Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 09:04 am GMT

PDB ID	:	5O0O
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 (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 (1)) were used in the production of this report:

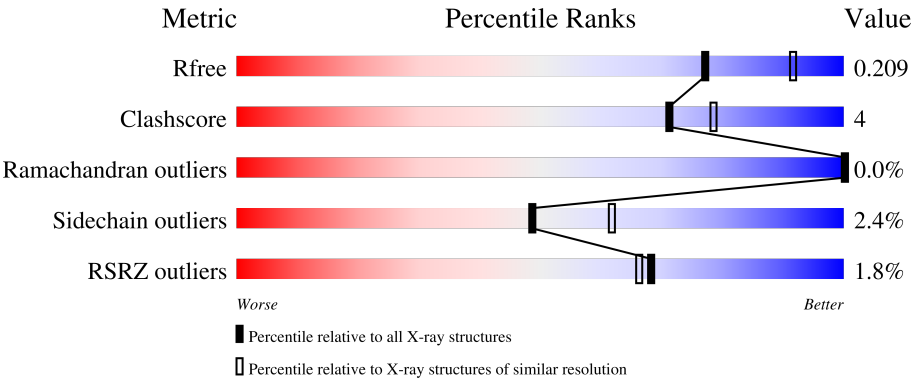
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	323	2% 89% 9% •
1	B	323	2% 87% 10% • •
1	C	323	% 85% 11% • •
1	D	323	3% 88% 10% •
1	E	323	2% 88% 10% •

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Mol	Chain	Length	Quality of chain
1	F	323	2% 86% 10%
1	G	323	2% 86% 10%
1	H	323	86% 10% 5%

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 (i)

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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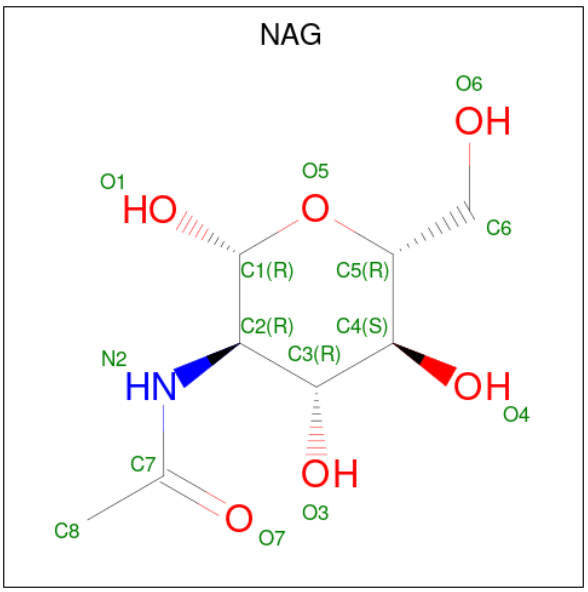
Chain	Residue	Modelled	Actual	Comment	Reference
E	342	HIS	-	expression tag	UNP Q99PI8
E	343	HIS	-	expression tag	UNP Q99PI8
E	344	HIS	-	expression tag	UNP Q99PI8
E	345	HIS	-	expression tag	UNP Q99PI8
E	346	HIS	-	expression tag	UNP Q99PI8
F	24	GLY	-	expression tag	UNP Q99PI8
F	25	SER	-	expression tag	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 (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



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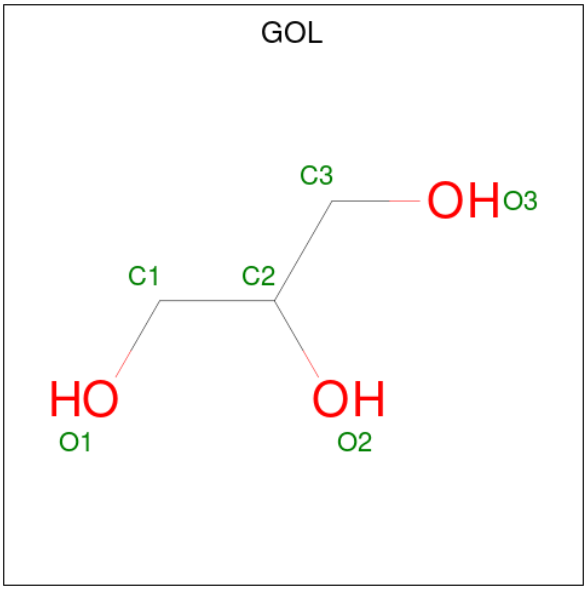
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C N O 14 8 1 5	0	0
2	E	1	Total C N O 14 8 1 5	0	0
2	F	1	Total C N O 14 8 1 5	0	0
2	F	1	Total C N O 14 8 1 5	0	0
2	F	1	Total C N O 14 8 1 5	0	0
2	G	1	Total C N O 14 8 1 5	0	0
2	G	1	Total C N O 14 8 1 5	0	0
2	G	1	Total C N O 14 8 1 5	0	0
2	H	1	Total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

