



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:57 PM BST

PDB ID : 3NJP
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 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 : 2.13.1
buster-report : 1.1.7 (2018)
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) : 2.13.1

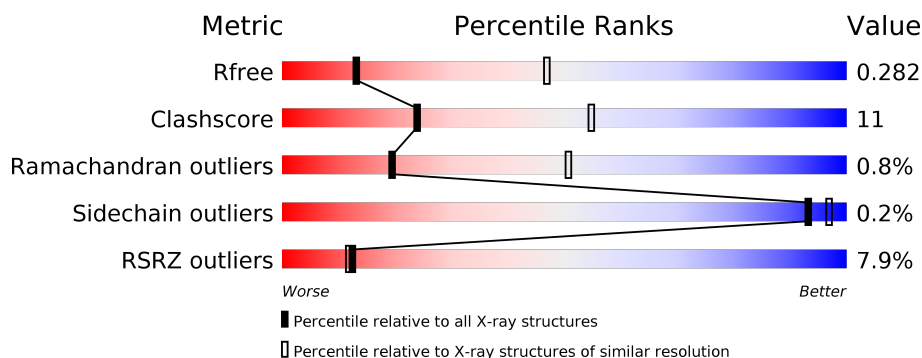
1 Overall quality at a glance

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	<div> <div>9%</div> <div> <div></div> <div>75%</div> <div>25%</div> </div> </div>
1	B	614	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>26%</div> </div> </div>
2	C	47	<div> <div></div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
2	D	47	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>23%</div> </div> </div>

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 crite-

ria:

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.

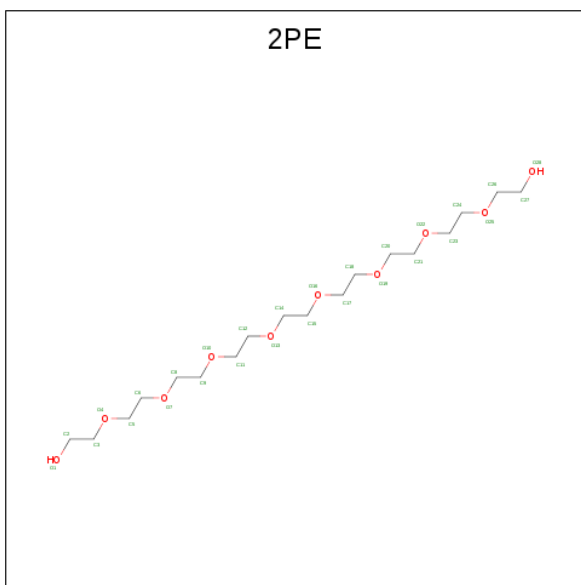
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	47	Total	C	N	O	S	0	0	0
			386	244	63	72	7			
2	D	47	Total	C	N	O	S	0	0	0
			386	244	63	72	7			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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 (three-letter code: 2PE) (formula: C₁₈H₃₈O₁₀).



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

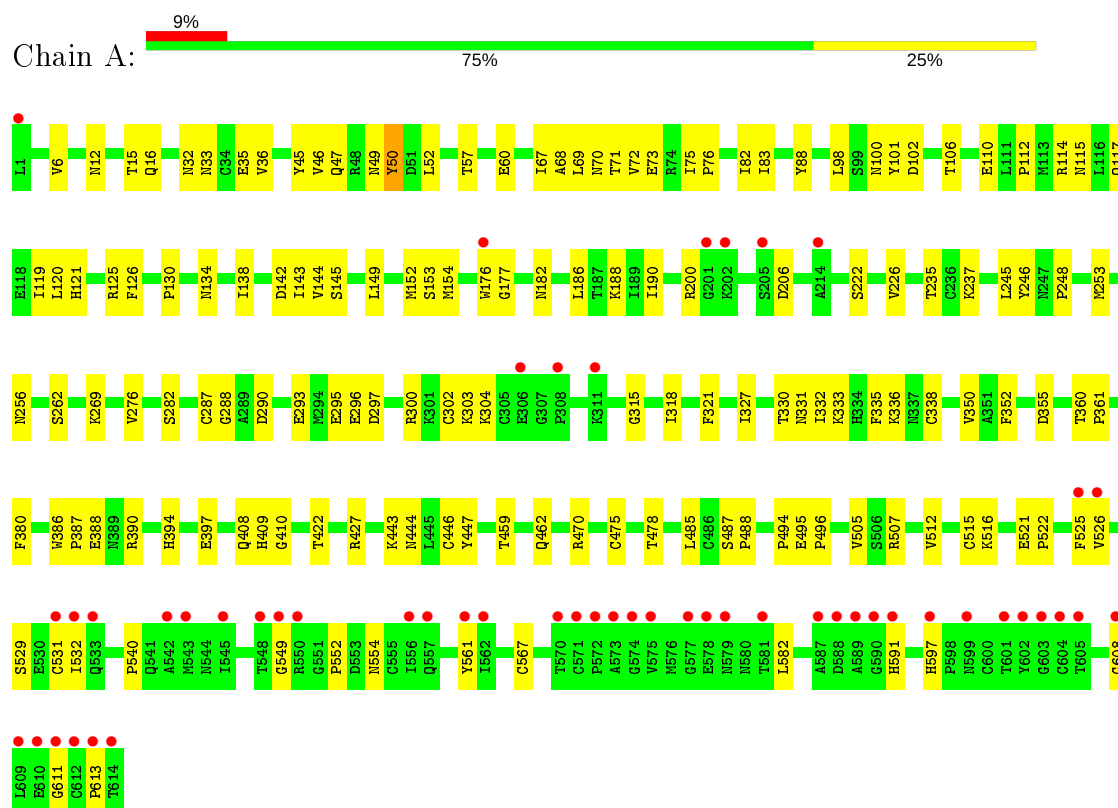
- Molecule 5 is water.

