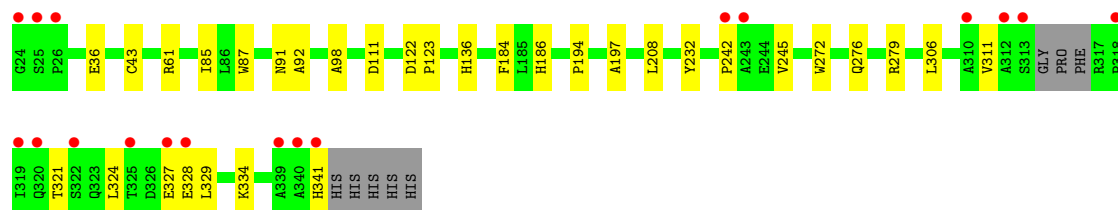
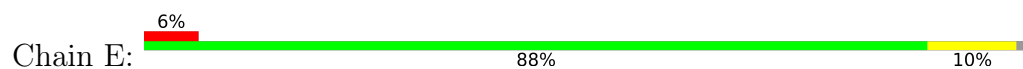
• Molecule 1: Reticulon-4 receptor



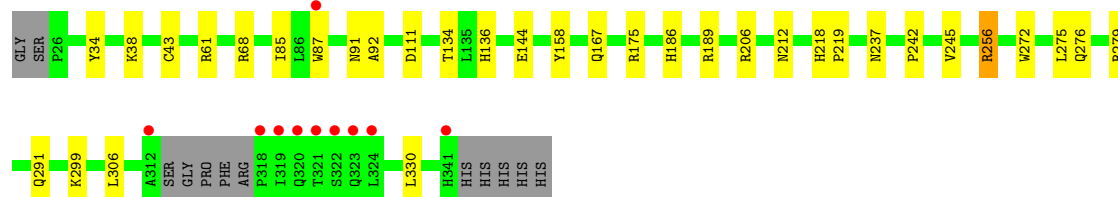
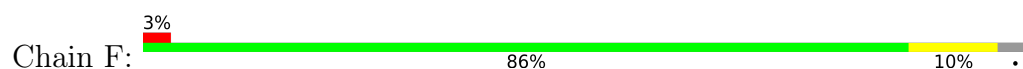
• Molecule 1: Reticulon-4 receptor



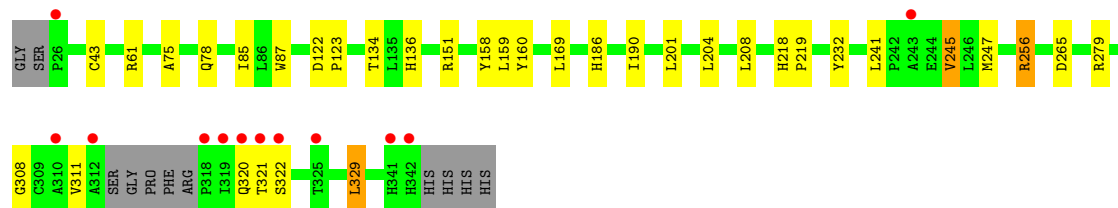
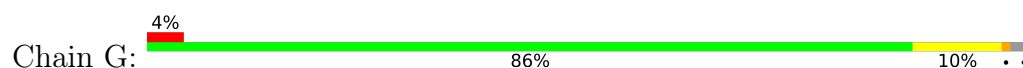
- Molecule 1: Reticulon-4 receptor



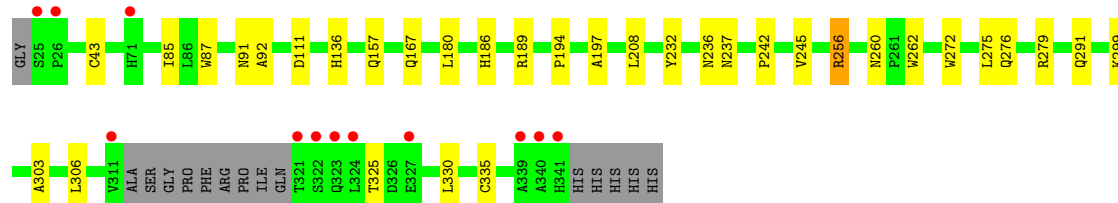
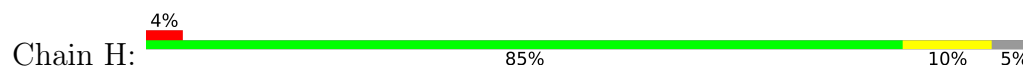
- Molecule 1: Reticulon-4 receptor



- Molecule 1: Reticulon-4 receptor



- Molecule 1: Reticulon-4 receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	168.49Å 168.49Å 256.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.39 – 2.20 70.39 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (70.39-2.20) 99.9 (70.39-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.167 , 0.207 0.171 , 0.209	Depositor DCC
R_{free} test set	9334 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.0	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	0.96	EDS
Total number of atoms	21913	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.42% 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: CL, GOL, 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	0.32	0/2527	0.69	2/3443 (0.1%)
1	B	0.33	0/2556	0.70	0/3483
1	C	0.32	0/2508	0.70	2/3415 (0.1%)
1	D	0.33	0/2531	0.67	0/3447
1	E	0.33	0/2540	0.69	0/3458
1	F	0.33	0/2514	0.69	0/3423
1	G	0.32	0/2503	0.68	2/3409 (0.1%)
1	H	0.31	0/2490	0.67	0/3392
All	All	0.32	0/20169	0.69	6/27470 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	247	MET	CA-C-N	-5.92	113.71	119.87
1	G	247	MET	C-N-CA	-5.92	113.71	119.87
1	A	218	HIS	CA-C-N	5.17	125.47	119.47
1	A	218	HIS	C-N-CA	5.17	125.47	119.47
1	C	122	ASP	CA-C-N	5.13	124.85	119.82
1	C	122	ASP	C-N-CA	5.13	124.85	119.82

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	2465	0	2432	19	0
1	B	2491	0	2456	22	0
1	C	2447	0	2414	19	0
1	D	2470	0	2438	18	0
1	E	2479	0	2443	18	0
1	F	2453	0	2424	21	0
1	G	2442	0	2413	17	0
1	H	2429	0	2390	18	0
2	A	42	0	39	0	0
2	B	42	0	39	0	0
2	C	42	0	39	0	0
2	D	42	0	39	0	0
2	E	42	0	39	0	0
2	F	42	0	39	2	0
2	G	42	0	39	0	0
2	H	42	0	39	0	0
3	A	18	0	24	5	0
3	B	6	0	8	1	0
3	D	6	0	8	1	0
3	F	6	0	8	2	0
3	H	6	0	8	0	0
4	A	12	0	0	5	0
4	B	13	0	0	5	0
4	C	14	0	0	5	0
4	D	9	0	0	4	0
4	E	11	0	0	1	0
4	F	13	0	0	3	0
4	G	12	0	0	2	0
4	H	10	0	0	2	0
5	A	243	0	0	4	0
5	B	230	0	0	3	0
5	C	204	0	0	1	0
5	D	249	0	0	1	0
5	E	200	0	0	0	0
5	F	258	0	0	3	0
5	G	194	0	0	0	0
5	H	187	0	0	1	0
All	All	21913	0	19778	145	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.

