



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 03:37 PM EDT

PDB ID : 6P8N  
Title : Crystal Structure of Antibody P-p1f1 in Complex with eOD-GT8  
Authors : Weidle, C.; Pancera, M.  
Deposited on : 2019-06-07  
Resolution : 3.20 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

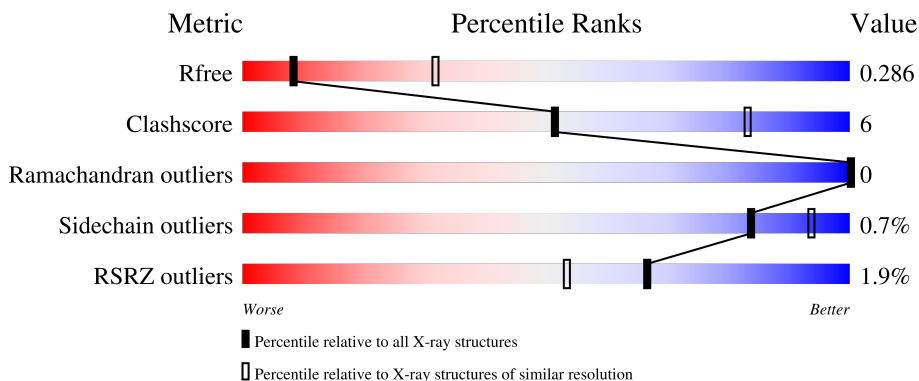
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\geq 3$ , 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	183	 6% 84% 8% 8%
1	C	183	 5% 80% 10% 9%
2	B	226	 85% 12% .
2	H	226	 88% 9% .
3	D	216	 82% 12% 6%

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Mol	Chain	Length	Quality of chain
3	L	216	 % 82% 12% 6%

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
5	NH4	C	202	-	-	-	X
6	EDO	H	301	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16725 atoms, of which 7970 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 Env outer domain eOD-GT8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	C	167	2091	716	945	207	215	8	0	0	0
1	A	168	2182	737	1006	208	223	8	0	0	0

- Molecule 2 is a protein called P-p1f1 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	H	221	3176	1032	1536	284	316	8	0	0	0
2	B	220	3174	1028	1538	282	318	8	0	0	0

- Molecule 3 is a protein called P-p1f1 Light Chain.

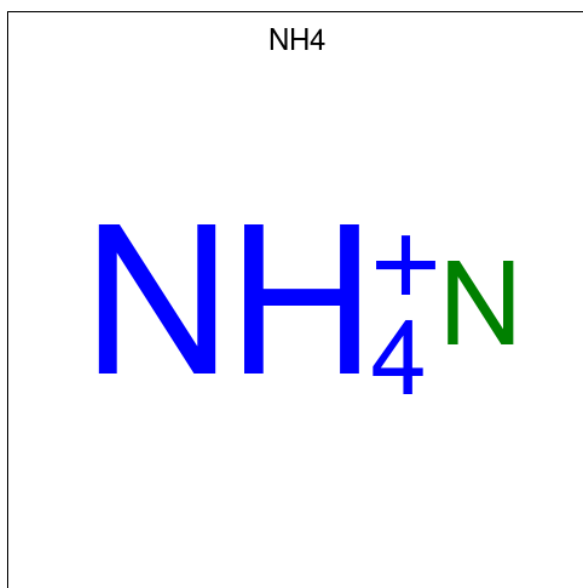
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	L	204	2961	962	1428	255	309	7	0	0	0
3	D	203	3019	972	1473	257	310	7	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	C	1	28	8	14	1	5	0	0

- Molecule 5 is AMMONIUM ION (three-letter code: NH4) (formula: H<sub>4</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	N		
5	C	1	5	4	1	0	0
5	B	1	5	4	1	0	0
5	B	1	5	4	1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	L	1	Total	C	H	O	0	0
			10	2	6	2		
6	L	1	Total	C	H	O	0	0
			10	2	6	2		

