



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:44 PM UTC

PDB ID : 3NJP / pdb_00003njp
Title : The Extracellular and Transmembrane Domain Interfaces in Epidermal Growth Factor Receptor Signaling
Authors : Lu, C.; Mi, L.-Z.; Grey, M.J.; Zhu, J.; Graef, E.; Yokoyama, S.; Springer, T.A.
Deposited on : 2010-06-17
Resolution : 3.30 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

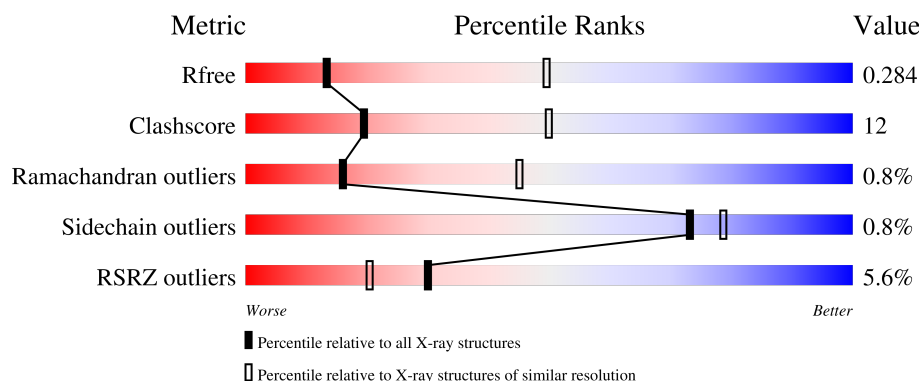
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	614	6% 73% 26%
1	B	614	5% 72% 27%
2	C	47	4% 89% 11%
2	D	47	4% 74% 26%

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
3	NAG	A	1172	X	-	-	-
3	NAG	A	1337	X	-	-	-
3	NAG	B	1504	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10567 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	614	Total	C	N	O	S	0	1	0
			4733	2921	844	908	60			
1	B	614	Total	C	N	O	S	0	1	0
			4730	2919	842	909	60			

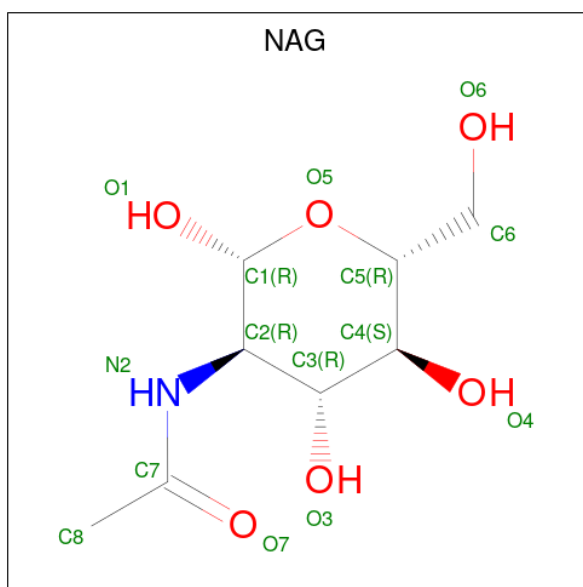
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	LYS	ASN	conflict	UNP P00533
B	516	LYS	ASN	conflict	UNP P00533

- Molecule 2 is a protein called Epidermal growth factor.

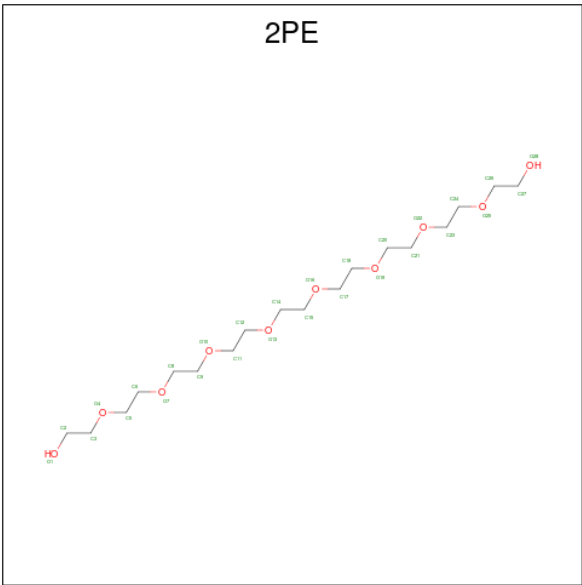
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	47	Total	C	N	O	S	0	0	0
			386	244	63	72	7			
2	D	47	Total	C	N	O	S	0	0	0
			386	244	63	72	7			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: C₁₈H₃₈O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			28	18	10		
4	B	1	Total	C	O	0	0
			28	18	10		
4	B	1	Total	C	O	0	0
			28	18	10		
4	D	1	Total	C	O	0	0
			28	18	10		
4	D	1	Total	C	O	0	0
			28	18	10		

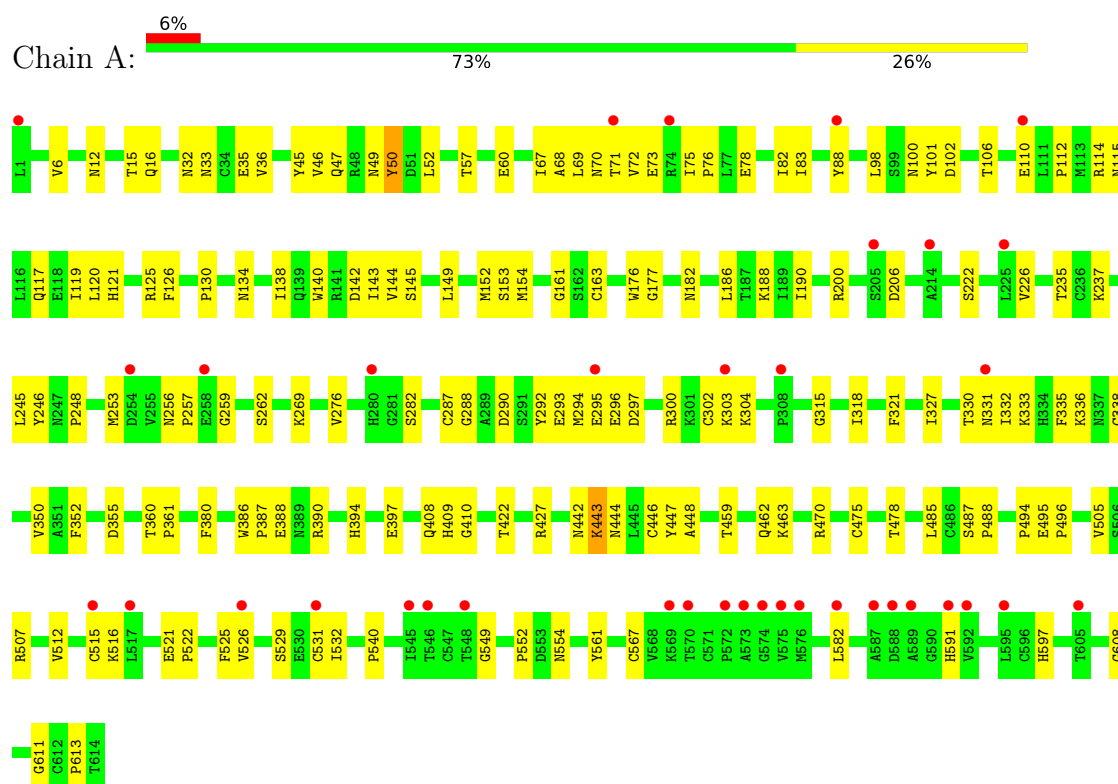
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	5	Total	O	0	0
			5	5		
5	C	5	Total	O	0	0
			5	5		
5	D	1	Total	O	0	0
			1	1		

