



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:52 PM UTC

PDB ID : 4XCN / pdb_00004xcn
Title : Crystal structure of human 4E10 Fab in complex with phosphatidic acid (06:0 PA); 2.9 Å resolution
Authors : Irimia, A.; Stanfield, R.L.; Wilson, I.A.
Deposited on : 2014-12-18
Resolution : 2.90 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

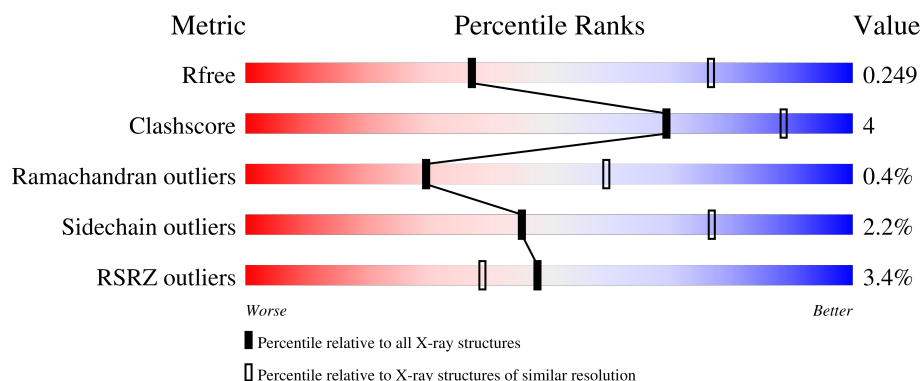
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	B	215	88% 11%
1	D	215	90% 9%
1	F	215	16% 85% 13% .
1	I	215	% 89% 10%
1	K	215	5% 90% 8% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	L	215	% 92% 7%
2	A	230	% 90% 9%
2	C	230	3% 86% 13%
2	E	230	5% 85% 9% 5%
2	G	230	3% 83% 13%
2	H	230	90% 9%
2	J	230	6% 86% 9% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20349 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 4E10 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	2	0
			1644	1020	284	335	5			
1	B	214	Total	C	N	O	S	0	2	0
			1641	1020	280	336	5			
1	D	214	Total	C	N	O	S	0	4	0
			1655	1028	282	340	5			
1	F	214	Total	C	N	O	S	0	2	0
			1594	985	277	327	5			
1	I	214	Total	C	N	O	S	0	1	0
			1606	995	274	332	5			
1	K	214	Total	C	N	O	S	0	0	0
			1600	995	274	327	4			

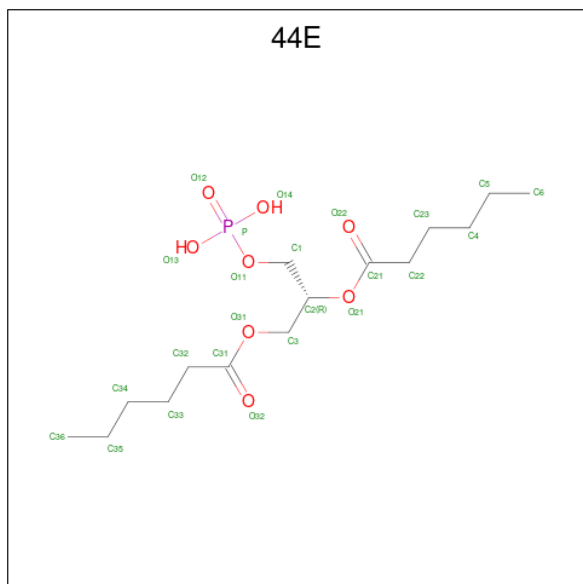
- Molecule 2 is a protein called 4E10 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	230	Total	C	N	O	S	0	4	0
			1704	1079	287	329	9			
2	A	227	Total	C	N	O	S	0	3	0
			1669	1061	276	324	8			
2	C	228	Total	C	N	O	S	0	2	0
			1660	1045	283	325	7			
2	E	218	Total	C	N	O	S	0	3	0
			1606	1015	271	313	7			
2	G	222	Total	C	N	O	S	0	4	0
			1608	1020	263	317	8			
2	J	219	Total	C	N	O	S	0	3	0
			1566	989	264	305	8			

- Molecule 3 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	C	O	0	0
			21	14	7		
3	B	1	Total	C	O	0	0
			21	14	7		
3	D	1	Total	C	O	0	0
			18	12	6		
3	F	1	Total	C	O	0	0
			6	4	2		
3	I	1	Total	C	O	0	0
			21	14	7		
3	K	1	Total	C	O	0	0
			18	12	6		

- Molecule 4 is (2R)-3-(phosphonoxy)propane-1,2-diyl dihexanoate (CCD ID: 44E) (formula: $C_{15}H_{29}O_8P$).



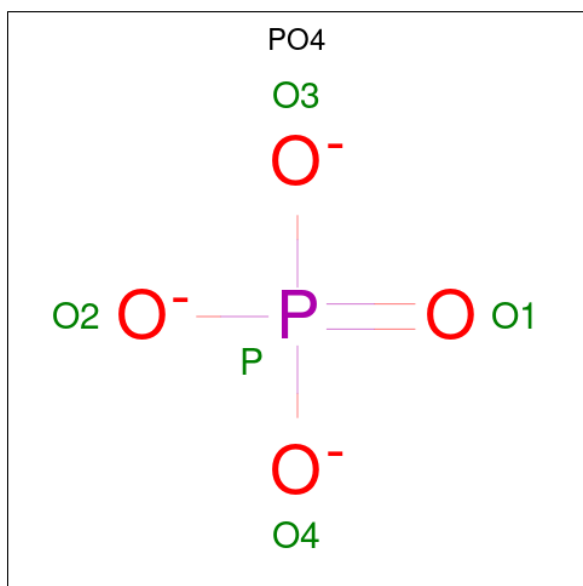
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	O	P	0	0
			21	12	8	1		
4	A	1	Total	C	O	P	0	0
			19	10	8	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	J	1	Total	O	P	0	0
			5	4	1		