- Molecule 3 is GLYCEROL (three-letter code: 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 (three-letter code: 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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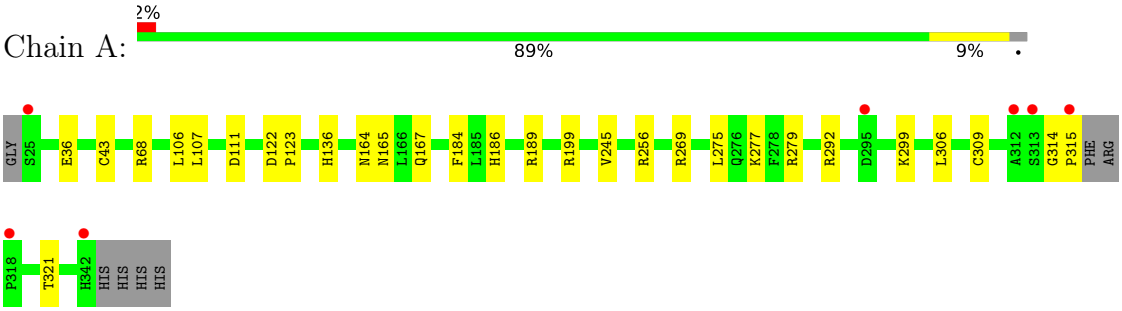
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	249	Total O 249 249	0	0
5	E	200	Total O 200 200	0	0
5	F	258	Total O 258 258	0	0
5	G	194	Total O 194 194	0	0
5	H	187	Total O 187 187	0	0

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.

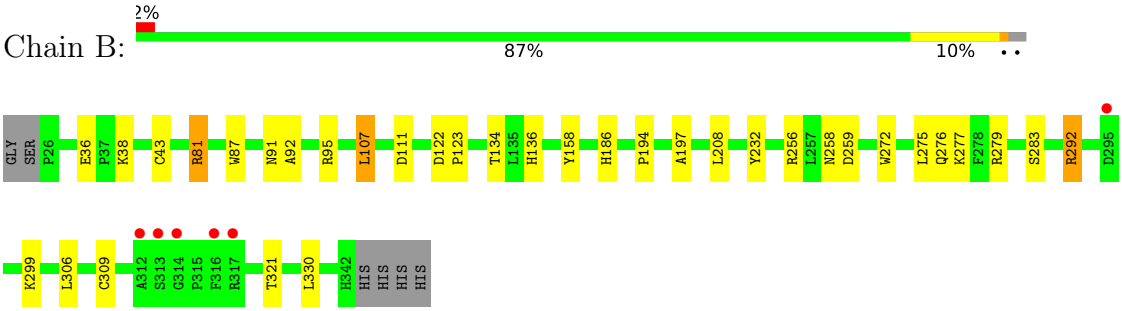
• Molecule 1: Reticulon-4 receptor

Chain A:



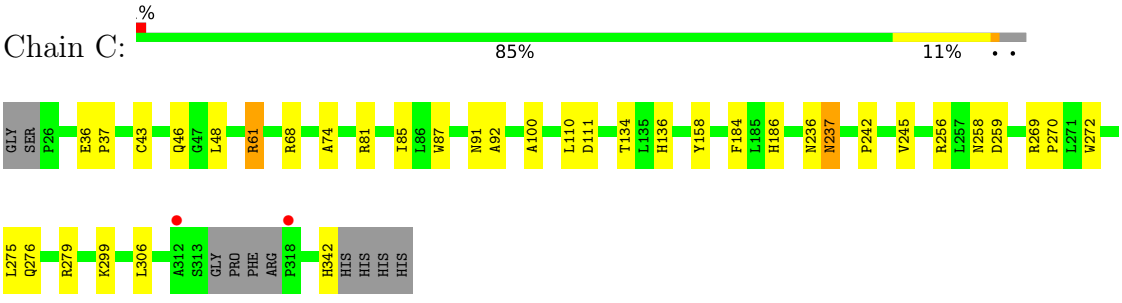
• Molecule 1: Reticulon-4 receptor

Chain B:



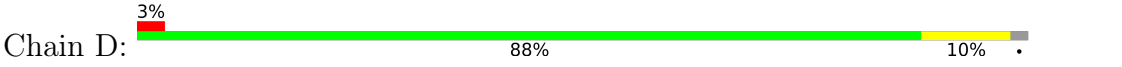
• Molecule 1: Reticulon-4 receptor

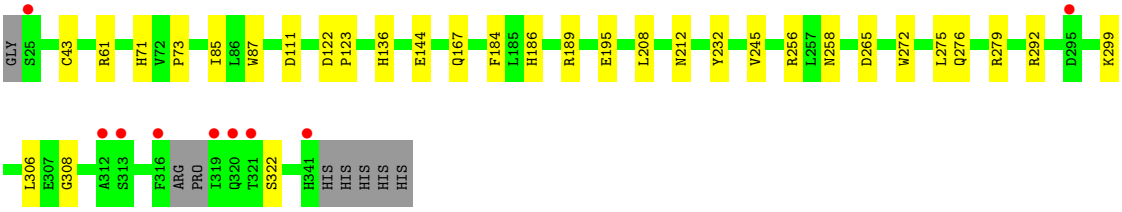
Chain C:



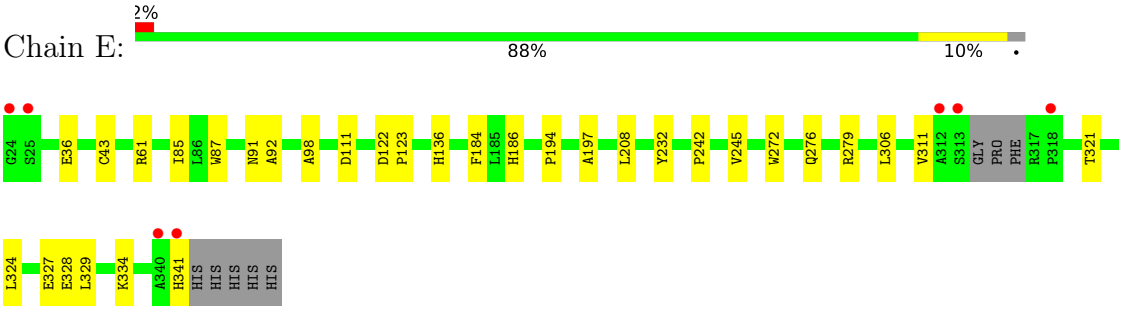
• Molecule 1: Reticulon-4 receptor

Chain D:

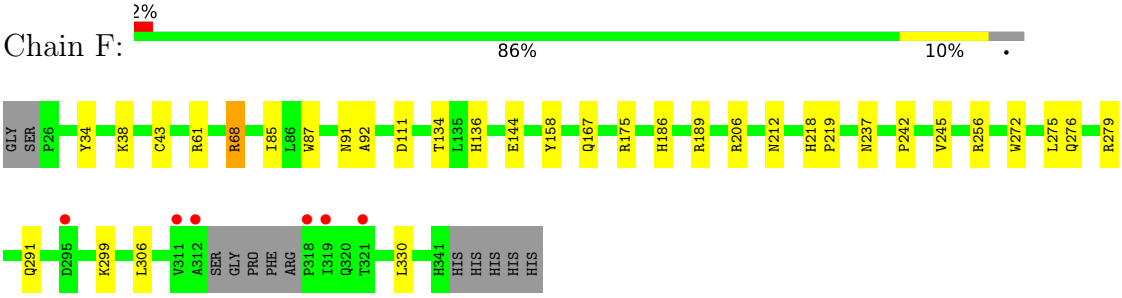




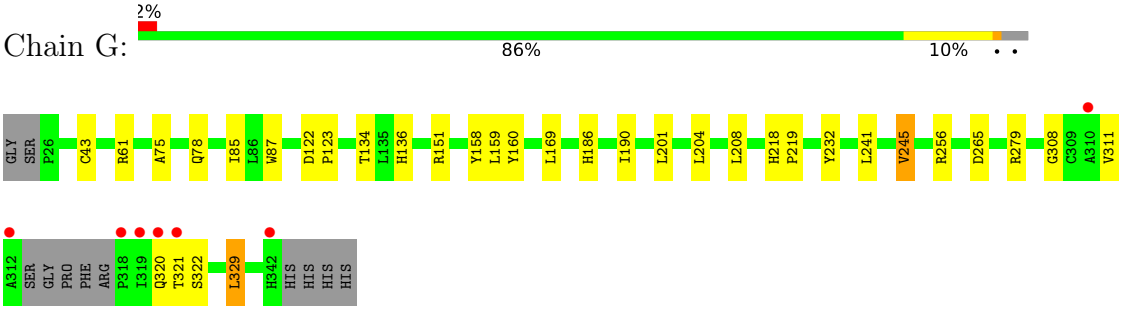
• Molecule 1: Reticulon-4 receptor



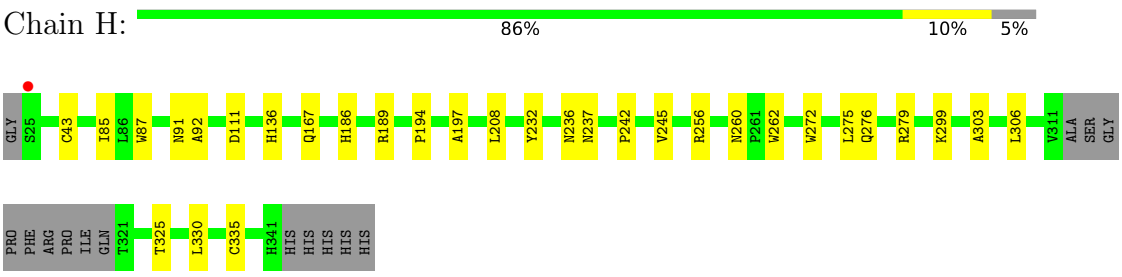
• Molecule 1: Reticulon-4 receptor



• Molecule 1: Reticulon-4 receptor



• Molecule 1: Reticulon-4 receptor



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.26 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.167 , 0.207 0.170 , 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 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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: CL, NAG, 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	0.25	0/2527	0.42	0/3443
1	B	0.25	0/2556	0.42	0/3483
1	C	0.25	0/2508	0.41	0/3415
1	D	0.26	0/2531	0.43	0/3447
1	E	0.25	0/2540	0.42	0/3458
1	F	0.26	0/2514	0.43	0/3423
1	G	0.24	0/2503	0.41	0/3409
1	H	0.24	0/2490	0.40	0/3392
All	All	0.25	0/20169	0.42	0/27470

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	2465	0	2432	17	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	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2453	0	2424	20	0
1	G	2442	0	2413	17	0
1	H	2429	0	2390	17	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	3	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	141	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 (141) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:38:LYS:NZ	5:B:508:HOH:O	2.49	0.45
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:184:PHE:HB3	4:A:417:CL:CL	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1	C	309/323 (96%)	297 (96%)	12 (4%)	0	100	100
1	D	312/323 (97%)	298 (96%)	13 (4%)	1 (0%)	41	46
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (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	269/275 (98%)	263 (98%)	6 (2%)	52	65
1	B	271/275 (98%)	264 (97%)	7 (3%)	46	58
1	C	267/275 (97%)	259 (97%)	8 (3%)	41	53
1	D	269/275 (98%)	263 (98%)	6 (2%)	52	65
1	E	270/275 (98%)	265 (98%)	5 (2%)	57	71
1	F	267/275 (97%)	259 (97%)	8 (3%)	41	53
1	G	266/275 (97%)	259 (97%)	7 (3%)	46	58
1	H	265/275 (96%)	260 (98%)	5 (2%)	57	71
All	All	2144/2200 (98%)	2092 (98%)	52 (2%)	49	62

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	43	CYS
1	A	107	LEU
1	A	245	VAL
1	A	292	ARG
1	A	306	LEU
1	B	36	GLU

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Mol	Chain	Res	Type
1	B	43	CYS
1	B	81	ARG
1	B	87	TRP
1	B	107	LEU
1	B	292	ARG
1	B	306	LEU
1	C	43	CYS
1	C	61	ARG
1	C	68	ARG
1	C	87	TRP
1	C	110	LEU
1	C	237	ASN
1	C	306	LEU
1	C	342	HIS
1	D	43	CYS
1	D	87	TRP
1	D	144	GLU
1	D	245	VAL
1	D	292	ARG
1	D	306	LEU
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	68	ARG
1	F	87	TRP
1	F	144	GLU
1	F	237	ASN
1	F	291	GLN
1	F	306	LEU
1	F	330	LEU
1	G	43	CYS
1	G	87	TRP
1	G	159	LEU
1	G	245	VAL
1	G	320	GLN
1	G	322	SER
1	G	329	LEU
1	H	43	CYS
1	H	87	TRP

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Mol	Chain	Res	Type
1	H	306	LEU
1	H	325	THR
1	H	330	LEU

