



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2021 – 04:10 PM EDT

PDB ID : 4OUR
Title : Crystal structure of Arabidopsis thaliana phytochrome B photosensory module
Authors : Sethe Burgie, E.; Bussell, A.N.; Walker, J.M.; Dubiel, K.; Vierstra, R.D.
Deposited on : 2014-02-18
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

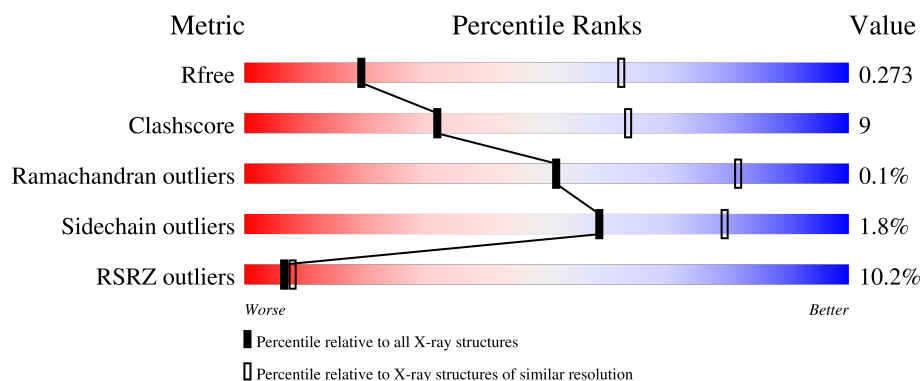
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	544	<div> <div>10%</div> <div>61%</div> <div>21%</div> <div>•</div> <div>18%</div> </div>
2	B	544	<div> <div>6%</div> <div>67%</div> <div>15%</div> <div>18%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	707	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7100 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 Phytochrome B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	1	0
			3494	2212	614	640	28			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	MET	-	expression tag	UNP P14713
A	625	SER	-	expression tag	UNP P14713
A	626	LEU	-	expression tag	UNP P14713
A	627	HIS	-	expression tag	UNP P14713
A	628	HIS	-	expression tag	UNP P14713
A	629	HIS	-	expression tag	UNP P14713
A	630	HIS	-	expression tag	UNP P14713
A	631	HIS	-	expression tag	UNP P14713
A	632	HIS	-	expression tag	UNP P14713

- Molecule 2 is a protein called Phytochrome B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	445	Total	C	N	O	S	0	1	0
			3438	2176	603	631	28			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	89	MET	-	expression tag	UNP P14713
B	498	UNK	GLU	SEE REMARK 999	UNP P14713
B	499	UNK	VAL	SEE REMARK 999	UNP P14713
B	500	UNK	GLN	SEE REMARK 999	UNP P14713
B	501	UNK	ILE	SEE REMARK 999	UNP P14713
B	502	UNK	LYS	SEE REMARK 999	UNP P14713
B	503	UNK	ASP	SEE REMARK 999	UNP P14713

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Chain	Residue	Modelled	Actual	Comment	Reference
B	504	UNK	VAL	SEE REMARK 999	UNP P14713
B	505	UNK	VAL	SEE REMARK 999	UNP P14713
B	506	UNK	GLU	SEE REMARK 999	UNP P14713
B	507	UNK	TRP	SEE REMARK 999	UNP P14713
B	508	UNK	LEU	SEE REMARK 999	UNP P14713
B	509	UNK	LEU	SEE REMARK 999	UNP P14713
B	510	UNK	ALA	SEE REMARK 999	UNP P14713
B	526	UNK	GLY	SEE REMARK 999	UNP P14713
B	527	UNK	TYR	SEE REMARK 999	UNP P14713
B	528	UNK	PRO	SEE REMARK 999	UNP P14713
B	529	UNK	GLY	SEE REMARK 999	UNP P14713
B	530	UNK	ALA	SEE REMARK 999	UNP P14713
B	531	UNK	ALA	SEE REMARK 999	UNP P14713
B	625	SER	-	expression tag	UNP P14713
B	626	LEU	-	expression tag	UNP P14713
B	627	HIS	-	expression tag	UNP P14713
B	628	HIS	-	expression tag	UNP P14713
B	629	HIS	-	expression tag	UNP P14713
B	630	HIS	-	expression tag	UNP P14713
B	631	HIS	-	expression tag	UNP P14713
B	632	HIS	-	expression tag	UNP P14713