All (145) 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:H:186:HIS:ND1	4:H:413:CL:CL	2.31	1.01
1:E:186:HIS:ND1	4:E:411:CL:CL	2.33	0.99
1:D:186:HIS:ND1	4:D:412:CL:CL	2.32	0.98
1:C:186:HIS:ND1	4:C:414:CL:CL	2.34	0.98
1:B:186:HIS:ND1	4:B:415:CL:CL	2.40	0.89
1:F:186:HIS:ND1	4:F:415:CL:CL	2.44	0.87
1:G:186:HIS:ND1	4:G:415:CL:CL	2.44	0.86
1:A:186:HIS:ND1	4:A:417:CL:CL	2.50	0.80
1:C:279:ARG:HG2	4:C:407:CL:CL	2.26	0.72
1:H:275:LEU:HD13	1:H:299:LYS:HG2	1.72	0.71
1:C:111:ASP:HA	1:C:136:HIS:HB2	1.71	0.71
1:D:256:ARG:HD2	4:D:406:CL:CL	2.29	0.69
1:F:111:ASP:HA	1:F:136:HIS:HB2	1.75	0.67
1:F:167:GLN:OE1	1:F:189:ARG:NH2	2.28	0.67
1:F:175:ARG:NH1	5:F:501:HOH:O	2.27	0.67
1:F:68:ARG:HD3	4:F:408:CL:CL	2.35	0.64
1:E:321:THR:HG23	1:E:329:LEU:HD11	1.80	0.64
1:A:111:ASP:HA	1:A:136:HIS:HB2	1.79	0.63
1:H:167:GLN:OE1	1:H:189:ARG:NH2	2.31	0.63
1:A:106:LEU:HD21	1:G:151:ARG:HH22	1.64	0.62
3:A:406:GOL:H12	1:H:335:CYS:HB3	1.81	0.62
5:A:501:HOH:O	1:H:279:ARG:NH1	2.33	0.62
1:G:256:ARG:HD2	4:G:407:CL:CL	2.38	0.61
1:A:256:ARG:HD2	4:A:408:CL:CL	2.37	0.60
1:F:256:ARG:HD2	4:F:407:CL:CL	2.39	0.60
1:A:279:ARG:NH1	5:A:501:HOH:O	2.24	0.60
1:C:256:ARG:HD2	4:C:406:CL:CL	2.39	0.60
1:B:111:ASP:HA	1:B:136:HIS:HB2	1.84	0.60
1:A:309:CYS:HB3	1:A:321:THR:HG21	1.84	0.59
1:A:167:GLN:OE1	1:A:189:ARG:NH2	2.36	0.59
1:C:81:ARG:NH2	5:C:501:HOH:O	2.26	0.59
1:D:111:ASP:HA	1:D:136:HIS:HB2	1.86	0.58
2:F:403:NAG:H3	2:F:403:NAG:H83	1.87	0.57
1:C:61:ARG:HD2	1:C:85:ILE:HD12	1.85	0.57
1:H:256:ARG:HD2	4:H:405:CL:CL	2.42	0.56
1:A:68:ARG:HD3	4:A:410:CL:CL	2.42	0.56
1:B:256:ARG:HD2	4:B:407:CL:CL	2.43	0.55
1:E:327:GLU:OE1	1:F:34:TYR:OH	2.15	0.54
1:D:167:GLN:OE1	1:D:189:ARG:NH2	2.40	0.54
1:F:275:LEU:HD13	1:F:299:LYS:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ARG:HD2	1:E:98:ALA:HB1	1.89	0.54
1:B:309:CYS:HB3	1:B:321:THR:HG21	1.90	0.54
1:H:303:ALA:O	5:H:501:HOH:O	2.18	0.54
1:D:184:PHE:HB3	4:D:412:CL:CL	2.45	0.53
1:D:195:GLU:OE2	5:D:501:HOH:O	2.18	0.53
1:G:136:HIS:HA	1:G:160:TYR:HB2	1.89	0.53
1:F:134:THR:HG22	1:F:158:TYR:HB2	1.89	0.53
1:C:134:THR:HG22	1:C:158:TYR:HB2	1.91	0.52
1:A:277:LYS:HD3	3:A:405:GOL:H11	1.92	0.51
1:E:341[A]:HIS:NE2	1:F:111:ASP:OD2	2.44	0.51
1:A:274:TRP:CD1	3:A:405:GOL:HO1	2.30	0.50
1:H:208:LEU:HD22	1:H:232:TYR:CD2	2.47	0.50
1:E:324:LEU:HD22	1:E:328:GLU:HG2	1.93	0.50
1:E:272:TRP:O	1:E:276:GLN:HG2	2.12	0.49
1:B:81:ARG:NH2	5:B:505:HOH:O	2.44	0.49
1:D:258:ASN:HB2	4:D:406:CL:CL	2.49	0.49
1:H:111:ASP:HA	1:H:136:HIS:HB2	1.93	0.49
1:C:36:GLU:HG3	1:C:37:PRO:HA	1.95	0.48
1:C:279:ARG:HD2	1:G:279:ARG:HD3	1.95	0.48
1:F:38:LYS:HB2	1:F:61:ARG:HD3	1.95	0.48
1:C:46:GLN:HB2	1:C:48:LEU:HG	1.94	0.48
1:D:61:ARG:HD2	1:D:85:ILE:HD12	1.94	0.48
1:C:258:ASN:OD1	1:C:259:ASP:N	2.44	0.48
1:E:334:LYS:NZ	1:F:134:THR:HG21	2.28	0.48
1:G:134:THR:HG22	1:G:158:TYR:HB2	1.95	0.48
2:F:403:NAG:HN2	3:F:404:GOL:H11	1.79	0.47
1:A:199:ARG:HB2	4:A:415:CL:CL	2.52	0.47
1:E:111:ASP:HA	1:E:136:HIS:HB2	1.97	0.47