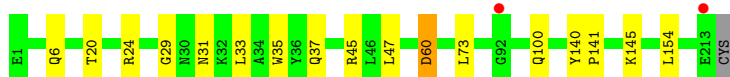
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	98	Total 98	O 98	0	0
7	H	95	Total 95	O 95	0	0
7	B	80	Total 80	O 80	0	0
7	A	67	Total 67	O 67	0	0
7	D	42	Total 42	O 42	0	0
7	C	64	Total 64	O 64	0	0
7	F	34	Total 34	O 34	0	0
7	E	30	Total 30	O 30	0	0
7	I	38	Total 38	O 38	0	0
7	G	42	Total 42	O 42	0	0
7	K	27	Total 27	O 27	0	0
7	J	13	Total 13	O 13	0	0

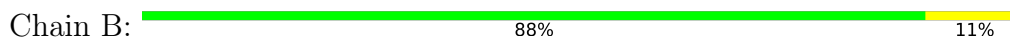
3 Residue-property plots [i](#)

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: 4E10 Fab light chain



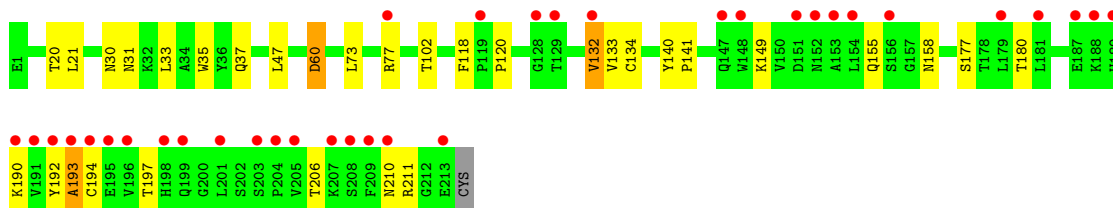
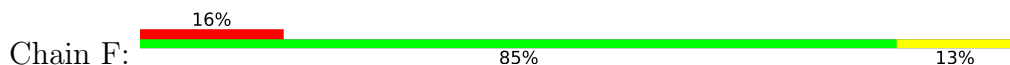
- Molecule 1: 4E10 Fab light chain



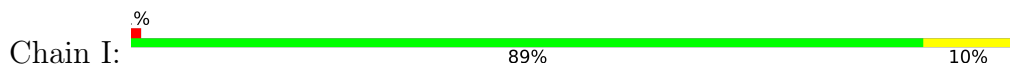
- Molecule 1: 4E10 Fab light chain



- Molecule 1: 4E10 Fab light chain

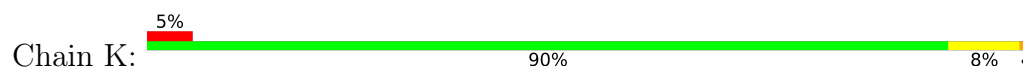


- Molecule 1: 4E10 Fab light chain





- Molecule 1: 4E10 Fab light chain



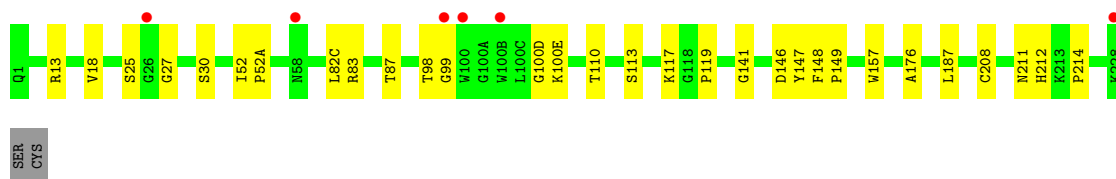
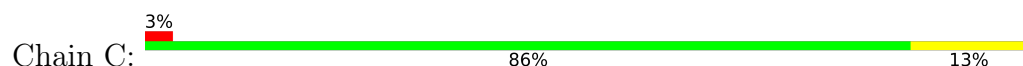
- Molecule 2: 4E10 Fab heavy chain



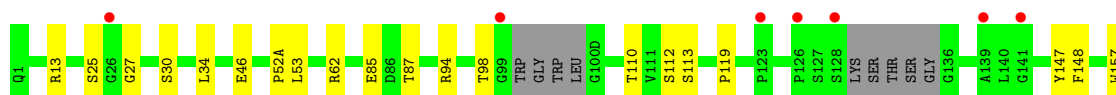
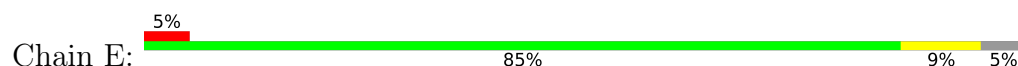
- Molecule 2: 4E10 Fab heavy chain