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



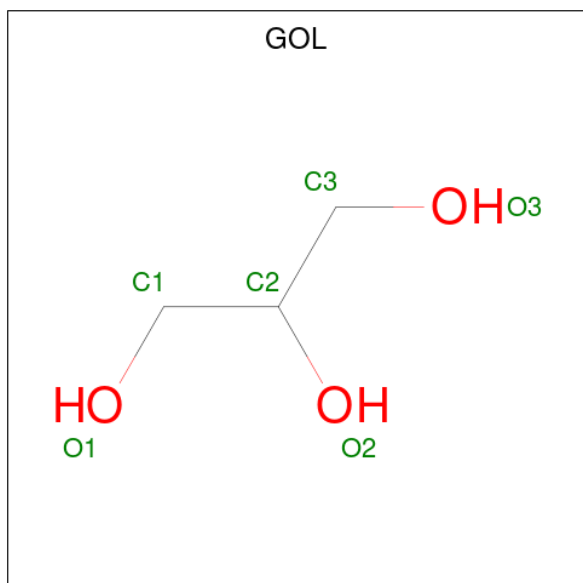
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



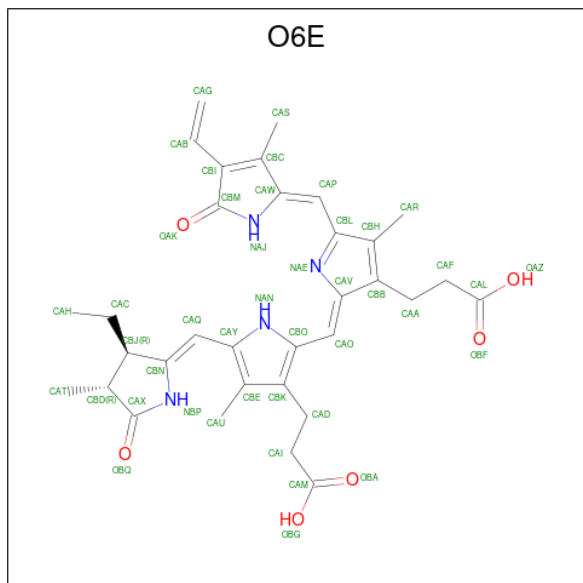
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is 3-[5-[(3 {R},4 {R})-3-ethyl-4-methyl-5-oxidanylidene-3,4-dihydropyrrol-2-yl)methyl]-2-[5-(4-ethyl-3-methyl-5-oxidanylidene-pyrrol-2-yl)methyl]-3-(3-hydroxy-3-oxopropyl)-4-methyl-1 {H}-pyrrol-2-yl)methyl]-4-methyl-1 {H}-pyrrol-3-yl]propanoic acid (three-letter code: O6E) (formula: C₃₃H₃₈N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 43	C 33	N 4	O 6	0	0
5	B	1	Total 43	C 33	N 4	O 6	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