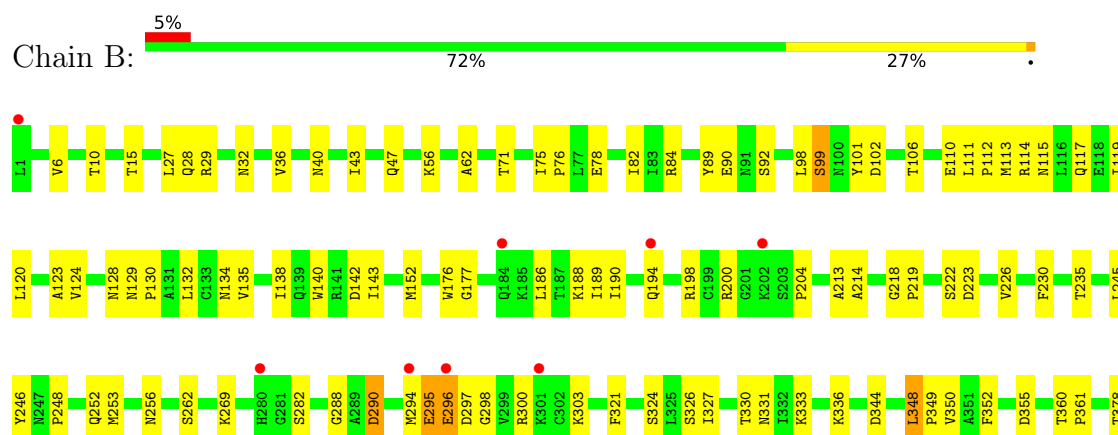
3 Residue-property plots

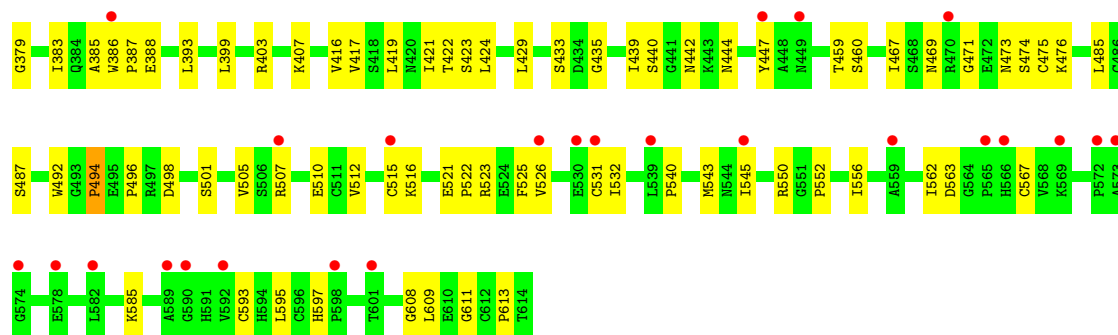
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Epidermal growth factor receptor

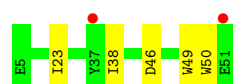
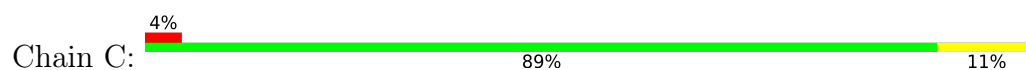


• Molecule 1: Epidermal growth factor receptor

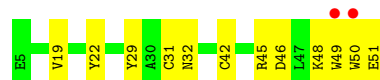
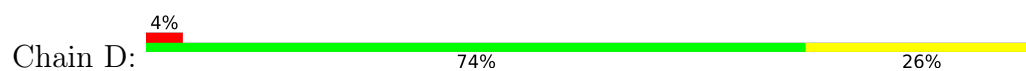




- Molecule 2: Epidermal growth factor



- Molecule 2: Epidermal growth factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	220.17Å 220.17Å 113.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.49 – 3.30 49.49 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.49-3.30) 98.2 (49.49-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.263 , 0.298 0.252 , 0.284	Depositor DCC
R_{free} test set	2322 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	92.1	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 121.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10567	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: 2PE, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/4828	0.72	0/6528
1	B	0.25	0/4825	0.71	2/6525 (0.0%)
2	C	0.24	0/397	0.63	0/536
2	D	0.23	0/397	0.63	0/536
All	All	0.25	0/10447	0.71	2/14125 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ASN	CA-C-N	5.21	124.83	119.05
1	B	129	ASN	C-N-CA	5.21	124.83	119.05

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	4733	0	4565	115	0
1	B	4730	0	4563	118	0
2	C	386	0	344	3	0
2	D	386	0	344	10	0
3	A	112	0	104	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	56	0	52	3	0
4	B	84	0	114	1	0
4	D	56	0	76	1	0
5	A	13	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	1	0	0	0	0
All	All	10567	0	10162	241	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 12.

