



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:46 AM UTC

PDB ID : 5ID7 / pdb_00005id7
Title : Crystal structure of human serum albumin in complex with phosphorodithioate derivative of myristoyl cyclic phosphatidic acid (cPA)
Authors : Sekula, B.; Bujacz, A.; Rytczak, P.; Bujacz, G.
Deposited on : 2016-02-24
Resolution : 2.26 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

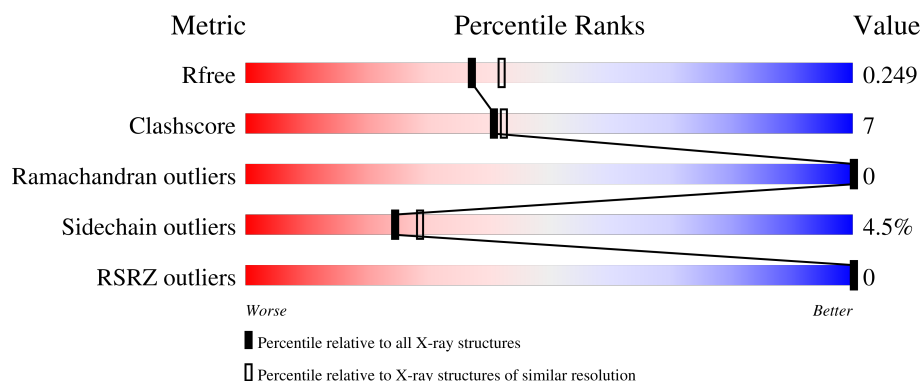
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	585	 80% 17% ..
1	B	585	 78% 20% ..

2 Entry composition [i](#)

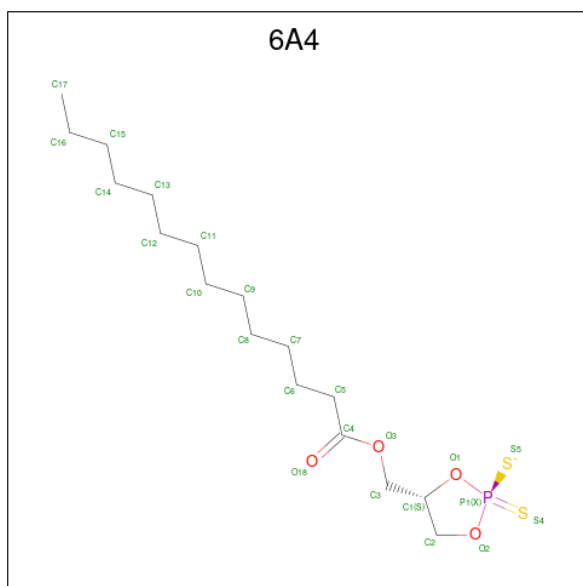
There are 5 unique types of molecules in this entry. The entry contains 9779 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	1	0
			4638	2928	786	883	41			
1	B	582	Total	C	N	O	S	0	1	0
			4636	2927	783	885	41			

- Molecule 2 is (4S)-2-sulfanylidene-4-[(tetradecanoyloxy)methyl]-1,3,2lambda 5 -dioxaphospholane-2-thiolate (CCD ID: 6A4) (formula: $C_{17}H_{32}O_4PS_2$).



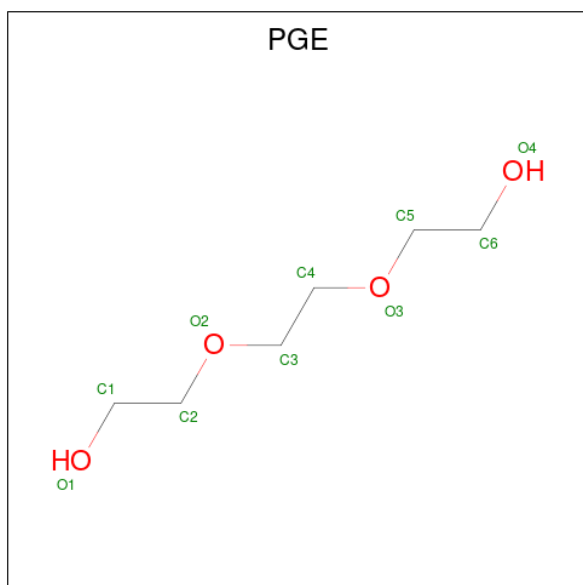
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	O	P	S	0	0
			24	17	4	1	2		
2	A	1	Total	C	O	P	S	0	0
			24	17	4	1	2		
2	A	1	Total	C	O	P	S	0	0
			24	17	4	1	2		
2	B	1	Total	C	O	P	S	0	0
			24	17	4	1	2		

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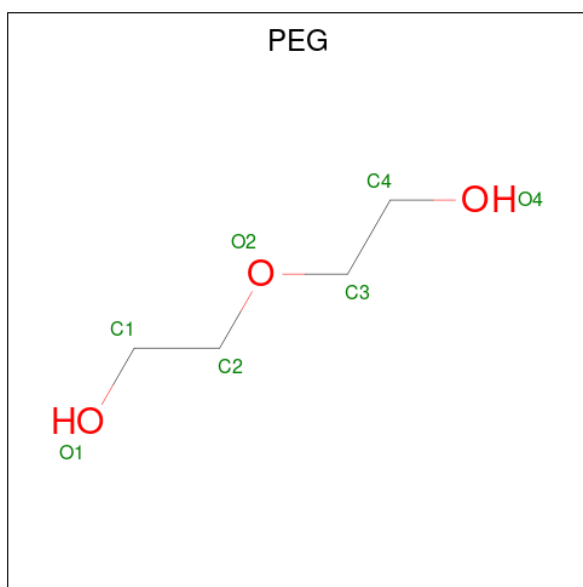
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	O	P	S	0	0
			24	17	4	1	2		
2	B	1	Total	C	O	P	S	0	0
			24	17	4	1	2		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

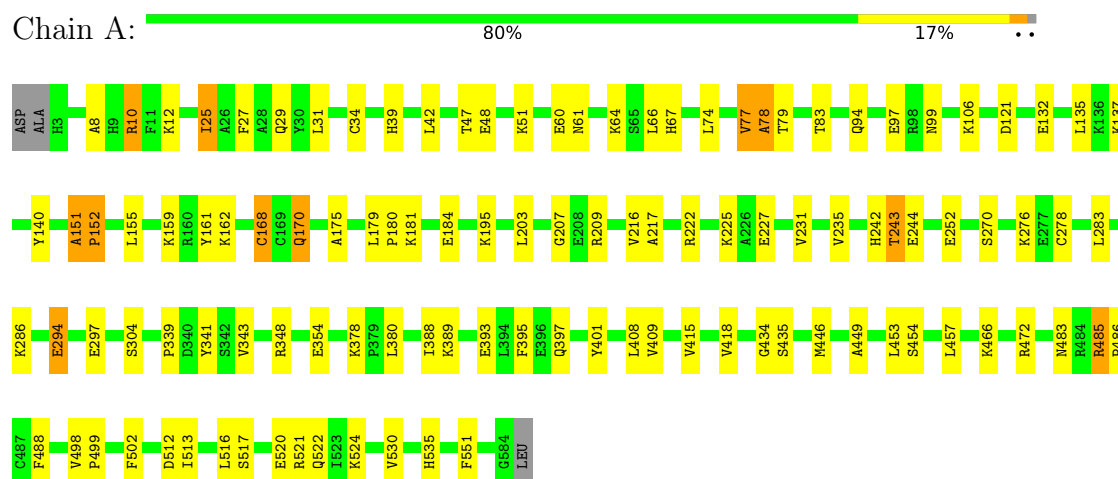
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	151	Total	O	0	0
			151	151		
5	B	159	Total	O	0	0
			159	159		