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 monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	GOL	A	405	-	5,5,5	0.38	0	5,5,5	0.29	0
3	GOL	H	404	-	5,5,5	0.38	0	5,5,5	0.32	0
2	NAG	H	403	1	14,14,15	0.36	0	17,19,21	0.45	0
2	NAG	D	401	1	14,14,15	0.33	0	17,19,21	0.36	0
3	GOL	D	404	-	5,5,5	0.36	0	5,5,5	0.27	0
2	NAG	B	401	1	14,14,15	0.23	0	17,19,21	0.80	0
3	GOL	B	404	-	5,5,5	0.37	0	5,5,5	0.35	0
2	NAG	G	403	1	14,14,15	0.30	0	17,19,21	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	F	401	1	14,14,15	0.35	0	17,19,21	0.55	0
2	NAG	F	403	1	14,14,15	0.52	0	17,19,21	1.32	2 (11%)
2	NAG	A	403	1	14,14,15	0.26	0	17,19,21	0.44	0
2	NAG	B	402	1	14,14,15	0.31	0	17,19,21	0.48	0
2	NAG	B	403	1	14,14,15	0.31	0	17,19,21	0.40	0
2	NAG	G	402	1	14,14,15	0.22	0	17,19,21	0.38	0
2	NAG	G	401	1	14,14,15	0.31	0	17,19,21	0.42	0
2	NAG	H	402	1	14,14,15	0.28	0	17,19,21	0.60	0
2	NAG	E	402	1	14,14,15	0.31	0	17,19,21	0.40	0
2	NAG	H	401	1	14,14,15	0.35	0	17,19,21	0.42	0
2	NAG	E	401	1	14,14,15	0.31	0	17,19,21	0.43	0
2	NAG	A	401	1	14,14,15	0.26	0	17,19,21	0.70	1 (5%)
3	GOL	A	406	-	5,5,5	0.36	0	5,5,5	0.22	0
2	NAG	A	402	1	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	E	403	1	14,14,15	0.31	0	17,19,21	0.38	0
3	GOL	F	404	-	5,5,5	0.38	0	5,5,5	0.29	0
2	NAG	C	402	1	14,14,15	0.20	0	17,19,21	0.50	0
2	NAG	D	403	1	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	D	402	1	14,14,15	0.20	0	17,19,21	0.50	0
2	NAG	C	403	1	14,14,15	0.21	0	17,19,21	0.41	0
2	NAG	F	402	1	14,14,15	0.17	0	17,19,21	0.53	0
3	GOL	A	404	-	5,5,5	0.38	0	5,5,5	0.14	0
2	NAG	C	401	1	14,14,15	0.27	0	17,19,21	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	405	-	-	3/4/4/4	-
3	GOL	H	404	-	-	0/4/4/4	-
2	NAG	H	403	1	-	0/6/23/26	0/1/1/1
2	NAG	D	401	1	-	2/6/23/26	0/1/1/1
3	GOL	D	404	-	-	4/4/4/4	-
2	NAG	B	401	1	-	3/6/23/26	0/1/1/1
3	GOL	B	404	-	-	4/4/4/4	-
2	NAG	G	403	1	-	0/6/23/26	0/1/1/1
2	NAG	F	401	1	-	2/6/23/26	0/1/1/1
2	NAG	F	403	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	403	1	-	2/6/23/26	0/1/1/1
2	NAG	B	402	1	-	2/6/23/26	0/1/1/1
2	NAG	B	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	G	401	1	-	2/6/23/26	0/1/1/1
2	NAG	H	402	1	-	1/6/23/26	0/1/1/1
2	NAG	E	402	1	-	0/6/23/26	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	A	401	1	-	0/6/23/26	0/1/1/1
3	GOL	A	406	-	-	2/4/4/4	-
2	NAG	A	402	1	-	3/6/23/26	0/1/1/1
2	NAG	E	403	1	-	2/6/23/26	0/1/1/1
3	GOL	F	404	-	-	2/4/4/4	-
2	NAG	C	402	1	-	2/6/23/26	0/1/1/1
2	NAG	D	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	403	1	-	2/6/23/26	0/1/1/1
2	NAG	F	402	1	-	0/6/23/26	0/1/1/1
3	GOL	A	404	-	-	2/4/4/4	-
2	NAG	C	401	1	-	0/6/23/26	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(^{o})	Ideal(^{o})
2	F	403	NAG	C2-N2-C7	4.39	129.16	122.90
2	A	401	NAG	C1-O5-C5	2.53	115.62	112.19
2	F	403	NAG	C1-C2-N2	2.05	113.98	110.49

There are no chirality outliers.