1:F:212:ASN:O	3:F:404:GOL:H12	2.14	0.47
1:B:134:THR:HG22	1:B:158:TYR:HB2	1.94	0.47
3:A:406:GOL:H11	5:A:673:HOH:O	2.15	0.47
1:B:292:ARG:HG2	4:B:409:CL:CL	2.52	0.47
1:C:184:PHE:HB3	4:C:414:CL:CL	2.52	0.47
1:F:206:ARG:NH1	5:F:505:HOH:O	2.48	0.46
1:D:272:TRP:O	1:D:276:GLN:HG2	2.15	0.46
1:G:241:LEU:HD22	1:G:245:VAL:HG11	1.97	0.46
1:A:275:LEU:HD13	1:A:299:LYS:HG2	1.98	0.46
1:D:208:LEU:HD22	1:D:232:TYR:CD2	2.50	0.46
1:F:279:ARG:HG2	5:F:681:HOH:O	2.14	0.46
5:B:512:HOH:O	1:D:276:GLN:HB2	2.16	0.45
1:E:61:ARG:HG2	1:E:85:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:PRO:O	1:E:245:VAL:HG12	2.16	0.45
1:G:208:LEU:HD22	1:G:232:TYR:CD2	2.51	0.45
1:B:279:ARG:HD3	1:H:279:ARG:HD2	1.98	0.45
1:A:279:ARG:HE	1:D:279:ARG:CZ	2.30	0.45
1:G:169:LEU:HG	1:G:190:ILE:HD13	1.99	0.45
1:E:91:ASN:HB3	1:E:92:ALA:H	1.63	0.45
1:H:242:PRO:O	1:H:245:VAL:HG12	2.17	0.44
1:C:91:ASN:HB3	1:C:92:ALA:H	1.68	0.44
1:E:208:LEU:HD22	1:E:232:TYR:CD2	2.52	0.44
1:H:272:TRP:O	1:H:276:GLN:HG2	2.18	0.44
1:B:330:LEU:HD13	1:H:85:ILE:HD13	1.99	0.44
1:B:95:ARG:NH1	4:B:412:CL:CL	2.84	0.44
4:C:407:CL:CL	1:E:279:ARG:NH1	2.88	0.44
1:D:71:HIS:CD2	1:D:73:PRO:HD3	2.53	0.44
1:D:275:LEU:HD13	1:D:299:LYS:HG2	1.99	0.44
1:H:194:PRO:HG2	1:H:197:ALA:HB2	2.00	0.43
1:B:258:ASN:OD1	1:B:259:ASP:N	2.49	0.43
1:B:283:SER:HB2	4:B:410:CL:CL	2.55	0.43
1:G:218:HIS:ND1	1:G:219:PRO:O	2.43	0.43
1:F:272:TRP:O	1:F:276:GLN:HG2	2.18	0.43
1:G:265:ASP:HB2	1:G:308:GLY:O	2.18	0.43
1:C:74:ALA:HA	1:C:100:ALA:HA	2.01	0.43
1:B:277:LYS:HD3	3:B:404:GOL:H31	2.01	0.43
1:B:208:LEU:HD22	1:B:232:TYR:CD2	2.54	0.43
1:G:329:LEU:HD12	1:G:329:LEU:HA	1.92	0.43
1:A:269:ARG:NH1	5:A:502:HOH:O	2.35	0.43
1:E:122:ASP:HA	1:E:123:PRO:HD3	1.87	0.42
1:B:122:ASP:HA	1:B:123:PRO:HD3	1.88	0.42
1:C:275:LEU:HD13	1:C:299:LYS:HG2	2.02	0.42
1:D:265:ASP:HB2	1:D:308:GLY:O	2.19	0.42
1:D:122:ASP:HA	1:D:123:PRO:HD3	1.86	0.42
1:F:218:HIS:CG	1:F:219:PRO:HD2	2.55	0.42
1:G:75:ALA:HB1	1:G:78:GLN:HB3	2.02	0.42
1:H:157:GLN:C	1:H:180:LEU:HD12	2.45	0.42
1:A:184:PHE:HB3	4:A:417:CL:CL	2.56	0.42
1:B:38:LYS:NZ	5:B:508:HOH:O	2.49	0.42
1:F:242:PRO:O	1:F:245:VAL:HG12	2.20	0.42
1:A:314:GLY:HA3	1:A:315:PRO:HD2	1.84	0.42
1:E:194:PRO:HG2	1:E:197:ALA:HB2	2.00	0.42
1:F:91:ASN:HB3	1:F:92:ALA:H	1.65	0.42
1:B:275:LEU:HD13	1:B:299:LYS:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:ASP:HA	1:G:123:PRO:HD3	1.88	0.42
1:B:91:ASN:HB3	1:B:92:ALA:H	1.67	0.41
1:H:236:ASN:HB3	1:H:237:ASN:H	1.78	0.41
1:C:272:TRP:O	1:C:276:GLN:HG2	2.20	0.41
1:B:272:TRP:O	1:B:276:GLN:HG2	2.19	0.41
1:C:269:ARG:HB2	1:C:270:PRO:HD3	2.03	0.41
1:E:334:LYS:HZ1	1:F:134:THR:HG21	1.86	0.41
1:H:260:ASN:HB2	1:H:262:TRP:NE1	2.35	0.41
1:C:236:ASN:HB3	1:C:237:ASN:H	1.69	0.41
1:G:61:ARG:HD2	1:G:85:ILE:HD12	2.02	0.41
1:B:107:LEU:HD12	1:B:107:LEU:HA	1.96	0.41
1:C:242:PRO:O	1:C:245:VAL:HG12	2.20	0.41
1:D:184:PHE:HD1	1:D:208:LEU:HD12	1.86	0.41
1:F:61:ARG:HG2	1:F:85:ILE:HB	2.02	0.41
1:A:122:ASP:HA	1:A:123:PRO:HD3	1.91	0.41