All (241) 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:A:521:GLU:HB2	1:A:522:PRO:HD3	1.51	0.91
2:D:45:ARG:HG2	2:D:45:ARG:HH11	1.35	0.90
1:B:521:GLU:HB3	1:B:522:PRO:HD3	1.57	0.84
1:B:505:VAL:HG23	1:B:512:VAL:HG23	1.62	0.79
1:B:422:THR:HA	1:B:444:ASN:O	1.87	0.74
1:B:194:GLN:HE21	1:B:204:PRO:HB3	1.55	0.72
1:B:222:SER:HB3	1:B:235:THR:HG22	1.72	0.72
1:B:447:TYR:OH	1:B:494:PRO:HG3	1.90	0.71
1:B:523:ARG:NH1	1:B:540:PRO:HB3	2.05	0.71
1:A:46:VAL:HG11	1:A:52:LEU:HD11	1.72	0.70
1:B:597:HIS:HB2	1:B:608:GLY:HA2	1.73	0.69
1:B:349:PRO:HG3	1:B:385:ALA:HB2	1.74	0.69
4:B:616:2PE:H171	4:B:617:2PE:H52	1.75	0.68
1:A:149:LEU:HA	1:A:152:MET:HG3	1.77	0.67
1:B:471:GLY:HA3	1:B:475:CYS:SG	2.34	0.67
2:D:45:ARG:HG2	2:D:45:ARG:NH1	2.09	0.67
1:B:523:ARG:HD2	1:B:540:PRO:HA	1.80	0.63
1:A:222:SER:HB3	1:A:235:THR:HG22	1.81	0.62
1:A:422:THR:HA	1:A:444:ASN:O	1.99	0.62
1:A:321:PHE:CE1	1:A:331:ASN:HB2	2.34	0.62
1:A:388:GLU:HB2	3:A:1420:NAG:O7	2.01	0.60
1:A:200:ARG:HB2	1:A:206:ASP:HB3	1.83	0.60
1:B:321:PHE:CE1	1:B:331:ASN:HB2	2.37	0.60
1:B:471:GLY:HA2	1:B:474:SER:HB3	1.83	0.59
1:B:82:ILE:HD12	1:B:213:ALA:HB1	1.84	0.59
1:A:70:ASN:HB3	1:A:72:VAL:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HD11	1:A:120:LEU:HG	1.84	0.58
1:A:110:GLU:HG2	1:A:112:PRO:HD3	1.86	0.58
1:B:295:GLU:HG2	1:B:296:GLU:H	1.68	0.58
1:A:352:PHE:CZ	1:A:387:PRO:HD3	2.38	0.57
1:B:245:LEU:HG	1:B:256:ASN:HB2	1.85	0.57
1:A:292:TYR:HE1	1:A:294:MET:HE2	1.69	0.57
1:B:532:ILE:HG21	1:B:550:ARG:HG2	1.86	0.57
1:B:124:VAL:H	1:B:152:MET:HG2	1.70	0.57
1:A:388:GLU:H	1:A:388:GLU:CD	2.13	0.57
1:B:496:PRO:HB2	1:B:510:GLU:HG3	1.85	0.57
1:B:62:ALA:O	1:B:84:ARG:HB2	2.04	0.56
1:A:552:PRO:HB2	1:A:567:CYS:H	1.70	0.56
2:D:45:ARG:HH22	2:D:51:GLU:HB2	1.69	0.56
1:B:84:ARG:HD3	1:B:120:LEU:HD12	1.86	0.56
1:B:123:ALA:HB1	1:B:152:MET:HG2	1.87	0.56
1:B:552:PRO:HB2	1:B:567:CYS:H	1.69	0.56
1:B:507:ARG:NH2	1:B:516:LYS:HG3	2.20	0.56
1:B:186:LEU:HD22	1:B:190:ILE:HD11	1.88	0.56
1:A:138:ILE:HG12	1:A:176:TRP:CE2	2.40	0.56
1:A:408:GLN:C	1:A:410:GLY:H	2.14	0.56
1:B:326:SER:HB2	1:B:348:LEU:HD22	1.87	0.56
1:A:447:TYR:OH	1:A:494:PRO:HG3	2.06	0.55
1:A:6:VAL:HG12	1:A:36:VAL:HB	1.88	0.55
1:B:135:VAL:HA	1:B:138:ILE:HD13	1.88	0.55
1:A:47:GLN:HA	1:A:71:THR:OG1	2.06	0.55
1:A:507:ARG:HH12	1:A:516:LYS:HE3	1.70	0.55
1:A:82:ILE:HG21	1:A:226:VAL:HG11	1.88	0.54
1:A:446:CYS:SG	1:A:470:ARG:HG2	2.48	0.54
1:A:549:GLY:HA3	1:A:554:ASN:OD1	2.08	0.54
1:B:543:MET:HE2	1:B:543:MET:HA	1.90	0.54
1:A:386:TRP:CG	1:A:387:PRO:HD2	2.43	0.53
1:B:117:GLN:HB2	1:B:214:ALA:HB1	1.91	0.53
1:B:563:ASP:HA	1:B:593:CYS:HB2	1.91	0.53
1:B:294:MET:HG2	1:B:303:LYS:HD2	1.90	0.53
1:A:46:VAL:HG12	1:A:72:VAL:HB	1.91	0.53
1:A:515:CYS:SG	1:A:526:VAL:HG22	2.49	0.53
1:B:134:ASN:OD1	1:B:177:GLY:HA2	2.09	0.53
1:B:419:LEU:HD13	1:B:421:ILE:HD11	1.91	0.53
1:B:102:ASP:HB2	1:B:106:THR:O	2.08	0.52
1:A:507:ARG:NH2	1:A:516:LYS:HG3	2.24	0.52
1:B:611:GLY:O	1:B:613:PRO:HD3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASP:CG	1:A:188:LYS:HB3	2.33	0.52
1:A:115:ASN:O	1:A:117:GLN:HG3	2.09	0.52
1:B:6:VAL:HG12	1:B:36:VAL:HB	1.89	0.52
1:B:378:THR:O	1:B:403:ARG:HB2	2.10	0.52
1:A:16:GLN:HB2	1:A:45:TYR:CE1	2.45	0.52
1:A:507:ARG:HD3	1:A:531:CYS:HB2	1.91	0.52
1:A:303:LYS:O	1:A:304:LYS:HD3	2.10	0.52
1:B:296:GLU:C	1:B:298:GLY:H	2.18	0.51
1:A:335:PHE:HA	1:A:338:CYS:SG	2.51	0.51
1:B:485:LEU:HD13	1:B:512:VAL:HA	1.92	0.51
1:A:235:THR:OG1	1:A:237:LYS:HE3	2.11	0.51
1:B:92:SER:OG	3:B:1151:NAG:H4	2.10	0.51
1:A:288:GLY:C	1:A:290:ASP:H	2.18	0.51
1:B:459:THR:HG22	1:B:460:SER:H	1.76	0.51
1:A:36:VAL:HG22	1:A:60:GLU:HG3	1.92	0.51
1:A:505:VAL:HG12	1:A:529:SER:HA	1.92	0.51
1:A:262:SER:H	1:A:282:SER:HA	1.76	0.51
1:A:282:SER:OG	1:B:253:MET:HE1	2.10	0.51
1:B:407:LYS:HD3	1:B:435:GLY:HA2	1.92	0.51
1:B:521:GLU:CB	1:B:522:PRO:HD3	2.36	0.50
1:B:545:ILE:HG13	1:B:556:ILE:HD11	1.94	0.50
1:B:262:SER:HB2	1:B:282:SER:HB3	1.93	0.50
1:A:186:LEU:HD12	1:A:186:LEU:H	1.77	0.50
2:D:22:TYR:HB2	2:D:29:TYR:CE2	2.47	0.50
2:D:48:LYS:O	2:D:49:TRP:CD2	2.65	0.50
1:B:421:ILE:HG22	1:B:423:SER:H	1.76	0.50
1:A:33:ASN:OD1	3:A:1032:NAG:H61	2.12	0.50
1:B:56:LYS:HG2	1:B:76:PRO:HB2	1.94	0.49
1:B:515:CYS:SG	1:B:526:VAL:HG22	2.52	0.49
1:A:505:VAL:HG23	1:A:512:VAL:HG23	1.94	0.49
1:A:245:LEU:HG	1:A:256:ASN:HB2	1.94	0.49
1:A:327:ILE:HD11	1:A:332:ILE:HG13	1.95	0.49
1:A:408:GLN:C	1:A:410:GLY:N	2.69	0.49
1:B:296:GLU:CD	1:B:297:ASP:H	2.21	0.49
1:A:88:TYR:OH	1:A:121:HIS:HB3	2.13	0.49
1:A:315:GLY:O	1:A:318:ILE:HG22	2.12	0.49
1:B:119:ILE:HG13	1:B:143:ILE:HG22	1.94	0.49
1:A:186:LEU:HB2	1:A:190:ILE:HD11	1.95	0.49
2:D:45:ARG:NH1	2:D:45:ARG:CG	2.75	0.49
1:B:388:GLU:CD	1:B:388:GLU:H	2.21	0.48
1:B:417:VAL:HA	1:B:440:SER:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:HIS:HB2	1:A:608:GLY:HA2	1.94	0.48
1:B:507:ARG:HD3	1:B:531:CYS:HB2	1.95	0.48
1:A:409:HIS:CE1	2:C:38:ILE:HD11	2.48	0.48
1:A:114:ARG:HD3	1:A:182:ASN:OD1	2.13	0.48
1:A:49:ASN:O	1:A:50:TYR:O	2.31	0.48
1:A:459:THR:O	1:A:462:GLN:HG3	2.14	0.48
1:B:142:ASP:CG	1:B:188:LYS:HB3	2.38	0.48
1:A:119:ILE:HG13	1:A:143:ILE:HG22	1.95	0.48
1:B:101:TYR:HE2	1:B:128:ASN:HB3	1.79	0.47
1:B:399:LEU:HD22	1:B:429:LEU:HD13	1.95	0.47
1:B:525:PHE:CE2	1:B:532:ILE:HB	2.49	0.47
1:B:262:SER:H	1:B:282:SER:HA	1.79	0.47
1:B:419:LEU:HB3	1:B:421:ILE:HG13	1.96	0.47
1:B:10:THR:O	1:B:40:ASN:HB2	2.14	0.47
1:A:303:LYS:NZ	1:A:303:LYS:HB3	2.30	0.47