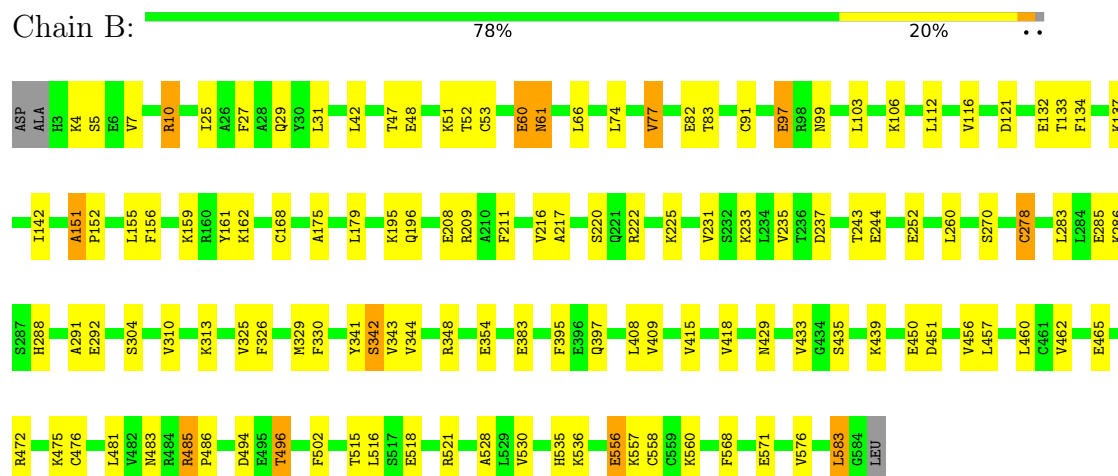
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Serum albumin



• Molecule 1: Serum albumin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	37.90Å 85.17Å 96.31Å 105.46° 89.78° 101.34°	Depositor
Resolution (Å)	45.90 – 2.26 45.90 – 2.26	Depositor EDS
% Data completeness (in resolution range)	93.6 (45.90-2.26) 86.8 (45.90-2.26)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.206 , 0.253 0.210 , 0.249	Depositor DCC
R_{free} test set	1012 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 20.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.247 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9779	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.19% 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: PEG, PGE, 6A4

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	1.30	7/4731 (0.1%)	1.24	18/6380 (0.3%)
1	B	1.30	11/4729 (0.2%)	1.24	19/6378 (0.3%)
All	All	1.30	18/9460 (0.2%)	1.24	37/12758 (0.3%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	462	VAL	C-O	-7.10	1.16	1.24
1	A	207	GLY	N-CA	6.45	1.51	1.45
1	B	341	TYR	CA-C	-6.27	1.44	1.52
1	A	378	LYS	C-O	-5.78	1.18	1.24
1	A	341	TYR	CA-C	-5.78	1.45	1.52
1	A	454	SER	N-CA	-5.74	1.39	1.46
1	A	78	ALA	CA-C	5.71	1.60	1.52
1	B	475	LYS	N-CA	-5.64	1.39	1.46
1	A	339	PRO	C-O	-5.62	1.16	1.24
1	B	220	SER	N-CA	-5.50	1.39	1.46
1	A	446	MET	C-O	-5.49	1.17	1.24
1	B	451	ASP	C-O	-5.48	1.17	1.24
1	B	528	ALA	N-CA	-5.39	1.39	1.46
1	B	310	VAL	CA-C	5.35	1.59	1.52
1	B	142	ILE	CA-C	-5.34	1.46	1.52
1	B	450	GLU	N-CA	-5.34	1.40	1.46
1	B	220	SER	CA-C	-5.19	1.46	1.52
1	B	476	CYS	CA-CB	-5.04	1.45	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	VAL	N-CA-C	-7.35	103.17	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	CYS	N-CA-C	6.61	120.55	112.23
1	A	78	ALA	CA-C-N	6.50	131.00	120.60
1	A	78	ALA	C-N-CA	6.50	131.00	120.60
1	B	383	GLU	CA-C-N	-6.47	113.02	119.56
1	B	383	GLU	C-N-CA	-6.47	113.02	119.56
1	A	121	ASP	CB-CA-C	-6.47	100.46	110.81
1	A	77	VAL	N-CA-CB	6.34	117.44	110.53
1	B	77	VAL	N-CA-CB	6.24	117.33	110.53
1	A	168	CYS	N-CA-C	6.08	118.87	111.82
1	B	409	VAL	N-CA-C	-6.01	104.47	110.30
1	B	91	CYS	N-CA-C	5.83	119.92	112.34
1	B	456	VAL	N-CA-C	-5.79	105.09	110.53
1	B	576	VAL	CB-CA-C	-5.66	104.50	112.14
1	A	151	ALA	CA-C-N	-5.66	113.85	119.56
1	A	151	ALA	C-N-CA	-5.66	113.85	119.56
1	B	151	ALA	CA-C-N	-5.65	113.80	119.56
1	B	151	ALA	C-N-CA	-5.65	113.80	119.56
1	B	27	PHE	N-CA-C	5.63	117.42	111.28
1	B	485	ARG	CA-C-N	-5.63	113.88	119.56
1	B	485	ARG	C-N-CA	-5.63	113.88	119.56
1	B	60	GLU	N-CA-C	5.61	118.38	109.96
1	A	27	PHE	N-CA-C	5.57	118.07	111.33
1	A	488	PHE	N-CA-C	5.48	117.69	111.11
1	A	397	GLN	N-CA-C	5.46	117.23	111.28
1	B	103	LEU	N-CA-C	5.45	117.22	111.28
1	A	485	ARG	CA-C-N	-5.44	113.43	119.19
1	A	485	ARG	C-N-CA	-5.44	113.43	119.19
1	B	342	SER	N-CA-C	-5.42	102.86	110.50
1	A	94	GLN	N-CA-C	-5.41	101.35	109.95
1	A	135	LEU	N-CA-C	5.31	116.75	111.07
1	B	397	GLN	N-CA-C	5.30	117.05	111.28
1	B	243	THR	N-CA-CB	5.29	117.90	110.12
1	A	25	ILE	CB-CA-C	-5.22	105.02	112.22
1	A	243	THR	N-CA-CB	5.16	117.71	110.12
1	B	278	CYS	N-CA-C	5.11	116.85	111.28
1	A	434	GLY	N-CA-C	-5.06	106.64	112.50

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	A	4638	0	4565	62	0
1	B	4636	0	4558	62	0
2	A	72	0	0	5	0
2	B	72	0	0	4	0
3	A	20	0	28	0	0
3	B	10	0	14	0	0
4	A	14	0	20	0	0
4	B	7	0	10	0	0
5	A	151	0	0	9	0
5	B	159	0	0	7	0
All	All	9779	0	9195	122	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 7.