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

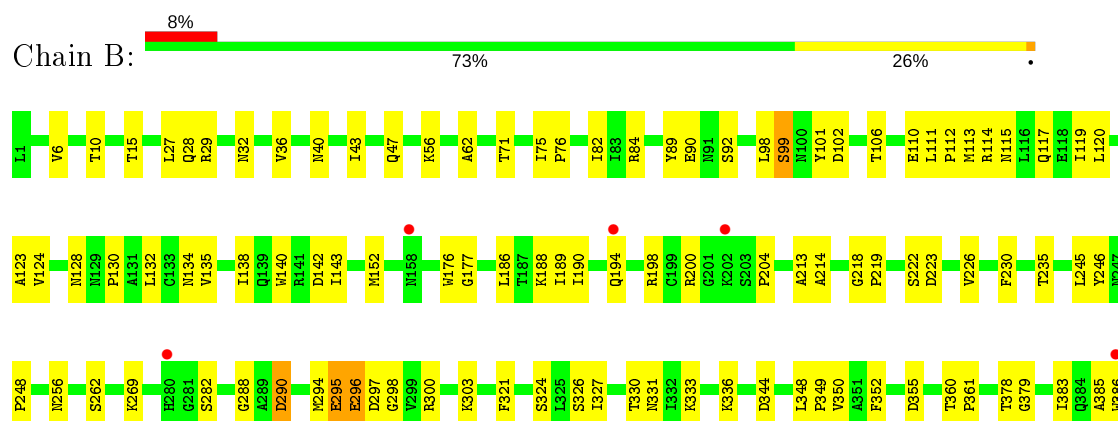
3 Residue-property plots [i](#)

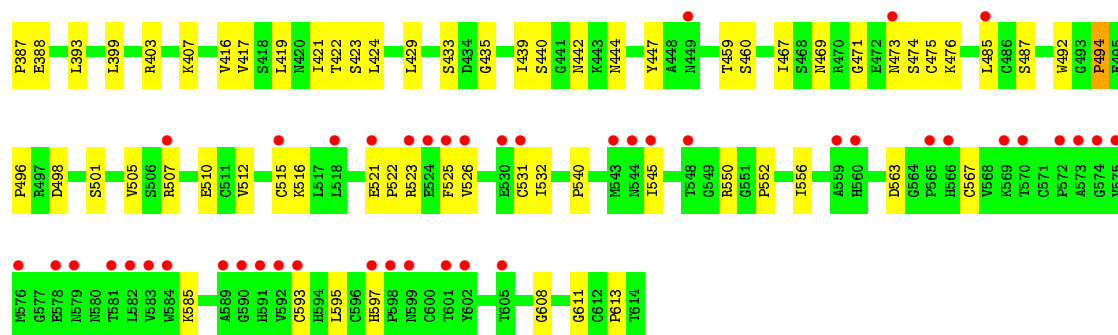
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Epidermal growth factor receptor





- Molecule 2: Epidermal growth factor

Chain C: 94% 6%



- Molecule 2: Epidermal growth factor

Chain D: 4% 77% 23%



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 0.251 , 0.282	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)	0.29 , 79.0	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	0.86	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	0.21	0/4828	0.38	0/6528
1	B	0.21	0/4825	0.38	0/6525
2	C	0.22	0/397	0.34	0/536
2	D	0.21	0/397	0.36	0/536
All	All	0.21	0/10447	0.38	0/14125

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	106	0
1	B	4730	0	4563	115	0
2	C	386	0	344	2	0
2	D	386	0	344	10	0
3	A	112	0	104	2	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	230	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 11.