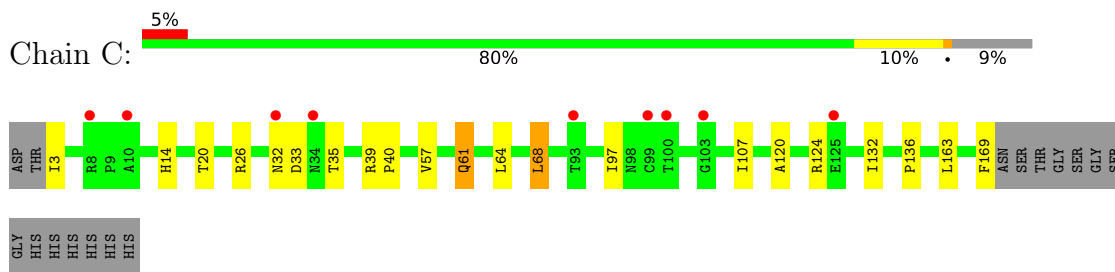
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	3	Total	O	0	0
			3	3		
7	H	10	Total	O	0	0
			10	10		
7	L	9	Total	O	0	0
			9	9		
7	A	5	Total	O	0	0
			5	5		
7	B	12	Total	O	0	0
			12	12		
7	D	10	Total	O	0	0
			10	10		

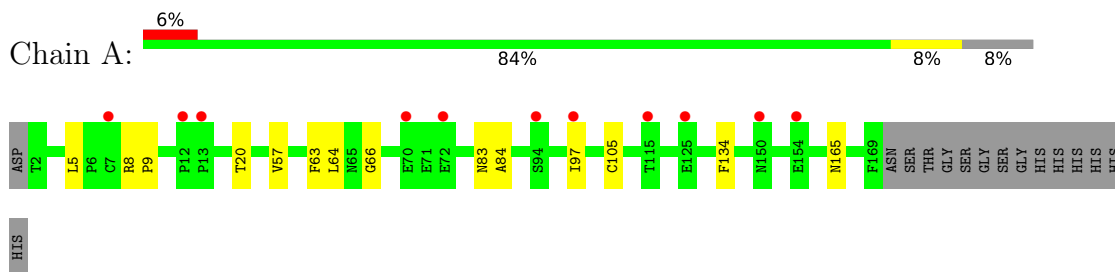
### 3 Residue-property plots [i](#)

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.

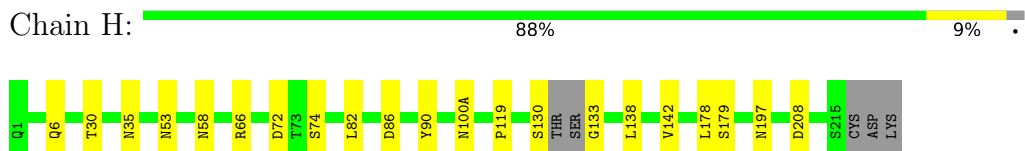
- Molecule 1: Env outer domain eOD-GT8



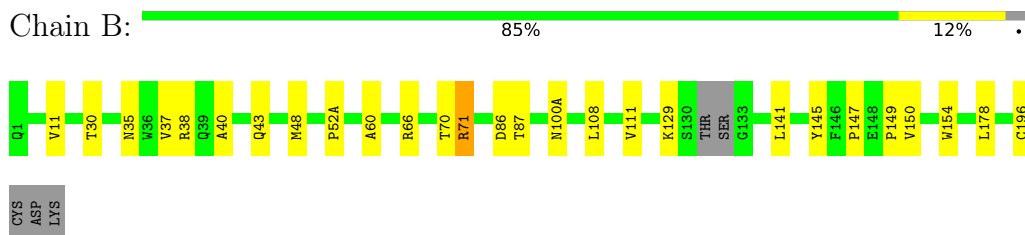
- Molecule 1: Env outer domain eOD-GT8




- Molecule 2: P-p1f1 Heavy Chain

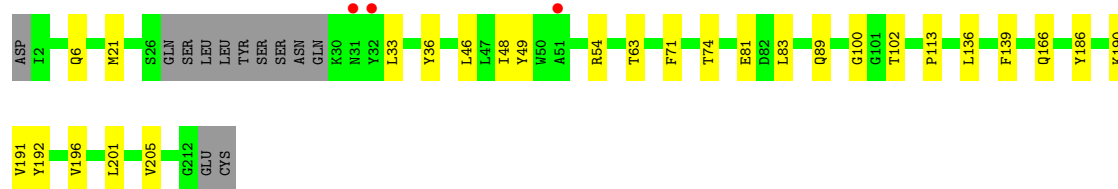


- Molecule 2: P-p1f1 Heavy Chain




- Molecule 3: P-p1f1 Light Chain

Chain L:  %



• Molecule 3: P-p1f1 Light Chain

Chain D:  %





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.88Å 92.41Å 223.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.16 – 3.20 41.16 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.9 (41.16-3.20) 96.0 (41.16-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 3.18Å)	Xtrriage
Refinement program	PHENIX (1.15.2_3472)	Depositor
R, $R_{free}$	0.226 , 0.287 0.225 , 0.286	Depositor DCC
$R_{free}$ test set	1024 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.2	Xtrriage
Anisotropy	0.068	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 72.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	16725	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2107e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, NH4, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/1204	0.43	0/1650
1	C	0.30	0/1174	0.52	1/1603 (0.1%)
2	B	0.26	0/1678	0.47	0/2290
2	H	0.26	0/1682	0.47	0/2294
3	D	0.26	0/1578	0.45	0/2140
3	L	0.27	0/1565	0.47	0/2127
All	All	0.26	0/8881	0.47	1/12104 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	LEU	CA-CB-CG	6.39	130.00	115.30