1:B:194:PRO:HG2	1:B:197:ALA:HB2	2.03	0.41
1:A:247:MET:HE1	3:A:405:GOL:H32	2.03	0.40
1:H:91:ASN:HB3	1:H:92:ALA:H	1.68	0.40
1:E:184:PHE:HD1	1:E:208:LEU:HD12	1.87	0.40
1:G:201:LEU:HD13	1:G:204:LEU:HD22	2.03	0.40
1:A:164:ASN:HB3	1:A:165:ASN:H	1.76	0.40
1:G:311:VAL:HG23	1:G:321:THR:HG22	2.04	0.40
1:D:212:ASN:O	3:D:404:GOL:H12	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	312/323 (97%)	297 (95%)	15 (5%)	0	100	100
1	B	316/323 (98%)	302 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	309/323 (96%)	297 (96%)	12 (4%)	0	100	100
1	D	312/323 (97%)	298 (96%)	13 (4%)	1 (0%)	36	42
1	E	312/323 (97%)	296 (95%)	16 (5%)	0	100	100
1	F	309/323 (96%)	294 (95%)	15 (5%)	0	100	100
1	G	308/323 (95%)	293 (95%)	15 (5%)	0	100	100
1	H	306/323 (95%)	293 (96%)	13 (4%)	0	100	100
All	All	2484/2584 (96%)	2370 (95%)	113 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	322	SER

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	269/275 (98%)	260 (97%)	9 (3%)	33	45
1	B	271/275 (98%)	266 (98%)	5 (2%)	51	68
1	C	267/275 (97%)	258 (97%)	9 (3%)	32	44
1	D	269/275 (98%)	263 (98%)	6 (2%)	45	61
1	E	270/275 (98%)	265 (98%)	5 (2%)	50	66
1	F	267/275 (97%)	259 (97%)	8 (3%)	36	49
1	G	266/275 (97%)	258 (97%)	8 (3%)	36	49
1	H	265/275 (96%)	258 (97%)	7 (3%)	40	55
All	All	2144/2200 (98%)	2087 (97%)	57 (3%)	39	53

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU

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Mol	Chain	Res	Type
1	A	43	CYS
1	A	61	ARG
1	A	68	ARG
1	A	107	LEU
1	A	245	VAL
1	A	253	GLN
1	A	256	ARG
1	A	306	LEU
1	B	36	GLU
1	B	43	CYS
1	B	107	LEU
1	B	256	ARG
1	B	306	LEU
1	C	36	GLU
1	C	43	CYS
1	C	61	ARG
1	C	87	TRP
1	C	110	LEU
1	C	237	ASN
1	C	256	ARG
1	C	306	LEU
1	C	342	HIS
1	D	43	CYS
1	D	87	TRP
1	D	245	VAL
1	D	256	ARG
1	D	306	LEU
1	D	319	ILE
1	E	36	GLU
1	E	43	CYS
1	E	87	TRP
1	E	306	LEU
1	E	311	VAL
1	F	43	CYS
1	F	87	TRP
1	F	144	GLU
1	F	237	ASN
1	F	256	ARG
1	F	291	GLN
1	F	306	LEU
1	F	330	LEU
1	G	43	CYS

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Mol	Chain	Res	Type
1	G	87	TRP
1	G	159	LEU
1	G	245	VAL
1	G	256	ARG
1	G	320	GLN
1	G	322	SER
1	G	329	LEU
1	H	43	CYS
1	H	87	TRP
1	H	256	ARG
1	H	291	GLN
1	H	306	LEU
1	H	325	THR
1	H	330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	HIS
1	A	288	ASN
1	A	341	HIS
1	B	65	HIS
1	B	196	HIS
1	C	196	HIS
1	C	213	HIS
1	D	46	GLN
1	D	320	GLN
1	D	341	HIS
1	E	157	GLN
1	F	196	HIS
1	G	35	ASN
1	G	65	HIS
1	G	202	HIS
1	H	210	HIS
1	H	211	GLN
1	H	291	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](#)

Of 125 ligands modelled in this entry, 94 are monoatomic - leaving 31 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	$\# Z > 2$
2	NAG	C	402	1	14,14,15	0.20	0	17,19,21	0.52	0
2	NAG	A	403	1	14,14,15	0.27	0	17,19,21	0.46	0
3	GOL	F	404	-	5,5,5	0.39	0	5,5,5	0.31	0
2	NAG	F	401	1	14,14,15	0.35	0	17,19,21	0.56	0
2	NAG	C	403	1	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	H	401	1	14,14,15	0.37	0	17,19,21	0.43	0
