Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2023 – 11:54 PM EDT

PDB ID	:	4XBG
Title	:	Crystal structure of human 4E10 Fab in complex with phosphatidic acid (06:0 PA): 2.73 A resolution
Authors	:	Irimia, A.; Stanfield, R.L.; Wilson, I.A.
Deposited on	:	2014-12-16
Resolution	:	2.73 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 (i) 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 (i)) were used in the production of this report:

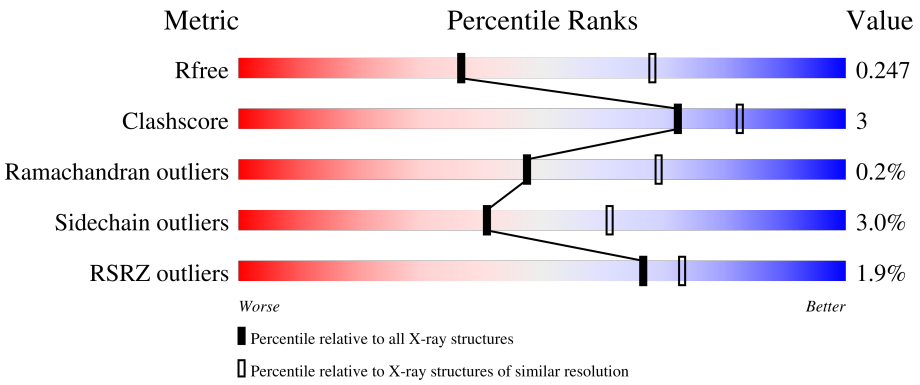
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 <=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	89% 10%
1	D	215	88% 11% •
1	F	215	5% 84% 13% ••
1	I	215	2% 87% 12% •
1	K	215	4% 88% 9% ••

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Mol	Chain	Length	Quality of chain
1	L	215	%, 93%, 6%
2	A	230	%, 86%, 12%
2	C	230	2%, 89%, 9%
2	E	230	%, 86%, 8%, 5%
2	G	230	%, 85%, 9%, 5%
2	H	230	%, 93%, 7%
2	J	230	4%, 84%, 10%, 6%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20282 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
			Total	C	N	O	S			
1	L	214	1648	1022	285	336	5	0	3	0
1	B	214	1659	1030	287	337	5	0	3	0
1	D	214	1671	1035	292	339	5	0	5	0
1	F	212	1600	990	279	327	4	0	1	0
1	I	214	1611	1000	276	330	5	0	1	0
1	K	212	1585	983	271	326	5	0	1	0

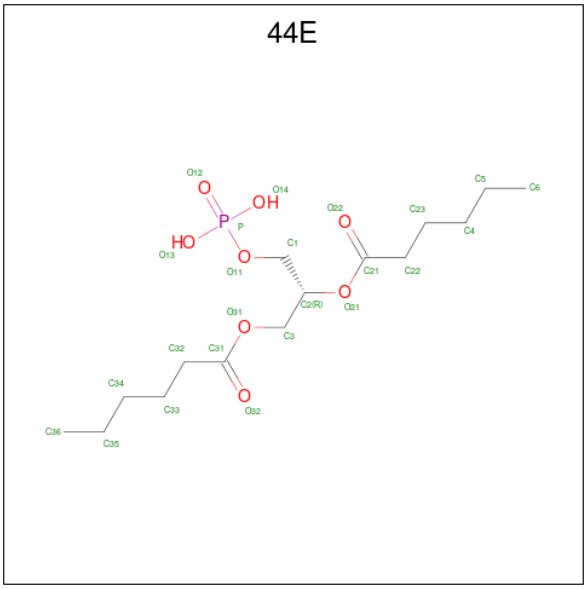
- Molecule 2 is a protein called 4E10 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	230	1716	1083	293	331	9	0	6	0
2	A	227	1709	1081	293	327	8	0	5	0
2	C	226	1648	1040	280	321	7	0	2	0
2	E	218	1602	1014	269	312	7	0	3	0
2	G	219	1606	1016	268	314	8	0	3	0
2	J	217	1553	984	256	305	8	0	3	0

- Molecule 3 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

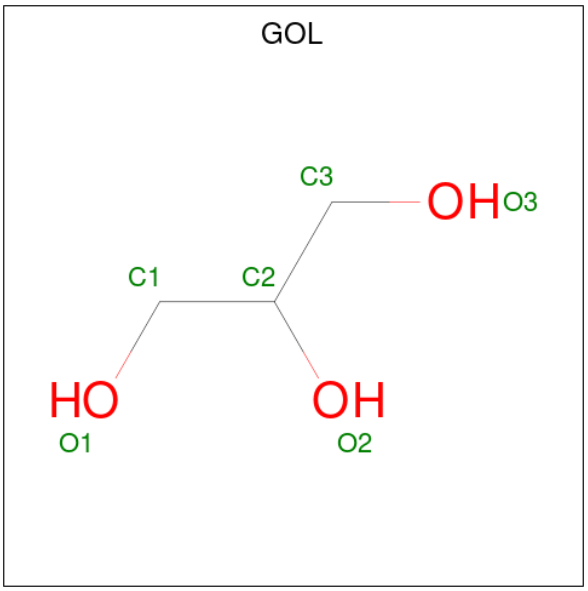
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	O		0	0
			21	14	7			
3	B	1	Total	C	O		0	0
			21	14	7			
3	D	1	Total	C	O		0	0
			18	12	6			
3	F	1	Total	C	O		0	0
			6	4	2			
3	I	1	Total	C	O		0	0
			21	14	7			
3	K	1	Total	C	O		0	0
			18	12	6			

- Molecule 4 is (2R)-3-(phosphonooxy)propane-1,2-diyl dihexanoate (three-letter code: 44E) (formula: $C_{15}H_{29}O_8P$).



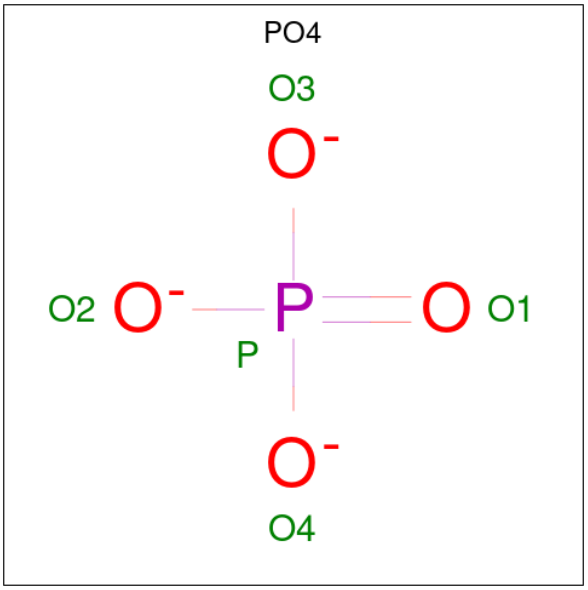
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	O	P	0	0
			17	8	8	1		
4	A	1	Total	C	O	P	0	0
			10	3	6	1		
4	A	1	Total	C	O	P	0	0
			16	9	6	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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

- Molecule 7 is water.