All (230) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LEU:HG	1:B:256:ASN:HB2	1.85	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: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: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:84:ARG:HD3	1:B:120:LEU:HD12	1.86	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: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: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
1:A:115:ASN:O	1:A:117:GLN:HG3	2.09	0.52
1:B:447:TYR:HH	1:B:494:PRO:HG3	1.75	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:A:335:PHE:HA	1:A:338:CYS:SG	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:388:GLU:CD	1:A:388:GLU:H	2.13	0.51
1:B:92:SER:OG	3:B:1151:NAG:H4	2.10	0.51
1:A:408:GLN:C	1:A:410:GLY:H	2.14	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: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:H	1:A:186:LEU:HD12	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:515:CYS:SG	1:B:526:VAL:HG22	2.52	0.49
1:B:56:LYS:HG2	1:B:76:PRO:HB2	1.94	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: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:CG	2:D:45:ARG:NH1	2.75	0.49
1:B:417:VAL:HA	1:B:440:SER:O	2.13	0.48
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:142:ASP:CG	1:A:188:LYS:HB3	2.33	0.48
1:A:459:THR:O	1:A:462:GLN:HG3	2.14	0.48
1:A:49:ASN:O	1:A:50:TYR:O	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:295:GLU:CG	1:A:300:ARG:HH11	2.28	0.47
1:B:296:GLU:C	1:B:298:GLY:H	2.18	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:132:LEU:HD11	1:B:135:VAL:HG21	1.98	0.46
1:A:288:GLY:C	1:A:290:ASP:H	2.18	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:O	1:A:190:ILE:HG22	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
1:B:75:ILE:HA	1:B:76:PRO:HD3	1.77	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:A:408:GLN:C	1:A:410:GLY:N	2.69	0.45
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:N	1:B:532:ILE:HD12	2.32	0.45
1:B:27:LEU:HD21	1:B:43:ILE:HG23	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:PHE:CZ	1:B:387:PRO:HD3	2.51	0.45
1:B:296:GLU:C	1:B:298:GLY:N	2.70	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:HD12	1:A:532:ILE:N	2.32	0.44
1:B:296:GLU:CD	1:B:297:ASP:H	2.21	0.44
1:B:327:ILE:O	1:B:327:ILE:HG23	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:253:MET:HE2	1:A:253:MET:HB2	1.67	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:330:THR:O	1:A:333:LYS:HG3	2.17	0.44
1:B:388:GLU:H	1:B:388:GLU:CD	2.21	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:O	1:A:478:THR:HG22	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:142:ASP:CG	1:B:188:LYS:HB3	2.38	0.43
1:B:29:ARG:HB3	2:D:49:TRP:CZ2	2.53	0.43
1:A:485:LEU:HD13	1:A:512:VAL:HA	2.00	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: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: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: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:A:72:VAL:HG22	1:A:73:GLU:N	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1151:NAG:H3	3:B:1151:NAG:O7	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:B:98:LEU:O	1:B:99:SER:C	2.58	0.42
1:A:287:CYS:SG	1:A:293:GLU:HG2	2.60	0.41
1:A:35:GLU:HA	1:A:57:THR:O	2.20	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:B:288:GLY:C	1:B:290:ASP:H	2.22	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: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:28:GLN:O	1:B:32:ASN:HB2	2.20	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:B:82:ILE:HG21	1:B:226:VAL:HG11	2.02	0.41
1:A:582:LEU:HD12	1:A:582:LEU:N	2.36	0.41
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:144:VAL:HG12	1:A:145:SER:N	2.36	0.40
1:A:380:PHE:C	1:A:380:PHE:CD1	2.94	0.40
1:A:83:ILE:O	1:A:119:ILE:HA	2.22	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

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	613/614 (100%)	531 (87%)	78 (13%)	4 (1%)	22	54
1	B	613/614 (100%)	531 (87%)	77 (13%)	5 (1%)	19	51
2	C	45/47 (96%)	40 (89%)	4 (9%)	1 (2%)	6	30
2	D	45/47 (96%)	40 (89%)	4 (9%)	1 (2%)	6	30
All	All	1316/1322 (100%)	1142 (87%)	163 (12%)	11 (1%)	19	51