1:B:295:GLU:HG2	1:B:296:GLU:N	2.28	0.47
1:B:383:ILE:HG22	1:B:419:LEU:HD11	1.96	0.47
1:A:125:ARG:HD2	1:A:153:SER:O	2.13	0.47
1:B:114:ARG:HA	1:B:176:TRP:CD1	2.49	0.47
1:B:459:THR:HG22	1:B:460:SER:N	2.29	0.47
1:A:295:GLU:CG	1:A:300:ARG:HH11	2.28	0.47
1:B:15:THR:HG23	2:D:31:CYS:O	2.14	0.47
1:B:47:GLN:HA	1:B:71:THR:OG1	2.15	0.47
1:A:276:VAL:HG11	1:A:302:CYS:SG	2.55	0.47
1:B:269:LYS:HD3	1:B:269:LYS:N	2.29	0.47
1:A:32:ASN:O	1:A:33:ASN:HB2	2.13	0.47
1:A:397:GLU:HG3	1:A:427:ARG:NH1	2.30	0.47
1:B:82:ILE:HD11	1:B:120:LEU:HG	1.97	0.47
1:B:89:TYR:CE2	1:B:90:GLU:HG2	2.51	0.46
1:B:98:LEU:O	1:B:99:SER:C	2.58	0.46
1:B:132:LEU:HD11	1:B:135:VAL:HG21	1.98	0.46
1:A:386:TRP:CD2	1:A:387:PRO:HD2	2.50	0.46
1:A:470:ARG:HG2	1:A:475:CYS:SG	2.55	0.46
1:B:330:THR:O	1:B:333:LYS:HG3	2.16	0.46
1:A:190:ILE:HG22	1:A:190:ILE:O	2.15	0.46
1:B:473:ASN:O	1:B:476:LYS:HG2	2.15	0.46
1:A:69:LEU:HD11	2:C:23:ILE:HD13	1.97	0.46
4:D:1:2PE:H142	4:D:1:2PE:H172	1.62	0.46
1:B:110:GLU:HG2	1:B:112:PRO:HG3	1.97	0.46
1:B:246:TYR:O	1:B:248:PRO:HD3	2.15	0.46
1:B:403:ARG:O	1:B:433:SER:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ILE:HA	1:B:76:PRO:HD3	1.77	0.46
1:B:288:GLY:C	1:B:290:ASP:H	2.22	0.46
1:A:397:GLU:HG3	1:A:427:ARG:HH11	1.80	0.46
1:A:350:VAL:HG22	1:A:355:ASP:HB2	1.98	0.46
1:B:393:LEU:HG	1:B:421:ILE:HD13	1.98	0.45
1:A:390:ARG:HG3	1:A:394:HIS:CE1	2.50	0.45
1:B:487:SER:HB3	1:B:501:SER:OG	2.17	0.45
1:B:532:ILE:HD12	1:B:532:ILE:N	2.32	0.45
1:B:27:LEU:HD21	1:B:43:ILE:HG23	1.97	0.45
1:B:296:GLU:C	1:B:298:GLY:N	2.70	0.45
1:B:447:TYR:CZ	1:B:494:PRO:HG3	2.51	0.45
1:A:102:ASP:HB2	1:A:106:THR:O	2.16	0.45
1:B:352:PHE:CZ	1:B:387:PRO:HD3	2.51	0.45
1:A:380:PHE:CD1	1:A:380:PHE:C	2.94	0.45
1:A:442:ASN:O	1:A:443:LYS:C	2.59	0.45
1:B:416:VAL:HB	1:B:439:ILE:HG23	1.98	0.45
1:B:442:ASN:O	1:B:469:ASN:HA	2.17	0.45
1:A:532:ILE:N	1:A:532:ILE:HD12	2.32	0.44
1:B:327:ILE:HG23	1:B:327:ILE:O	2.17	0.44
1:B:186:LEU:HD23	1:B:189:ILE:HD11	2.00	0.44
1:A:248:PRO:HG3	1:B:230:PHE:CZ	2.52	0.44
1:B:324:SER:HB3	3:B:1328:NAG:H4	1.99	0.44
1:A:36:VAL:HG22	1:A:60:GLU:CG	2.47	0.44
1:B:295:GLU:HB2	1:B:300:ARG:HH11	1.82	0.44
1:A:246:TYR:O	1:A:248:PRO:HD3	2.18	0.44
1:A:257:PRO:C	1:A:259:GLY:H	2.25	0.44
1:A:288:GLY:C	1:A:290:ASP:N	2.75	0.44
1:A:330:THR:O	1:A:333:LYS:HG3	2.17	0.44
1:A:295:GLU:HG3	1:A:300:ARG:NH1	2.33	0.44
1:B:115:ASN:O	1:B:117:GLN:HG3	2.18	0.43
1:A:478:THR:HG22	1:A:478:THR:O	2.18	0.43
1:A:611:GLY:O	1:A:613:PRO:HD3	2.18	0.43
1:A:262:SER:HB2	1:A:282:SER:CB	2.48	0.43
1:B:29:ARG:HB3	2:D:49:TRP:CZ2	2.53	0.43
1:A:446:CYS:C	1:A:448:ALA:H	2.26	0.43
1:A:485:LEU:HD13	1:A:512:VAL:HA	2.00	0.43
2:C:46:ASP:CG	2:C:49:TRP:HD1	2.27	0.43
1:A:186:LEU:HB2	1:A:190:ILE:CD1	2.48	0.43
1:B:516:LYS:CD	1:B:522:PRO:HD2	2.48	0.43
1:A:140:TRP:NE1	1:A:154:MET:HE1	2.33	0.43
1:B:609:LEU:C	1:B:611:GLY:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ILE:HG22	1:A:100:ASN:HD21	1.84	0.43
1:B:200:ARG:HH12	1:B:219:PRO:HD3	1.84	0.43
1:A:75:ILE:HA	1:A:76:PRO:HD3	1.81	0.42
1:A:253:MET:HE2	1:A:253:MET:HB2	1.88	0.42
1:A:12:ASN:HB3	1:A:15:THR:HB	2.01	0.42
1:B:585:LYS:HG2	1:B:595:LEU:HA	2.01	0.42
1:A:296:GLU:O	1:A:297:ASP:HB2	2.20	0.42
1:B:360:THR:HA	1:B:361:PRO:HD3	1.84	0.42
1:B:386:TRP:CG	1:B:387:PRO:HD2	2.55	0.42
1:B:424:LEU:HD13	1:B:492:TRP:HZ3	1.84	0.42
1:A:72:VAL:HG22	1:A:73:GLU:N	2.34	0.42
1:A:101:TYR:HB3	1:A:130:PRO:HD2	2.01	0.42
1:A:262:SER:HB2	1:A:282:SER:HB3	2.01	0.42
1:A:360:THR:HA	1:A:361:PRO:HD3	1.89	0.42
1:B:117:GLN:O	1:B:143:ILE:HA	2.19	0.42
1:B:344:ASP:OD1	1:B:379:GLY:HA3	2.19	0.42
3:B:1151:NAG:O7	3:B:1151:NAG:H3	2.19	0.42
1:A:295:GLU:HG3	1:A:300:ARG:HH11	1.83	0.42
1:A:487:SER:OG	1:A:488:PRO:HD2	2.20	0.42
1:A:561:TYR:HA	1:A:591:HIS:HB3	2.01	0.42
1:B:492:TRP:N	1:B:498:ASP:O	2.52	0.42
1:A:35:GLU:HA	1:A:57:THR:O	2.20	0.41
1:A:287:CYS:SG	1:A:293:GLU:HG2	2.60	0.41
1:B:194:GLN:NE2	1:B:204:PRO:HB3	2.31	0.41
1:A:126:PHE:HB2	1:A:154:MET:HB2	2.01	0.41
1:A:525:PHE:CE2	1:A:532:ILE:HB	2.55	0.41
1:B:188:LYS:HB2	1:B:198:ARG:NH1	2.35	0.41
1:A:126:PHE:H	1:A:154:MET:HB3	1.84	0.41
1:A:253:MET:HE1	1:B:282:SER:OG	2.20	0.41
1:A:161:GLY:C	1:A:163:CYS:H	2.29	0.41
1:A:134:ASN:OD1	1:A:177:GLY:HA2	2.21	0.41
1:A:269:LYS:HD3	1:A:269:LYS:N	2.35	0.41
1:A:507:ARG:NH1	1:A:516:LYS:HE3	2.35	0.41
1:A:521:GLU:CB	1:A:522:PRO:HD3	2.35	0.41
1:B:28:GLN:O	1:B:32:ASN:HB2	2.20	0.41
1:B:101:TYR:HB3	1:B:130:PRO:HD2	2.02	0.41
1:B:111:LEU:HG	1:B:113:MET:HG3	2.03	0.41
1:B:467:ILE:HD11	2:D:51:GLU:H	1.86	0.41
1:A:177:GLY:HA3	1:A:182:ASN:HD22	1.86	0.41
1:A:582:LEU:N	1:A:582:LEU:HD12	2.36	0.41
1:B:82:ILE:HG21	1:B:226:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLY:N	1:B:223:ASP:HB3	2.36	0.41
1:B:89:TYR:CD2	1:B:90:GLU:HG2	2.56	0.41
1:A:495:GLU:HA	1:A:496:PRO:HD3	1.94	0.40
1:B:138:ILE:HG22	1:B:140:TRP:CD1	2.56	0.40
2:D:19:VAL:CG2	2:D:32:ASN:HB3	2.51	0.40
1:A:83:ILE:O	1:A:119:ILE:HA	2.22	0.40
1:A:144:VAL:HG12	1:A:145:SER:N	2.36	0.40
1:A:68:ALA:HA	1:A:98:LEU:O	2.22	0.40
1:B:262:SER:HB2	1:B:282:SER:CB	2.51	0.40
1:B:350:VAL:HG22	1:B:355:ASP:HB2	2.03	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	613/614 (100%)	531 (87%)	78 (13%)	4 (1%)	18	49
1	B	613/614 (100%)	531 (87%)	77 (13%)	5 (1%)	16	45
2	C	45/47 (96%)	40 (89%)	4 (9%)	1 (2%)	5	26
2	D	45/47 (96%)	40 (89%)	4 (9%)	1 (2%)	5	26
All	All	1316/1322 (100%)	1142 (87%)	163 (12%)	11 (1%)	16	45