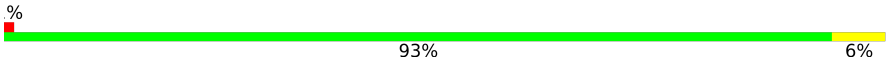
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	L	72	72	72	0	0
			Total	O		
7	H	63	63	63	0	0
			Total	O		
7	B	73	73	73	0	0
			Total	O		
7	A	72	72	72	0	0
			Total	O		
7	D	35	35	35	0	0
			Total	O		
7	C	41	41	41	0	0
			Total	O		
7	F	34	34	34	0	0
			Total	O		
7	E	32	32	32	0	0
			Total	O		
7	I	19	19	19	0	0
			Total	O		
7	G	35	35	35	0	0
			Total	O		
7	K	14	14	14	0	0
			Total	O		
7	J	4	4	4	0	0

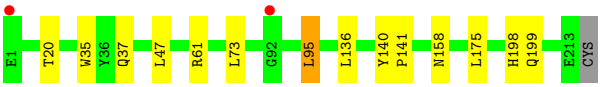
3 Residue-property plots (i)

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

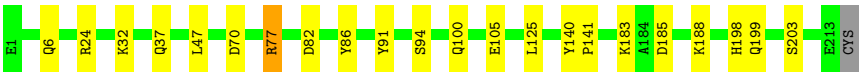
Chain L:





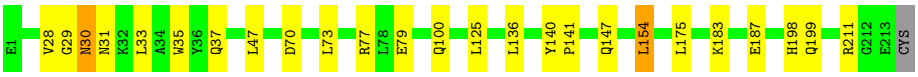
- Molecule 1: 4E10 Fab light chain

Chain B:



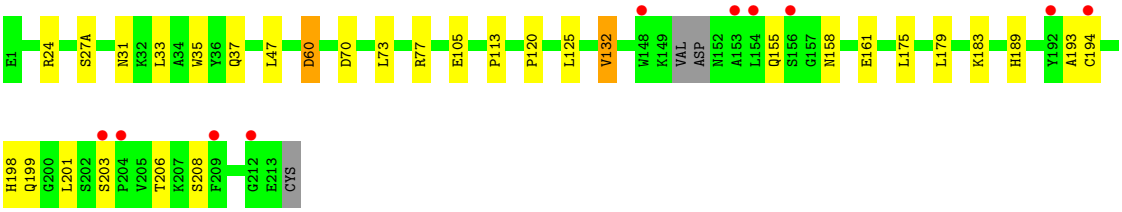
- Molecule 1: 4E10 Fab light chain

Chain D:



- Molecule 1: 4E10 Fab light chain

Chain F:



- Molecule 1: 4E10 Fab light chain

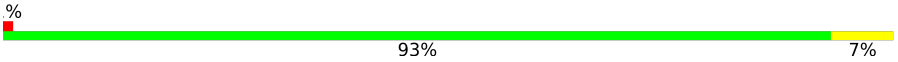
Chain I:

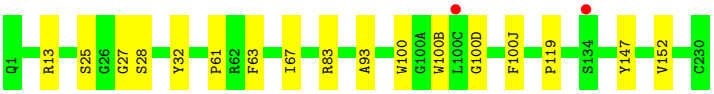
• Molecule 1: 4E10 Fab light chain

Chain K:

• Molecule 2: 4E10 Fab heavy chain

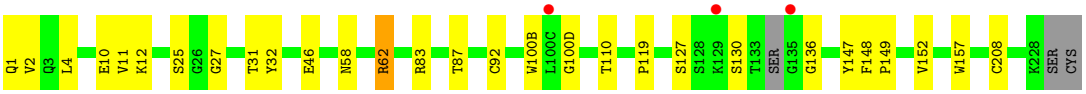
Chain H:





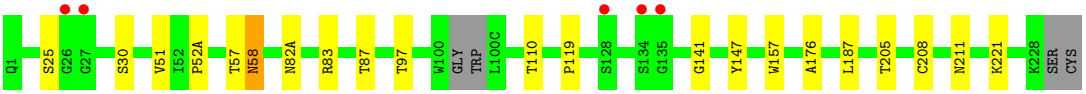
• Molecule 2: 4E10 Fab heavy chain

Chain A:



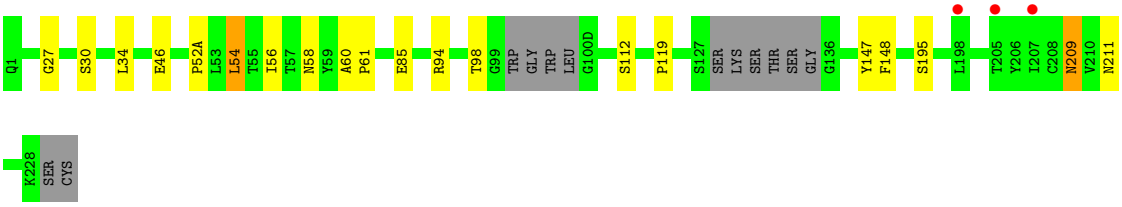
• Molecule 2: 4E10 Fab heavy chain

Chain C:



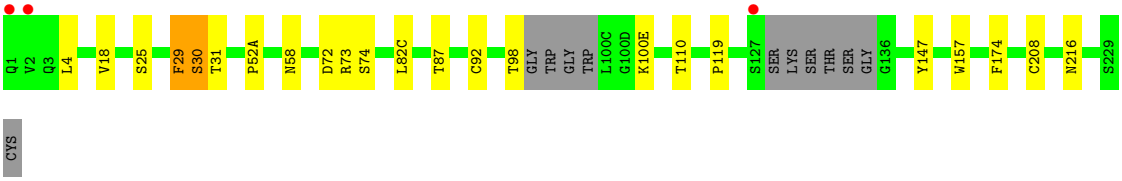
• Molecule 2: 4E10 Fab heavy chain

Chain E:



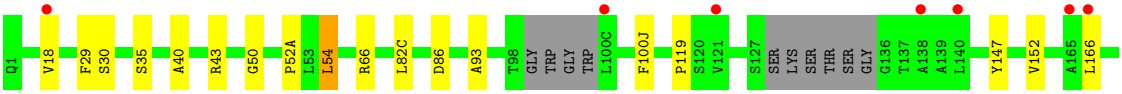
• Molecule 2: 4E10 Fab heavy chain

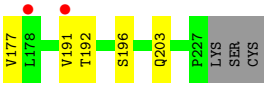
Chain G:



- Molecule 2: 4E10 Fab heavy chain

Chain J:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	149.56Å 149.56Å 470.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.24 – 2.73 39.24 – 2.73	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.24-2.73) 97.6 (39.24-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.202 , 0.246 0.205 , 0.247	Depositor DCC
R_{free} test set	4060 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20282	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.3657e-03.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: UNL, GOL, 44E, PO4

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	0.26	0/1695	0.44	0/2297
1	D	0.25	0/1710	0.45	0/2319
1	F	0.25	0/1632	0.48	0/2218
1	I	0.25	0/1647	0.44	0/2240
1	K	0.25	0/1621	0.47	0/2210
1	L	0.25	0/1684	0.45	0/2285
2	A	0.26	0/1760	0.46	0/2401
2	C	0.27	0/1692	0.45	0/2311
2	E	0.24	0/1648	0.45	0/2252
2	G	0.24	0/1652	0.47	0/2259
2	H	0.25	0/1774	0.47	0/2424
2	J	0.23	0/1599	0.45	0/2197
All	All	0.25	0/20114	0.46	0/27413

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	B	1659	0	1610	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1671	0	1617	12	0
1	F	1600	0	1501	16	0
1	I	1611	0	1525	15	0
1	K	1585	0	1481	12	0
1	L	1648	0	1587	10	0
2	A	1709	0	1701	13	0
2	C	1648	0	1622	9	0
2	E	1602	0	1576	9	0
2	G	1606	0	1572	12	0
2	H	1716	0	1698	8	0
2	J	1553	0	1479	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	26	0	24	0	0
4	H	17	0	9	1	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	C	5	0	0	0	0
6	E	5	0	0	0	0
6	G	5	0	0	0	0
6	J	5	0	0	1	0
7	A	72	0	0	0	0
7	B	73	0	0	0	0
7	C	41	0	0	1	0
7	D	35	0	0	0	0
7	E	32	0	0	2	0
7	F	34	0	0	0	0
7	G	35	0	0	0	0
7	H	63	0	0	0	0
7	I	19	0	0	0	0
7	J	4	0	0	0	0
7	K	14	0	0	1	0
7	L	72	0	0	0	0
All	All	20282	0	19018	133	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 3.