2	NAG	E	401	1	14,14,15	0.33	0	17,19,21	0.44	0
2	NAG	D	403	1	14,14,15	0.26	0	17,19,21	0.45	0
2	NAG	G	402	1	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	A	402	1	14,14,15	0.25	0	17,19,21	0.47	0
3	GOL	B	404	-	5,5,5	0.38	0	5,5,5	0.38	0
2	NAG	A	401	1	14,14,15	0.28	0	17,19,21	0.72	1 (5%)
3	GOL	A	404	-	5,5,5	0.39	0	5,5,5	0.16	0
3	GOL	H	404	-	5,5,5	0.38	0	5,5,5	0.35	0
2	NAG	E	403	1	14,14,15	0.33	0	17,19,21	0.40	0
2	NAG	G	403	1	14,14,15	0.31	0	17,19,21	0.35	0
2	NAG	F	403	1	14,14,15	0.56	0	17,19,21	1.40	2 (11%)
3	GOL	A	405	-	5,5,5	0.39	0	5,5,5	0.30	0
2	NAG	B	402	1	14,14,15	0.33	0	17,19,21	0.50	0
2	NAG	B	401	1	14,14,15	0.23	0	17,19,21	0.84	0
2	NAG	H	402	1	14,14,15	0.29	0	17,19,21	0.63	0
3	GOL	D	404	-	5,5,5	0.37	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	G	401	1	14,14,15	0.33	0	17,19,21	0.44	0
2	NAG	F	402	1	14,14,15	0.17	0	17,19,21	0.55	0
2	NAG	B	403	1	14,14,15	0.33	0	17,19,21	0.42	0
2	NAG	D	402	1	14,14,15	0.20	0	17,19,21	0.52	0
2	NAG	C	401	1	14,14,15	0.28	0	17,19,21	0.53	0
3	GOL	A	406	-	5,5,5	0.37	0	5,5,5	0.24	0
2	NAG	H	403	1	14,14,15	0.39	0	17,19,21	0.47	0
2	NAG	E	402	1	14,14,15	0.32	0	17,19,21	0.41	0
2	NAG	D	401	1	14,14,15	0.35	0	17,19,21	0.38	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
2	NAG	C	402	1	-	2/6/23/26	0/1/1/1
2	NAG	A	403	1	-	2/6/23/26	0/1/1/1
3	GOL	F	404	-	-	2/4/4/4	-
2	NAG	F	401	1	-	2/6/23/26	0/1/1/1
2	NAG	C	403	1	-	2/6/23/26	0/1/1/1
2	NAG	H	401	1	-	0/6/23/26	0/1/1/1
2	NAG	E	401	1	-	2/6/23/26	0/1/1/1
2	NAG	D	403	1	-	2/6/23/26	0/1/1/1
2	NAG	G	402	1	-	0/6/23/26	0/1/1/1
2	NAG	A	402	1	-	3/6/23/26	0/1/1/1
3	GOL	B	404	-	-	4/4/4/4	-
2	NAG	A	401	1	-	0/6/23/26	0/1/1/1
3	GOL	A	404	-	-	2/4/4/4	-
3	GOL	H	404	-	-	0/4/4/4	-
2	NAG	E	403	1	-	2/6/23/26	0/1/1/1
2	NAG	G	403	1	-	0/6/23/26	0/1/1/1
2	NAG	F	403	1	-	6/6/23/26	0/1/1/1
3	GOL	A	405	-	-	3/4/4/4	-
2	NAG	B	402	1	-	2/6/23/26	0/1/1/1
2	NAG	B	401	1	-	4/6/23/26	0/1/1/1
2	NAG	H	402	1	-	2/6/23/26	0/1/1/1
3	GOL	D	404	-	-	4/4/4/4	-
2	NAG	G	401	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	402	1	-	0/6/23/26	0/1/1/1
2	NAG	B	403	1	-	2/6/23/26	0/1/1/1
2	NAG	D	402	1	-	2/6/23/26	0/1/1/1
2	NAG	C	401	1	-	0/6/23/26	0/1/1/1
3	GOL	A	406	-	-	2/4/4/4	-
2	NAG	H	403	1	-	0/6/23/26	0/1/1/1
2	NAG	E	402	1	-	0/6/23/26	0/1/1/1
2	NAG	D	401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	403	NAG	C2-N2-C7	4.67	129.16	122.90
2	A	401	NAG	C1-O5-C5	2.56	115.62	112.19
2	F	403	NAG	C1-C2-N2	2.25	113.98	110.43

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	GOL	O1-C1-C2-C3
3	A	405	GOL	O1-C1-C2-O2
3	A	405	GOL	O1-C1-C2-C3
3	A	406	GOL	C1-C2-C3-O3
3	B	404	GOL	O1-C1-C2-O2
3	B	404	GOL	O1-C1-C2-C3
3	B	404	GOL	C1-C2-C3-O3
3	D	404	GOL	O1-C1-C2-C3
3	D	404	GOL	C1-C2-C3-O3
3	F	404	GOL	O1-C1-C2-C3
2	A	403	NAG	O5-C5-C6-O6
2	B	403	NAG	O5-C5-C6-O6
2	F	403	NAG	O5-C5-C6-O6
2	E	403	NAG	O5-C5-C6-O6
2	C	403	NAG	O5-C5-C6-O6
2	B	403	NAG	C4-C5-C6-O6
2	D	402	NAG	C4-C5-C6-O6
2	A	403	NAG	C4-C5-C6-O6
