



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:59 AM UTC

PDB ID : 8BF4 / pdb_00008bf4
Title : Crystal structure of Mouse Plexin-B1 (20-535) in complex with VHH15 and VHH14
Authors : Cowan, R.; Hall, G.; Carr, M.
Deposited on : 2022-10-24
Resolution : 2.15 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

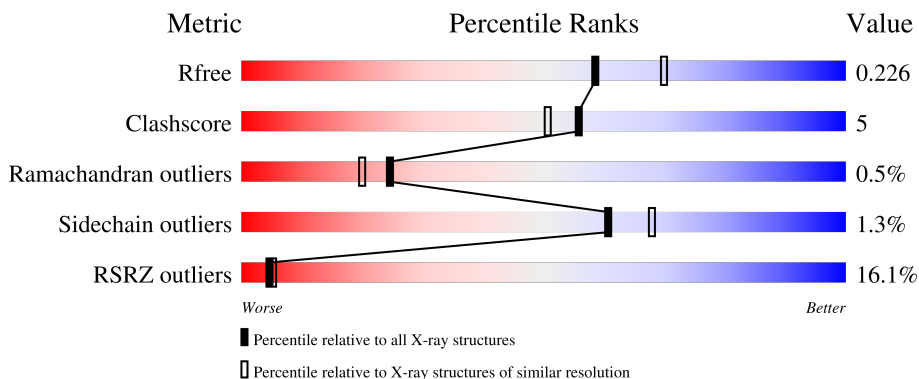
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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.



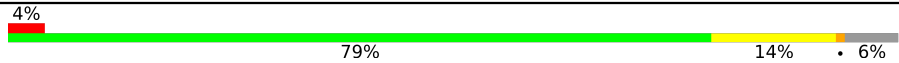
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	124	
1	D	124	
2	C	523	
2	F	523	
3	B	130	

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Mol	Chain	Length	Quality of chain
3	E	130	

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	NAG	F	604	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11421 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 VHH14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	117	876	548	152	171	5	0	0	0
1	A	107	811	507	140	159	5	0	0	0

- Molecule 2 is a protein called Plexin-B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	491	3719	2347	650	701	21	0	1	0
2	C	483	3661	2306	640	694	21	0	0	0

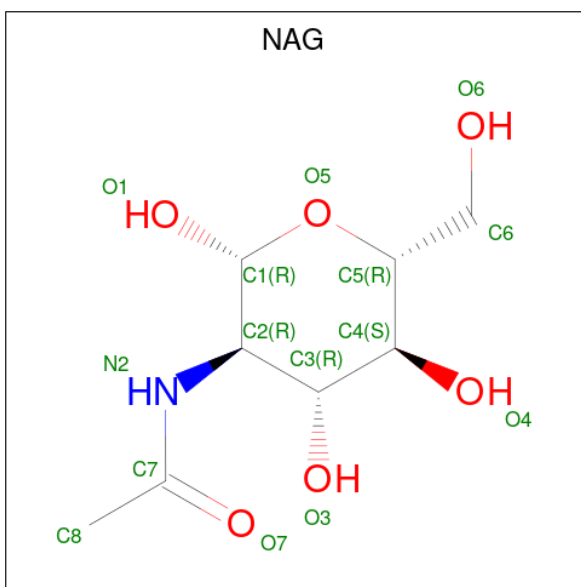
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	536	LYS	-	expression tag	UNP Q8CJH3
F	537	HIS	-	expression tag	UNP Q8CJH3
F	538	HIS	-	expression tag	UNP Q8CJH3
F	539	HIS	-	expression tag	UNP Q8CJH3
F	540	HIS	-	expression tag	UNP Q8CJH3
F	541	HIS	-	expression tag	UNP Q8CJH3
F	542	HIS	-	expression tag	UNP Q8CJH3
C	536	LYS	-	expression tag	UNP Q8CJH3
C	537	HIS	-	expression tag	UNP Q8CJH3
C	538	HIS	-	expression tag	UNP Q8CJH3
C	539	HIS	-	expression tag	UNP Q8CJH3
C	540	HIS	-	expression tag	UNP Q8CJH3
C	541	HIS	-	expression tag	UNP Q8CJH3
C	542	HIS	-	expression tag	UNP Q8CJH3

- Molecule 3 is a protein called VHH15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	122	Total 927	C 576	N 162	O 183	S 6	0	0	0
3	B	123	Total 932	C 579	N 163	O 184	S 6	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