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
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%)	537 (100%)	0	100	100
1	B	537/536 (100%)	536 (100%)	1 (0%)	93	97
2	C	41/41 (100%)	41 (100%)	0	100	100
2	D	41/41 (100%)	40 (98%)	1 (2%)	49	73
All	All	1156/1154 (100%)	1154 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	290	ASP
2	D	50	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	409	HIS
1	B	33	ASN
1	B	194	GLN
1	B	280	HIS
1	B	408	GLN

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](#)

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	1049	1	14,14,15	0.57	0	17,19,21	0.74	1 (5%)
3	NAG	A	1328	1	14,14,15	0.49	0	17,19,21	0.80	0
4	2PE	B	615	-	27,27,27	0.54	0	26,26,26	0.38	0
3	NAG	A	1172	1	14,14,15	0.51	0	17,19,21	0.80	1 (5%)
4	2PE	B	616	-	27,27,27	0.53	0	26,26,26	0.32	0
3	NAG	A	1420	1	14,14,15	0.52	0	17,19,21	0.74	0
3	NAG	A	1337	1	14,14,15	0.52	0	17,19,21	0.72	0
3	NAG	B	1328	1	14,14,15	0.50	0	17,19,21	0.87	0
3	NAG	A	1151	1	14,14,15	0.48	0	17,19,21	0.92	1 (5%)
4	2PE	D	1	-	27,27,27	0.50	0	26,26,26	0.30	0
4	2PE	B	617	-	27,27,27	0.54	0	26,26,26	0.29	0
3	NAG	B	1151	1	14,14,15	0.46	0	17,19,21	0.78	1 (5%)
3	NAG	B	1032	1	14,14,15	0.48	0	17,19,21	0.93	1 (5%)
3	NAG	A	1504	1	14,14,15	0.51	0	17,19,21	0.79	0
3	NAG	B	1504	1	14,14,15	0.52	0	17,19,21	0.71	0
3	NAG	A	1032	1	14,14,15	0.49	0	17,19,21	1.06	1 (5%)
4	2PE	D	52	-	27,27,27	0.53	0	26,26,26	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1337	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	1049	1	-	2/6/23/26	0/1/1/1
4	2PE	B	615	-	-	18/25/25/25	-
3	NAG	A	1172	1	1/1/5/7	0/6/23/26	0/1/1/1
4	2PE	B	616	-	-	10/25/25/25	-
3	NAG	A	1420	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1151	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1328	1	-	2/6/23/26	0/1/1/1

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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	-	-	13/25/25/25	-
4	2PE	B	617	-	-	13/25/25/25	-
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
3	NAG	A	1504	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1504	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	A	1032	1	-	3/6/23/26	0/1/1/1
4	2PE	D	52	-	-	10/25/25/25	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1032	NAG	C1-O5-C5	3.64	117.13	112.19
3	B	1032	NAG	C1-O5-C5	2.68	115.83	112.19
3	A	1151	NAG	C1-O5-C5	2.33	115.35	112.19
3	A	1172	NAG	C1-O5-C5	2.20	115.18	112.19
3	A	1049	NAG	O5-C5-C6	2.13	110.54	107.20
3	B	1151	NAG	C1-O5-C5	2.11	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 (79) 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	O19-C20-C21-O22
4	D	1	2PE	O13-C14-C15-O16
4	D	52	2PE	O7-C8-C9-O10
4	B	615	2PE	O10-C11-C12-O13
3	B	1328	NAG	O5-C5-C6-O6
4	B	617	2PE	O7-C8-C9-O10

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

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Mol	Chain	Res	Type	Atoms
4	D	1	2PE	C20-C21-O22-C23
4	D	52	2PE	C8-C9-O10-C11
4	B	616	2PE	C20-C21-O22-C23
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	B	617	2PE	O4-C5-C6-O7
4	D	52	2PE	C12-C11-O10-C9
4	D	1	2PE	O16-C17-C18-O19
4	B	616	2PE	C5-C6-O7-C8
4	D	1	2PE	C15-C14-O13-C12
3	A	1032	NAG	C1-C2-N2-C7
4	B	615	2PE	C8-C9-O10-C11
3	A	1032	NAG	C3-C2-N2-C7
4	B	615	2PE	O1-C2-C3-O4
4	B	617	2PE	O1-C2-C3-O4
4	D	52	2PE	O13-C14-C15-O16
4	B	617	2PE	O22-C23-C24-O25
4	B	617	2PE	C20-C21-O22-C23
4	B	615	2PE	C9-C8-O7-C6
4	B	616	2PE	O10-C11-C12-O13
4	B	615	2PE	O22-C23-C24-O25
4	D	1	2PE	O10-C11-C12-O13
4	B	615	2PE	O16-C17-C18-O19
4	B	616	2PE	O19-C20-C21-O22
4	D	1	2PE	O7-C8-C9-O10