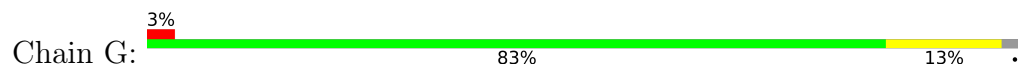
- Molecule 2: 4E10 Fab heavy chain



- Molecule 2: 4E10 Fab heavy chain

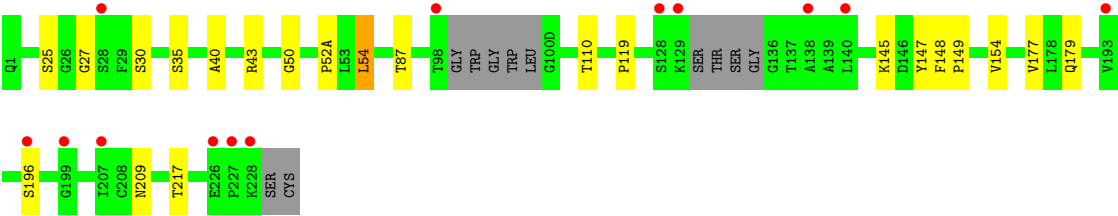
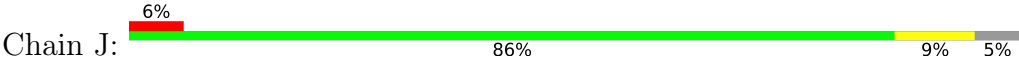


- Molecule 2: 4E10 Fab heavy chain





● Molecule 2: 4E10 Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	149.89Å 149.89Å 469.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.06 – 2.90 49.06 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.06-2.90) 98.1 (49.06-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.193 , 0.246 0.201 , 0.249	Depositor DCC
R_{free} test set	3443 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20349	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.10% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 44E, PO4, UNL