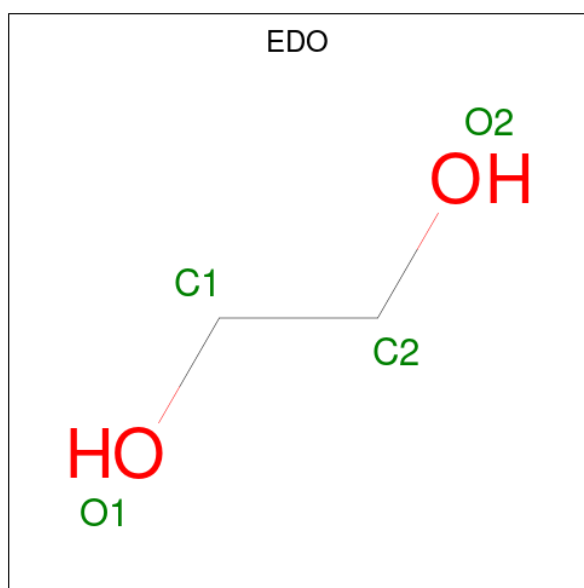


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	F	1	Total 14	C 8	N 1	O 5	0	0
4	F	1	Total 14	C 8	N 1	O 5	0	0
4	F	1	Total 14	C 8	N 1	O 5	0	0
4	F	1	Total 14	C 8	N 1	O 5	0	0
4	C	1	Total 14	C 8	N 1	O 5	0	0
4	C	1	Total 14	C 8	N 1	O 5	0	0
4	C	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total Cl 1 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

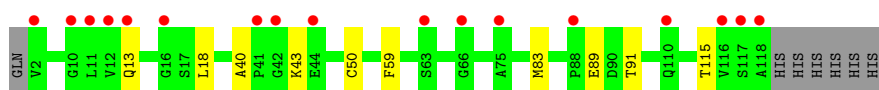
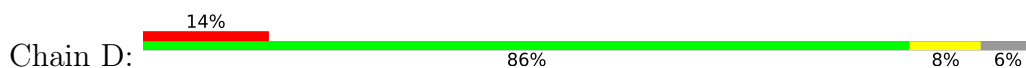
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	27	Total O 27 27	0	0
7	F	168	Total O 168 168	0	0
7	E	29	Total O 29 29	0	0
7	A	20	Total O 20 20	0	0
7	C	125	Total O 125 125	0	0
7	B	23	Total O 23 23	0	0

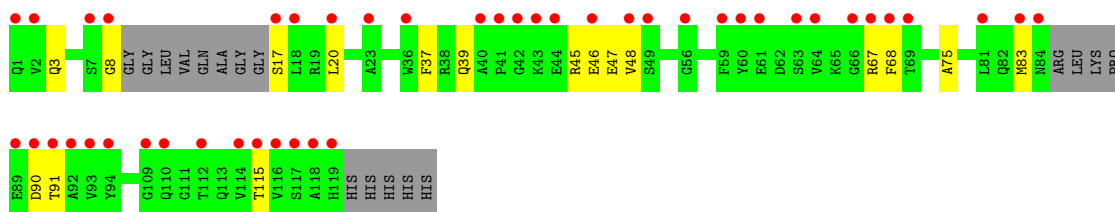
3 Residue-property plots i

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.

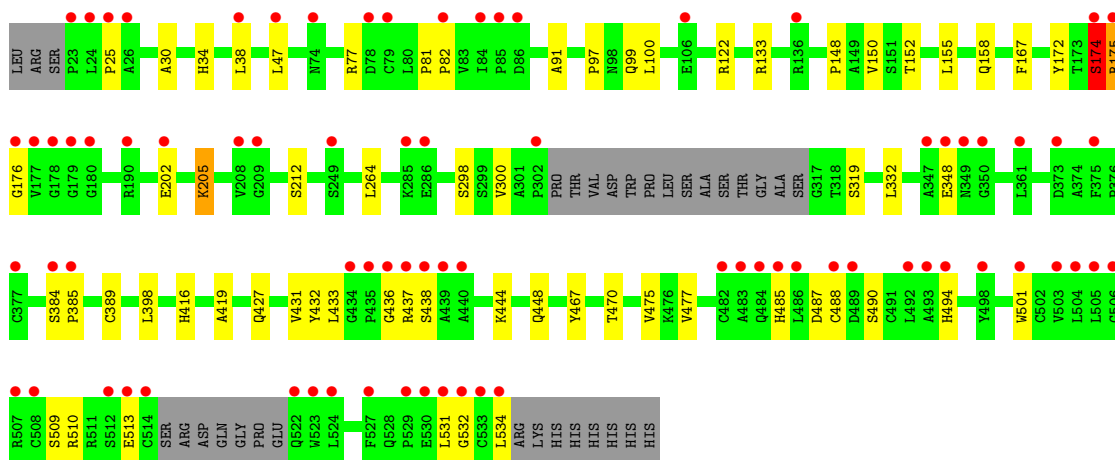
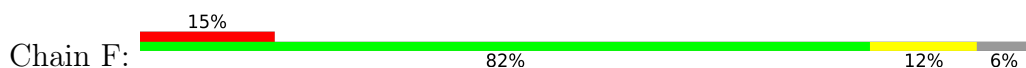
- Molecule 1: VHH14