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	TYR
1	A	336	LYS
1	B	99	SER
1	B	295	GLU
2	D	46	ASP

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Mol	Chain	Res	Type
1	A	443	LYS
1	B	336	LYS
1	B	296	GLU
2	C	50	TRP
1	A	540	PRO
1	B	494	PRO

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	537/536 (100%)	535 (100%)	2 (0%)	84	84
1	B	537/536 (100%)	532 (99%)	5 (1%)	70	78
2	C	41/41 (100%)	41 (100%)	0	100	100
2	D	41/41 (100%)	39 (95%)	2 (5%)	22	51
All	All	1156/1154 (100%)	1147 (99%)	9 (1%)	73	79

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	463	LYS
1	B	78	GLU
1	B	252	GLN
1	B	290	ASP
1	B	348	LEU
1	B	562	ILE
2	D	42	CYS
2	D	50	TRP

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

Mol	Chain	Res	Type
1	A	157	GLN

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Mol	Chain	Res	Type
1	A	409	HIS
1	B	33	ASN
1	B	49	ASN
1	B	121	HIS
1	B	210	ASN
1	B	359	HIS
1	B	408	GLN
1	B	444	ASN
1	B	594	HIS
2	D	32	ASN

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](#)

17 ligands are modelled in this entry.

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	NAG	A	1151	1	14,14,15	0.47	0	17,19,21	0.87	1 (5%)
4	2PE	D	1	-	27,27,27	0.50	0	26,26,26	0.30	0
3	NAG	A	1032	1	14,14,15	0.48	0	17,19,21	1.06	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1337	1	14,14,15	0.51	0	17,19,21	0.68	0
3	NAG	B	1151	1	14,14,15	0.46	0	17,19,21	0.74	1 (5%)
3	NAG	B	1504	1	14,14,15	0.51	0	17,19,21	0.68	0
4	2PE	D	52	-	27,27,27	0.53	0	26,26,26	0.33	0
3	NAG	A	1328	1	14,14,15	0.48	0	17,19,21	0.77	0
3	NAG	B	1032	1	14,14,15	0.48	0	17,19,21	0.89	1 (5%)
4	2PE	B	617	-	27,27,27	0.54	0	26,26,26	0.29	0
4	2PE	B	616	-	27,27,27	0.53	0	26,26,26	0.32	0
3	NAG	A	1420	1	14,14,15	0.51	0	17,19,21	0.70	0
3	NAG	B	1328	1	14,14,15	0.48	0	17,19,21	0.84	0
3	NAG	A	1049	1	14,14,15	0.56	0	17,19,21	0.65	0
4	2PE	B	615	-	27,27,27	0.54	0	26,26,26	0.38	0
3	NAG	A	1504	1	14,14,15	0.50	0	17,19,21	0.75	0
3	NAG	A	1172	1	14,14,15	0.50	0	17,19,21	0.76	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1151	1	-	0/6/23/26	0/1/1/1
4	2PE	D	1	-	-	11/25/25/25	-
3	NAG	A	1032	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1337	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	1151	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1504	1	1/1/5/7	3/6/23/26	0/1/1/1
4	2PE	D	52	-	-	10/25/25/25	-
3	NAG	A	1328	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1032	1	-	2/6/23/26	0/1/1/1
4	2PE	B	617	-	-	13/25/25/25	-
4	2PE	B	616	-	-	9/25/25/25	-
3	NAG	A	1420	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1328	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1049	1	-	2/6/23/26	0/1/1/1
4	2PE	B	615	-	-	16/25/25/25	-
3	NAG	A	1504	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1172	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1032	NAG	C1-O5-C5	3.69	117.13	112.19
3	B	1032	NAG	C1-O5-C5	2.72	115.83	112.19
3	A	1151	NAG	C1-O5-C5	2.36	115.35	112.19
3	A	1172	NAG	C1-O5-C5	2.23	115.18	112.19
3	B	1151	NAG	C1-O5-C5	2.13	115.05	112.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1172	NAG	C1
3	A	1337	NAG	C1
3	B	1504	NAG	C1