All (53) 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

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Mol	Chain	Res	Type	Atoms
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	B	403	NAG	C4-C5-C6-O6
2	C	403	NAG	O5-C5-C6-O6
2	D	402	NAG	C4-C5-C6-O6
2	A	403	NAG	C4-C5-C6-O6
2	F	403	NAG	C4-C5-C6-O6
2	D	402	NAG	O5-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	D	401	NAG	O5-C5-C6-O6
2	B	402	NAG	O5-C5-C6-O6
2	C	403	NAG	C4-C5-C6-O6
2	D	401	NAG	C4-C5-C6-O6
2	E	401	NAG	O5-C5-C6-O6
2	E	403	NAG	C4-C5-C6-O6
2	E	401	NAG	C4-C5-C6-O6
2	F	401	NAG	C4-C5-C6-O6
2	B	402	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	F	401	NAG	O5-C5-C6-O6
2	G	401	NAG	C4-C5-C6-O6
2	G	401	NAG	O5-C5-C6-O6
3	F	404	GOL	O1-C1-C2-O2
2	A	402	NAG	O5-C5-C6-O6
2	B	401	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	401	NAG	O5-C5-C6-O6
2	C	402	NAG	C4-C5-C6-O6
2	B	401	NAG	C3-C2-N2-C7
2	H	402	NAG	C3-C2-N2-C7
3	A	405	GOL	C1-C2-C3-O3
2	C	402	NAG	O5-C5-C6-O6
2	F	403	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	GOL	1	0
3	D	404	GOL	1	0
3	B	404	GOL	1	0
2	F	403	NAG	2	0
3	A	406	GOL	2	0
3	F	404	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, 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	316/323 (97%)	-0.36	7 (2%)	62	59	21, 36, 61, 125	0
1	B	317/323 (98%)	-0.45	6 (1%)	66	65	24, 35, 61, 135	0
1	C	313/323 (96%)	-0.41	2 (0%)	89	88	24, 36, 73, 131	0
1	D	315/323 (97%)	-0.31	9 (2%)	51	49	20, 30, 80, 127	0
1	E	315/323 (97%)	-0.30	7 (2%)	62	59	23, 36, 73, 136	0
1	F	311/323 (96%)	-0.36	6 (1%)	66	65	18, 30, 67, 130	0
1	G	312/323 (96%)	-0.37	7 (2%)	62	59	24, 38, 69, 134	0
1	H	308/323 (95%)	-0.36	1 (0%)	94	93	22, 38, 73, 131	0
All	All	2507/2584 (97%)	-0.36	45 (1%)	68	66	18, 35, 71, 136	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	ALA	10.1
1	A	315	PRO	7.3
1	B	317	ARG	7.0
1	E	340	ALA	6.9
1	A	313	SER	6.3
1	B	316	PHE	6.3
1	H	25	SER	6.2
1	F	319	ILE	5.7
1	D	316	PHE	5.4
1	A	25	SER	5.2
1	E	25	SER	5.1
1	E	312	ALA	5.0
1	C	312	ALA	4.8
1	D	25	SER	4.7
1	G	319	ILE	4.6
1	E	24	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	320	GLN	4.3
1	G	320	GLN	4.3
1	G	321	THR	4.1
1	E	341[A]	HIS	4.0
1	C	318	PRO	3.9
1	B	313	SER	3.7
1	G	318	PRO	3.5
1	D	313	SER	3.5
1	F	295	ASP	3.4
1	G	312	ALA	3.2
1	B	295	ASP	3.2
1	F	312	ALA	3.2
1	B	314	GLY	3.0
1	D	321	THR	2.9
1	D	319	ILE	2.8
1	E	318	PRO	2.8
1	E	313	SER	2.7
1	D	312	ALA	2.7
1	D	295	ASP	2.7
1	F	318	PRO	2.6
1	F	321	THR	2.6
1	A	318	PRO	2.4
1	D	341	HIS	2.3
1	G	342	HIS	2.2
1	A	295	ASP	2.2
1	G	310	ALA	2.2
1	B	312	ALA	2.1
1	F	311	VAL	2.1
1	A	342	HIS	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 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, 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