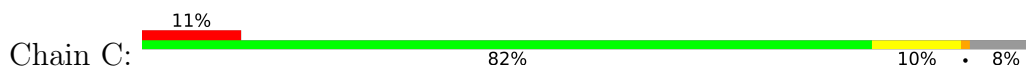
- Molecule 1: VHH14

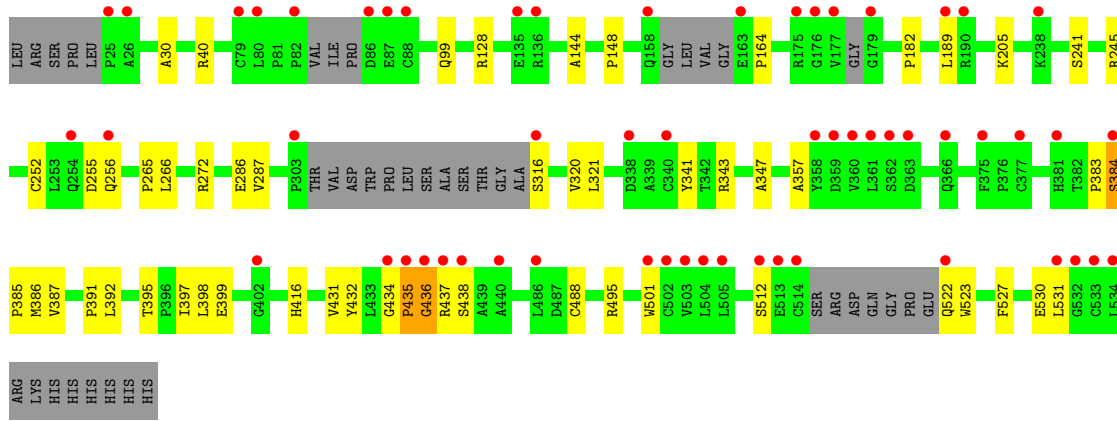


- Molecule 2: Plexin-B1

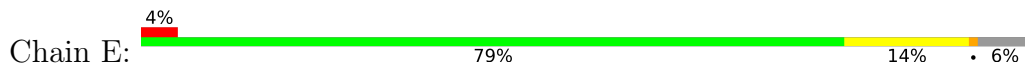


- Molecule 2: Plexin-B1

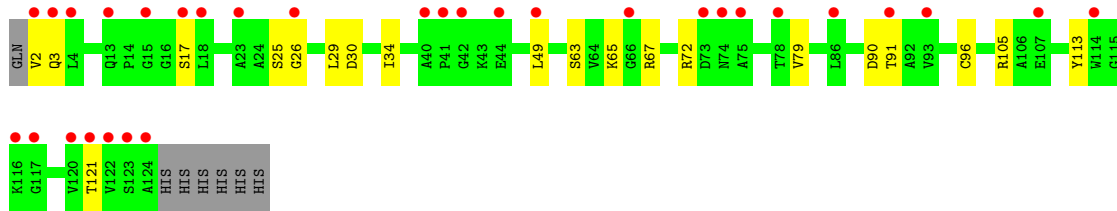
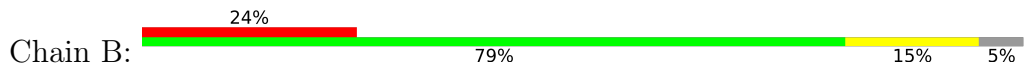




● Molecule 3: VHH15



● Molecule 3: VHH15



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.27Å 109.23Å 95.48Å 90.00° 90.70° 90.00°	Depositor
Resolution (Å)	95.26 – 2.15 95.26 – 2.15	Depositor EDS
% Data completeness (in resolution range)	72.1 (95.26-2.15) 70.4 (95.26-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.14Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.211 , 0.228 0.210 , 0.226	Depositor DCC
R_{free} test set	2021 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtrriage
Anisotropy	0.091	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.005 for l,k,-h 0.024 for h,-k,-l 0.016 for l,-k,h	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11421	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: EDO, NAG, CL