All (122) 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:25:ILE:O	1:A:29:GLN:HG3	1.81	0.81
1:B:25:ILE:O	1:B:29:GLN:HG3	1.82	0.79
1:A:348:ARG:NH1	2:A:601:6A4:S4	2.53	0.79
1:B:326:PHE:HA	1:B:329:MET:HE3	1.64	0.77
1:A:78:ALA:HB3	1:B:515:THR:CG2	2.21	0.70
1:A:294:GLU:HG3	5:A:798:HOH:O	1.90	0.70
1:B:116:VAL:HB	5:B:784:HOH:O	1.94	0.67
1:A:61:ASN:OD1	1:A:64:LYS:HE3	1.96	0.64
1:B:156:PHE:CE1	1:B:285:GLU:HG2	2.35	0.62
1:A:276:LYS:HG2	5:A:721:HOH:O	1.99	0.61
1:A:78:ALA:HB3	1:B:515:THR:HG23	1.81	0.61
1:A:10:ARG:HG3	1:A:66:LEU:HD11	1.83	0.60
1:A:517:SER:OG	1:A:520:GLU:HG3	2.02	0.60
1:B:472:ARG:HD2	5:B:708:HOH:O	2.02	0.58
1:A:137:LYS:HE2	5:A:841:HOH:O	2.03	0.58
1:A:217:ALA:HB3	1:A:343:VAL:HG13	1.84	0.58
1:B:222:ARG:NH1	1:B:291:ALA:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ALA:O	1:B:179:LEU:HG	2.04	0.57
1:B:10:ARG:HG3	1:B:66:LEU:HD11	1.85	0.56
1:A:155:LEU:HG	1:A:159:LYS:HE3	1.87	0.56
1:A:222[B]:ARG:HG2	1:A:222[B]:ARG:HH11	1.70	0.56
1:B:155:LEU:HG	1:B:159:LYS:HE3	1.86	0.56
1:A:175:ALA:O	1:A:179:LEU:HG	2.05	0.56
1:B:217:ALA:HB3	1:B:343:VAL:HG13	1.86	0.56
1:A:8:ALA:O	1:A:12:LYS:HE3	2.05	0.55
1:A:512:ASP:HB2	1:A:516:LEU:HD21	1.88	0.55
1:B:342:SER:OG	2:B:601:6A4:S5	2.64	0.55
1:B:325:VAL:HG12	1:B:329:MET:HE2	1.89	0.55
1:B:485:ARG:HB3	2:B:601:6A4:S4	2.48	0.54
1:A:395:PHE:CZ	1:A:435:SER:HA	2.43	0.53
1:B:483:ASN:C	1:B:486:PRO:HD2	2.34	0.52
1:A:79:THR:HG23	1:A:83:THR:OG1	2.09	0.52
1:B:216:VAL:CG2	1:B:235:VAL:HG21	2.39	0.52
1:A:244:GLU:OE2	1:A:252:GLU:HB3	2.09	0.52
1:B:536:LYS:HG3	1:B:583:LEU:HD23	1.91	0.52
1:A:457:LEU:HD12	2:A:603:6A4:S5	2.50	0.52
1:A:216:VAL:CG2	1:A:235:VAL:HG21	2.39	0.52
1:B:494:ASP:OD1	1:B:496:THR:HG23	2.12	0.50
1:A:551:PHE:CD2	2:A:602:6A4:O18	2.65	0.50
1:A:242:HIS:C	5:A:713:HOH:O	2.54	0.50
1:A:485:ARG:NE	2:A:601:6A4:S4	2.75	0.49
1:A:512:ASP:OD1	1:A:513:ILE:N	2.46	0.49
1:A:203:LEU:CD2	5:A:713:HOH:O	2.61	0.48
1:B:61:ASN:HD22	1:B:61:ASN:N	2.09	0.48
1:B:395:PHE:CZ	1:B:435:SER:HA	2.48	0.48
1:A:31:LEU:HD11	1:A:74:LEU:HD23	1.95	0.48
1:A:67:HIS:CE1	1:A:252:GLU:OE2	2.67	0.48
1:B:60:GLU:HG3	1:B:61:ASN:HD22	1.80	0.47
1:A:170:GLN:O	1:A:170:GLN:HG3	2.15	0.47
1:A:34:CYS:SG	1:A:79:THR:HG21	2.55	0.47
1:B:556:GLU:OE2	1:B:560:LYS:HD2	2.14	0.47
1:A:483:ASN:C	1:A:486:PRO:HD2	2.40	0.47
1:A:415:VAL:HG12	1:A:418:VAL:HG23	1.96	0.47
1:B:209:ARG:NH2	1:B:354:GLU:OE1	2.47	0.47
1:B:415:VAL:HG12	1:B:418:VAL:HG23	1.95	0.47
1:A:551:PHE:CE2	2:A:602:6A4:O18	2.67	0.46
1:A:34:CYS:HB2	1:A:39:HIS:HE1	1.81	0.46
1:B:233:LYS:NZ	1:B:237:ASP:OD2	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:PHE:HA	1:B:329:MET:CE	2.40	0.46
1:A:513:ILE:O	1:A:521:ARG:HD3	2.15	0.46
1:B:31:LEU:HD11	1:B:74:LEU:HD23	1.97	0.46
1:B:60:GLU:HG3	1:B:61:ASN:ND2	2.30	0.46
1:A:502:PHE:HB2	1:A:535:HIS:CE1	2.51	0.46
1:A:47:THR:O	1:A:51:LYS:HG2	2.16	0.46
1:B:47:THR:O	1:B:51:LYS:HG2	2.16	0.46
1:A:472:ARG:HD2	5:A:789:HOH:O	2.16	0.45
1:B:216:VAL:HG23	1:B:235:VAL:HG21	1.98	0.45
1:B:7:VAL:HG12	5:B:737:HOH:O	2.15	0.45
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.99	0.45
1:A:209:ARG:NH2	1:A:354:GLU:OE1	2.49	0.44
1:A:60:GLU:O	1:A:61:ASN:HB2	2.18	0.44
1:A:516:LEU:CD1	1:A:524:LYS:HE3	2.48	0.44
1:A:161:TYR:O	1:A:162:LYS:C	2.61	0.44
1:B:439:LYS:HB3	5:B:824:HOH:O	2.17	0.44
1:B:161:TYR:O	1:B:162:LYS:C	2.61	0.43
1:A:216:VAL:HG23	1:A:235:VAL:HG21	1.99	0.43
1:B:237:ASP:HB3	1:B:260:LEU:HD13	1.99	0.43
1:A:34:CYS:HB2	1:A:39:HIS:CE1	2.53	0.43
1:B:133:THR:O	1:B:134:PHE:C	2.61	0.43
1:A:243:THR:N	5:A:713:HOH:O	2.51	0.43
1:A:408:LEU:HD22	1:A:530:VAL:CG2	2.48	0.43
1:A:401:TYR:CE1	1:A:522:GLN:HG2	2.54	0.43
1:B:97:GLU:HB3	5:B:849:HOH:O	2.18	0.43
1:B:83:THR:HG21	5:B:811:HOH:O	2.19	0.43
1:B:208:GLU:O	1:B:209:ARG:C	2.61	0.43
1:B:288:HIS:NE2	1:B:292:GLU:OE1	2.52	0.43
1:B:112:LEU:HB2	5:B:836:HOH:O	2.18	0.43
1:B:502:PHE:HB2	1:B:535:HIS:CE1	2.54	0.43
1:B:244:GLU:OE2	1:B:252:GLU:HB3	2.18	0.42
1:B:52:THR:OG1	1:B:53:CYS:N	2.53	0.42
1:A:485:ARG:O	1:A:485:ARG:HD2	2.19	0.42
1:A:278:CYS:O	1:A:286:LYS:HG3	2.20	0.42
1:B:408:LEU:HD22	1:B:530:VAL:CG2	2.48	0.42
1:A:216:VAL:HG22	1:A:235:VAL:HG21	2.01	0.42
1:B:558:CYS:HB3	1:B:568:PHE:CE2	2.55	0.42
1:A:180:PRO:O	1:A:184:GLU:HG2	2.20	0.42
1:B:557:LYS:HE2	1:B:571:GLU:HG3	2.02	0.42
1:A:151:ALA:HB3	1:A:152:PRO:HD3	2.03	0.41
1:B:60:GLU:CG	1:B:61:ASN:ND2	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:VAL:HG23	1:B:481:LEU:CD2	2.51	0.41
1:B:348:ARG:NH1	2:B:601:6A4:S4	2.78	0.41
1:B:457:LEU:HD12	2:B:603:6A4:S5	2.59	0.41
1:B:278:CYS:O	1:B:286:LYS:HG3	2.20	0.41
1:A:195:LYS:HE3	1:A:195:LYS:HB2	1.91	0.41
1:A:222[B]:ARG:HG2	1:A:222[B]:ARG:NH1	2.33	0.41
1:A:389:LYS:O	1:A:393:GLU:HG3	2.20	0.41
1:B:429:ASN:O	1:B:433:VAL:HG23	2.20	0.41
1:B:485:ARG:O	1:B:485:ARG:HD2	2.19	0.41
1:A:242:HIS:HB3	5:A:713:HOH:O	2.20	0.41
1:B:216:VAL:HG22	1:B:235:VAL:HG21	2.02	0.41
1:B:485:ARG:N	1:B:486:PRO:CD	2.84	0.41
1:A:516:LEU:HD11	1:A:524:LYS:HE3	2.02	0.41
1:B:231:VAL:O	1:B:235:VAL:HG23	2.21	0.41
1:A:498:VAL:O	1:A:499:PRO:C	2.61	0.41
1:B:211:PHE:CD1	1:B:211:PHE:C	2.98	0.41
1:A:227:GLU:HG2	5:A:709:HOH:O	2.20	0.41
1:B:195:LYS:HE3	1:B:195:LYS:HB2	1.94	0.41
1:B:516:LEU:O	1:B:521:ARG:NH2	2.54	0.41
1:A:168:CYS:SG	1:A:181:LYS:HD2	2.61	0.40
1:A:449:ALA:O	1:A:453:LEU:HB2	2.21	0.40
1:B:330:PHE:CD1	1:B:330:PHE:C	2.99	0.40
1:A:231:VAL:O	1:A:235:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	581/585 (99%)	558 (96%)	23 (4%)	0	100	100
1	B	581/585 (99%)	550 (95%)	31 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1162/1170 (99%)	1108 (95%)	54 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	510/511 (100%)	490 (96%)	20 (4%)	28	35
1	B	510/511 (100%)	484 (95%)	26 (5%)	21	23
All	All	1020/1022 (100%)	974 (96%)	46 (4%)	24	29