2	D	402	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	F	403	NAG	C4-C5-C6-O6
2	D	401	NAG	O5-C5-C6-O6
2	B	402	NAG	O5-C5-C6-O6
2	D	401	NAG	C4-C5-C6-O6
2	E	403	NAG	C4-C5-C6-O6
2	A	402	NAG	C8-C7-N2-C2
2	A	402	NAG	O7-C7-N2-C2
2	D	403	NAG	C8-C7-N2-C2
2	D	403	NAG	O7-C7-N2-C2
2	F	403	NAG	C8-C7-N2-C2
2	F	403	NAG	O7-C7-N2-C2
2	E	401	NAG	O5-C5-C6-O6
2	C	403	NAG	C4-C5-C6-O6
2	E	401	NAG	C4-C5-C6-O6
2	F	401	NAG	C4-C5-C6-O6
3	A	404	GOL	O1-C1-C2-O2
3	A	406	GOL	O2-C2-C3-O3
3	B	404	GOL	O2-C2-C3-O3
3	D	404	GOL	O1-C1-C2-O2
3	D	404	GOL	O2-C2-C3-O3
2	B	402	NAG	C4-C5-C6-O6
2	F	401	NAG	O5-C5-C6-O6
2	G	401	NAG	C4-C5-C6-O6
3	F	404	GOL	O1-C1-C2-O2
2	G	401	NAG	O5-C5-C6-O6
2	A	402	NAG	O5-C5-C6-O6
2	B	401	NAG	C4-C5-C6-O6
2	B	401	NAG	C3-C2-N2-C7
2	H	402	NAG	C3-C2-N2-C7
2	C	402	NAG	C4-C5-C6-O6
2	B	401	NAG	O5-C5-C6-O6
2	C	402	NAG	O5-C5-C6-O6
3	A	405	GOL	C1-C2-C3-O3
2	B	401	NAG	C1-C2-N2-C7
2	F	403	NAG	C1-C2-N2-C7
2	H	402	NAG	C1-C2-N2-C7
2	F	403	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	404	GOL	2	0
3	B	404	GOL	1	0
2	F	403	NAG	2	0
3	A	405	GOL	3	0
3	D	404	GOL	1	0
3	A	406	GOL	2	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, 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	316/323 (97%)	-0.28	10 (3%)	50	47	21, 36, 61, 125	0
1	B	317/323 (98%)	-0.33	9 (2%)	55	52	15, 35, 61, 135	1 (0%)
1	C	313/323 (96%)	-0.23	12 (3%)	44	41	24, 36, 73, 131	0
1	D	315/323 (97%)	-0.32	19 (6%)	27	24	20, 30, 80, 127	1 (0%)
1	E	315/323 (97%)	-0.16	18 (5%)	29	26	16, 36, 70, 136	2 (0%)
1	F	311/323 (96%)	-0.37	10 (3%)	50	47	14, 30, 67, 130	2 (0%)
1	G	312/323 (96%)	-0.16	12 (3%)	44	41	24, 38, 69, 134	0
1	H	308/323 (95%)	-0.18	12 (3%)	43	40	18, 38, 73, 131	2 (0%)
All	All	2507/2584 (97%)	-0.25	102 (4%)	41	38	14, 35, 71, 136	8 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	PRO	10.1
1	G	318	PRO	10.0
1	A	312	ALA	8.6
1	E	341[A]	HIS	7.2
1	F	312	ALA	7.1
1	F	318	PRO	6.9
1	E	340	ALA	6.9
1	B	316	PHE	6.8
1	C	318	PRO	6.8
1	D	319	ILE	6.7
1	G	312	ALA	6.1
1	G	342	HIS	6.0
1	G	319	ILE	6.0
1	H	341	HIS	5.8
1	D	316	PHE	5.5
1	G	26	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
1	F	319	ILE	5.3
1	G	321	THR	5.1
1	A	313	SER	4.7
1	E	312	ALA	4.7
1	B	26	PRO	4.6
1	B	318	PRO	4.5
1	C	319	ILE	4.5
1	C	342	HIS	4.5
1	D	341	HIS	4.4
1	C	26	PRO	4.4
1	A	342	HIS	4.3
1	H	26	PRO	4.3
1	F	341	HIS	4.2
1	H	321	THR	4.2
1	E	313	SER	4.2
1	D	340	ALA	4.2
1	A	314	GLY	4.2
1	E	24	GLY	4.1
1	B	342	HIS	4.1
1	H	322	SER	4.1
1	G	320	GLN	4.0
1	D	315	PRO	4.0
1	B	317	ARG	3.9
1	F	322	SER	3.9
1	G	322	SER	3.9
1	F	321	THR	3.9
1	A	318	PRO	3.8
1	G	310	ALA	3.7
1	E	339	ALA	3.7
1	B	313	SER	3.6
1	H	340	ALA	3.6
1	E	25	SER	3.6
1	H	25	SER	3.6
1	H	323	GLN	3.6
1	C	320	GLN	3.3
1	G	341	HIS	3.3
1	D	25	SER	3.3
1	E	318	PRO	3.2
1	D	321	THR	3.2
1	C	313	SER	3.0
1	D	243	ALA	3.0
1	B	315	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	341	HIS	2.8
1	D	320	GLN	2.8
1	D	324	LEU	2.8
1	E	243	ALA	2.8
1	C	321	THR	2.8
1	G	243	ALA	2.8
1	B	314	GLY	2.8
1	E	26	PRO	2.8
1	C	312	ALA	2.8