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	0.20	0/825	0.38	0/1114
1	D	0.23	0/892	0.41	0/1206
2	C	0.28	0/3749	0.47	1/5120 (0.0%)
2	F	0.34	1/3815 (0.0%)	0.56	1/5216 (0.0%)
3	B	0.22	0/950	0.42	0/1282
3	E	0.28	0/945	0.41	0/1275
All	All	0.29	1/11176 (0.0%)	0.49	2/15213 (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
2	C	0	3
2	F	0	5
3	B	0	1
3	E	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	174	SER	C-N	-7.30	1.21	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	175	ARG	N-CA-C	-10.40	96.83	112.54
2	C	436	GLY	N-CA-C	-5.71	99.64	113.18

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	105	ARG	Sidechain
2	C	245	ARG	Sidechain
2	C	40	ARG	Sidechain
2	C	435	PRO	Peptide
3	E	105	ARG	Sidechain
2	F	122	ARG	Sidechain
2	F	133	ARG	Sidechain
2	F	174	SER	Mainchain
2	F	175	ARG	Sidechain
2	F	384	SER	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	811	0	762	11	0
1	D	876	0	839	5	0
2	C	3661	0	3551	33	1
2	F	3719	0	3622	34	1
3	B	932	0	888	11	0
3	E	927	0	883	11	0
4	C	42	0	39	1	0
4	F	56	0	52	2	0
5	F	1	0	0	0	0
6	C	4	0	6	0	0
7	A	20	0	0	0	0
7	B	23	0	0	0	0
7	C	125	0	0	3	0
7	D	27	0	0	0	0
7	E	29	0	0	0	0
7	F	168	0	0	2	0
All	All	11421	0	10642	101	1

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 5.