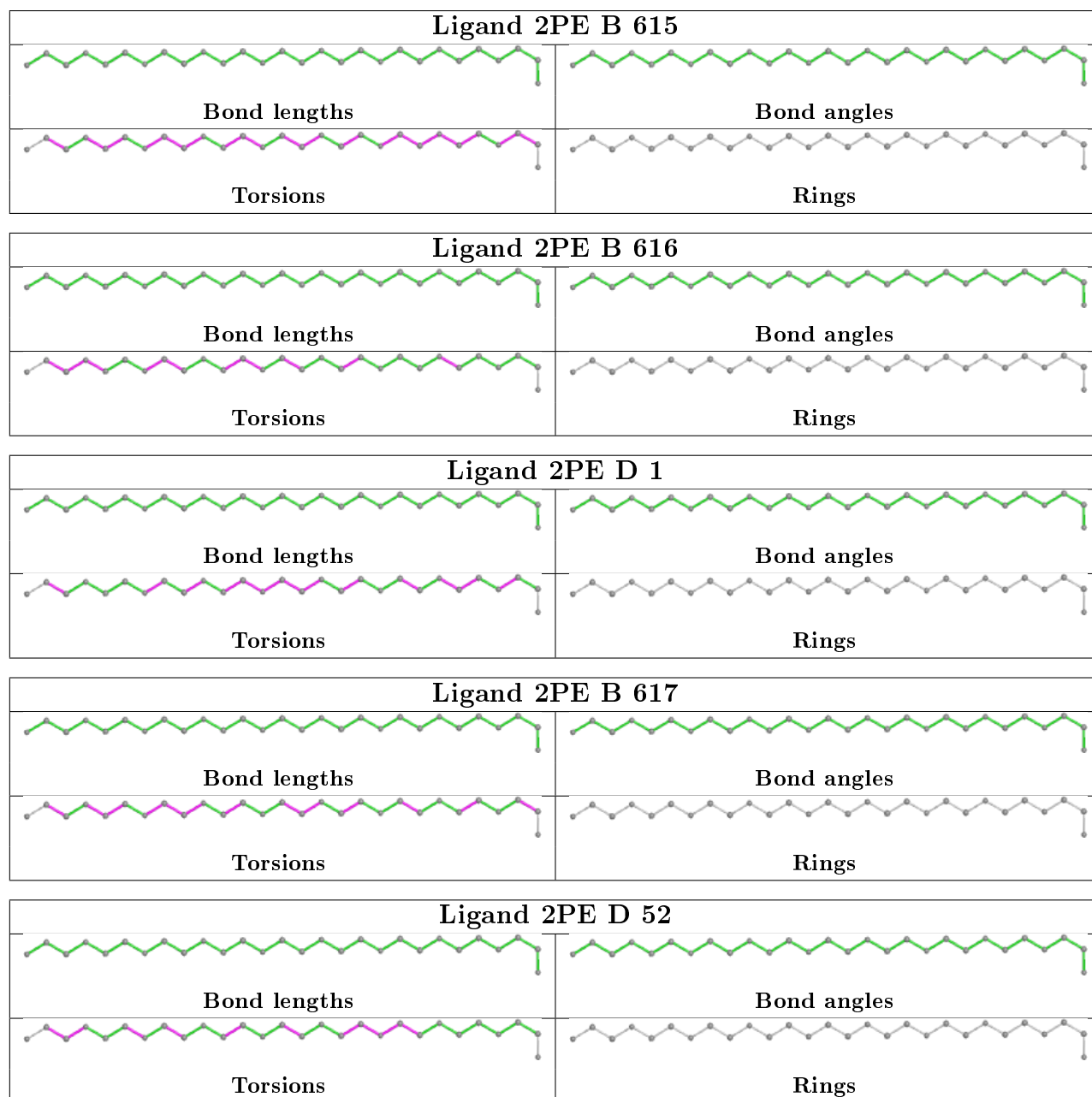
There are no ring outliers.