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

Mol	Chain	Res	Type
1	A	10	ARG
1	A	42	LEU
1	A	48	GLU
1	A	77	VAL
1	A	97	GLU
1	A	99	ASN
1	A	106	LYS
1	A	132	GLU
1	A	140	TYR
1	A	152	PRO
1	A	170	GLN
1	A	225	LYS
1	A	270	SER
1	A	283	LEU
1	A	294	GLU
1	A	297	GLU
1	A	304	SER
1	A	380	LEU
1	A	388	ILE
1	A	466	LYS

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Mol	Chain	Res	Type
1	B	4	LYS
1	B	5	SER
1	B	10	ARG
1	B	42	LEU
1	B	48	GLU
1	B	61	ASN
1	B	77	VAL
1	B	82	GLU
1	B	97	GLU
1	B	99	ASN
1	B	106	LYS
1	B	121	ASP
1	B	132	GLU
1	B	137	LYS
1	B	196	GLN
1	B	225	LYS
1	B	270	SER
1	B	283	LEU
1	B	304	SER
1	B	313	LYS
1	B	460	LEU
1	B	465	GLU
1	B	496	THR
1	B	518	GLU
1	B	556	GLU
1	B	583	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	99	ASN
1	B	61	ASN
1	B	99	ASN
1	B	170	GLN
1	B	268	GLN
1	B	385	GLN
1	B	503	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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$
2	6A4	A	603	-	22,24,24	1.26	2 (9%)	24,29,29	1.39	3 (12%)
3	PGE	A	604	-	9,9,9	0.46	0	8,8,8	0.58	0
2	6A4	B	602	-	22,24,24	1.03	2 (9%)	24,29,29	1.36	3 (12%)
4	PEG	A	607	-	6,6,6	0.62	0	5,5,5	0.39	0
3	PGE	A	606	-	9,9,9	0.62	0	8,8,8	0.84	0
4	PEG	A	605	-	6,6,6	0.73	0	5,5,5	0.73	0
2	6A4	A	601	-	22,24,24	1.17	1 (4%)	24,29,29	1.18	3 (12%)
2	6A4	B	603	-	22,24,24	1.11	2 (9%)	24,29,29	1.35	4 (16%)
3	PGE	B	604	-	9,9,9	0.48	0	8,8,8	0.39	0
4	PEG	B	605	-	6,6,6	0.72	0	5,5,5	0.90	0
2	6A4	A	602	-	22,24,24	1.13	2 (9%)	24,29,29	1.38	4 (16%)
2	6A4	B	601	-	22,24,24	1.07	1 (4%)	24,29,29	1.10	3 (12%)