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	B	0.32	0/1677	0.75	0/2276
1	D	0.30	0/1694	0.72	0/2299
1	F	0.33	0/1627	0.83	4/2214 (0.2%)
1	I	0.29	0/1642	0.70	0/2235
1	K	0.30	0/1633	0.72	0/2223
1	L	0.31	0/1680	0.72	0/2279
2	A	0.32	0/1720	0.79	1/2353 (0.0%)
2	C	0.30	0/1705	0.76	1/2331 (0.0%)
2	E	0.30	0/1652	0.75	0/2257
2	G	0.33	0/1657	0.76	0/2267
2	H	0.32	0/1759	0.78	1/2403 (0.0%)
2	J	0.30	0/1612	0.75	0/2213
All	All	0.31	0/20058	0.75	7/27350 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	30	SER	N-CA-C	6.80	118.69	111.28
1	F	193	ALA	CA-C-N	6.45	133.30	121.70
1	F	193	ALA	C-N-CA	6.45	133.30	121.70
2	H	30	SER	N-CA-C	5.84	118.43	111.71
1	F	211	ARG	N-CA-C	5.72	118.48	109.96
1	F	192	TYR	N-CA-C	5.36	117.15	108.41
2	C	98	THR	N-CA-C	-5.21	107.47	113.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1641	0	1575	14	0
1	D	1655	0	1586	11	0
1	F	1594	0	1469	16	0
1	I	1606	0	1497	11	0
1	K	1600	0	1511	9	0
1	L	1644	0	1588	10	0
2	A	1669	0	1636	9	0
2	C	1660	0	1627	17	0
2	E	1606	0	1581	10	0
2	G	1608	0	1557	15	0
2	H	1704	0	1691	15	0
2	J	1566	0	1476	10	0
3	B	21	0	0	0	0
3	D	18	0	0	0	0
3	F	6	0	0	0	0
3	I	21	0	0	0	0
3	K	18	0	0	0	0
3	L	21	0	0	0	0
4	A	19	0	18	0	0
4	H	21	0	20	0	0
5	A	6	0	8	0	0
6	C	5	0	0	0	0
6	E	5	0	0	0	0
6	J	5	0	0	0	0
7	A	67	0	0	0	0
7	B	80	0	0	0	0
7	C	64	0	0	0	0
7	D	42	0	0	0	0
7	E	30	0	0	0	0
7	F	34	0	0	0	0
7	G	42	0	0	0	0
7	H	95	0	0	0	0
7	I	38	0	0	1	0
7	J	13	0	0	0	0
7	K	27	0	0	0	0
7	L	98	0	0	2	0
All	All	20349	0	18840	136	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (136) 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)
2:H:3:GLN:NE2	1:D:53:SER:OG	2.15	0.79
1:F:120:PRO:HD3	1:F:132:VAL:HG13	1.70	0.73
2:A:117:LYS:NZ	2:A:146:ASP:O	2.22	0.72
1:F:60:ASP:OD1	1:F:60:ASP:N	2.25	0.70
1:K:151:ASP:HA	1:K:191:VAL:HG13	1.74	0.69
2:E:30:SER:HB2	2:E:53:LEU:HB2	1.75	0.68
1:L:24:ARG:NH2	1:B:1:GLU:OE1	2.27	0.67
1:I:32:LYS:HD2	1:I:92:GLY:HA2	1.76	0.67
1:K:60:ASP:OD2	1:K:60:ASP:N	2.28	0.67
2:G:10:GLU:HG2	2:G:12:LYS:HE2	1.78	0.66
1:B:185:ASP:HA	1:B:188:LYS:HE3	1.75	0.66
2:J:30:SER:HA	2:J:52(A):PRO:HB2	1.78	0.66
1:I:60:ASP:OD1	1:I:60:ASP:N	2.28	0.65
2:C:117:LYS:NZ	2:C:146:ASP:O	2.29	0.64
2:A:87:THR:HG23	2:A:110:THR:HA	1.79	0.64
1:F:193:ALA:HA	1:F:194:CYS:HB3	1.78	0.63
2:C:87:THR:HG23	2:C:110:THR:HA	1.82	0.61
2:E:30:SER:HA	2:E:52(A):PRO:HB2	1.82	0.61
2:G:66:ARG:NH2	2:G:82(A):ASN:O	2.31	0.60
2:J:87:THR:HG23	2:J:110:THR:HA	1.82	0.60
1:F:149:LYS:N	1:F:193:ALA:O	2.23	0.59
2:E:87:THR:HG23	2:E:110:THR:HA	1.85	0.59
2:H:27:GLY:HA2	2:H:100:TRP:NE1	2.18	0.58
2:A:127:SER:HB3	2:A:130:SER:HB3	1.85	0.58
2:E:46:GLU:OE2	2:E:62:ARG:NH1	2.36	0.58
2:A:119:PRO:HB3	2:A:147:TYR:HB3	1.86	0.57
2:G:87:THR:HG23	2:G:110:THR:HA	1.87	0.57
1:F:134[B]:CYS:SG	1:F:177:SER:HB3	2.45	0.57
2:G:72:ASP:OD1	2:G:74:SER:OG	2.22	0.56
1:F:194:CYS:O	1:F:206:THR:HG23	2.06	0.55
1:I:140:TYR:CD2	1:I:141:PRO:HA	2.41	0.55
1:L:45:ARG:NH1	1:D:60:ASP:OD2	2.41	0.54
1:K:37:GLN:HB2	1:K:47:LEU:HD11	1.88	0.54
2:J:119:PRO:HB3	2:J:147:TYR:HB3	1.89	0.54
2:H:211:ASN:ND2	2:H:218:LYS:HD3	2.23	0.53
2:C:176:ALA:HB2	2:C:187:LEU:HD23	1.90	0.53
2:H:211:ASN:HD22	2:H:218:LYS:HD3	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:66:ARG:HD2	2:G:82(B):SER:HB2	1.91	0.53
2:H:27:GLY:HA2	2:H:100:TRP:HE1	1.73	0.52
1:F:155:GLN:OE1	1:F:158:ASN:ND2	2.41	0.52
1:K:6:GLN:O	1:K:100:GLN:NE2	2.42	0.52
1:B:94:SER:O	2:A:58:ASN:ND2	2.34	0.52
2:C:119:PRO:HB3	2:C:147:TYR:HB3	1.91	0.52
1:I:37:GLN:HB2	1:I:47:LEU:HD11	1.93	0.51
2:H:93:ALA:HB1	2:H:100(J):PHE:HB3	1.91	0.51
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.91	0.51
2:J:40:ALA:HB3	2:J:43:ARG:HG3	1.94	0.50
1:L:6:GLN:O	1:L:100:GLN:NE2	2.45	0.50
2:C:30:SER:HA	2:C:52(A):PRO:HB2	1.94	0.50
1:I:94:SER:O	2:G:58:ASN:ND2	2.43	0.49
1:B:37:GLN:HB2	1:B:47:LEU:HD11	1.94	0.49
1:B:19:ALA:HB2	1:B:78:LEU:HD11	1.94	0.49
1:D:32:LYS:HD2	1:D:91:TYR:CE2	2.48	0.49
2:H:117:LYS:HG2	2:H:118:GLY:O	2.13	0.48
1:D:37:GLN:HB2	1:D:47:LEU:HD11	1.95	0.48
1:L:45:ARG:NH2	7:L:424:HOH:O	2.46	0.48
2:H:100:TRP:CE2	2:C:99:GLY:HA2	2.49	0.48
2:G:18:VAL:HB	2:G:82(C):LEU:HD11	1.96	0.48