All (101) 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)
3:B:91:THR:HG23	3:B:121:THR:HA	1.62	0.81
2:C:384:SER:HB3	2:C:385:PRO:HD3	1.61	0.80
1:A:91:THR:HG23	1:A:115:THR:HA	1.69	0.75
2:F:448:GLN:NE2	2:F:470:THR:OG1	2.20	0.75
2:F:487:ASP:OD1	2:F:490:SER:N	2.21	0.74
1:A:3:GLN:HE22	2:C:241:SER:H	1.36	0.74
2:F:389:CYS:SG	7:F:861:HOH:O	2.51	0.69
3:E:67:ARG:NH2	3:E:90:ASP:OD2	2.26	0.68
2:F:38:LEU:HD11	2:F:47:LEU:HD22	1.75	0.68
2:F:348:GLU:OE1	2:F:348:GLU:N	2.24	0.67
2:C:272:ARG:O	2:C:272:ARG:NH1	2.28	0.67
2:C:436:GLY:O	2:C:438:SER:N	2.27	0.67
2:F:158:GLN:NE2	7:F:703:HOH:O	2.28	0.66
3:B:2:VAL:HG22	3:B:26:GLY:HA3	1.77	0.64
3:E:29:LEU:HD22	3:E:34:ILE:HD11	1.80	0.63
1:A:39:GLN:OE1	1:A:45:ARG:NH2	2.32	0.63
3:E:63:SER:O	3:E:67:ARG:NH1	2.35	0.60
1:D:91:THR:HG23	1:D:115:THR:HA	1.84	0.59
2:C:357:ALA:HB2	2:C:387:VAL:HB	1.85	0.58
3:B:67:ARG:NH2	3:B:90:ASP:OD2	2.37	0.57
2:C:343:ARG:HH21	2:C:347:ALA:HA	1.68	0.57
2:C:488:CYS:HG	2:C:501:TRP:CG	2.22	0.57
2:C:286:GLU:OE1	2:C:286:GLU:N	2.30	0.56
2:C:320:VAL:HG12	2:C:399:GLU:HG2	1.86	0.56
2:C:128:ARG:NH1	7:C:704:HOH:O	2.35	0.56
2:F:398:LEU:HD22	2:F:431:VAL:HG11	1.87	0.55
1:A:46:GLU:HG2	1:A:47:GLU:N	2.22	0.55
2:F:91:ALA:HB3	4:F:604:NAG:H62	1.88	0.55
2:C:266:LEU:HD23	2:C:392:LEU:HB3	1.89	0.54
3:E:49:LEU:HD21	3:E:60:TYR:CD2	2.43	0.54
2:F:436:GLY:O	2:F:438:SER:N	2.41	0.53
2:F:427:GLN:HE21	2:F:444:LYS:HD2	1.72	0.53
2:C:341:TYR:CD1	2:C:383:PRO:HD2	2.44	0.53
2:F:172:TYR:CZ	2:F:174:SER:HB2	2.44	0.52
2:C:434:GLY:O	2:C:436:GLY:N	2.39	0.52
2:C:148:PRO:HG2	3:B:113:TYR:OH	2.10	0.52
2:F:485:HIS:CE1	2:F:494:HIS:HD1	2.29	0.51
2:C:265:PRO:HG2	2:C:391:PRO:HA	1.91	0.51
2:C:30:ALA:HA	4:C:601:NAG:H82	1.93	0.51
3:B:29:LEU:HG	3:B:34:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100:LEU:HD13	2:F:152:THR:HG22	1.93	0.50
1:D:18:LEU:HB3	1:D:83:MET:HE2	1.93	0.49
1:A:17:SER:N	1:A:83:MET:O	2.45	0.49
3:E:12:VAL:HG12	1:A:75:ALA:HB1	1.95	0.49
2:C:495:ARG:NH1	2:C:527:PHE:O	2.44	0.49
2:F:34:HIS:CG	3:E:100:SER:HB2	2.48	0.49
2:F:77:ARG:O	2:F:176:GLY:HA2	2.13	0.48
2:F:97:PRO:HG2	2:F:148:PRO:HB3	1.97	0.47
2:F:298:SER:OG	2:F:319:SER:OG	2.31	0.47
1:D:40:ALA:HB3	1:D:43:LYS:HD3	1.96	0.47
2:F:172:TYR:CE1	2:F:174:SER:HB2	2.49	0.47