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	2PE	C14-C15-O16-C17
4	B	617	2PE	C23-C24-O25-C26
4	B	615	2PE	O7-C8-C9-O10
4	D	52	2PE	O7-C8-C9-O10
4	D	52	2PE	O19-C20-C21-O22
4	D	1	2PE	O13-C14-C15-O16
3	B	1328	NAG	O5-C5-C6-O6
4	B	615	2PE	O10-C11-C12-O13
4	B	617	2PE	O7-C8-C9-O10
4	D	1	2PE	O4-C5-C6-O7
3	B	1032	NAG	C8-C7-N2-C2
3	B	1032	NAG	O7-C7-N2-C2
3	B	1504	NAG	C8-C7-N2-C2
3	B	1504	NAG	O7-C7-N2-C2
3	A	1049	NAG	O5-C5-C6-O6
4	B	615	2PE	O19-C20-C21-O22
4	B	615	2PE	O4-C5-C6-O7
4	B	615	2PE	O13-C14-C15-O16
4	B	616	2PE	C27-C26-O25-C24
4	D	52	2PE	O10-C11-C12-O13
3	A	1420	NAG	O5-C5-C6-O6
4	B	616	2PE	O25-C26-C27-O28
4	B	617	2PE	O25-C26-C27-O28
3	B	1328	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	616	2PE	O16-C17-C18-O19
4	B	616	2PE	O13-C14-C15-O16
4	B	615	2PE	O25-C26-C27-O28
4	D	1	2PE	O25-C26-C27-O28
3	B	1504	NAG	O5-C5-C6-O6
4	B	617	2PE	O19-C20-C21-O22
3	A	1032	NAG	O5-C5-C6-O6
3	B	1151	NAG	O5-C5-C6-O6
3	B	1151	NAG	C3-C2-N2-C7
3	A	1032	NAG	C1-C2-N2-C7
4	D	1	2PE	C5-C6-O7-C8
4	B	615	2PE	C18-C17-O16-C15
4	B	615	2PE	C20-C21-O22-C23
4	B	615	2PE	C15-C14-O13-C12
4	B	617	2PE	C21-C20-O19-C18
4	D	1	2PE	C21-C20-O19-C18
3	A	1049	NAG	C4-C5-C6-O6
4	D	1	2PE	C2-C3-O4-C5
4	B	615	2PE	C2-C3-O4-C5
4	D	52	2PE	C24-C23-O22-C21
4	D	52	2PE	O16-C17-C18-O19
4	B	616	2PE	C18-C17-O16-C15
4	D	52	2PE	O25-C26-C27-O28
4	B	617	2PE	O10-C11-C12-O13
4	B	615	2PE	C21-C20-O19-C18
4	B	616	2PE	C23-C24-O25-C26
4	D	1	2PE	C18-C17-O16-C15
4	D	1	2PE	C20-C21-O22-C23
4	B	616	2PE	C20-C21-O22-C23
4	D	52	2PE	C27-C26-O25-C24
4	D	52	2PE	C8-C9-O10-C11
4	B	617	2PE	O13-C14-C15-O16
4	B	615	2PE	C23-C24-O25-C26
4	B	617	2PE	C15-C14-O13-C12
4	B	615	2PE	C5-C6-O7-C8
4	B	617	2PE	O16-C17-C18-O19
4	D	52	2PE	C12-C11-O10-C9
3	A	1032	NAG	C3-C2-N2-C7
4	B	617	2PE	O4-C5-C6-O7
4	B	616	2PE	C5-C6-O7-C8
4	D	1	2PE	C15-C14-O13-C12
4	D	1	2PE	O16-C17-C18-O19

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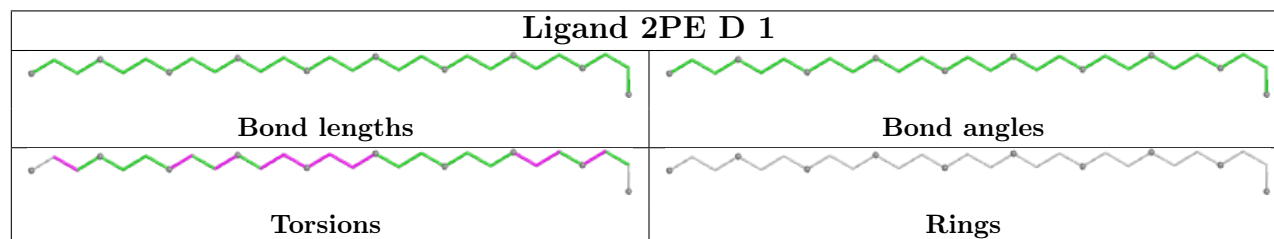
Mol	Chain	Res	Type	Atoms
4	B	615	2PE	C8-C9-O10-C11
4	B	615	2PE	O1-C2-C3-O4
4	B	617	2PE	C20-C21-O22-C23
4	B	617	2PE	O1-C2-C3-O4
4	B	615	2PE	C9-C8-O7-C6
4	D	52	2PE	O13-C14-C15-O16
4	B	617	2PE	O22-C23-C24-O25
4	B	616	2PE	O10-C11-C12-O13