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
2	6A4	A	603	-	-	11/18/29/29	0/1/1/1
3	PGE	A	604	-	-	4/7/7/7	-
2	6A4	B	602	-	-	11/18/29/29	0/1/1/1
4	PEG	A	607	-	-	3/4/4/4	-
3	PGE	A	606	-	-	3/7/7/7	-
4	PEG	A	605	-	-	1/4/4/4	-
2	6A4	A	601	-	-	7/18/29/29	0/1/1/1
2	6A4	B	603	-	-	7/18/29/29	0/1/1/1
3	PGE	B	604	-	-	4/7/7/7	-
4	PEG	B	605	-	-	0/4/4/4	-
2	6A4	A	602	-	-	9/18/29/29	0/1/1/1
2	6A4	B	601	-	-	9/18/29/29	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	6A4	O3-C4	4.75	1.47	1.33
2	A	603	6A4	O3-C4	4.67	1.47	1.33
2	B	603	6A4	O3-C4	4.24	1.45	1.33
2	B	601	6A4	O3-C4	4.08	1.45	1.33
2	A	602	6A4	O3-C4	3.90	1.44	1.33
2	B	602	6A4	O3-C4	3.74	1.44	1.33
2	A	602	6A4	P1-S4	2.69	1.99	1.93
2	A	603	6A4	P1-S4	2.61	1.99	1.93
2	B	602	6A4	P1-S4	2.49	1.98	1.93
2	B	603	6A4	P1-S4	2.30	1.98	1.93

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	6A4	O2-P1-S5	4.14	118.12	106.42
2	B	603	6A4	O2-P1-S5	4.05	117.87	106.42
2	B	602	6A4	O3-C4-C5	3.56	122.69	111.83
2	A	601	6A4	O3-C4-C5	3.17	121.51	111.83
2	B	601	6A4	O3-C4-C5	3.13	121.37	111.83
2	A	603	6A4	O3-C4-C5	3.09	121.26	111.83
2	A	602	6A4	O3-C4-C5	3.09	121.25	111.83
2	A	602	6A4	O1-P1-S5	2.79	114.09	106.61
2	B	602	6A4	O3-C4-O18	-2.60	117.12	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	603	6A4	O3-C4-C5	2.59	119.74	111.83
2	B	601	6A4	O3-C4-O18	-2.54	117.28	123.63
2	A	601	6A4	O2-P1-S5	2.45	113.36	106.42
2	B	603	6A4	O1-C1-C2	2.44	108.08	103.05
2	A	602	6A4	O3-C4-O18	-2.43	117.55	123.63
2	A	603	6A4	C3-O3-C4	2.36	125.76	117.12
2	A	602	6A4	C14-C13-C12	-2.36	102.42	114.37
2	B	602	6A4	O1-P1-S5	2.27	112.71	106.61
2	B	601	6A4	O1-C1-C2	2.08	107.35	103.05
2	A	601	6A4	O1-C1-C2	2.06	107.30	103.05
2	B	603	6A4	O3-C4-O18	-2.03	118.55	123.63

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	6A4	O1-C1-C3-O3
2	A	602	6A4	C2-C1-C3-O3
2	A	603	6A4	O1-C1-C3-O3
2	A	603	6A4	C2-C1-C3-O3
2	B	602	6A4	O1-C1-C3-O3
2	B	602	6A4	C2-C1-C3-O3
2	B	603	6A4	C2-C1-C3-O3
2	B	601	6A4	O18-C4-O3-C3
2	B	601	6A4	C5-C4-O3-C3
2	A	601	6A4	C5-C4-O3-C3
2	A	601	6A4	O18-C4-O3-C3
2	A	602	6A4	O18-C4-O3-C3
2	A	603	6A4	C12-C13-C14-C15
3	A	606	PGE	O3-C5-C6-O4
2	B	602	6A4	C4-C5-C6-C7
2	B	603	6A4	C4-C5-C6-C7
3	A	604	PGE	O3-C5-C6-O4
3	A	606	PGE	O1-C1-C2-O2
3	B	604	PGE	O3-C5-C6-O4
2	A	602	6A4	C5-C4-O3-C3
2	B	601	6A4	C10-C11-C12-C13
2	B	602	6A4	C7-C8-C9-C10
2	A	602	6A4	C5-C6-C7-C8
2	B	601	6A4	C12-C13-C14-C15
2	B	602	6A4	C6-C7-C8-C9
2	A	601	6A4	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	A	604	PGE	O1-C1-C2-O2
4	A	607	PEG	O2-C3-C4-O4
2	B	601	6A4	C5-C6-C7-C8
2	A	601	6A4	C5-C6-C7-C8
2	B	602	6A4	C11-C10-C9-C8
3	B	604	PGE	O2-C3-C4-O3
2	A	603	6A4	C11-C10-C9-C8
2	B	602	6A4	C5-C6-C7-C8
4	A	605	PEG	O2-C3-C4-O4
2	A	602	6A4	C6-C7-C8-C9
2	A	603	6A4	C14-C15-C16-C17
2	B	601	6A4	C11-C10-C9-C8
2	A	603	6A4	C10-C11-C12-C13
2	B	603	6A4	C7-C8-C9-C10
2	A	603	6A4	C13-C14-C15-C16
2	A	601	6A4	C6-C7-C8-C9
3	A	604	PGE	O2-C3-C4-O3
2	A	603	6A4	C9-C10-C11-C12
2	B	602	6A4	C9-C10-C11-C12
2	B	602	6A4	O18-C4-O3-C3
2	A	603	6A4	O18-C4-O3-C3
2	A	602	6A4	C9-C10-C11-C12
3	A	606	PGE	C4-C3-O2-C2
4	A	607	PEG	O1-C1-C2-O2
2	B	603	6A4	C14-C15-C16-C17
2	A	601	6A4	C12-C13-C14-C15
2	A	603	6A4	C5-C4-O3-C3
3	A	604	PGE	C1-C2-O2-C3
2	B	603	6A4	C11-C10-C9-C8
2	B	603	6A4	C11-C12-C13-C14
2	A	602	6A4	C10-C11-C12-C13
4	A	607	PEG	C1-C2-O2-C3
2	B	601	6A4	C7-C8-C9-C10
3	B	604	PGE	C3-C4-O3-C5
2	A	603	6A4	C7-C8-C9-C10
2	A	602	6A4	C4-C5-C6-C7
2	B	602	6A4	C13-C14-C15-C16
3	B	604	PGE	C1-C2-O2-C3
2	B	601	6A4	C13-C14-C15-C16
2	A	601	6A4	C10-C11-C12-C13
2	B	603	6A4	O1-C1-C3-O3
2	B	602	6A4	C5-C4-O3-C3