3:E:34:ILE:HG21	3:E:79:VAL:HG11	1.97	0.47
2:C:384:SER:HB3	2:C:385:PRO:CD	2.39	0.47
2:F:488:CYS:HG	2:F:501:TRP:CD1	2.33	0.47
1:D:89:GLU:H	1:D:89:GLU:CD	2.23	0.46
2:F:47:LEU:HD11	2:F:467:TYR:CZ	2.49	0.46
2:C:416:HIS:HB3	2:C:432:TYR:HE1	1.81	0.46
2:C:398:LEU:HD22	2:C:431:VAL:HG11	1.98	0.46
2:C:182:PRO:HG3	2:C:205:LYS:HD3	1.98	0.46
3:E:28:ARG:HE	3:E:28:ARG:HB3	1.64	0.46
2:F:416:HIS:HB3	2:F:432:TYR:HE1	1.81	0.45
3:B:63:SER:O	3:B:67:ARG:NH1	2.49	0.45
2:C:286:GLU:HG2	2:C:287:VAL:H	1.81	0.45
2:F:419:ALA:HB2	2:F:433:LEU:HD11	1.99	0.44
2:C:164:PRO:HG2	2:C:189:LEU:HB2	1.99	0.44
2:C:522:GLN:HB3	2:C:523:TRP:H	1.63	0.44
2:C:99:GLN:HG2	2:C:144:ALA:HB1	1.99	0.43
2:F:202:GLU:O	2:F:205:LYS:NZ	2.50	0.43
2:C:488:CYS:HG	2:C:501:TRP:CD1	2.36	0.43
2:F:81:PRO:HA	2:F:82:PRO:C	2.43	0.43
1:A:37:PHE:HA	1:A:48:VAL:HG23	2.01	0.43
2:F:30:ALA:HA	4:F:601:NAG:H82	2.01	0.43
3:B:30:ASP:N	3:B:30:ASP:OD1	2.52	0.42
2:F:510:ARG:HB2	2:F:513:GLU:OE1	2.19	0.42
3:B:29:LEU:O	3:B:72:ARG:NH2	2.52	0.42
2:C:252:CYS:HB2	2:C:255:ASP:HB2	2.02	0.42
3:E:91:THR:HG23	3:E:121:THR:HA	2.02	0.42
3:E:116:LYS:HD3	3:E:116:LYS:HA	1.95	0.41
2:F:475:VAL:HG12	2:F:477:VAL:HG23	2.01	0.41
2:F:488:CYS:HG	2:F:501:TRP:CG	2.38	0.41
2:F:264:LEU:HD22	2:F:332:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLU:HG2	1:A:47:GLU:H	1.86	0.41
2:C:531:LEU:HD12	2:C:531:LEU:HA	1.71	0.41
1:A:8:GLY:HA3	1:A:20:LEU:HD23	2.03	0.41
2:C:321:LEU:O	2:C:397:ILE:HG12	2.21	0.41
1:D:50:CYS:HB3	1:D:59:PHE:HB3	2.03	0.41
2:F:99:GLN:NE2	2:F:150:VAL:O	2.54	0.41
2:F:172:TYR:CZ	2:F:212:SER:HB2	2.56	0.41
3:E:67:ARG:HH22	3:E:90:ASP:CG	2.28	0.41
1:A:67:ARG:NH1	1:A:90:ASP:OD2	2.53	0.41
1:A:68:PHE:CE2	1:A:83:MET:HG2	2.56	0.41
2:C:256:GLN:OE1	7:C:701:HOH:O	2.22	0.41
2:F:531:LEU:HB3	2:F:532:GLY:H	1.69	0.41
3:B:3:GLN:HB2	3:B:25:SER:OG	2.20	0.41
3:B:29:LEU:HD23	3:B:79:VAL:HG23	2.02	0.40
3:B:65:LYS:HA	3:B:65:LYS:HD2	1.85	0.40
2:F:433:LEU:O	2:F:438:SER:HA	2.22	0.40
2:C:182:PRO:CG	2:C:205:LYS:HD3	2.51	0.40
2:C:99:GLN:NE2	7:C:718:HOH:O	2.54	0.40
2:F:155:LEU:HG	2:F:167:PHE:HB2	2.04	0.40
2:C:386:MET:HE3	2:C:386:MET:HB2	1.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:534:LEU:CD1	2:C:530:GLU:O[1_654]	2.12	0.08