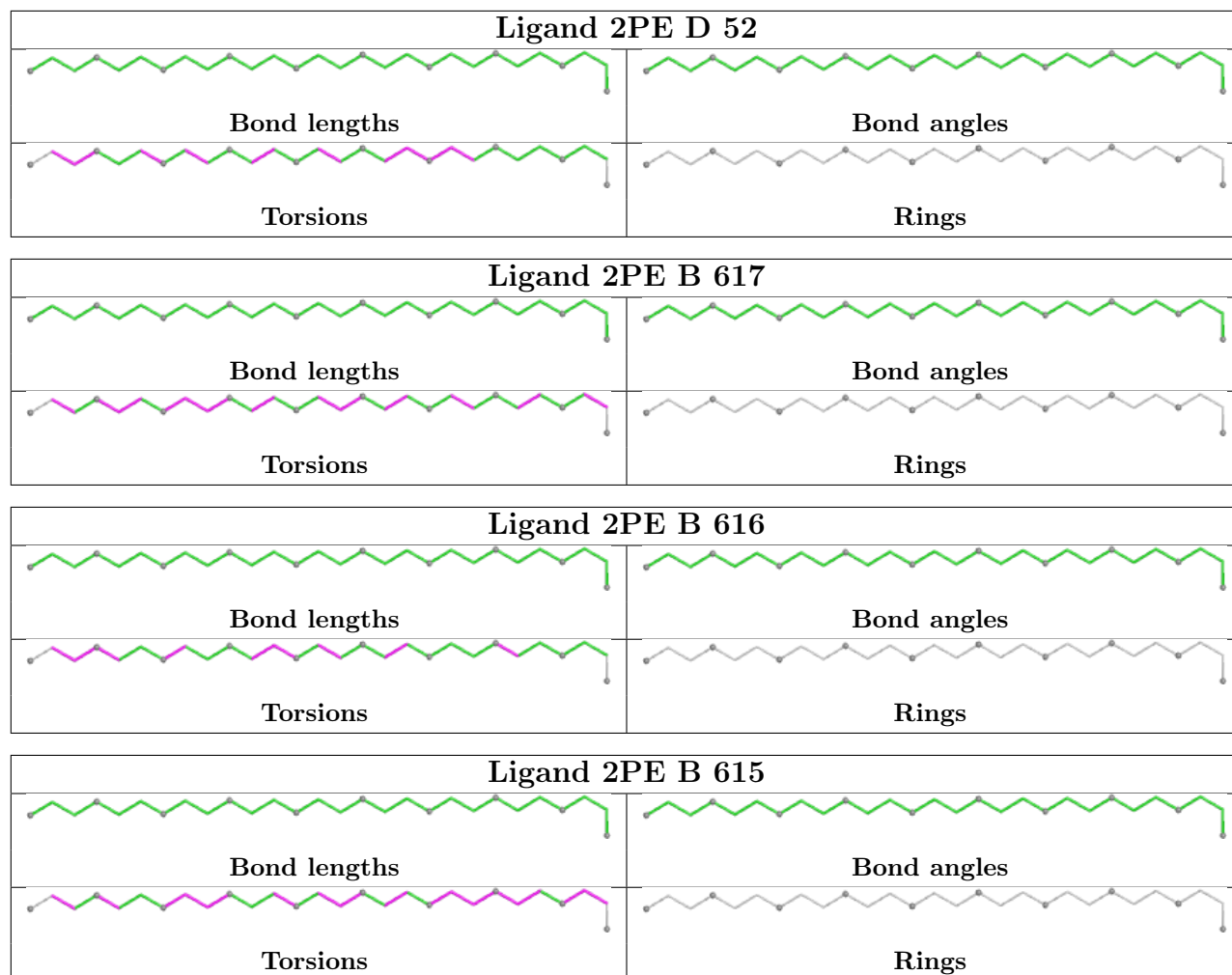
There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	2PE	1	0
3	A	1032	NAG	1	0
3	B	1151	NAG	2	0
4	B	617	2PE	1	0
4	B	616	2PE	1	0
3	A	1420	NAG	1	0
3	B	1328	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	614/614 (100%)	0.35	37 (6%)	27	19	57, 110, 241, 303	1 (0%)
1	B	614/614 (100%)	0.31	33 (5%)	31	21	65, 117, 222, 268	1 (0%)
2	C	47/47 (100%)	0.20	2 (4%)	40	25	81, 98, 131, 163	0
2	D	47/47 (100%)	0.24	2 (4%)	40	25	81, 111, 154, 184	0
All	All	1322/1322 (100%)	0.32	74 (5%)	30	20	57, 113, 228, 303	2 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	587	ALA	5.1
1	A	517	LEU	4.7
1	A	605	THR	4.6
2	D	50	TRP	4.3
1	B	574	GLY	4.2
1	B	565	PRO	4.0
1	A	570	THR	3.9
1	B	294	MET	3.8
1	B	566	HIS	3.7
1	A	74[B]	ARG	3.4
1	B	572	PRO	3.4
1	A	582	LEU	3.3
1	B	578	GLU	3.3
1	A	588	ASP	3.3
1	A	1	LEU	3.3
1	B	1	LEU	3.0
1	A	303	LYS	3.0
1	A	545	ILE	3.0
1	A	595	LEU	3.0
1	B	582	LEU	3.0
1	B	449	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	601	THR	2.9
1	B	530	GLU	2.9
1	B	569	LYS	2.9
2	C	51	GLU	2.9
1	A	589	ALA	2.9
1	B	507	ARG	2.9
1	A	546	THR	2.8
2	C	37	TYR	2.8
1	B	280	HIS	2.8
1	A	569	LYS	2.7
1	A	254	ASP	2.7
1	B	592	VAL	2.7
1	B	194	GLN	2.6
1	A	331	ASN	2.5
1	A	572	PRO	2.5
1	A	548	THR	2.5
1	B	598	PRO	2.5
1	A	280	HIS	2.4
1	A	526	VAL	2.4
1	B	184	GLN	2.4
1	B	470	ARG	2.4
2	D	49	TRP	2.4
1	B	531	CYS	2.4
1	A	88	TYR	2.4
1	A	591	HIS	2.3
1	B	301	LYS	2.3
1	A	214	ALA	2.3
1	A	205	SER	2.3
1	B	296	GLU	2.3
1	B	545	ILE	2.3
1	B	386	TRP	2.3
1	B	590	GLY	2.3
1	B	559	ALA	2.3
1	A	515	CYS	2.3
1	B	447	TYR	2.2
1	A	71	THR	2.2
1	A	110	GLU	2.2
1	A	225	LEU	2.2
1	B	526	VAL	2.2
1	B	539	LEU	2.2
1	A	573	ALA	2.2
1	B	589	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	573	ALA	2.1
1	B	202	LYS	2.1
1	A	576	MET	2.1
1	A	575	VAL	2.1
1	B	515	CYS	2.1
1	A	308	PRO	2.1
1	A	531	CYS	2.1
1	A	295	GLU	2.1
1	A	258	GLU	2.1
1	A	574	GLY	2.0
1	A	592	VAL	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($\text{\AA}^2$)	Q<0.9
3	NAG	A	1172	14/15	0.24	0.17	123,135,143,144	0
3	NAG	A	1504	14/15	0.47	0.16	152,159,166,168	0
3	NAG	A	1049	14/15	0.54	0.15	130,153,165,166	0
3	NAG	B	1504	14/15	0.54	0.09	170,178,191,191	0
3	NAG	A	1337	14/15	0.55	0.16	147,155,158,158	0
4	2PE	D	52	28/28	0.61	0.22	110,124,137,143	0
4	2PE	D	1	28/28	0.63	0.15	116,139,157,157	0
3	NAG	A	1151	14/15	0.70	0.15	101,109,116,119	0
3	NAG	A	1420	14/15	0.71	0.11	144,148,176,178	0
4	2PE	B	615	28/28	0.71	0.16	88,105,147,157	0
3	NAG	B	1032	14/15	0.73	0.16	115,127,138,147	0
4	2PE	B	617	28/28	0.73	0.16	79,97,115,119	0