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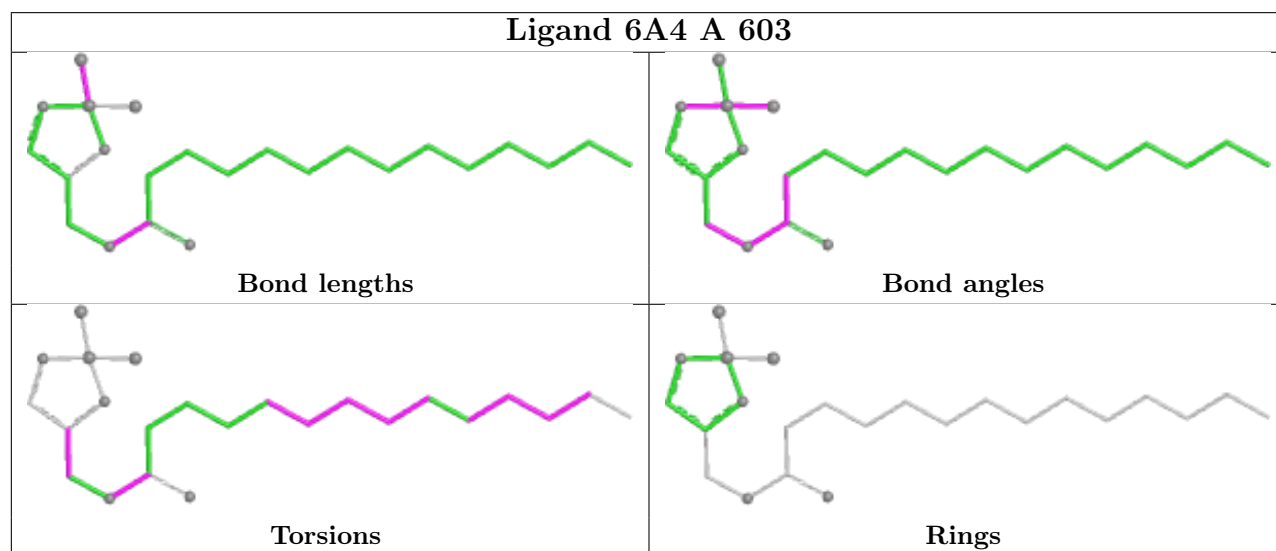
Mol	Chain	Res	Type	Atoms
2	B	601	6A4	C9-C10-C11-C12

There are no ring outliers.

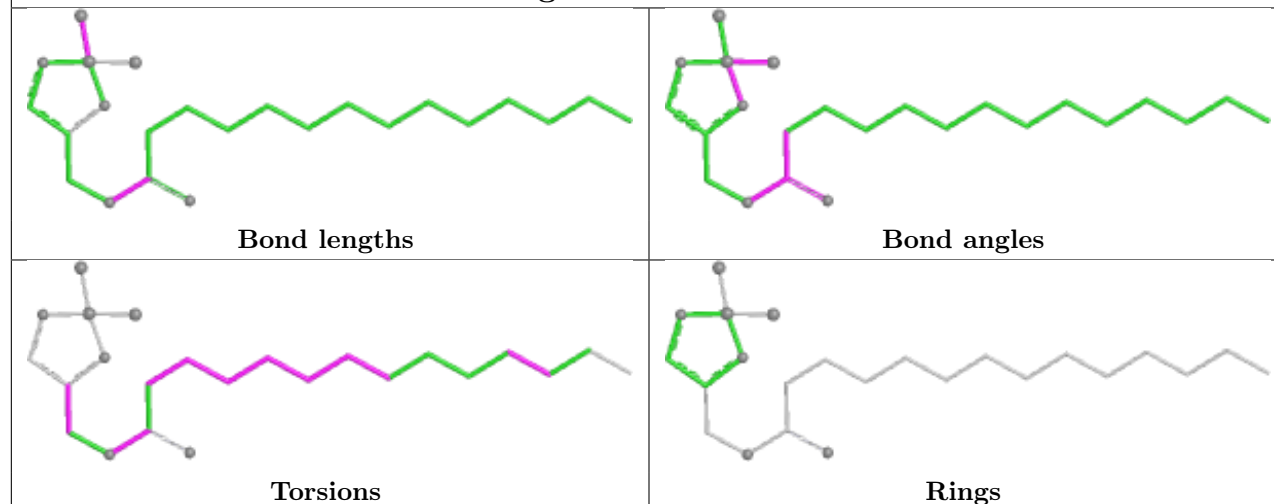
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	6A4	1	0
2	A	601	6A4	2	0
2	B	603	6A4	1	0
2	A	602	6A4	2	0
2	B	601	6A4	3	0

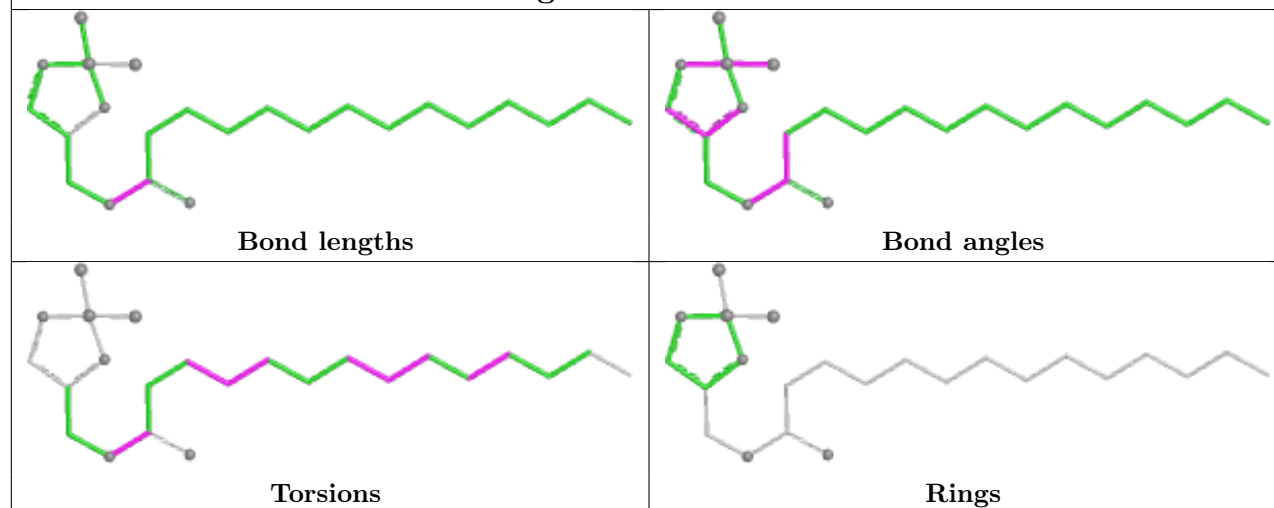
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