1	H	339	ALA	2.8
1	D	295	ASP	2.7
1	H	324	LEU	2.7
1	E	327	GLU	2.7
1	E	319	ILE	2.7
1	D	312	ALA	2.6
1	D	322	SER	2.6
1	F	323	GLN	2.6
1	H	311	VAL	2.6
1	E	322	SER	2.6
1	H	327	GLU	2.5
1	D	326	ASP	2.5
1	D	327	GLU	2.5
1	D	26	PRO	2.5
1	E	325	THR	2.5
1	B	295	ASP	2.5
1	C	323	GLN	2.5
1	C	322	SER	2.4
1	F	87	TRP	2.4
1	D	323	GLN	2.4
1	A	25	SER	2.4
1	H	71[A]	HIS	2.4
1	G	325	THR	2.3
1	E	320	GLN	2.3
1	D	314	GLY	2.3
1	E	328	GLU	2.3
1	E	242	PRO	2.2
1	E	310	ALA	2.2
1	D	313	SER	2.2
1	F	320	GLN	2.2
1	A	216	ARG	2.1
1	A	26	PRO	2.1
1	A	341	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	311	VAL	2.1
1	F	324	LEU	2.1

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(Å ²)	Q<0.9
2	NAG	B	403	14/15	0.39	0.21	71,90,98,100	0
2	NAG	G	403	14/15	0.42	0.18	70,83,89,91	0
2	NAG	C	403	14/15	0.49	0.25	88,102,110,113	0
2	NAG	F	403	14/15	0.55	0.21	88,96,104,104	0
2	NAG	A	403	14/15	0.57	0.20	73,85,89,89	0
2	NAG	H	403	14/15	0.58	0.19	71,78,87,91	0
2	NAG	E	403	14/15	0.59	0.18	72,79,87,90	0
2	NAG	D	403	14/15	0.65	0.18	68,79,84,86	0
2	NAG	B	402	14/15	0.70	0.19	58,73,88,91	0
3	GOL	A	406	6/6	0.71	0.27	63,78,81,83	0
2	NAG	H	402	14/15	0.72	0.19	61,79,86,90	0
3	GOL	A	404	6/6	0.76	0.28	93,96,97,98	0
2	NAG	E	402	14/15	0.76	0.17	65,73,80,82	0
2	NAG	A	402	14/15	0.77	0.16	52,65,82,84	0
2	NAG	F	402	14/15	0.77	0.17	51,63,75,78	0
2	NAG	D	402	14/15	0.78	0.17	55,68,83,85	0
2	NAG	G	402	14/15	0.80	0.14	44,68,75,76	0
2	NAG	C	402	14/15	0.80	0.16	55,69,81,81	0
3	GOL	H	404	6/6	0.80	0.21	64,72,74,75	0
3	GOL	A	405	6/6	0.83	0.21	43,62,65,69	0
3	GOL	F	404	6/6	0.84	0.21	68,75,77,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	404	6/6	0.84	0.19	51,69,73,77	0
4	CL	A	416	1/1	0.84	0.24	89,89,89,89	0
2	NAG	B	401	14/15	0.85	0.12	39,47,55,60	0
3	GOL	B	404	6/6	0.85	0.25	57,70,75,75	0
4	CL	E	412	1/1	0.87	0.18	72,72,72,72	0
4	CL	E	414	1/1	0.87	0.20	104,104,104,104	0
2	NAG	A	401	14/15	0.88	0.10	35,50,58,61	0
2	NAG	G	401	14/15	0.88	0.10	40,46,51,52	0
4	CL	G	405	1/1	0.88	0.16	75,75,75,75	0
4	CL	C	417	1/1	0.89	0.14	72,72,72,72	0
4	CL	H	414	1/1	0.89	0.28	104,104,104,104	0
4	CL	F	412	1/1	0.90	0.14	63,63,63,63	0
4	CL	E	413	1/1	0.90	0.27	82,82,82,82	0
2	NAG	E	401	14/15	0.90	0.09	40,47,57,58	0
4	CL	B	416	1/1	0.91	0.13	60,60,60,60	0
4	CL	C	413	1/1	0.91	0.14	66,66,66,66	0
2	NAG	H	401	14/15	0.91	0.08	34,46,50,52	0
4	CL	C	411	1/1	0.92	0.13	62,62,62,62	0
2	NAG	C	401	14/15	0.93	0.08	31,45,50,55	0
4	CL	H	407	1/1	0.93	0.20	67,67,67,67	0
2	NAG	F	401	14/15	0.93	0.08	28,40,51,57	0
4	CL	C	416	1/1	0.94	0.15	90,90,90,90	0
4	CL	B	409	1/1	0.94	0.13	62,62,62,62	0
4	CL	F	414	1/1	0.94	0.10	50,50,50,50	0
4	CL	E	410	1/1	0.94	0.11	47,47,47,47	0
4	CL	G	412	1/1	0.94	0.11	60,60,60,60	0
4	CL	G	413	1/1	0.94	0.10	72,72,72,72	0
4	CL	C	412	1/1	0.94	0.11	50,50,50,50	0
4	CL	A	415	1/1	0.94	0.11	68,68,68,68	0
4	CL	G	410	1/1	0.95	0.10	62,62,62,62	0
4	CL	G	411	1/1	0.95	0.10	67,67,67,67	0
2	NAG	D	401	14/15	0.95	0.06	28,38,43,49	0
4	CL	B	410	1/1	0.95	0.10	62,62,62,62	0