1:K:29:GLY:C	1:K:31:ASN:H	2.21	0.48
2:E:13:ARG:NH2	2:E:113:SER:O	2.46	0.47
2:H:212:HIS:CD2	2:H:214:PRO:HD2	2.49	0.47
1:D:31:ASN:O	1:D:33:LEU:N	2.44	0.47
2:J:54:LEU:HD13	2:J:54:LEU:HA	1.69	0.47
2:J:119:PRO:HD2	2:J:217:THR:HG21	1.96	0.47
2:E:119:PRO:HB3	2:E:147:TYR:HB3	1.96	0.47
1:K:23:CYS:HB2	1:K:35:TRP:CH2	2.50	0.47
2:C:99:GLY:HA3	2:C:100(D):GLY:HA2	1.95	0.47
1:D:145:LYS:HB3	1:D:197:THR:OG1	2.15	0.47
2:C:100(D):GLY:O	2:C:100(E):LYS:HD2	2.16	0.46
2:G:157:TRP:CH2	2:G:208[B]:CYS:HB3	2.51	0.46
2:J:145:LYS:NZ	2:J:179:GLN:OE1	2.46	0.46
2:E:209:ASN:OD1	2:E:209:ASN:N	2.48	0.46
2:C:13:ARG:NH2	2:C:113:SER:O	2.49	0.46
1:I:134:CYS:HB2	1:I:148:TRP:CZ2	2.51	0.46
1:B:30:ASN:O	1:B:31:ASN:HB2	2.16	0.45
2:C:148:PHE:HA	2:C:149:PRO:HA	1.75	0.45
2:E:112:SER:HB3	2:E:148:PHE:CZ	2.52	0.45
2:H:100:TRP:NE1	2:C:99:GLY:HA2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:TRP:HB2	1:B:48:ILE:HB	1.99	0.45
1:D:21:LEU:HD23	1:D:102:THR:HB	2.00	0.45
1:F:37:GLN:HB2	1:F:47:LEU:HD11	1.98	0.45
1:F:140:TYR:CD2	1:F:141:PRO:HA	2.52	0.44
1:L:140:TYR:CG	1:L:141:PRO:HA	2.52	0.44
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.99	0.44
2:C:157:TRP:CH2	2:C:208[B]:CYS:HB3	2.52	0.44
1:D:140:TYR:CG	1:D:141:PRO:HA	2.52	0.44
2:C:18:VAL:HB	2:C:82(C):LEU:HD11	1.99	0.44
1:B:15:PRO:HB2	1:F:77:ARG:HH22	1.83	0.44
1:F:35:TRP:CD2	1:F:73:LEU:HB2	2.53	0.44
1:D:35:TRP:CE2	1:D:73:LEU:HB2	2.52	0.44
2:E:157:TRP:CH2	2:E:208:CYS:HB3	2.52	0.44
1:F:190:LYS:O	1:F:210:ASN:HA	2.18	0.43
2:J:154:VAL:HA	2:J:209:ASN:O	2.19	0.43
2:H:30:SER:HB3	2:H:53:LEU:HB2	2.01	0.43
2:C:212:HIS:CD2	2:C:214:PRO:HD2	2.53	0.43
1:I:120:PRO:HD3	1:I:132:VAL:HG22	2.01	0.43
2:G:148:PHE:HA	2:G:149:PRO:HA	1.81	0.43
1:F:30:ASN:O	1:F:31:ASN:HB2	2.17	0.43
2:J:148:PHE:HA	2:J:149:PRO:HA	1.76	0.43
1:L:35:TRP:CE2	1:L:73:LEU:HB2	2.54	0.43
1:B:89:GLN:HB2	1:B:98:PHE:CD1	2.54	0.43
1:B:140:TYR:CG	1:B:141:PRO:HA	2.54	0.43
2:A:157:TRP:CH2	2:A:208[B]:CYS:HB3	2.54	0.42
2:G:29:PHE:CE2	2:G:52(A):PRO:HB3	2.54	0.42
1:D:140:TYR:CD2	1:D:141:PRO:HA	2.54	0.42
2:H:48:MET:HE2	2:H:67:ILE:HD12	2.01	0.42
2:J:35:SER:HA	2:J:50:GLY:HA2	2.01	0.42
2:G:12:LYS:O	2:G:111:VAL:HA	2.20	0.42
1:B:15:PRO:HB2	1:F:77:ARG:HH12	1.84	0.42
1:K:32:LYS:HD2	1:K:91:TYR:CE2	2.54	0.42
2:C:176:ALA:HA	2:C:187:LEU:HB3	2.00	0.42
2:H:87:THR:HG23	2:H:110:THR:HA	2.01	0.42
1:D:49:TYR:O	1:D:53:SER:HB2	2.20	0.42
2:G:145:LYS:NZ	2:G:179:GLN:OE1	2.52	0.42
1:L:35:TRP:CD2	1:L:73:LEU:HB2	2.54	0.42
1:B:38:GLN:O	1:B:84:ALA:HB1	2.20	0.42
1:B:61:ARG:HA	1:K:77:ARG:NH1	2.35	0.42
2:A:2:VAL:HG22	2:A:27:GLY:HA3	2.02	0.42
2:H:32:TYR:OH	2:H:100(D):GLY:HA3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ASP:O	1:B:86:TYR:OH	2.36	0.41
2:G:176:ALA:HA	2:G:187:LEU:HB3	2.01	0.41
1:L:60:ASP:OD1	1:I:77:ARG:NE	2.35	0.41
2:C:141:GLY:HA2	2:C:157:TRP:CZ2	2.55	0.41
1:F:21:LEU:HD23	1:F:102:THR:HB	2.01	0.41
1:I:107:LYS:HA	1:I:140:TYR:OH	2.21	0.41
2:G:127:SER:C	2:G:129:LYS:H	2.29	0.41
2:C:52:ILE:HA	2:C:52(A):PRO:HD3	1.86	0.41
1:F:118:PHE:HB2	1:F:133:VAL:HG12	2.03	0.41
1:I:124:GLN:HG2	1:I:129:THR:O	2.21	0.41
1:L:145:LYS:NZ	7:L:497:HOH:O	2.54	0.40
2:A:157:TRP:CH2	2:A:208[A]:CYS:HB3	2.57	0.40
1:I:142:ARG:HD2	7:I:423:HOH:O	2.21	0.40
1:K:35:TRP:HB2	1:K:48:ILE:HB	2.04	0.40
2:G:34:LEU:HD11	2:G:92[B]:CYS:SG	2.62	0.40
2:A:133:THR:HB	2:A:137:THR:O	2.20	0.40
2:E:34:LEU:HD23	2:E:94:ARG:HG2	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	B	214/215 (100%)	205 (96%)	9 (4%)	0	100	100
1	D	216/215 (100%)	206 (95%)	9 (4%)	1 (0%)	24	54
1	F	214/215 (100%)	202 (94%)	12 (6%)	0	100	100
1	I	213/215 (99%)	203 (95%)	9 (4%)	1 (0%)	24	54
1	K	212/215 (99%)	203 (96%)	9 (4%)	0	100	100
1	L	214/215 (100%)	203 (95%)	9 (4%)	2 (1%)	14	41
2	A	226/230 (98%)	221 (98%)	4 (2%)	1 (0%)	30	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	228/230 (99%)	222 (97%)	5 (2%)	1 (0%)	30	59
2	E	215/230 (94%)	209 (97%)	5 (2%)	1 (0%)	24	54
2	G	220/230 (96%)	211 (96%)	7 (3%)	2 (1%)	14	41
2	H	232/230 (101%)	226 (97%)	5 (2%)	1 (0%)	30	59
2	J	216/230 (94%)	211 (98%)	4 (2%)	1 (0%)	24	54
All	All	2620/2670 (98%)	2522 (96%)	87 (3%)	11 (0%)	30	59