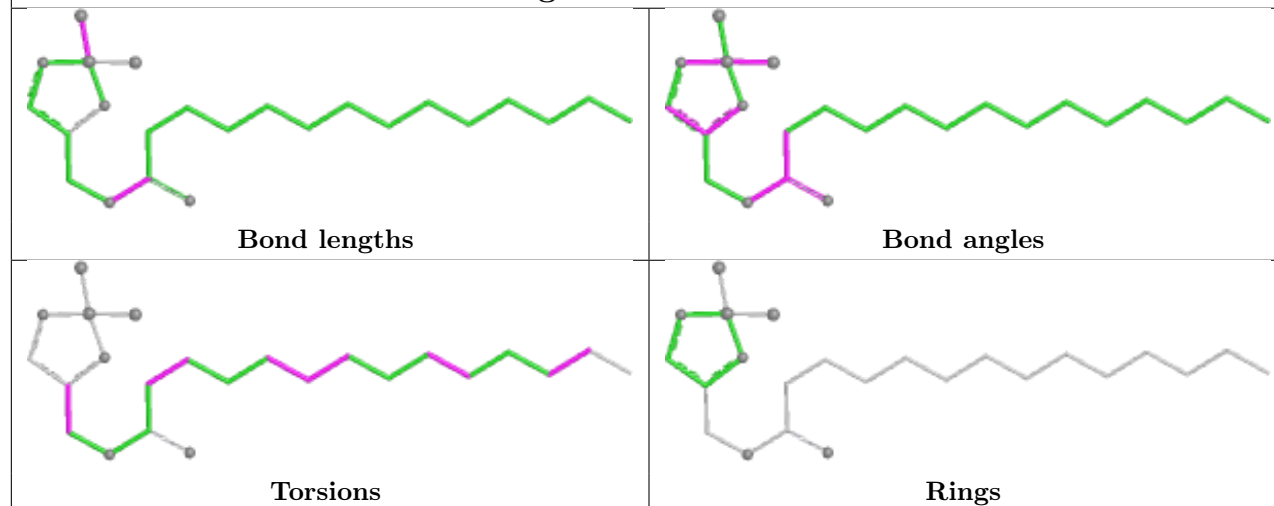
Ligand 6A4 B 602

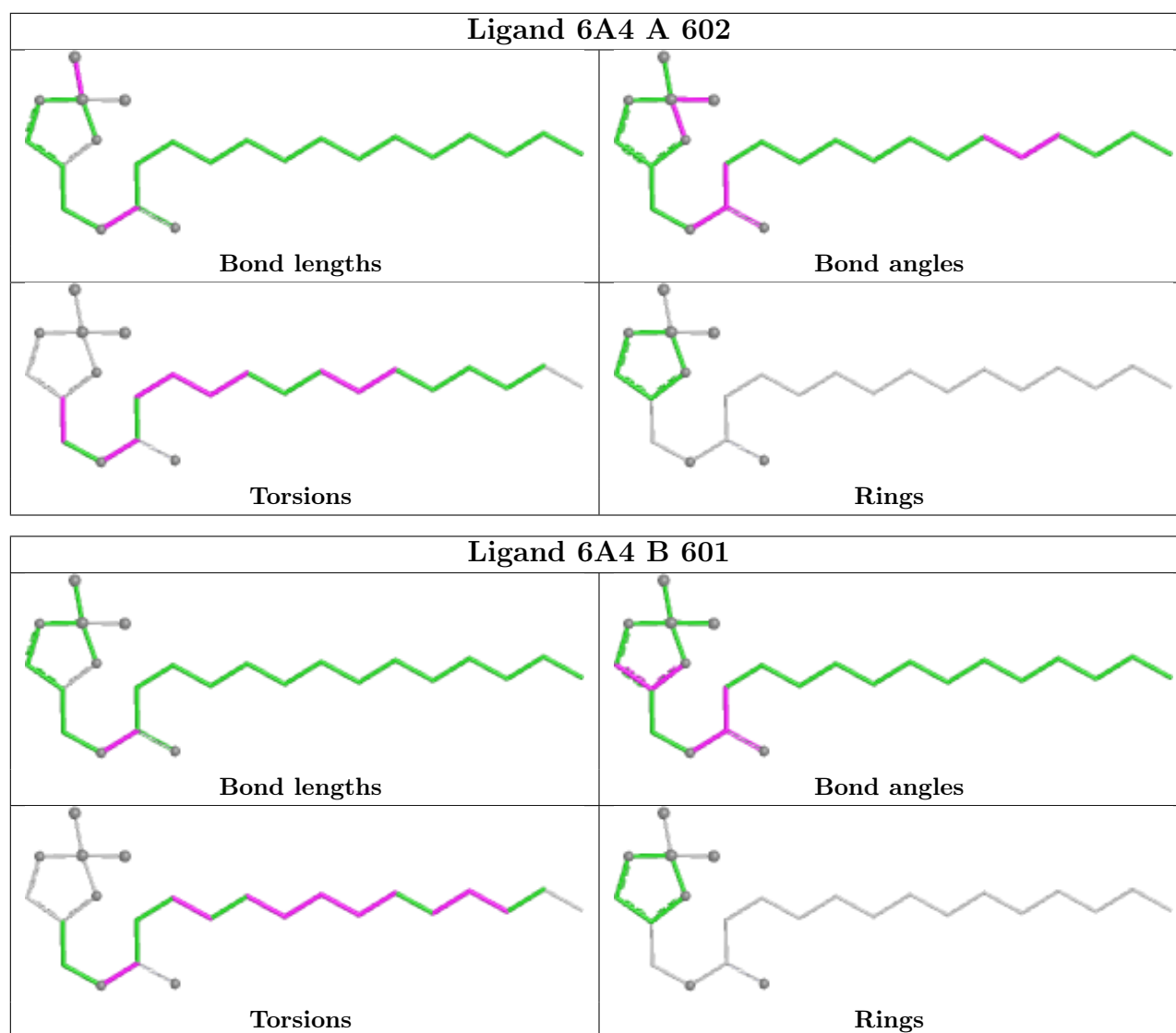


Ligand 6A4 A 601



Ligand 6A4 B 603





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	A	582/585 (99%)	-1.44	0 100 100	18, 45, 77, 95	1 (0%)
1	B	582/585 (99%)	-1.48	0 100 100	22, 44, 69, 102	1 (0%)
All	All	1164/1170 (99%)	-1.46	0 100 100	18, 44, 73, 102	2 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PGE	A	606	10/10	0.98	0.05	36,40,42,43	0
2	6A4	A	602	24/24	0.99	0.03	26,33,54,59	0
2	6A4	A	603	24/24	0.99	0.04	34,52,59,60	0
2	6A4	B	601	24/24	0.99	0.04	33,53,74,80	0
2	6A4	B	602	24/24	0.99	0.03	29,39,56,69	0
2	6A4	B	603	24/24	0.99	0.05	42,70,80,83	0
3	PGE	A	604	10/10	0.99	0.03	42,45,48,55	0

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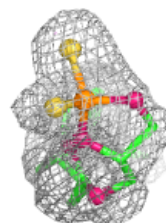
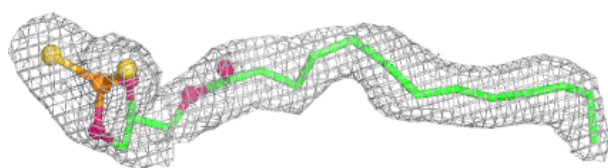
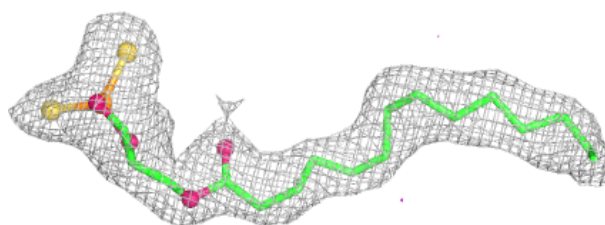
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	6A4	A	601	24/24	0.99	0.05	33,52,60,68	0
3	PGE	B	604	10/10	0.99	0.04	56,57,64,65	0
4	PEG	A	605	7/7	0.99	0.05	41,46,51,52	0
4	PEG	A	607	7/7	0.99	0.04	46,51,55,58	0
4	PEG	B	605	7/7	0.99	0.04	30,31,36,38	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.