3	GOL	A	404	6/6	0.56	0.25	93,96,97,98	0
3	GOL	A	406	6/6	0.60	0.40	63,78,81,83	0
2	NAG	C	403	14/15	0.61	0.38	88,102,110,113	0
2	NAG	B	403	14/15	0.66	0.33	71,90,98,100	0
3	GOL	D	404	6/6	0.66	0.25	51,69,73,77	0
3	GOL	H	404	6/6	0.66	0.29	64,72,74,75	0
2	NAG	F	403	14/15	0.68	0.35	88,96,104,104	0
4	CL	A	416	1/1	0.69	0.24	89,89,89,89	0
2	NAG	H	403	14/15	0.72	0.31	71,78,87,91	0
2	NAG	A	403	14/15	0.72	0.26	73,85,89,89	0
3	GOL	F	404	6/6	0.75	0.30	68,75,77,78	0
2	NAG	B	402	14/15	0.76	0.18	58,73,88,91	0
3	GOL	B	404	6/6	0.76	0.29	57,70,75,75	0
2	NAG	E	403	14/15	0.77	0.32	72,79,87,90	0
2	NAG	E	402	14/15	0.77	0.21	65,73,80,82	0
2	NAG	H	402	14/15	0.79	0.21	61,79,86,90	0
3	GOL	A	405	6/6	0.80	0.41	43,62,65,69	0
2	NAG	C	402	14/15	0.82	0.19	55,69,81,81	0
4	CL	H	414	1/1	0.82	0.30	104,104,104,104	0
2	NAG	G	403	14/15	0.83	0.36	70,83,89,91	0
4	CL	G	405	1/1	0.84	0.10	75,75,75,75	0
2	NAG	G	402	14/15	0.85	0.19	44,68,75,76	0
4	CL	C	413	1/1	0.85	0.10	66,66,66,66	0
2	NAG	D	403	14/15	0.86	0.29	68,79,84,86	0
4	CL	C	417	1/1	0.86	0.09	72,72,72,72	0
2	NAG	A	402	14/15	0.87	0.16	52,65,82,84	0
4	CL	G	413	1/1	0.87	0.10	72,72,72,72	0
4	CL	E	412	1/1	0.87	0.18	72,72,72,72	0
2	NAG	F	402	14/15	0.88	0.14	51,63,75,78	0
2	NAG	B	401	14/15	0.88	0.15	39,47,55,60	0
2	NAG	D	402	14/15	0.89	0.16	55,68,83,85	0
4	CL	C	409	1/1	0.89	0.12	65,65,65,65	0
4	CL	F	412	1/1	0.91	0.10	63,63,63,63	0
4	CL	B	416	1/1	0.91	0.08	60,60,60,60	0
4	CL	G	412	1/1	0.91	0.07	60,60,60,60	0
4	CL	B	417	1/1	0.91	0.09	58,58,58,58	0
4	CL	A	411	1/1	0.91	0.11	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	E	414	1/1	0.92	0.21	104,104,104,104	0
2	NAG	G	401	14/15	0.92	0.12	40,46,51,52	0
4	CL	B	409	1/1	0.92	0.07	62,62,62,62	0
4	CL	G	410	1/1	0.93	0.06	62,62,62,62	0
4	CL	G	411	1/1	0.93	0.11	67,67,67,67	0
4	CL	C	411	1/1	0.93	0.14	62,62,62,62	0
4	CL	B	410	1/1	0.93	0.08	62,62,62,62	0
4	CL	E	413	1/1	0.93	0.21	82,82,82,82	0
4	CL	H	407	1/1	0.94	0.20	67,67,67,67	0
4	CL	B	405	1/1	0.94	0.10	47,47,47,47	0
2	NAG	A	401	14/15	0.95	0.14	35,50,58,61	0
4	CL	F	414	1/1	0.95	0.10	50,50,50,50	0
4	CL	F	417	1/1	0.95	0.08	58,58,58,58	0
4	CL	C	412	1/1	0.95	0.07	50,50,50,50	0
2	NAG	C	401	14/15	0.95	0.11	31,45,50,55	0
4	CL	A	415	1/1	0.95	0.11	68,68,68,68	0
2	NAG	F	401	14/15	0.95	0.13	28,40,51,57	0
2	NAG	E	401	14/15	0.95	0.13	40,47,57,58	0
4	CL	C	410	1/1	0.95	0.11	60,60,60,60	0
4	CL	H	413	1/1	0.95	0.10	41,41,41,41	0
4	CL	F	406	1/1	0.95	0.08	47,47,47,47	0
2	NAG	D	401	14/15	0.96	0.09	28,38,43,49	0
4	CL	E	410	1/1	0.96	0.08	47,47,47,47	0
4	CL	H	406	1/1	0.96	0.08	55,55,55,55	0