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	30	SER
2	H	27	GLY
2	A	27	GLY
1	D	29	GLY
2	G	100(D)	GLY
2	C	27	GLY
1	I	29	GLY
1	L	31	ASN
1	L	29	GLY
2	E	27	GLY
2	J	27	GLY

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	B	183/185 (99%)	181 (99%)	2 (1%)	65	88
1	D	185/185 (100%)	182 (98%)	3 (2%)	55	83
1	F	169/185 (91%)	163 (96%)	6 (4%)	31	65
1	I	174/185 (94%)	169 (97%)	5 (3%)	37	71
1	K	174/185 (94%)	167 (96%)	7 (4%)	28	62
1	L	185/185 (100%)	181 (98%)	4 (2%)	45	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	184/189 (97%)	179 (97%)	5 (3%)	39	73
2	C	182/189 (96%)	179 (98%)	3 (2%)	55	83
2	E	178/189 (94%)	174 (98%)	4 (2%)	45	77
2	G	175/189 (93%)	174 (99%)	1 (1%)	78	93
2	H	191/189 (101%)	189 (99%)	2 (1%)	68	89
2	J	164/189 (87%)	160 (98%)	4 (2%)	43	75
All	All	2144/2244 (96%)	2098 (98%)	46 (2%)	45	77

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	THR
1	L	33	LEU
1	L	60	ASP
1	L	154	LEU
2	H	25	SER
2	H	83	ARG
1	B	107	LYS
1	B	154	LEU
2	A	1	GLN
2	A	55	THR
2	A	128	SER
2	A	152	VAL
2	A	188	SER
1	D	20	THR
1	D	33	LEU
1	D	100	GLN
2	C	25	SER
2	C	83	ARG
2	C	211	ASN
1	F	20	THR
1	F	33	LEU
1	F	60	ASP
1	F	132	VAL
1	F	180	THR
1	F	197	THR
2	E	25	SER
2	E	85	GLU
2	E	98	THR
2	E	209	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	20	THR
1	I	33	LEU
1	I	60	ASP
1	I	100	GLN
1	I	197	THR
2	G	98	THR
1	K	33	LEU
1	K	60	ASP
1	K	106	VAL
1	K	129	THR
1	K	191	VAL
1	K	197	THR
1	K	203	SER
2	J	25	SER
2	J	54	LEU
2	J	177	VAL
2	J	196	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	3	GLN
2	H	82(A)	ASN
2	H	102	HIS
2	H	211	ASN
1	B	160	GLN
1	F	37	GLN
2	E	58	ASN
2	E	82(A)	ASN
2	E	102	HIS
1	I	160	GLN
2	G	64	GLN
2	J	82(A)	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are unknown - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	44E	H	301	-	20,20,23	0.45	0	23,25,28	0.96	0
6	PO4	E	301	-	4,4,4	0.95	0	6,6,6	0.45	0
6	PO4	C	301	-	4,4,4	0.94	0	6,6,6	0.47	0
6	PO4	J	301	-	4,4,4	0.93	0	6,6,6	0.47	0
5	GOL	A	302	-	5,5,5	0.39	0	5,5,5	0.32	0
4	44E	A	301	-	18,18,23	0.43	0	19,22,28	0.74	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
5	GOL	A	302	-	-	3/4/4/4	-
4	44E	H	301	-	-	13/22/22/25	-
4	44E	A	301	-	-	6/19/19/25	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

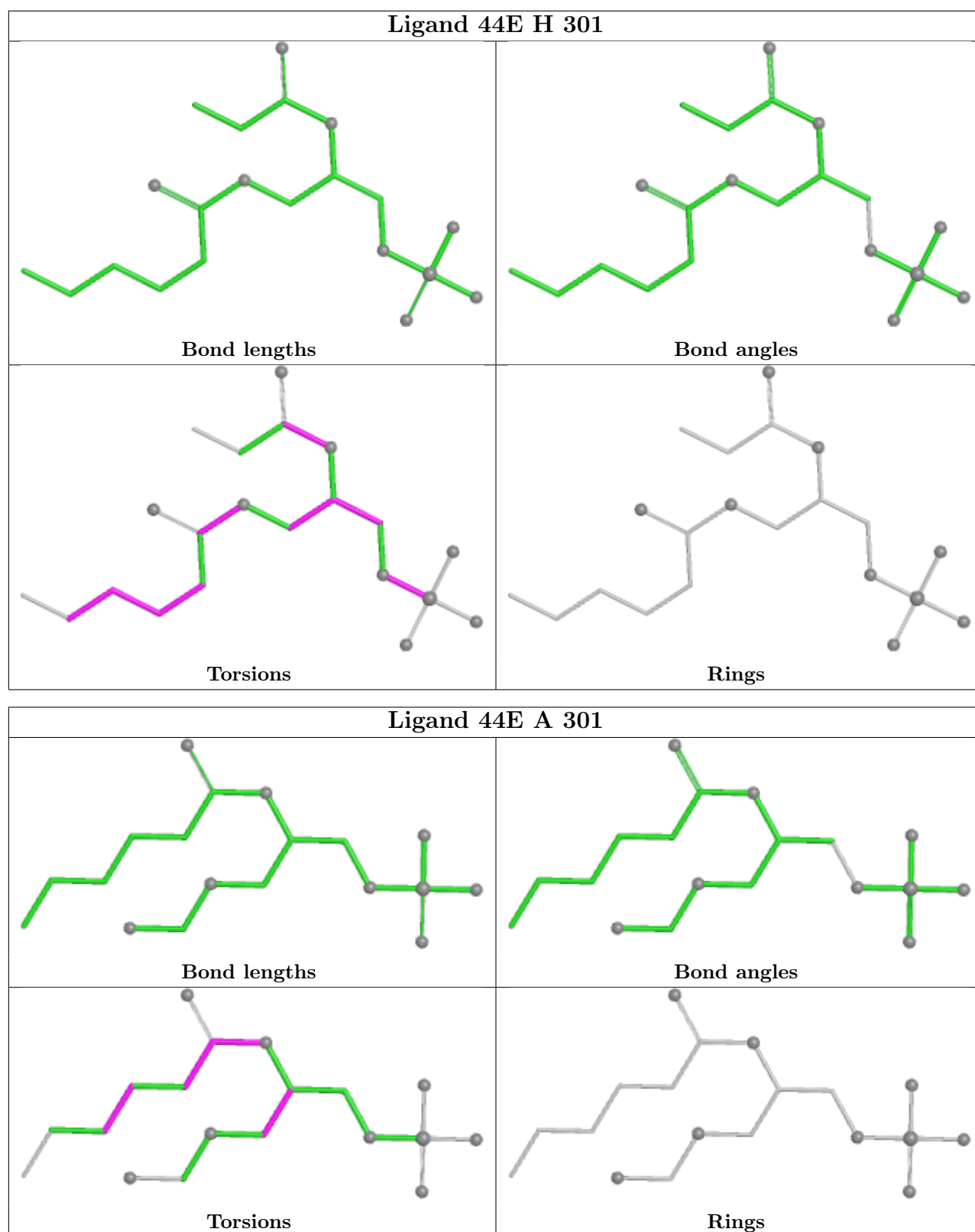
All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	44E	C1-O11-P-O13
4	H	301	44E	C1-O11-P-O14
4	H	301	44E	O32-C31-O31-C3
4	H	301	44E	C32-C31-O31-C3
4	A	301	44E	O22-C21-O21-C2
4	A	301	44E	C22-C21-O21-C2
4	H	301	44E	C31-C32-C33-C34
4	A	301	44E	O21-C2-C3-O31
4	H	301	44E	C33-C34-C35-C36
4	H	301	44E	C32-C33-C34-C35
4	H	301	44E	O21-C2-C3-O31
4	A	301	44E	C22-C23-C4-C5
4	H	301	44E	O11-C1-C2-O21
4	H	301	44E	C1-C2-C3-O31
5	A	302	GOL	O2-C2-C3-O3
4	A	301	44E	C1-C2-C3-O31
4	H	301	44E	O22-C21-O21-C2
5	A	302	GOL	O1-C1-C2-O2
4	H	301	44E	O11-C1-C2-C3
4	H	301	44E	C1-O11-P-O12
5	A	302	GOL	O1-C1-C2-C3
4	A	301	44E	O22-C21-C22-C23