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	1176	1006	1005	11	0
1	C	1146	945	944	23	0
2	B	1636	1538	1538	15	1
2	H	1640	1536	1535	12	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1546	1473	1473	15	0
3	L	1533	1428	1428	16	0
4	C	14	14	13	3	0
5	B	2	8	0	0	0
5	C	1	4	0	0	0
6	H	4	6	6	0	0
6	L	8	12	12	0	1
7	A	5	0	0	0	0
7	B	12	0	0	0	0
7	C	3	0	0	0	0
7	D	10	0	0	0	0
7	H	10	0	0	0	0
7	L	9	0	0	0	0
All	All	8755	7970	7954	93	2

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 6.

All (93) 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:D:136:LEU:HD21	3:D:196:VAL:HG21	1.56	0.84
3:L:6:GLN:NE2	3:L:100:GLY:O	2.18	0.75
1:C:97:ILE:HA	1:C:107:ILE:HG22	1.70	0.74
1:C:20:THR:HG22	1:C:68:LEU:HD21	1.68	0.73
2:H:130:SER:HG	2:H:133:GLY:N	1.85	0.73
4:C:201:NAG:O7	4:C:201:NAG:O3	2.05	0.72
1:C:14:HIS:O	4:C:201:NAG:O3	2.08	0.71
1:C:40:PRO:CB	1:C:61:GLN:OE1	2.38	0.71
2:B:66:ARG:NH2	2:B:86:ASP:OD2	2.25	0.70
3:L:83:LEU:HD11	3:L:166:GLN:HB3	1.77	0.66
2:B:108:LEU:HD23	2:B:149:PRO:HD3	1.79	0.65
3:D:33:LEU:HD22	3:D:71:PHE:CG	2.32	0.65
3:D:136:LEU:HD21	3:D:196:VAL:CG2	2.25	0.64
2:H:66:ARG:NH1	2:H:86:ASP:OD2	2.31	0.64
3:L:21:MET:SD	3:L:102:THR:HG21	2.38	0.63
3:L:190:LYS:HG3	3:L:191:VAL:HG23	1.81	0.62
3:L:33:LEU:HD22	3:L:71:PHE:CG	2.34	0.62
1:C:20:THR:HG22	1:C:68:LEU:CD2	2.29	0.62
3:D:6:GLN:OE1	3:D:88:CYS:N	2.32	0.62
1:C:124:ARG:NH2	1:C:169:PHE:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:130:SER:OG	2:H:133:GLY:N	2.36	0.59
1:C:107:ILE:HD11	1:C:163:LEU:HD21	1.87	0.56
3:L:186:TYR:O	3:L:192:TYR:OH	2.23	0.56
1:C:40:PRO:HG3	1:C:61:GLN:OE1	2.06	0.56
3:D:25:SER:O	3:D:69:THR:OG1	2.24	0.56
1:C:40:PRO:CG	1:C:61:GLN:OE1	2.54	0.56
2:B:35:ASN:ND2	2:B:100(A):ASN:OD1	2.32	0.55
1:C:26:ARG:O	2:H:58:ASN:ND2	2.39	0.55
1:C:57:VAL:HG11	1:C:64:LEU:CB	2.37	0.55
1:C:40:PRO:HB3	1:C:61:GLN:OE1	2.07	0.54
3:L:136:LEU:HD21	3:L:196:VAL:HG13	1.89	0.54
2:B:87:THR:HG22	2:B:111:VAL:H	1.73	0.54
3:D:201:LEU:HD13	3:D:205:VAL:HG23	1.91	0.53
2:H:72:ASP:OD1	2:H:74:SER:OG	2.24	0.52
3:L:201:LEU:HD13	3:L:205:VAL:HG23	1.92	0.52
3:L:81:GLU:N	3:L:81:GLU:OE1	2.43	0.52
3:D:147:GLN:NE2	3:D:195:GLU:OE1	2.43	0.52
3:L:63:THR:OG1	3:L:74:THR:OG1	2.29	0.51
1:C:20:THR:CG2	1:C:68:LEU:CD2	2.87	0.51