7 monomers are involved in 7 short contacts:

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.49	53 (8%)	10 10	70, 110, 241, 303	0
1	B	614/614 (100%)	0.34	50 (8%)	12 11	65, 117, 222, 268	0
2	C	47/47 (100%)	0.11	0	100 100	81, 98, 131, 163	0
2	D	47/47 (100%)	0.06	2 (4%)	35 34	81, 111, 154, 184	0
All	All	1322/1322 (100%)	0.39	105 (7%)	12 12	65, 113, 228, 303	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	573	ALA	10.9
1	A	605	THR	10.9
1	A	587	ALA	9.7
1	A	589	ALA	8.3
1	A	588	ASP	8.2
1	B	578	GLU	8.2
1	B	572	PRO	7.3
1	B	601	THR	7.3
1	B	574	GLY	7.2
1	A	602	TYR	6.7
1	A	570	THR	6.7
1	A	601	THR	6.6
1	A	574	GLY	6.1
1	B	591	HIS	5.4
1	A	591	HIS	5.3
1	B	573	ALA	5.3
1	B	579	ASN	5.1
1	B	575	VAL	5.0
1	B	583	VAL	5.0
1	A	590	GLY	4.9
1	A	545	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	526	VAL	4.7
1	A	613	PRO	4.5
1	A	612	CYS	4.4
1	B	597	HIS	4.4
1	A	556	ILE	4.3
1	A	571	CYS	4.3
1	A	575	VAL	4.1
1	B	543	MET	4.0
1	A	525	PHE	4.0
1	B	526	VAL	3.9
1	A	533	GLN	3.9
1	B	485	LEU	3.9
1	B	599	ASN	3.9
1	B	565	PRO	3.9
1	A	543	MET	3.8
1	B	566	HIS	3.8
1	B	582	LEU	3.8
1	B	545	ILE	3.7
1	A	578	GLU	3.7
1	A	603	GLY	3.6
1	A	562	ILE	3.6
1	A	561	TYR	3.5
1	B	598	PRO	3.5
1	B	531	CYS	3.4
1	B	593	CYS	3.4
1	B	523	ARG	3.4
1	B	592	VAL	3.4
1	B	590	GLY	3.3
1	A	214	ALA	3.3
1	A	572	PRO	3.3
1	A	581	THR	3.3
1	A	306	GLU	3.3
1	A	610	GLU	3.3
1	B	521	GLU	3.2
1	A	599	ASN	3.1
1	B	158	ASN	3.1
1	A	611	GLY	3.1
1	A	308	PRO	3.1
1	B	576	MET	3.0
1	A	614	THR	3.0
1	B	507	ARG	3.0
1	B	194	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	280	HIS	2.9
1	A	542	ALA	2.9
1	A	550	ARG	2.8
1	A	579	ASN	2.8
1	B	589	ALA	2.7
1	A	597	HIS	2.7
1	B	569	LYS	2.7
1	B	581	THR	2.7
1	A	549	GLY	2.6
1	B	525	PHE	2.5
1	A	532	ILE	2.5
1	A	577	GLY	2.5
1	B	449	ASN	2.4
1	B	530	GLU	2.4
1	B	548	THR	2.4
1	A	202	LYS	2.4
1	B	570	THR	2.4
1	B	473	ASN	2.3
1	B	602	TYR	2.3
1	B	584	TRP	2.3
1	B	605	THR	2.3
1	A	557	GLN	2.3
1	B	560	HIS	2.3
1	B	515	CYS	2.3
1	B	202	LYS	2.2
2	D	10	HIS	2.2
1	A	609	LEU	2.2
1	B	524	GLU	2.2
1	A	201	GLY	2.1
1	A	604	CYS	2.1
1	A	205	SER	2.1
1	A	176	TRP	2.1
1	A	531	CYS	2.1
1	A	1	LEU	2.1
1	A	608	GLY	2.1
1	A	548	THR	2.1
1	A	311	LYS	2.1
1	B	544	ASN	2.0
2	D	8	LEU	2.0
1	B	518	LEU	2.0
1	B	386	TRP	2.0
1	B	559	ALA	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](#)