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	101/124 (82%)	94 (93%)	7 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	115/124 (93%)	112 (97%)	3 (3%)	0	100	100
2	C	471/523 (90%)	454 (96%)	14 (3%)	3 (1%)	21	15
2	F	486/523 (93%)	461 (95%)	21 (4%)	4 (1%)	16	10
3	B	121/130 (93%)	113 (93%)	8 (7%)	0	100	100
3	E	120/130 (92%)	118 (98%)	2 (2%)	0	100	100
All	All	1414/1554 (91%)	1352 (96%)	55 (4%)	7 (0%)	24	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	385	PRO
2	C	384	SER
2	F	174	SER
2	F	437	ARG
2	C	437	ARG
2	F	25	PRO
2	C	435	PRO

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	83/96 (86%)	83 (100%)	0	100	100
1	D	89/96 (93%)	88 (99%)	1 (1%)	65	72
2	C	397/430 (92%)	394 (99%)	3 (1%)	73	79
2	F	403/430 (94%)	400 (99%)	3 (1%)	76	82
3	B	97/104 (93%)	94 (97%)	3 (3%)	35	37
3	E	97/104 (93%)	92 (95%)	5 (5%)	21	17
All	All	1166/1260 (92%)	1151 (99%)	15 (1%)	61	68

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	13	GLN
2	F	205	LYS
2	F	300	VAL
2	F	509	SER
3	E	34	ILE
3	E	44	GLU
3	E	46	GLU
3	E	78	THR
3	E	96	CYS
2	C	316	SER
2	C	395	THR
2	C	512	SER
3	B	17	SER
3	B	49	LEU
3	B	96	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	82	GLN
2	F	256	GLN
2	F	404	GLN
2	F	427	GLN
2	F	448	GLN
2	F	465	HIS
2	F	471	GLN
3	E	104	GLN
1	A	3	GLN
2	C	331	GLN
2	C	494	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	NAG	F	604	2	14,14,15	0.37	0	17,19,21	0.90	1 (5%)
4	NAG	F	603	2	14,14,15	0.37	0	17,19,21	0.77	0
4	NAG	C	601	2	14,14,15	0.41	0	17,19,21	0.50	0
4	NAG	C	602	2	14,14,15	0.40	0	17,19,21	0.49	0
4	NAG	C	603	2	14,14,15	0.17	0	17,19,21	0.46	0
4	NAG	F	602	2	14,14,15	0.31	0	17,19,21	0.51	0
4	NAG	F	601	2	14,14,15	0.45	0	17,19,21	0.66	0
6	EDO	C	604	-	3,3,3	0.46	0	2,2,2	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	603	2	-	4/6/23/26	0/1/1/1
4	NAG	F	604	2	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	C	601	2	-	0/6/23/26	0/1/1/1
4	NAG	C	602	2	-	0/6/23/26	0/1/1/1
4	NAG	C	603	2	-	2/6/23/26	0/1/1/1
4	NAG	F	602	2	-	2/6/23/26	0/1/1/1
4	NAG	F	601	2	-	0/6/23/26	0/1/1/1
6	EDO	C	604	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	604	NAG	O5-C1-C2	2.49	115.15	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	604	NAG	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	603	NAG	C8-C7-N2-C2
4	F	603	NAG	O7-C7-N2-C2
4	F	602	NAG	O5-C5-C6-O6
4	F	602	NAG	C4-C5-C6-O6
4	F	604	NAG	C8-C7-N2-C2
4	F	604	NAG	O7-C7-N2-C2
4	C	603	NAG	C4-C5-C6-O6
4	F	603	NAG	O5-C5-C6-O6
4	C	603	NAG	O5-C5-C6-O6
4	F	603	NAG	C3-C2-N2-C7
6	C	604	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	604	NAG	1	0
4	C	601	NAG	1	0
4	F	601	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	107/124 (86%)	2.02	45 (42%) 0 1	40, 62, 83, 91	0
1	D	117/124 (94%)	1.08	17 (14%) 6 6	35, 50, 69, 81	0
2	C	483/523 (92%)	0.77	57 (11%) 9 10	24, 42, 71, 103	0
2	F	491/523 (93%)	0.81	78 (15%) 5 5	20, 39, 78, 91	1 (0%)
3	B	123/130 (94%)	1.51	31 (25%) 1 2	30, 54, 77, 89	0
3	E	122/130 (93%)	0.49	5 (4%) 41 46	26, 42, 57, 69	0
All	All	1443/1554 (92%)	0.94	233 (16%) 4 5	20, 44, 77, 103	1 (0%)