4	CL	A	411	1/1	0.95	0.11	67,67,67,67	0
4	CL	H	412	1/1	0.95	0.14	56,56,56,56	0
4	CL	H	413	1/1	0.95	0.08	41,41,41,41	0
4	CL	C	409	1/1	0.95	0.13	65,65,65,65	0
4	CL	F	406	1/1	0.96	0.10	47,47,47,47	0
4	CL	B	417	1/1	0.96	0.09	58,58,58,58	0
4	CL	C	407	1/1	0.96	0.13	51,51,51,51	0
4	CL	G	414	1/1	0.96	0.10	51,51,51,51	0
4	CL	H	406	1/1	0.96	0.07	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	F	416	1/1	0.96	0.08	65,65,65,65	0
4	CL	C	408	1/1	0.96	0.10	66,66,66,66	0
4	CL	G	406	1/1	0.96	0.11	52,52,52,52	0
4	CL	D	413	1/1	0.96	0.10	58,58,58,58	0
4	CL	B	408	1/1	0.97	0.09	45,45,45,45	0
4	CL	F	407	1/1	0.97	0.14	44,44,44,44	0
4	CL	F	411	1/1	0.97	0.12	59,59,59,59	0
4	CL	A	407	1/1	0.97	0.06	52,52,52,52	0
4	CL	F	413	1/1	0.97	0.10	67,67,67,67	0
4	CL	A	413	1/1	0.97	0.06	52,52,52,52	0
4	CL	B	412	1/1	0.97	0.08	46,46,46,46	0
4	CL	F	417	1/1	0.97	0.11	58,58,58,58	0
4	CL	A	414	1/1	0.97	0.09	57,57,57,57	0
4	CL	A	408	1/1	0.97	0.08	45,45,45,45	0
4	CL	D	411	1/1	0.97	0.11	51,51,51,51	0
4	CL	D	412	1/1	0.97	0.08	41,41,41,41	0
4	CL	C	404	1/1	0.97	0.06	43,43,43,43	0
4	CL	E	404	1/1	0.97	0.06	44,44,44,44	0
4	CL	E	405	1/1	0.97	0.07	55,55,55,55	0
4	CL	E	406	1/1	0.97	0.07	43,43,43,43	0
4	CL	C	405	1/1	0.97	0.10	56,56,56,56	0
4	CL	H	409	1/1	0.97	0.09	44,44,44,44	0
4	CL	H	410	1/1	0.97	0.14	50,50,50,50	0
4	CL	C	406	1/1	0.97	0.11	46,46,46,46	0
4	CL	A	409	1/1	0.97	0.13	50,50,50,50	0
4	CL	B	405	1/1	0.97	0.06	47,47,47,47	0
4	CL	B	413	1/1	0.98	0.07	48,48,48,48	0
4	CL	F	415	1/1	0.98	0.06	36,36,36,36	0
4	CL	C	414	1/1	0.98	0.07	40,40,40,40	0
4	CL	E	407	1/1	0.98	0.05	54,54,54,54	0
4	CL	G	404	1/1	0.98	0.08	50,50,50,50	0
4	CL	E	408	1/1	0.98	0.12	50,50,50,50	0
4	CL	E	409	1/1	0.98	0.08	38,38,38,38	0
4	CL	G	407	1/1	0.98	0.06	46,46,46,46	0
4	CL	G	408	1/1	0.98	0.04	42,42,42,42	0
4	CL	G	409	1/1	0.98	0.12	51,51,51,51	0
4	CL	B	414	1/1	0.98	0.08	40,40,40,40	0
4	CL	E	411	1/1	0.98	0.06	40,40,40,40	0
4	CL	A	410	1/1	0.98	0.11	48,48,48,48	0
4	CL	D	406	1/1	0.98	0.07	35,35,35,35	0
4	CL	D	409	1/1	0.98	0.10	38,38,38,38	0
4	CL	H	405	1/1	0.98	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	F	405	1/1	0.98	0.06	47,47,47,47	0
4	CL	D	410	1/1	0.98	0.07	44,44,44,44	0
4	CL	H	408	1/1	0.98	0.06	50,50,50,50	0
4	CL	B	406	1/1	0.98	0.06	56,56,56,56	0
4	CL	F	409	1/1	0.98	0.07	39,39,39,39	0
4	CL	H	411	1/1	0.98	0.06	42,42,42,42	0
4	CL	C	410	1/1	0.98	0.07	60,60,60,60	0
4	CL	B	411	1/1	0.98	0.07	49,49,49,49	0
4	CL	A	412	1/1	0.98	0.14	50,50,50,50	0
4	CL	G	415	1/1	0.99	0.06	37,37,37,37	0
4	CL	A	417	1/1	0.99	0.06	37,37,37,37	0
4	CL	F	410	1/1	0.99	0.07	44,44,44,44	0
4	CL	D	405	1/1	0.99	0.07	43,43,43,43	0
4	CL	B	415	1/1	0.99	0.04	41,41,41,41	0
4	CL	D	407	1/1	0.99	0.05	31,31,31,31	0
4	CL	D	408	1/1	0.99	0.07	34,34,34,34	0
4	CL	A	418	1/1	0.99	0.11	31,31,31,31	0
4	CL	C	415	1/1	0.99	0.10	42,42,42,42	0
4	CL	B	407	1/1	0.99	0.09	46,46,46,46	0
4	CL	F	408	1/1	0.99	0.04	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.