All (133) 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:A:127:SER:HB3	2:A:130:SER:HB3	1.59	0.85
1:D:77[B]:ARG:NH2	1:D:79:GLU:OE2	2.19	0.76
2:A:46:GLU:OE2	2:A:62[B]:ARG:NH2	2.22	0.73
1:I:32:LYS:HD2	1:I:92:GLY:HA2	1.72	0.70
1:B:24:ARG:NH1	1:B:70:ASP:OD1	2.23	0.70
2:A:31:THR:HG21	2:A:100(B):TRP:HA	1.76	0.68
2:C:58:ASN:ND2	7:C:401:HOH:O	2.27	0.67
1:L:95:LEU:HD11	2:H:61:PRO:HD3	1.77	0.67
1:I:145:LYS:HB3	1:I:197:THR:HG23	1.79	0.65
1:K:19:ALA:HB2	1:K:78:LEU:HD21	1.79	0.64
2:J:119:PRO:HB3	2:J:147:TYR:HB3	1.79	0.64
1:B:185:ASP:HA	1:B:188:LYS:HE3	1.80	0.63
1:F:120:PRO:HD3	1:F:132:VAL:HG13	1.79	0.63
2:E:30:SER:HA	2:E:52(A):PRO:HB2	1.81	0.63
1:K:186:TYR:O	1:K:192:TYR:OH	2.16	0.63
1:B:94:SER:O	2:A:58:ASN:ND2	2.32	0.61
1:I:37:GLN:HB2	1:I:47:LEU:HD11	1.81	0.61
2:C:30:SER:HA	2:C:52(A):PRO:HB2	1.83	0.61
2:H:27:GLY:HA2	2:H:100:TRP:NE1	2.15	0.61
2:C:51:VAL:HG23	2:C:57:THR:HG22	1.83	0.60
2:E:58:ASN:ND2	7:E:403:HOH:O	2.34	0.58
2:G:72:ASP:OD1	2:G:74:SER:OG	2.21	0.58
1:K:37:GLN:HB2	1:K:47:LEU:HD11	1.86	0.58
2:J:30:SER:HA	2:J:52(A):PRO:HB2	1.86	0.58
2:H:28:SER:HB3	2:H:32:TYR:HE2	1.68	0.58
2:G:30:SER:HA	2:G:52(A):PRO:HB2	1.86	0.57
1:F:155:GLN:OE1	1:F:158:ASN:ND2	2.36	0.55
1:B:37:GLN:HB2	1:B:47:LEU:HD11	1.89	0.55
2:J:66:ARG:NH1	2:J:86:ASP:OD2	2.41	0.54
1:K:3:VAL:H	1:K:26:SER:HB3	1.73	0.53
1:B:77:ARG:NH2	7:K:402:HOH:O	2.42	0.53
1:D:136:LEU:HB2	1:D:175:LEU:HB3	1.91	0.53
2:A:2:VAL:HG22	2:A:27:GLY:HA3	1.91	0.53
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.92	0.52
1:K:118:PHE:HB2	1:K:133:VAL:HG23	1.91	0.52
1:K:17:GLU:HG2	1:K:18:ARG:H	1.74	0.52
1:F:60:ASP:OD1	1:F:60:ASP:N	2.33	0.51
2:J:18:VAL:HB	2:J:82(C):LEU:HD11	1.91	0.51
1:I:94:SER:O	2:G:58:ASN:ND2	2.38	0.51
1:D:31:ASN:O	1:D:33:LEU:N	2.44	0.51
1:F:37:GLN:HB2	1:F:47:LEU:HD11	1.93	0.51
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:140:TYR:CD1	1:I:141:PRO:HA	2.46	0.50
2:C:176:ALA:HB2	2:C:187:LEU:HD23	1.93	0.49
2:E:34:LEU:HD23	2:E:94:ARG:HG2	1.93	0.49
2:E:46:GLU:OE1	7:E:401:HOH:O	2.20	0.49
2:J:40:ALA:HB3	2:J:43:ARG:HG3	1.93	0.49
2:H:32:TYR:OH	2:H:100(D):GLY:HA3	2.13	0.49
1:D:28:VAL:O	1:D:30:ASN:N	2.46	0.49
1:K:150:VAL:HG13	1:K:192:TYR:CE1	2.47	0.48
1:L:35:TRP:CD2	1:L:73:LEU:HB2	2.48	0.48
2:A:119:PRO:HB3	2:A:147:TYR:HB3	1.95	0.48
1:D:37:GLN:HB2	1:D:47:LEU:HD11	1.94	0.48
1:F:193:ALA:HA	1:F:194:CYS:HB3	1.94	0.48
2:C:119:PRO:HB3	2:C:147:TYR:HB3	1.95	0.48
1:D:187:GLU:O	1:D:211:ARG:NH2	2.47	0.48
2:G:30:SER:OG	2:G:73:ARG:NH1	2.45	0.48
2:E:209:ASN:N	2:E:209:ASN:OD1	2.47	0.47
1:K:5:THR:HA	1:K:100:GLN:HE22	1.79	0.47
1:I:140:TYR:CG	1:I:141:PRO:HA	2.50	0.47
1:F:113:PRO:HD3	1:F:198:HIS:ND1	2.30	0.47
1:F:158:ASN:OD1	1:F:158:ASN:N	2.48	0.47
1:F:161:GLU:OE2	1:F:175:LEU:HD11	2.15	0.47
2:E:119:PRO:HB3	2:E:147:TYR:HB3	1.96	0.47
2:J:29:PHE:N	6:J:301:PO4:O1	2.44	0.47
2:J:35:SER:HA	2:J:50:GLY:HA2	1.97	0.47
1:L:158:ASN:OD1	1:L:158:ASN:N	2.47	0.46
1:B:140:TYR:CD1	1:B:141:PRO:HA	2.50	0.46
2:G:18:VAL:HB	2:G:82(C):LEU:HD11	1.97	0.46
1:I:162:SER:OG	2:G:174:PHE:HB3	2.15	0.46
1:I:198:HIS:CG	1:I:199:GLN:H	2.33	0.46
1:L:136:LEU:HB2	1:L:175:LEU:HB3	1.96	0.46
2:E:54:LEU:HB2	2:E:56:ILE:HG13	1.98	0.46
1:B:198:HIS:CG	1:B:199:GLN:H	2.34	0.46
1:D:198:HIS:CG	1:D:199:GLN:H	2.33	0.46
2:A:148:PHE:HA	2:A:149:PRO:HA	1.78	0.46
2:A:10:GLU:HG2	2:A:12:LYS:HD3	1.97	0.45
1:L:198:HIS:CG	1:L:199:GLN:H	2.34	0.45
1:F:198:HIS:CG	1:F:199:GLN:H	2.33	0.45
1:L:61:ARG:HH12	1:D:77[B]:ARG:CZ	2.30	0.45
2:A:11:VAL:HG21	2:A:149:PRO:HG3	1.99	0.45
1:D:35:TRP:CE2	1:D:73:LEU:HB2	2.52	0.45
2:J:54:LEU:HD13	2:J:54:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:O	1:B:183:LYS:HD2	2.17	0.44
1:F:194:CYS:O	1:F:206:THR:HG23	2.18	0.44
1:K:158:ASN:OD1	1:K:158:ASN:N	2.51	0.44
1:K:187:GLU:H	1:K:187:GLU:HG2	1.65	0.44
2:C:87:THR:HG23	2:C:110:THR:HA	2.00	0.43
2:J:166:LEU:HD21	2:J:191:VAL:HG21	2.01	0.43
1:K:150:VAL:HG13	1:K:192:TYR:HE1	1.83	0.43
1:F:35:TRP:CD2	1:F:73:LEU:HB2	2.53	0.43
1:I:158:ASN:OD1	1:I:158:ASN:N	2.51	0.43
2:A:157:TRP:CH2	2:A:208[B]:CYS:HB3	2.53	0.43
1:K:126:LYS:HB2	1:K:126:LYS:HE3	1.79	0.43
1:L:35:TRP:CE2	1:L:73:LEU:HB2	2.54	0.43
1:B:6:GLN:O	1:B:100:GLN:NE2	2.47	0.43
1:L:140:TYR:CG	1:L:141:PRO:HA	2.54	0.42
1:F:125:LEU:O	1:F:183:LYS:HD2	2.20	0.42
1:D:125:LEU:O	1:D:183:LYS:HD2	2.19	0.42
1:D:140:TYR:CG	1:D:141:PRO:HA	2.55	0.42
1:D:147:GLN:HG2	1:D:154:LEU:HD21	2.01	0.42
1:B:32:LYS:HD2	1:B:91:TYR:CE2	2.54	0.42
2:E:112:SER:HB3	2:E:148:PHE:CZ	2.54	0.42
1:I:82:ASP:O	1:I:86:TYR:OH	2.24	0.42
2:H:100(B):TRP:CD1	4:H:301:44E:H11	2.55	0.42
2:G:157:TRP:CH2	2:G:208[B]:CYS:HB3	2.54	0.42
1:I:15:PRO:HD3	1:I:106:VAL:HG13	2.01	0.42
1:I:134:CYS:HB2	1:I:148:TRP:CZ2	2.55	0.42
2:G:4:LEU:HD13	2:G:92[B]:CYS:SG	2.60	0.42
2:C:157:TRP:CH2	2:C:208[B]:CYS:HB3	2.55	0.42
2:C:208[A]:CYS:SG	2:C:221:LYS:HB3	2.60	0.42
2:E:60:ALA:HA	2:E:61:PRO:HD3	1.95	0.42
1:B:82:ASP:O	1:B:86:TYR:OH	2.32	0.41
1:I:54:ARG:HA	1:I:55:PRO:HD3	1.93	0.41
2:C:141:GLY:HA2	2:C:157:TRP:CH2	2.56	0.41
1:I:32:LYS:HB3	1:I:91:TYR:CE2	2.56	0.41
2:G:119:PRO:HB3	2:G:147:TYR:HB3	2.01	0.41
2:J:93:ALA:HB1	2:J:100(J):PHE:HB3	2.02	0.41
1:F:198:HIS:CG	1:F:199:GLN:N	2.88	0.41
1:B:140:TYR:CG	1:B:141:PRO:HA	2.55	0.41
2:G:100(E):LYS:HD3	2:G:100(E):LYS:HA	1.90	0.41
1:F:155:GLN:HB3	1:F:158:ASN:OD1	2.20	0.41
2:H:63:PHE:O	2:H:67:ILE:HG22	2.21	0.41
2:A:4:LEU:HD13	2:A:92[B]:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:VAL:HG23	1:F:179:LEU:HB3	2.03	0.41
2:G:87:THR:HG23	2:G:110:THR:HA	2.03	0.40
1:L:140:TYR:CD1	1:L:141:PRO:HA	2.55	0.40
2:H:93:ALA:HB1	2:H:100(J):PHE:HB3	2.04	0.40
2:A:32:TYR:OH	2:A:100(D):GLY:HA3	2.21	0.40
2:A:87:THR:HG23	2:A:110:THR:HA	2.03	0.40
1:F:31:ASN:O	1:F:33:LEU:N	2.51	0.40
1:I:124:GLN:HG2	1:I:129:THR:O	2.22	0.40
2:G:29:PHE:O	2:G:31:THR:N	2.54	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	B	215/215 (100%)	208 (97%)	7 (3%)	0	100	100
1	D	217/215 (101%)	208 (96%)	7 (3%)	2 (1%)	17	32
1	F	209/215 (97%)	196 (94%)	13 (6%)	0	100	100
1	I	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
1	K	211/215 (98%)	203 (96%)	8 (4%)	0	100	100
1	L	215/215 (100%)	208 (97%)	7 (3%)	0	100	100
2	A	228/230 (99%)	221 (97%)	6 (3%)	1 (0%)	34	55
2	C	224/230 (97%)	218 (97%)	6 (3%)	0	100	100
2	E	215/230 (94%)	209 (97%)	5 (2%)	1 (0%)	29	48
2	G	216/230 (94%)	209 (97%)	5 (2%)	2 (1%)	17	32
2	H	234/230 (102%)	230 (98%)	4 (2%)	0	100	100
2	J	214/230 (93%)	209 (98%)	5 (2%)	0	100	100
All	All	2611/2670 (98%)	2524 (97%)	81 (3%)	6 (0%)	47	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	30	SER
1	D	29	GLY
2	A	136	GLY
1	D	30	ASN
2	E	27	GLY
2	G	29	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	187/185 (101%)	184 (98%)	3 (2%)	62	78
1	D	188/185 (102%)	185 (98%)	3 (2%)	62	78
1	F	173/185 (94%)	162 (94%)	11 (6%)	17	31
1	I	177/185 (96%)	171 (97%)	6 (3%)	37	58
1	K	173/185 (94%)	164 (95%)	9 (5%)	23	39
1	L	185/185 (100%)	183 (99%)	2 (1%)	73	84
2	A	191/189 (101%)	185 (97%)	6 (3%)	40	60
2	C	181/189 (96%)	174 (96%)	7 (4%)	32	53
2	E	177/189 (94%)	171 (97%)	6 (3%)	37	58
2	G	178/189 (94%)	175 (98%)	3 (2%)	60	76
2	H	192/189 (102%)	187 (97%)	5 (3%)	46	66
2	J	167/189 (88%)	161 (96%)	6 (4%)	35	55
All	All	2169/2244 (97%)	2102 (97%)	67 (3%)	41	60