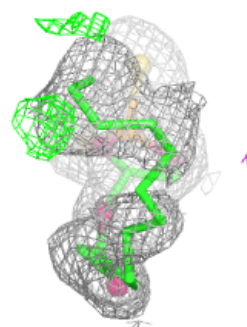
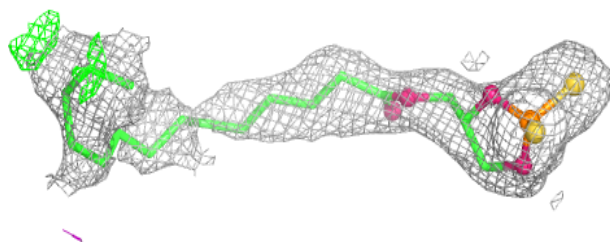
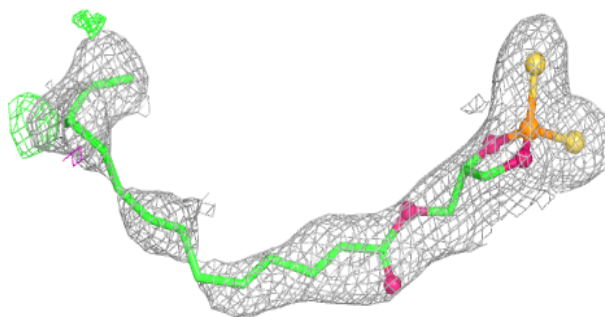
Electron density around 6A4 A 602:

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

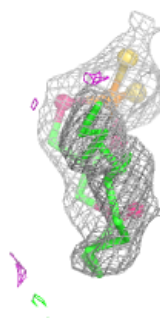
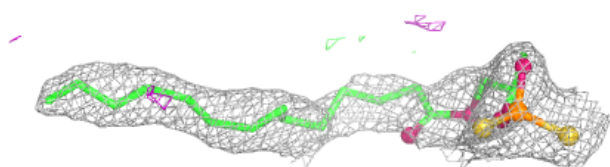
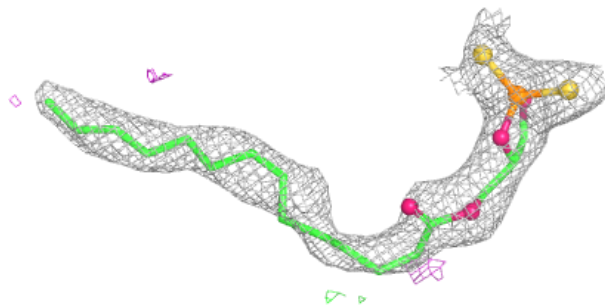


Electron density around 6A4 A 603:

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

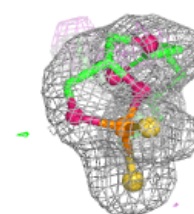
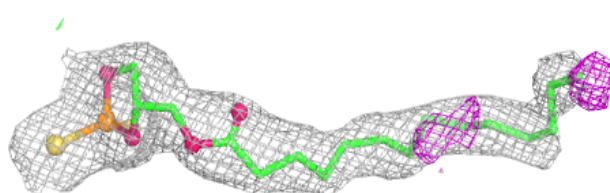
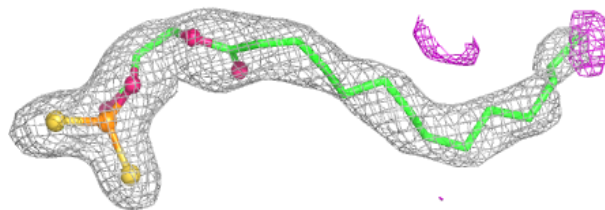
**Electron density around 6A4 B 601:**

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

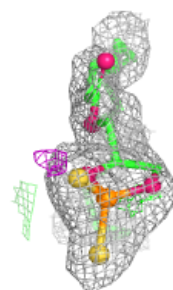
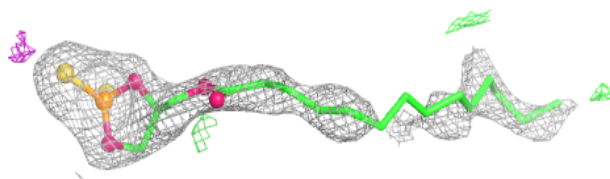
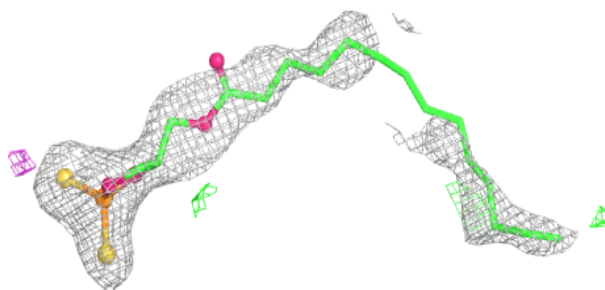


Electron density around 6A4 B 602:

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

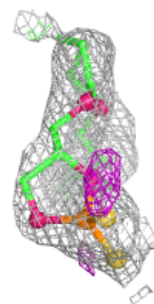
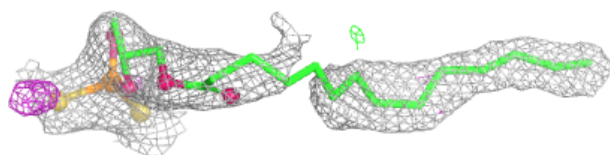
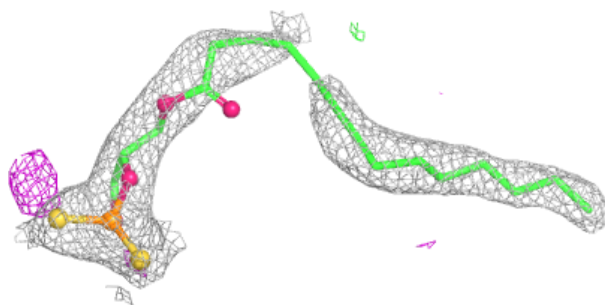
**Electron density around 6A4 B 603:**

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



Electron density around 6A4 A 601:

$2mF_o-DF_c$ (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.