4	CL	G	406	1/1	0.96	0.06	52,52,52,52	0
4	CL	H	410	1/1	0.96	0.07	50,50,50,50	0
2	NAG	H	401	14/15	0.96	0.11	34,46,50,52	0
4	CL	A	413	1/1	0.96	0.06	52,52,52,52	0
4	CL	C	414	1/1	0.97	0.06	40,40,40,40	0
4	CL	C	416	1/1	0.97	0.13	90,90,90,90	0
4	CL	A	409	1/1	0.97	0.08	50,50,50,50	0
4	CL	D	413	1/1	0.97	0.08	58,58,58,58	0
4	CL	E	405	1/1	0.97	0.08	55,55,55,55	0
4	CL	E	406	1/1	0.97	0.08	43,43,43,43	0
4	CL	G	404	1/1	0.97	0.11	50,50,50,50	0
4	CL	H	412	1/1	0.97	0.11	56,56,56,56	0
4	CL	B	413	1/1	0.97	0.09	48,48,48,48	0
4	CL	A	414	1/1	0.97	0.12	57,57,57,57	0
4	CL	F	407	1/1	0.98	0.12	44,44,44,44	0
4	CL	F	411	1/1	0.98	0.17	59,59,59,59	0
4	CL	C	407	1/1	0.98	0.14	51,51,51,51	0
4	CL	F	413	1/1	0.98	0.08	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	D	409	1/1	0.98	0.07	38,38,38,38	0
4	CL	F	415	1/1	0.98	0.10	36,36,36,36	0
4	CL	D	410	1/1	0.98	0.11	44,44,44,44	0
4	CL	D	411	1/1	0.98	0.09	51,51,51,51	0
4	CL	D	412	1/1	0.98	0.10	41,41,41,41	0
4	CL	C	408	1/1	0.98	0.06	66,66,66,66	0
4	CL	G	407	1/1	0.98	0.07	46,46,46,46	0
4	CL	G	409	1/1	0.98	0.10	51,51,51,51	0
4	CL	E	404	1/1	0.98	0.10	44,44,44,44	0
4	CL	B	412	1/1	0.98	0.08	46,46,46,46	0
4	CL	B	408	1/1	0.98	0.08	45,45,45,45	0
4	CL	E	407	1/1	0.98	0.10	54,54,54,54	0
4	CL	G	414	1/1	0.98	0.07	51,51,51,51	0
4	CL	H	405	1/1	0.98	0.08	48,48,48,48	0
4	CL	B	414	1/1	0.98	0.06	40,40,40,40	0
4	CL	A	408	1/1	0.98	0.07	45,45,45,45	0
4	CL	H	408	1/1	0.98	0.09	50,50,50,50	0
4	CL	H	409	1/1	0.98	0.16	44,44,44,44	0
4	CL	A	407	1/1	0.98	0.09	52,52,52,52	0
4	CL	H	411	1/1	0.98	0.10	42,42,42,42	0
4	CL	C	404	1/1	0.98	0.11	43,43,43,43	0
4	CL	F	405	1/1	0.98	0.12	47,47,47,47	0
4	CL	C	405	1/1	0.98	0.09	56,56,56,56	0
4	CL	D	407	1/1	0.99	0.11	31,31,31,31	0
4	CL	D	408	1/1	0.99	0.10	34,34,34,34	0
4	CL	G	408	1/1	0.99	0.11	42,42,42,42	0
4	CL	B	411	1/1	0.99	0.06	49,49,49,49	0
4	CL	B	406	1/1	0.99	0.07	56,56,56,56	0
4	CL	A	412	1/1	0.99	0.09	50,50,50,50	0
4	CL	C	406	1/1	0.99	0.09	46,46,46,46	0
4	CL	F	408	1/1	0.99	0.10	36,36,36,36	0
4	CL	F	409	1/1	0.99	0.10	39,39,39,39	0
4	CL	G	415	1/1	0.99	0.09	37,37,37,37	0
4	CL	F	410	1/1	0.99	0.08	44,44,44,44	0
4	CL	A	417	1/1	0.99	0.08	37,37,37,37	0
4	CL	C	415	1/1	0.99	0.06	42,42,42,42	0
4	CL	B	415	1/1	0.99	0.10	41,41,41,41	0
4	CL	A	410	1/1	0.99	0.07	48,48,48,48	0
4	CL	D	405	1/1	0.99	0.14	43,43,43,43	0
4	CL	F	416	1/1	0.99	0.08	65,65,65,65	0
4	CL	E	409	1/1	0.99	0.07	38,38,38,38	0
4	CL	D	406	1/1	0.99	0.07	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	E	411	1/1	0.99	0.10	40,40,40,40	0
4	CL	E	408	1/1	1.00	0.10	50,50,50,50	0
4	CL	B	407	1/1	1.00	0.07	46,46,46,46	0
4	CL	A	418	1/1	1.00	0.08	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.