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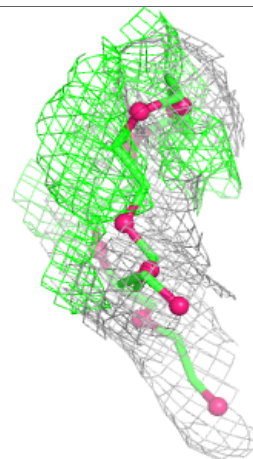
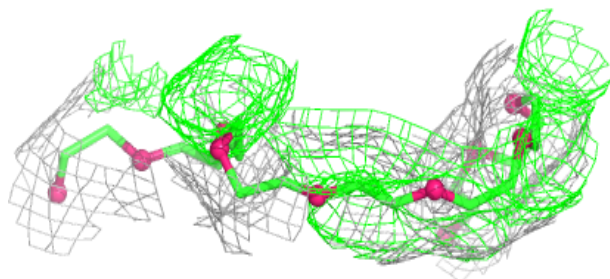
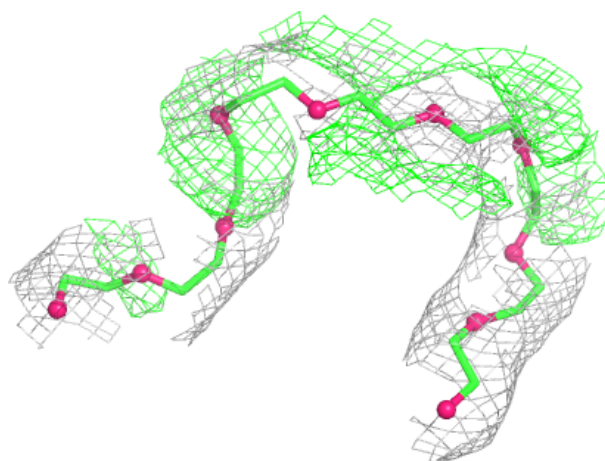
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	B	1151	14/15	0.77	0.10	142,149,164,165	0
3	NAG	A	1032	14/15	0.77	0.11	108,120,129,132	0
4	2PE	B	616	28/28	0.82	0.12	84,105,115,118	0
3	NAG	B	1328	14/15	0.94	0.11	69,81,95,98	0
3	NAG	A	1328	14/15	0.97	0.08	70,79,88,91	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

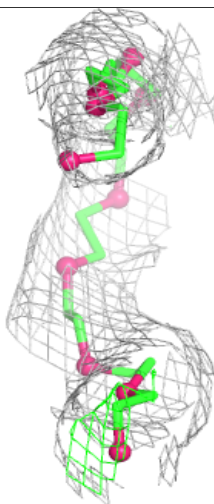
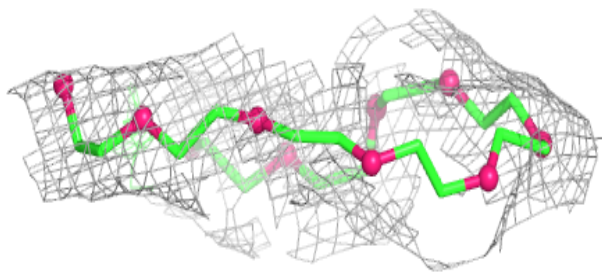
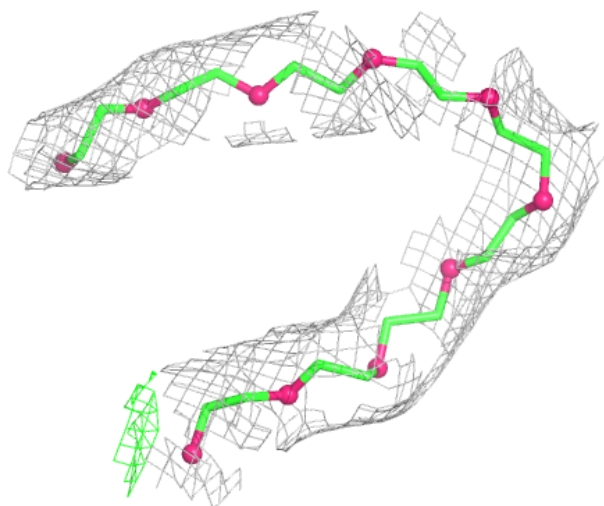
Electron density around 2PE D 52:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



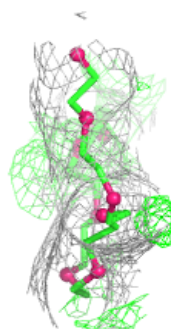
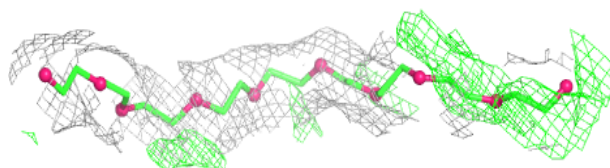
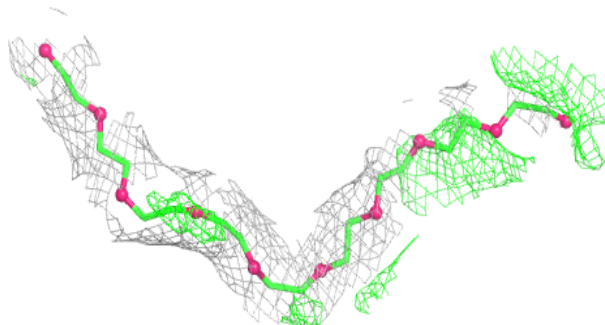
Electron density around 2PE D 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

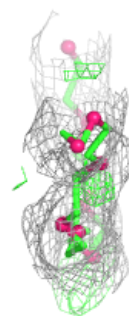
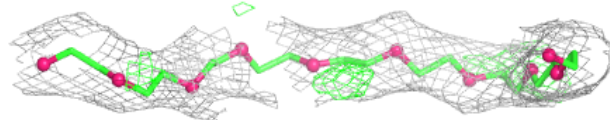
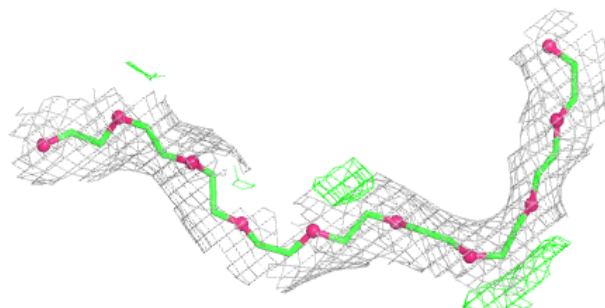


Electron density around 2PE B 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

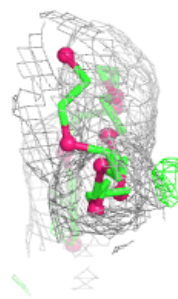
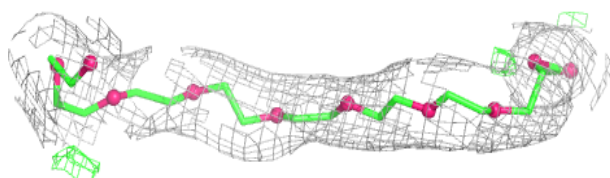
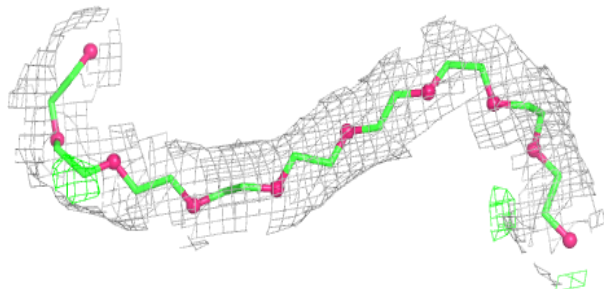
**Electron density around 2PE B 617:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 2PE B 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.