1:C:3:ILE:N	1:C:107:ILE:O	2.44	0.51
2:H:119:PRO:HB2	2:H:142:VAL:HG13	1.93	0.50
1:A:8:ARG:CB	1:A:9:PRO:HD3	2.40	0.50
3:L:36:TYR:CE1	3:L:46:LEU:HD13	2.47	0.49
1:C:20:THR:HB	1:C:68:LEU:HD23	1.94	0.49
2:B:11:VAL:HG22	2:B:147:PRO:HG3	1.93	0.49
1:A:8:ARG:CB	1:A:9:PRO:CD	2.91	0.48
2:H:35:ASN:ND2	2:H:100(A):ASN:OD1	2.44	0.47
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.94	0.47
3:L:113:PRO:CA	3:L:139:PHE:HB3	2.45	0.47
2:H:197:ASN:ND2	2:H:208:ASP:OD2	2.45	0.47
2:H:6:GLN:NE2	2:H:90:TYR:O	2.39	0.46
2:B:48:MET:O	2:B:60:ALA:N	2.47	0.46
1:C:107:ILE:HD11	1:C:163:LEU:CD2	2.46	0.45
3:L:33:LEU:HD12	3:L:89:GLN:O	2.17	0.45
1:A:5:LEU:HD23	1:A:5:LEU:H	1.82	0.45
1:A:64:LEU:HD22	1:A:97:ILE:CD1	2.48	0.44
2:B:145:TYR:CE2	2:B:150:VAL:HG23	2.53	0.44
3:D:163:VAL:HG22	3:D:175:LEU:HD12	1.99	0.44
3:L:46:LEU:HD21	3:L:49:TYR:HB3	2.00	0.44
1:A:20:THR:HG21	1:A:66:GLY:C	2.38	0.44
1:A:134:PHE:O	1:A:165:ASN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:THR:HB	1:C:68:LEU:CD2	2.48	0.43
1:C:57:VAL:HG13	1:C:57:VAL:O	2.18	0.43
1:A:5:LEU:HD21	1:A:105:CYS:HB2	1.99	0.43
3:D:165:GLU:OE1	3:D:166:GLN:N	2.45	0.43
2:B:30:THR:HA	2:B:52(A):PRO:HB2	2.00	0.43
2:B:70:THR:HG22	2:B:71:ARG:N	2.34	0.42
3:D:186:TYR:O	3:D:192:TYR:OH	2.33	0.42
2:B:70:THR:HG22	2:B:71:ARG:H	1.84	0.42
2:H:66:ARG:NH2	2:H:82:LEU:HD21	2.35	0.42
2:B:141:LEU:HD12	2:B:178:LEU:O	2.19	0.42
3:D:50:TRP:O	3:D:51:ALA:HB3	2.20	0.42
3:D:182:SER:O	3:D:186:TYR:N	2.50	0.42
2:B:40:ALA:HB3	2:B:43:GLN:HB2	2.02	0.42
3:L:48:ILE:HD13	3:L:54:ARG:HA	2.02	0.41
2:B:154:TRP:CH2	2:B:196:CYS:SG	3.13	0.41
1:C:39:ARG:NH1	1:C:136:PRO:O	2.46	0.41
1:C:57:VAL:CG1	1:C:64:LEU:O	2.69	0.41
1:C:57:VAL:HG12	1:C:64:LEU:O	2.20	0.41
2:H:30:THR:O	2:H:53:ASN:ND2	2.52	0.41
1:A:83:ASN:OD1	1:A:84:ALA:N	2.54	0.41
2:B:37:VAL:HG12	2:B:38:ARG:N	2.35	0.41
1:A:57:VAL:HG11	1:A:64:LEU:HB2	2.02	0.41
2:B:196:CYS:O	2:B:208:ASP:HA	2.21	0.41
1:A:20:THR:HG22	1:A:20:THR:O	2.21	0.41
1:C:33:ASP:O	1:C:35:THR:N	2.53	0.41
4:C:201:NAG:O7	4:C:201:NAG:C3	2.69	0.41
3:D:179:LEU:HD23	3:D:179:LEU:O	2.20	0.41
3:L:113:PRO:HA	3:L:139:PHE:HB3	2.02	0.40
3:D:190:LYS:HG2	3:D:191:VAL:HG23	2.02	0.40
2:H:178:LEU:HD12	2:H:179:SER:N	2.37	0.40
1:C:120:ALA:O	1:C:132:ILE:HD12	2.20	0.40
1:A:63:PHE:O	1:A:64:LEU:HD23	2.21	0.40