There are no ring outliers.

No monomer is involved in short contacts.

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	B	214/215 (99%)	-0.28	1 (0%) 87 83	12, 21, 37, 56	2 (0%)
1	D	214/215 (99%)	-0.23	0 100 100	14, 27, 41, 60	4 (1%)
1	F	214/215 (99%)	0.64	35 (16%) 4 3	14, 41, 77, 84	2 (0%)
1	I	214/215 (99%)	0.17	2 (0%) 81 75	25, 39, 54, 66	1 (0%)
1	K	214/215 (99%)	0.58	11 (5%) 33 26	25, 49, 79, 90	0
1	L	214/215 (99%)	-0.31	2 (0%) 81 75	9, 24, 46, 60	2 (0%)
2	A	227/230 (98%)	-0.37	3 (1%) 75 67	10, 20, 43, 67	3 (1%)
2	C	228/230 (99%)	-0.18	6 (2%) 57 48	14, 25, 59, 71	2 (0%)
2	E	218/230 (94%)	0.16	11 (5%) 34 27	14, 31, 74, 94	3 (1%)
2	G	222/230 (96%)	0.04	6 (2%) 56 47	19, 35, 60, 84	4 (1%)
2	H	230/230 (100%)	-0.31	0 100 100	11, 21, 44, 65	4 (1%)
2	J	219/230 (95%)	0.70	13 (5%) 28 22	22, 58, 81, 96	3 (1%)
All	All	2628/2670 (98%)	0.05	90 (3%) 48 39	9, 31, 70, 96	30 (1%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	100(C)	LEU	5.1
1	K	213	GLU	4.6
2	C	100	TRP	4.2
1	F	190	LYS	3.8
1	F	204	PRO	3.7
1	F	209	PHE	3.7
1	F	210	ASN	3.7
2	C	100(B)	TRP	3.6
1	F	205	VAL	3.5
1	K	11	GLN	3.4
1	F	194	CYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	201	LEU	3.1
1	F	192	TYR	3.0
1	F	203	SER	3.0
1	B	79	GLU	3.0
1	F	151	ASP	3.0
1	K	203	SER	3.0
2	A	135	GLY	2.9
2	E	141	GLY	2.9
1	F	153	ALA	2.9
2	E	99	GLY	2.9
1	F	77	ARG	2.9
1	I	202	SER	2.9
1	F	187	GLU	2.8
1	F	156	SER	2.8
2	J	128	SER	2.8
2	J	226	GLU	2.8
2	E	26	GLY	2.8
1	F	195	GLU	2.7
2	A	133	THR	2.7
1	F	208	SER	2.7
1	F	213	GLU	2.7
2	E	128	SER	2.7
1	F	129	THR	2.7
2	E	200	THR	2.6
1	F	193	ALA	2.6
2	A	128	SER	2.6
1	I	77	ARG	2.6
2	G	26	GLY	2.6
1	F	132	VAL	2.6
2	J	140	LEU	2.6
2	J	28	SER	2.6
1	F	188	LYS	2.6
1	L	92	GLY	2.6
2	J	227	PRO	2.6
1	K	192	TYR	2.5
1	F	198	HIS	2.5
1	K	30	ASN	2.5
2	E	123	PRO	2.4
2	E	197	SER	2.4
1	L	213	GLU	2.4
2	E	198	LEU	2.4
1	F	119	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	204	PRO	2.4
1	F	148	TRP	2.4
2	E	139	ALA	2.4
2	J	98	THR	2.4
1	F	196	VAL	2.4
2	G	27	GLY	2.4
1	F	152	ASN	2.3
1	K	186	TYR	2.3
1	F	147	GLN	2.3
2	J	228	LYS	2.3
2	C	99	GLY	2.3
1	F	179	LEU	2.3
1	F	181	LEU	2.2
2	G	1	GLN	2.2
2	J	199	GLY	2.2
2	C	228	LYS	2.2
1	F	191	VAL	2.2
1	F	128	GLY	2.2
2	J	138	ALA	2.2
1	F	199	GLN	2.1
2	E	126	PRO	2.1
2	J	193	VAL	2.1
1	F	207	LYS	2.1
1	K	202	SER	2.1
2	G	130	SER	2.1
2	J	207	ILE	2.1
2	J	196	SER	2.1
2	C	26	GLY	2.1
1	K	143	GLU	2.1
2	C	58	ASN	2.1
2	E	199	GLY	2.1
1	F	154	LEU	2.0
1	K	70	ASP	2.0
1	F	189	HIS	2.0
1	K	191	VAL	2.0
2	G	30	SER	2.0
2	J	129	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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](#)