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	THR
1	L	95	LEU
2	H	13	ARG

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Mol	Chain	Res	Type
2	H	25	SER
2	H	83[A]	ARG
2	H	83[B]	ARG
2	H	152	VAL
1	B	77	ARG
1	B	105	GLU
1	B	203	SER
2	A	1	GLN
2	A	25	SER
2	A	62[A]	ARG
2	A	62[B]	ARG
2	A	83	ARG
2	A	152	VAL
1	D	70	ASP
1	D	100	GLN
1	D	154	LEU
2	C	25	SER
2	C	58	ASN
2	C	82(A)	ASN
2	C	83	ARG
2	C	97	THR
2	C	205	THR
2	C	211	ASN
1	F	24	ARG
1	F	27(A)	SER
1	F	60	ASP
1	F	70	ASP
1	F	77	ARG
1	F	105	GLU
1	F	132	VAL
1	F	189	HIS
1	F	201	LEU
1	F	203	SER
1	F	208	SER
2	E	54	LEU
2	E	85	GLU
2	E	98	THR
2	E	195	SER
2	E	209	ASN
2	E	211	ASN
1	I	100	GLN
1	I	105	GLU

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Mol	Chain	Res	Type
1	I	154	LEU
1	I	156	SER
1	I	162	SER
1	I	197	THR
2	G	25	SER
2	G	98	THR
2	G	216	ASN
1	K	1	GLU
1	K	11	GLN
1	K	20	THR
1	K	100	GLN
1	K	126	LYS
1	K	129	THR
1	K	133	VAL
1	K	187	GLU
1	K	197	THR
2	J	54	LEU
2	J	152	VAL
2	J	177	VAL
2	J	192	THR
2	J	196	SER
2	J	203	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	124	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)

Of 15 ligands modelled in this entry, 6 are unknown - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PO4	C	301	-	4,4,4	0.91	0	6,6,6	0.43	0
6	PO4	G	301	-	4,4,4	0.92	0	6,6,6	0.42	0
4	44E	H	301	-	16,16,23	0.50	0	20,21,28	0.72	0
4	44E	A	301	-	9,9,23	0.66	0	11,12,28	0.62	0
5	GOL	A	303	-	5,5,5	0.35	0	5,5,5	0.30	0
5	GOL	B	302	-	5,5,5	0.36	0	5,5,5	0.24	0
6	PO4	E	301	-	4,4,4	0.89	0	6,6,6	0.45	0
6	PO4	J	301	-	4,4,4	0.87	0	6,6,6	0.48	0
4	44E	A	302	-	15,15,23	0.46	0	18,18,28	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	44E	H	301	-	-	6/17/17/25	-
4	44E	A	301	-	-	2/8/8/25	-
5	GOL	A	303	-	-	2/4/4/4	-
5	GOL	B	302	-	-	4/4/4/4	-
4	44E	A	302	-	-	3/14/14/25	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	302	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	B	302	GOL	C1-C2-C3-O3
5	A	303	GOL	O1-C1-C2-C3
4	H	301	44E	O32-C31-O31-C3
4	H	301	44E	C22-C21-O21-C2
5	B	302	GOL	O1-C1-C2-O2
5	B	302	GOL	O2-C2-C3-O3
4	H	301	44E	C32-C31-O31-C3
5	A	303	GOL	O1-C1-C2-O2
4	H	301	44E	O11-C1-C2-C3
4	H	301	44E	O11-C1-C2-O21
4	A	301	44E	O11-C1-C2-O21
4	A	302	44E	O32-C31-O31-C3
4	A	301	44E	C2-C1-O11-P
4	H	301	44E	C1-C2-C3-O31
4	A	302	44E	O31-C31-C32-C33
4	A	302	44E	O32-C31-C32-C33

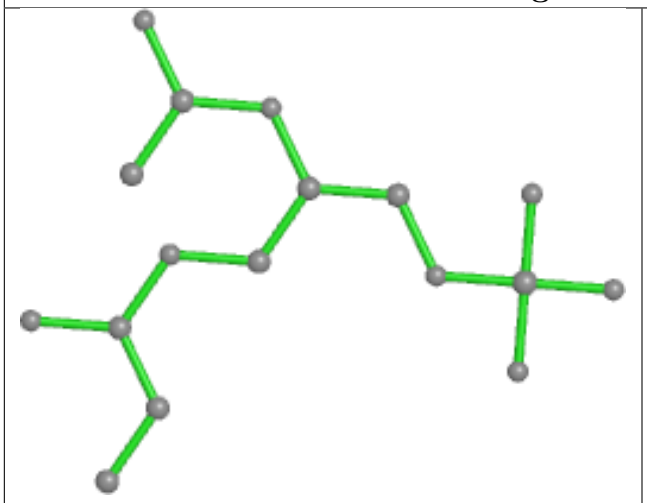
There are no ring outliers.