All (2) 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)
6:L:301:EDO:O2	6:L:301:EDO:O2[2_555]	2.03	0.17
2:H:133:GLY:N	2:B:111:VAL:O[2_645]	2.14	0.06

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	166/183 (91%)	149 (90%)	17 (10%)	0	100	100
1	C	165/183 (90%)	144 (87%)	21 (13%)	0	100	100
2	B	216/226 (96%)	203 (94%)	13 (6%)	0	100	100
2	H	217/226 (96%)	204 (94%)	13 (6%)	0	100	100
3	D	199/216 (92%)	186 (94%)	13 (6%)	0	100	100
3	L	200/216 (93%)	188 (94%)	12 (6%)	0	100	100
All	All	1163/1250 (93%)	1074 (92%)	89 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	108/158 (68%)	108 (100%)	0	100	100
1	C	98/158 (62%)	96 (98%)	2 (2%)	55	80
2	B	173/191 (91%)	171 (99%)	2 (1%)	71	88
2	H	170/191 (89%)	169 (99%)	1 (1%)	86	94
3	D	169/191 (88%)	168 (99%)	1 (1%)	86	94
3	L	163/191 (85%)	163 (100%)	0	100	100
All	All	881/1080 (82%)	875 (99%)	6 (1%)	84	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	32	ASN
1	C	61	GLN
2	H	138	LEU
2	B	71	ARG
2	B	129	LYS
3	D	190	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are modelled with single atom - leaving 4 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	$\# Z  > 2$
6	EDO	L	301	-	3,3,3	0.47	0	2,2,2	0.36	0
6	EDO	L	302	-	3,3,3	0.47	0	2,2,2	0.30	0
6	EDO	H	301	-	3,3,3	0.48	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	201	1	14,14,15	1.64	2 (14%)	17,19,21	1.54	3 (17%)

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
6	EDO	L	301	-	-	0/1/1/1	-
6	EDO	L	302	-	-	0/1/1/1	-
6	EDO	H	301	-	-	0/1/1/1	-
4	NAG	C	201	1	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	201	NAG	C7-N2	3.84	1.47	1.34
4	C	201	NAG	O5-C1	3.05	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	201	NAG	C4-C3-C2	3.45	116.07	111.02
4	C	201	NAG	C3-C4-C5	3.14	115.84	110.24
4	C	201	NAG	C8-C7-N2	2.26	119.92	116.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	201	NAG	C3-C2-N2-C7
4	C	201	NAG	O5-C5-C6-O6
4	C	201	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	301	EDO	0	1
4	C	201	NAG	3	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	168/183 (91%)	0.37	11 (6%) 18 11	55, 91, 128, 150	0
1	C	167/183 (91%)	0.30	9 (5%) 25 14	56, 90, 120, 162	0
2	B	220/226 (97%)	-0.19	0 100 100	28, 50, 74, 84	0
2	H	221/226 (97%)	-0.17	0 100 100	35, 54, 83, 99	0
3	D	203/216 (93%)	-0.20	0 100 100	30, 52, 79, 101	0
3	L	204/216 (94%)	0.01	3 (1%) 73 61	29, 59, 91, 121	0
All	All	1183/1250 (94%)	-0.01	23 (1%) 66 53	28, 60, 112, 162	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100	THR	4.9
1	A	70	GLU	3.6
1	C	93	THR	3.0
3	L	31	ASN	3.0
1	C	10	ALA	2.9
1	C	99	CYS	2.7
1	C	32	ASN	2.7
3	L	51	ALA	2.6
1	C	34	ASN	2.6
1	A	97	ILE	2.5
1	A	7	CYS	2.5
1	A	12	PRO	2.4
1	A	94	SER	2.4
1	A	150	ASN	2.4
1	A	13	PRO	2.4
1	A	154	GLU	2.3
1	C	125	GLU	2.3
1	C	8	ARG	2.2
1	A	125	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	103	GLY	2.2
1	A	72	GLU	2.1
1	A	115	THR	2.0
3	L	32	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	EDO	H	301	4/4	0.43	0.57	200,269,325,325	10
5	NH4	C	202	1/1	0.61	0.84	54,65,65,65	0
5	NH4	B	302	1/1	0.81	0.20	45,54,54,54	5
4	NAG	C	201	14/15	0.82	0.28	102,118,140,142	0
6	EDO	L	301	4/4	0.84	0.24	40,56,72,72	0
6	EDO	L	302	4/4	0.86	0.17	35,42,52,52	0
5	NH4	B	301	1/1	0.92	0.29	31,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.