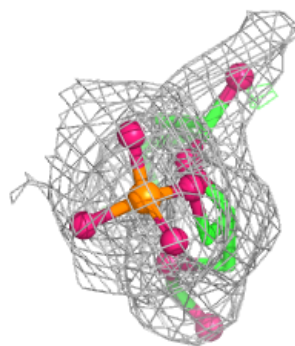
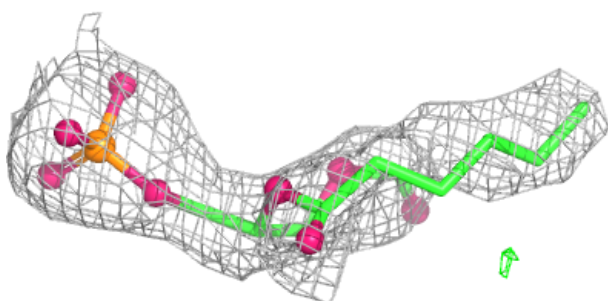
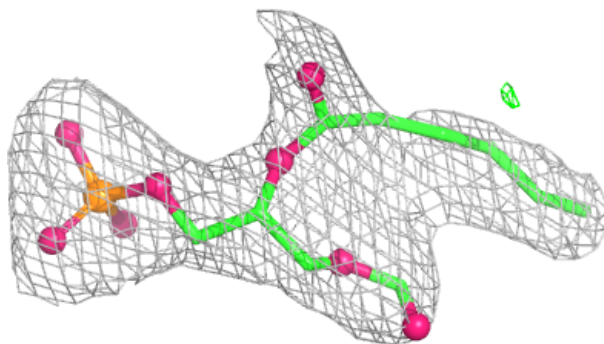
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	PO4	E	301	5/5	0.73	0.19	60,61,75,80	0
6	PO4	J	301	5/5	0.77	0.17	74,74,81,99	0
3	UNL	D	301	18/-	0.82	0.15	31,40,49,49	0
6	PO4	C	301	5/5	0.82	0.15	62,68,90,97	0
3	UNL	K	301	18/-	0.86	0.13	35,41,52,55	0
3	UNL	F	301	6/-	0.89	0.14	33,35,42,50	0
3	UNL	B	301	21/-	0.90	0.10	18,28,35,38	0
3	UNL	I	301	21/-	0.90	0.10	28,36,41,43	0
4	44E	A	301	19/24	0.91	0.13	36,50,66,68	0
3	UNL	L	301	21/-	0.91	0.10	10,23,29,38	0
5	GOL	A	302	6/6	0.92	0.16	18,26,30,30	0
4	44E	H	301	21/24	0.92	0.13	26,44,51,66	0

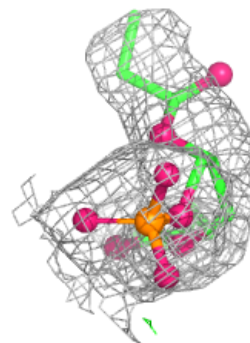
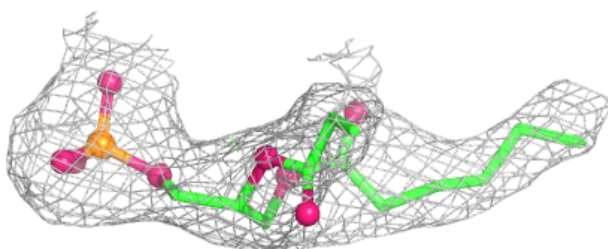
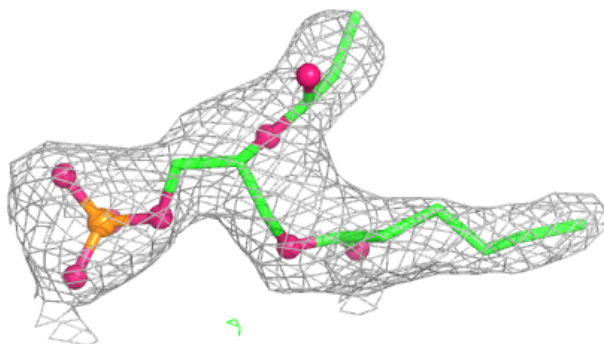
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 44E A 301:

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

**Electron density around 44E H 301:**

$2mF_o-DF_c$ (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.