2 monomers are involved in 2 short contacts:

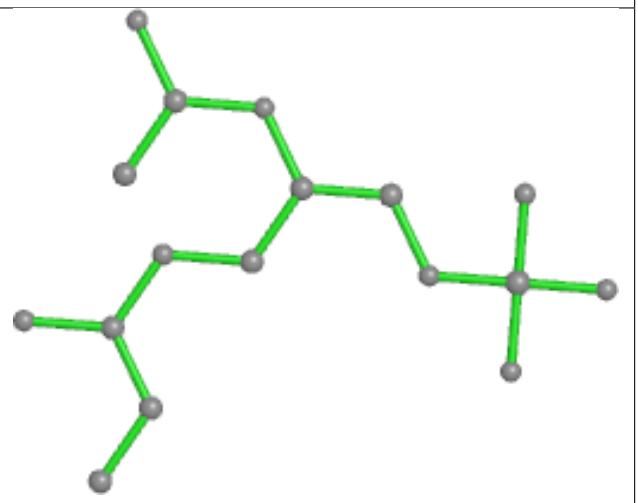
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	301	44E	1	0
6	J	301	PO4	1	0

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 then 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.

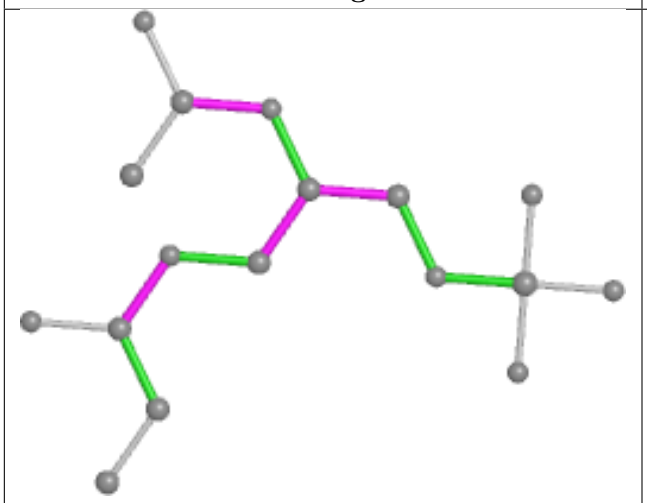
Ligand 44E H 301



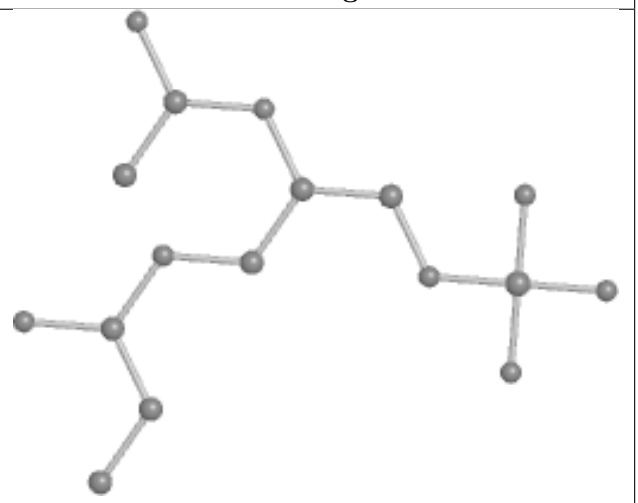
Bond lengths



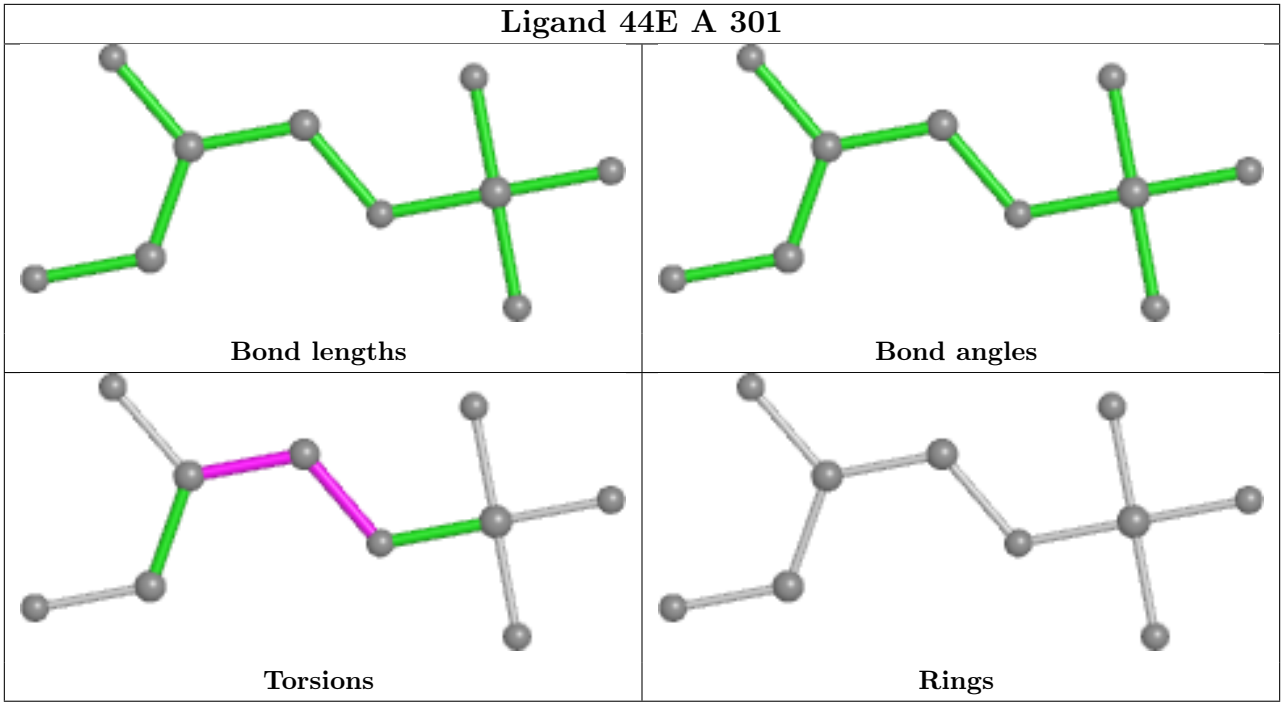
Bond angles

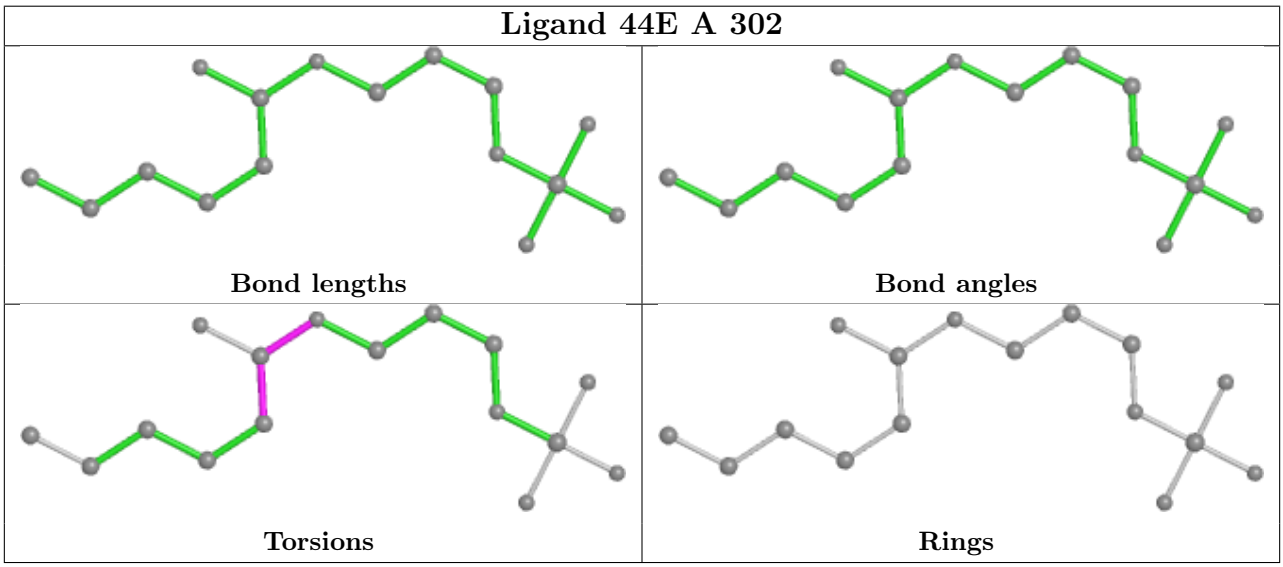


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	B	214/215 (99%)	-0.33	0	100	100	20, 33, 51, 76	0
1	D	214/215 (99%)	-0.25	0	100	100	26, 43, 61, 73	0
1	F	212/215 (98%)	0.17	10 (4%)	31	34	27, 54, 95, 107	0
1	I	214/215 (99%)	0.07	4 (1%)	66	73	38, 60, 80, 96	0
1	K	212/215 (98%)	0.23	9 (4%)	36	39	43, 72, 100, 107	0
1	L	214/215 (99%)	-0.27	2 (0%)	84	88	24, 37, 58, 80	0
2	A	227/230 (98%)	-0.27	3 (1%)	77	82	19, 31, 63, 89	0
2	C	226/230 (98%)	-0.24	5 (2%)	62	69	26, 40, 81, 100	0
2	E	218/230 (94%)	-0.10	3 (1%)	75	80	25, 43, 86, 104	0
2	G	219/230 (95%)	-0.03	3 (1%)	75	80	32, 52, 74, 106	0
2	H	230/230 (100%)	-0.25	2 (0%)	84	88	20, 34, 65, 86	0