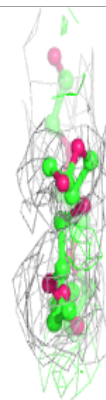
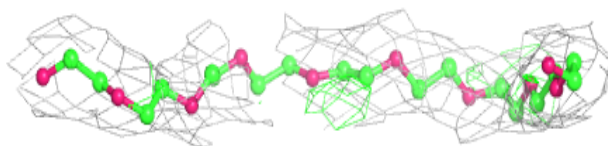
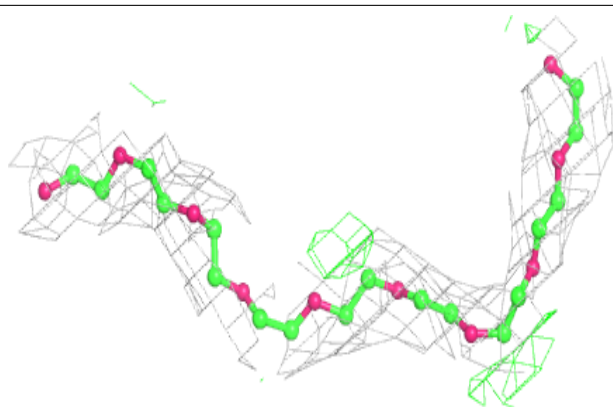
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	2PE	B	617	28/28	0.70	0.21	79,97,115,119	0
4	2PE	B	615	28/28	0.72	0.17	88,105,147,157	0
4	2PE	D	52	28/28	0.74	0.16	110,124,137,143	0
3	NAG	A	1049	14/15	0.75	0.40	130,153,165,166	0
3	NAG	A	1151	14/15	0.77	0.28	101,109,116,119	0
4	2PE	D	1	28/28	0.79	0.18	116,139,157,157	0
3	NAG	A	1172	14/15	0.81	0.17	123,135,143,144	0
3	NAG	B	1032	14/15	0.81	0.25	115,127,138,147	0
3	NAG	B	1504	14/15	0.83	0.37	170,178,191,191	0
3	NAG	A	1337	14/15	0.84	0.40	147,155,158,158	0
3	NAG	A	1032	14/15	0.85	0.22	108,120,129,132	0
3	NAG	A	1420	14/15	0.86	0.30	144,148,176,178	0
3	NAG	B	1151	14/15	0.86	0.15	142,149,164,165	0
3	NAG	A	1504	14/15	0.87	0.40	152,159,166,168	0
4	2PE	B	616	28/28	0.87	0.15	84,105,115,118	0
3	NAG	A	1328	14/15	0.91	0.30	70,79,88,91	0
3	NAG	B	1328	14/15	0.94	0.26	69,81,95,98	0

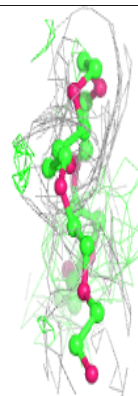
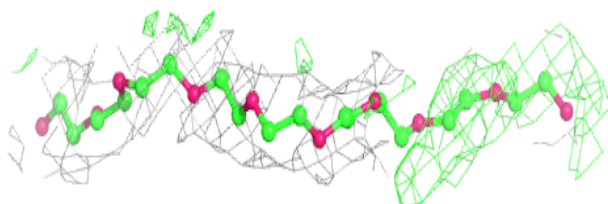
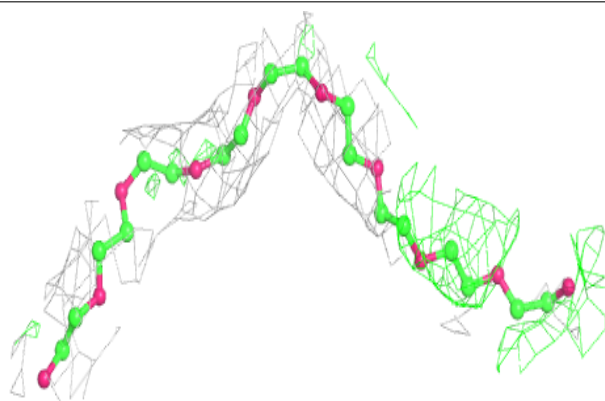
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2PE 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)