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	23	PRO	6.8
2	C	177	VAL	6.7
1	A	116	VAL	6.4
1	A	118	ALA	6.2
2	F	24	LEU	6.2
2	C	25	PRO	5.8
1	A	40	ALA	5.7
1	A	8	GLY	5.3
2	F	504	LEU	5.3
2	F	436	GLY	5.3
2	F	177	VAL	5.2
2	F	486	LEU	5.2
2	C	361	LEU	5.0
2	F	174	SER	5.0
3	B	40	ALA	5.0
1	A	18	LEU	5.0
1	A	41	PRO	4.9
2	C	384	SER	4.9
1	D	2	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
2	C	435	PRO	4.8
3	B	122	VAL	4.7
2	F	25	PRO	4.6
2	F	506	GLY	4.6
2	F	438	SER	4.6
2	C	504	LEU	4.5
1	A	2	VAL	4.5
2	F	439	ALA	4.5
3	B	26	GLY	4.4
1	D	118	ALA	4.4
3	B	124	ALA	4.4
2	C	503	VAL	4.2
2	F	385	PRO	4.2
2	C	514	CYS	4.2
1	A	59	PHE	4.2
3	B	2	VAL	4.2
2	C	176	GLY	4.2
1	A	84	ASN	4.2
2	C	534	LEU	4.2
1	A	68	PHE	4.1
2	F	175	ARG	4.1
2	F	84	ILE	4.1
1	D	13	GLN	4.1
2	F	435	PRO	4.1
2	F	503	VAL	4.1
1	A	89	GLU	4.0
1	A	114	VAL	4.0
1	A	42	GLY	4.0
2	C	436	GLY	4.0
1	A	119	HIS	3.9
2	C	501	TRP	3.9
2	F	522	GLN	3.9
3	B	41	PRO	3.9
2	F	26	ALA	3.8
2	F	176	GLY	3.8
1	A	63	SER	3.7
1	D	11	LEU	3.7
2	F	440	ALA	3.7
2	F	190	ARG	3.7
2	C	381	HIS	3.6
2	C	163	GLU	3.6
1	A	92	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	F	384	SER	3.6
2	C	26	ALA	3.6
2	C	303	PRO	3.6
2	F	531	LEU	3.6
2	F	507	ARG	3.5
2	C	179	GLY	3.5
1	A	117	SER	3.5
2	C	502	CYS	3.5
2	C	533	CYS	3.5
1	A	64	VAL	3.5
3	B	114	TRP	3.5
2	F	514	CYS	3.4
2	C	82	PRO	3.4
3	B	123	SER	3.4
2	F	501	TRP	3.3
1	D	41	PRO	3.3
1	A	66	GLY	3.3
2	F	534	LEU	3.3
1	D	75	ALA	3.3
1	A	20	LEU	3.3
2	F	202	GLU	3.3
2	F	78	ASP	3.2
1	A	17	SER	3.2
2	F	533	CYS	3.2
2	C	136	ARG	3.2
1	D	44	GLU	3.2
3	B	42	GLY	3.2
2	C	256	GLN	3.2
3	B	3	GLN	3.2
3	B	93	VAL	3.1
3	B	75	ALA	3.1
1	A	91	THR	3.1
2	C	158	GLN	3.1
2	F	523	TRP	3.1
1	D	12	VAL	3.1
1	A	43	LYS	3.1
1	A	1	GLN	3.0
1	A	60	TYR	3.0
2	F	529	PRO	3.0
3	E	123	SER	3.0
2	F	532	GLY	3.0
3	B	66	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	302	PRO	3.0
2	F	498	TYR	3.0
2	C	531	LEU	3.0
2	F	178	GLY	3.0
2	F	179	GLY	2.9
1	A	115	THR	2.9
3	E	114	TRP	2.9
2	F	208	VAL	2.9
1	D	16	GLY	2.9
2	C	522	GLN	2.9
2	F	373	ASP	2.8
1	A	109	GLY	2.8
2	C	86	ASP	2.8
2	F	361	LEU	2.8
1	A	67	ARG	2.8
2	C	437	ARG	2.8
1	A	81	LEU	2.8
2	F	377	CYS	2.8
2	C	360	VAL	2.8
2	F	492	LEU	2.7
3	E	109	TYR	2.7
2	C	438	SER	2.7
2	C	505	LEU	2.7
2	F	484	GLN	2.7
2	F	482	CYS	2.7
2	F	285	LYS	2.7
1	A	110	GLN	2.7
2	F	524	LEU	2.6
1	A	94	TYR	2.6
2	C	79	CYS	2.6
2	F	483	ALA	2.6
3	B	74	ASN	2.6
3	B	73	ASP	2.6
3	B	13	GLN	2.6
2	F	437	ARG	2.6
2	C	190	ARG	2.6
3	B	107	GLU	2.6
2	F	79	CYS	2.6
2	F	512	SER	2.6
2	F	488	CYS	2.5
1	A	69	THR	2.5
2	F	347	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	117	SER	2.5
2	F	434	GLY	2.5
2	C	254	GLN	2.5
3	B	86	LEU	2.5
2	C	512	SER	2.5
2	C	434	GLY	2.5
2	F	348	GLU	2.4
2	F	136	ARG	2.4
2	F	286	GLU	2.4
1	A	90	ASP	2.4
1	D	63	SER	2.4
2	F	505	LEU	2.4
2	F	350	GLY	2.4
3	B	15	GLY	2.4
2	C	88	CYS	2.4
2	C	80	LEU	2.4
2	F	530	GLU	2.4
3	B	23	ALA	2.3
3	B	44	GLU	2.3
2	C	532	GLY	2.3
1	A	7	SER	2.3
2	F	494	HIS	2.3
3	B	121	THR	2.3
1	A	44	GLU	2.3
2	F	508	CYS	2.3
2	F	513	GLU	2.3
2	F	47	LEU	2.3
2	F	527	PHE	2.3
1	A	112	THR	2.3
2	F	82	PRO	2.3
2	F	349	ASN	2.3
1	A	83	MET	2.3
2	C	316	SER	2.3
2	C	362	SER	2.3
1	A	93	VAL	2.3
2	F	489	ASP	2.3
3	E	18	LEU	2.3
2	F	249	SER	2.2
2	C	366	GLN	2.2
2	C	338	ASP	2.2
1	D	10	GLY	2.2
1	A	61	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	485	HIS	2.2
3	B	17	SER	2.2
3	B	78	THR	2.2
1	D	116	VAL	2.2
3	B	116	LYS	2.2
3	B	117	GLY	2.2
1	A	23	ALA	2.2
3	B	49	LEU	2.2
2	C	358	TYR	2.2
3	E	65	LYS	2.2
1	D	88	PRO	2.2
3	B	91	THR	2.2
2	C	359	ASP	2.2
2	C	87	GLU	2.2
2	F	85	PRO	2.1
2	F	375	PHE	2.1
2	C	135	GLU	2.1
2	C	513	GLU	2.1
1	A	48	VAL	2.1
2	F	493	ALA	2.1
2	C	340	CYS	2.1
2	C	486	LEU	2.1
1	A	46	GLU	2.1
2	F	106	GLU	2.1
1	A	49	SER	2.1
2	F	38	LEU	2.1
1	D	66	GLY	2.1
2	C	402	GLY	2.1
1	A	36	TRP	2.1
2	C	440	ALA	2.1
2	F	86	ASP	2.1
2	C	363	ASP	2.1
2	C	175	ARG	2.1
2	F	209	GLY	2.1
2	F	74	ASN	2.0
2	C	377	CYS	2.0
2	C	238	LYS	2.0
1	D	42	GLY	2.0
2	C	375	PHE	2.0
3	B	120	VAL	2.0
1	D	110	GLN	2.0
2	C	189	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	B	4	LEU	2.0
3	B	18	LEU	2.0
1	A	56	GLY	2.0
2	F	180	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	F	604	14/15	0.33	0.25	66,77,83,86	0
4	NAG	F	603	14/15	0.69	0.17	64,69,78,80	0
4	NAG	C	603	14/15	0.86	0.12	46,53,70,72	0
4	NAG	C	602	14/15	0.87	0.10	45,52,60,62	0
4	NAG	F	602	14/15	0.88	0.09	38,47,56,58	0
6	EDO	C	604	4/4	0.90	0.23	36,39,50,54	0
4	NAG	F	601	14/15	0.92	0.09	33,35,44,49	0
4	NAG	C	601	14/15	0.93	0.08	33,39,43,46	0
5	CL	F	605	1/1	0.98	0.10	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.