2	J	217/230 (94%)	0.48	9 (4%)	37	41	45, 79, 102, 115	0
All	All	2617/2670 (98%)	-0.07	50 (1%)	66	73	19, 46, 90, 115	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	100(C)	LEU	5.0
2	C	134	SER	4.6
1	F	154	LEU	4.4
1	K	150	VAL	4.2
1	F	203	SER	4.1
2	C	135	GLY	3.6
1	K	189	HIS	3.5
2	A	100(C)	LEU	3.5
1	F	194	CYS	3.4
2	J	138	ALA	3.3
1	I	202	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	J	140	LEU	3.1
1	I	200	GLY	3.0
2	C	128	SER	2.9
2	J	166	LEU	2.9
1	F	212	GLY	2.8
2	C	27	GLY	2.7
1	I	201	LEU	2.7
1	L	1	GLU	2.7
1	K	203	SER	2.7
1	F	148	TRP	2.6
2	J	121	VAL	2.6
1	F	156	SER	2.6
1	K	192	TYR	2.6
1	F	209	PHE	2.5
2	E	198	LEU	2.5
2	J	191	VAL	2.5
2	H	134	SER	2.4
1	F	204	PRO	2.4
2	G	2	VAL	2.4
2	G	1	GLN	2.4
2	J	165	ALA	2.4
1	F	192	TYR	2.3
2	E	207	ILE	2.3
1	K	202	SER	2.3
2	J	18	VAL	2.3
2	C	26	GLY	2.2
1	I	185	ASP	2.2
2	A	129	LYS	2.2
1	K	209	PHE	2.2
1	L	92	GLY	2.2
1	K	186	TYR	2.2
2	G	127	SER	2.2
1	K	152	ASN	2.2
2	H	100(C)	LEU	2.1
2	A	135	GLY	2.1
2	E	205	THR	2.1
2	J	178	LEU	2.1
1	F	153	ALA	2.1
1	K	154	LEU	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)

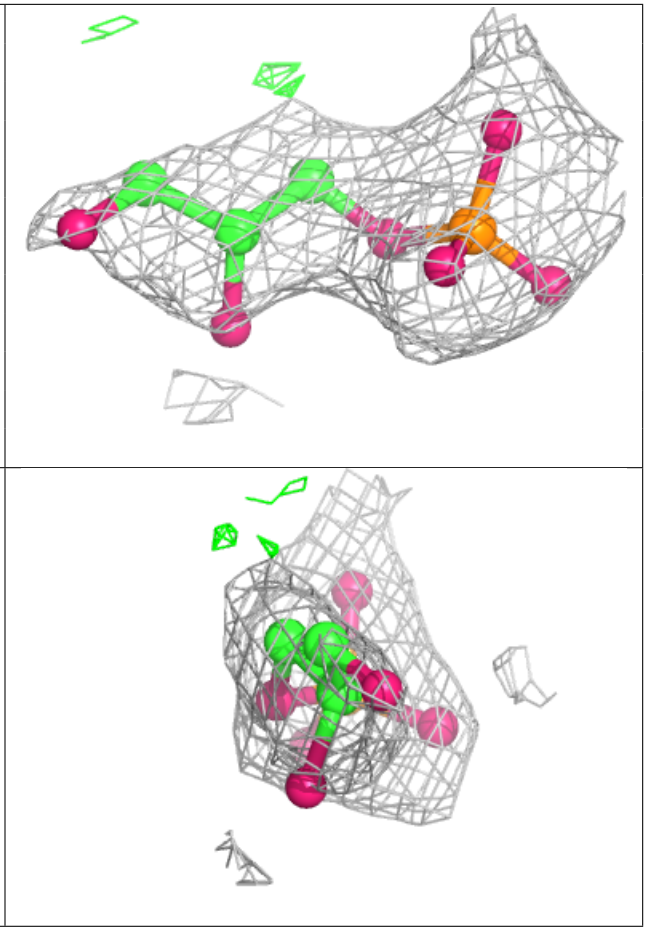
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