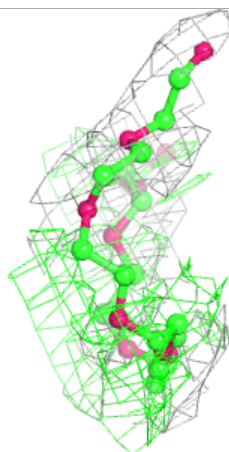
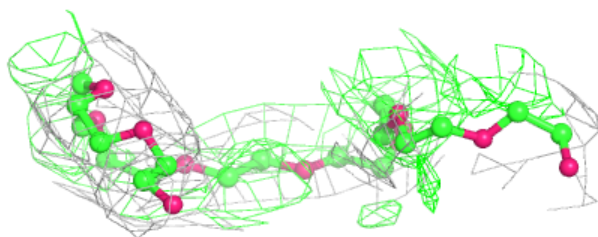
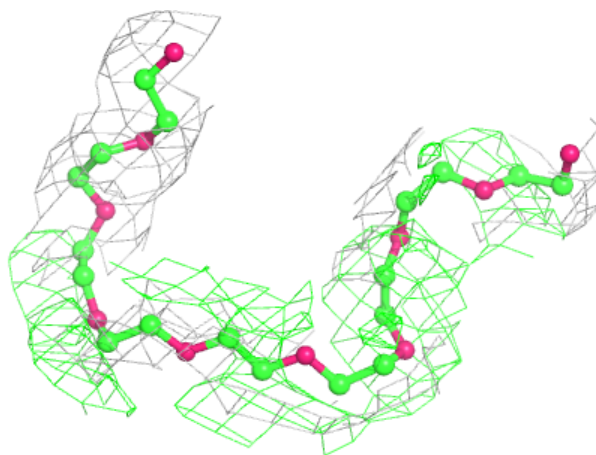
**Electron density around 2PE B 615:**

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



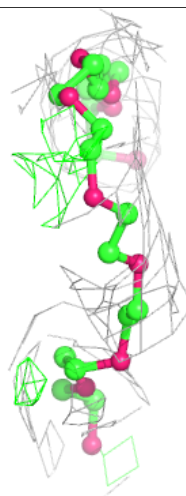
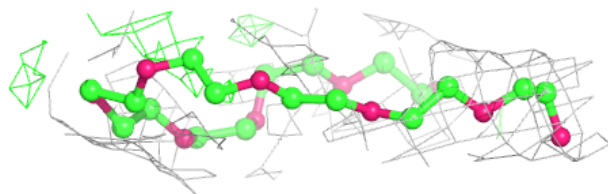
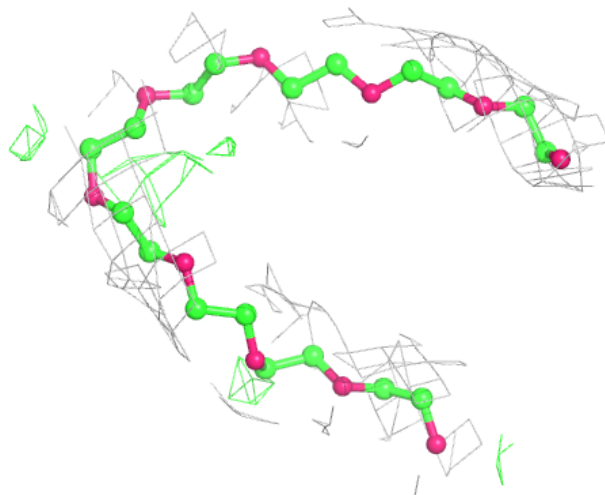
Electron density around 2PE D 52:

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



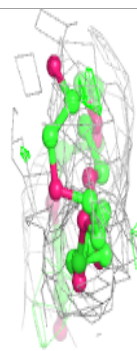
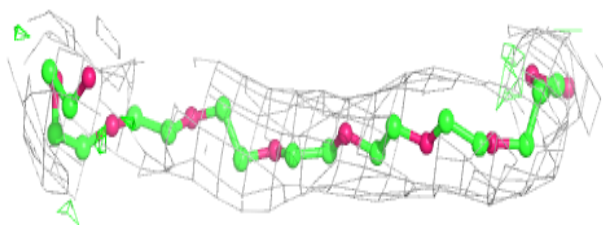
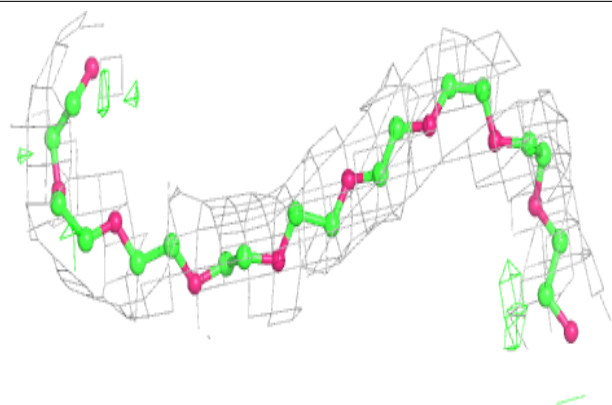
Electron density around 2PE D 1:

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



Electron density around 2PE B 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.