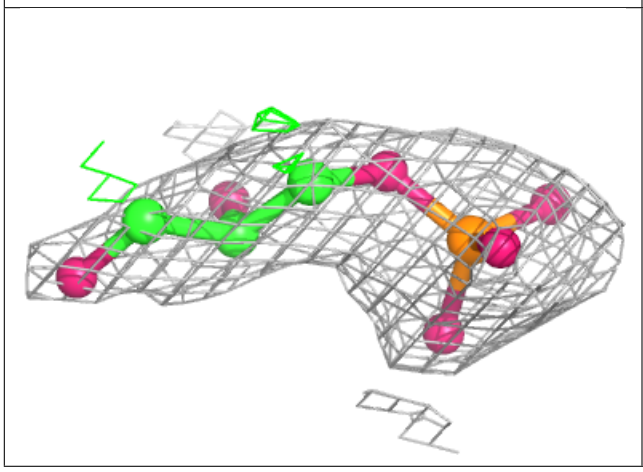
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	303	6/6	0.72	0.28	45,52,61,68	0
4	44E	A	301	10/24	0.83	0.22	74,79,95,115	0
6	PO4	C	301	5/5	0.83	0.18	88,90,99,109	0
6	PO4	J	301	5/5	0.86	0.17	72,85,89,98	0
3	UNL	D	301	18/-	0.87	0.25	45,55,65,65	0
5	GOL	B	302	6/6	0.88	0.24	26,43,46,46	0
3	UNL	K	301	18/-	0.89	0.16	50,66,78,86	0
3	UNL	F	301	6/-	0.89	0.21	46,50,64,69	0
3	UNL	I	301	21/-	0.90	0.19	45,55,63,65	0
6	PO4	E	301	5/5	0.91	0.21	64,69,96,112	0
6	PO4	G	301	5/5	0.91	0.15	76,81,96,96	0
4	44E	H	301	17/24	0.91	0.24	49,71,85,87	0
3	UNL	L	301	21/-	0.93	0.16	23,34,43,51	0
3	UNL	B	301	21/-	0.93	0.15	30,41,51,59	0
4	44E	A	302	16/24	0.93	0.23	46,70,80,82	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:

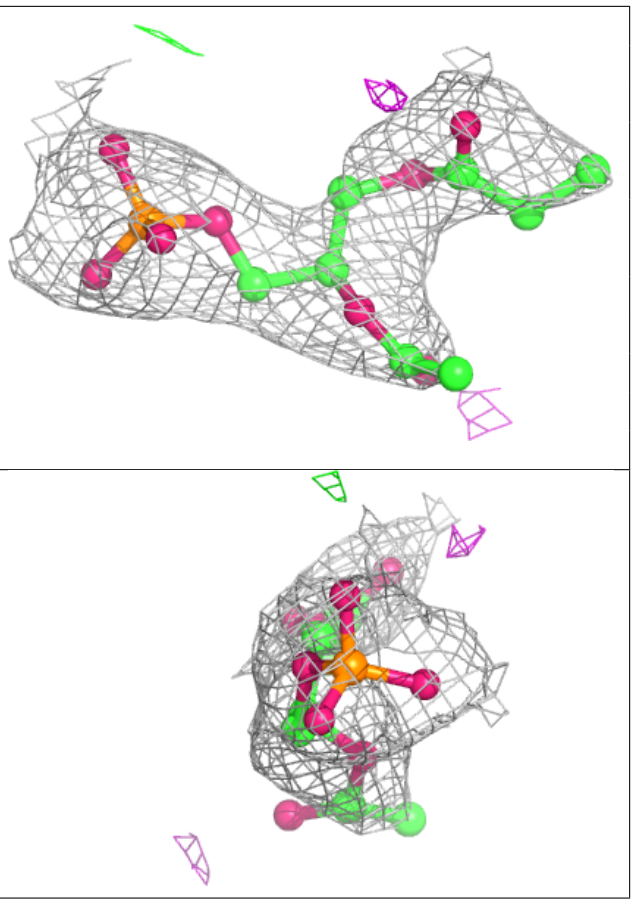
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





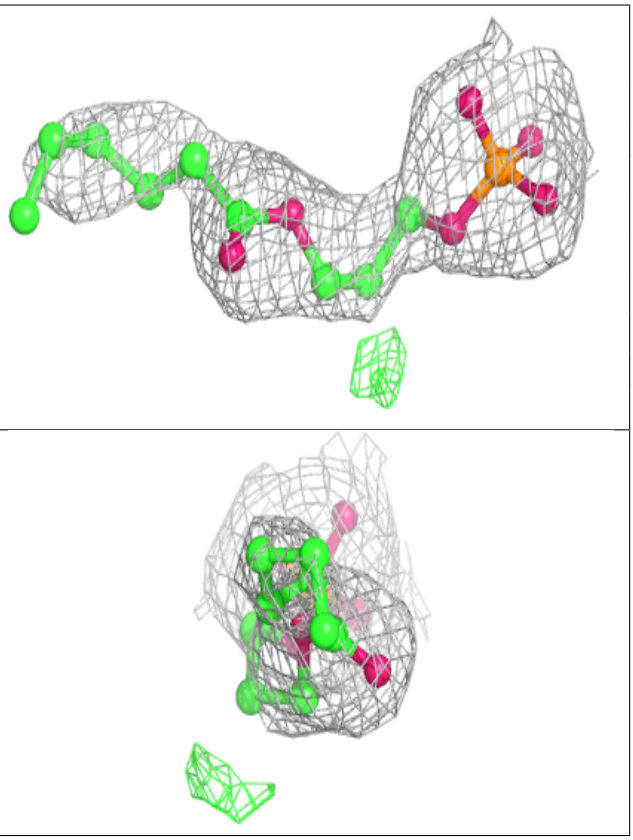
Electron density around 44E H 301:

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



Electron density around 44E A 302:

$2mF_o$-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.