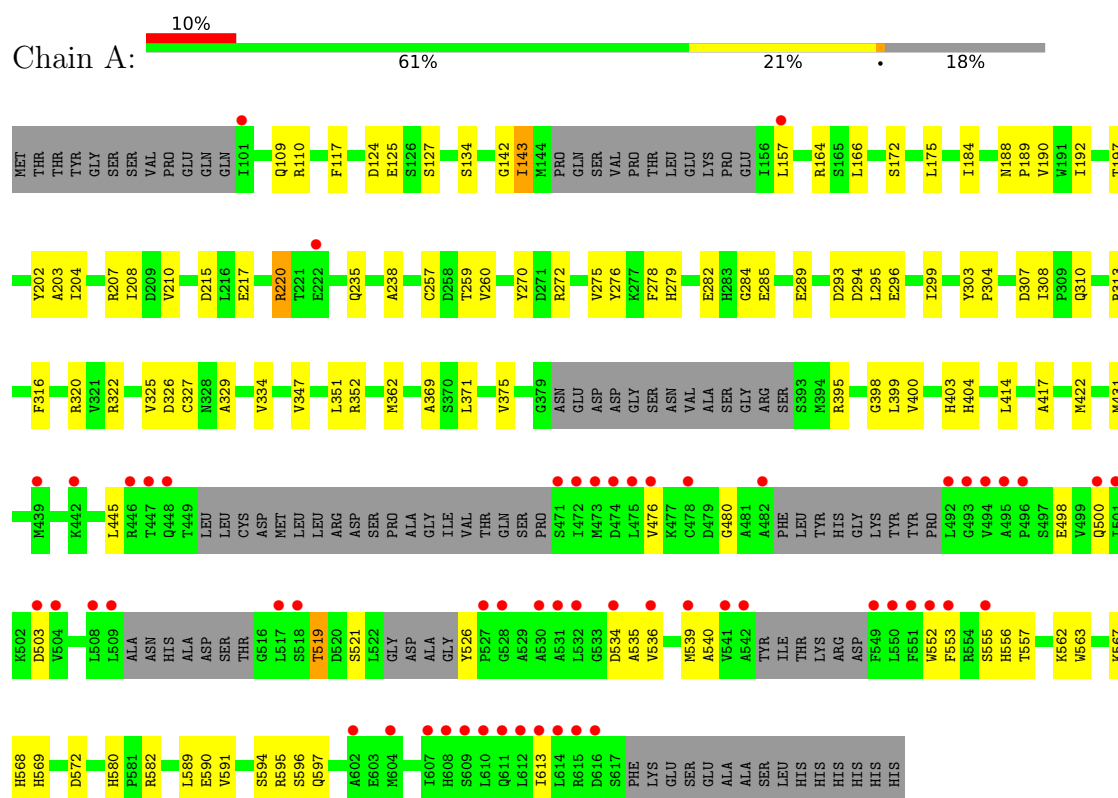
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	O	0	0
			2	2		
7	B	3	Total	O	0	0
			3	3		

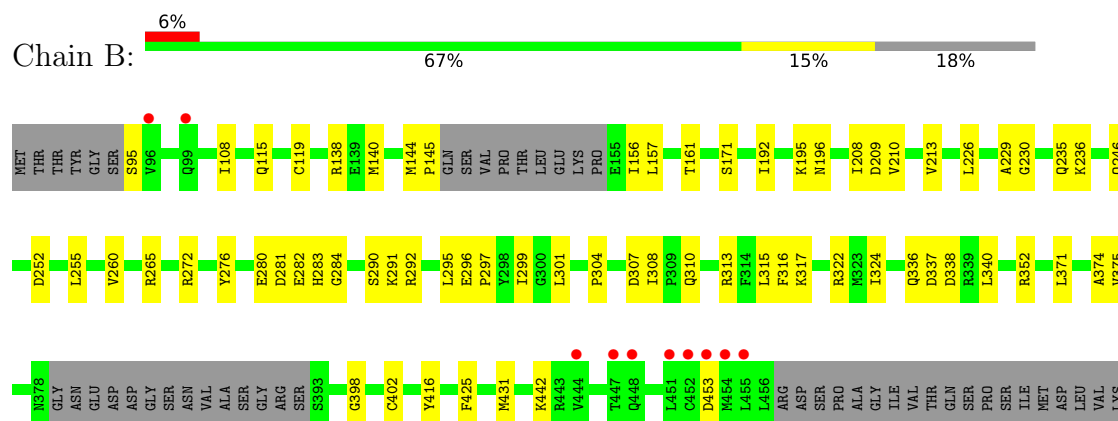
3 Residue-property plots

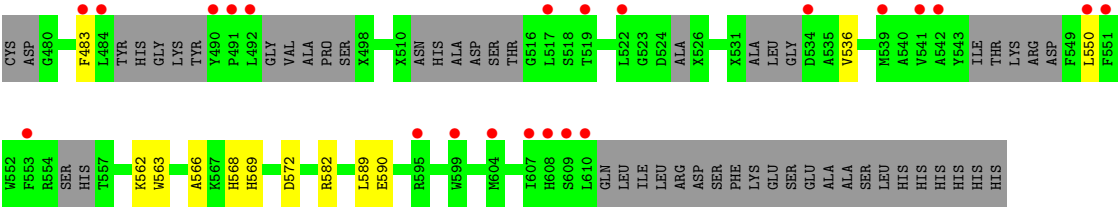
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: Phytochrome B





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.50Å 127.50Å 300.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 3.40 49.57 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.56-3.40) 91.3 (49.57-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.242 , 0.270 0.247 , 0.273	Depositor DCC
R_{free} test set	1751 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7100	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, SO4, PGE, O6E

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.21	0/3557	0.37	0/4805
2	B	0.21	0/3406	0.36	0/4599
All	All	0.21	0/6963	0.37	0/9404

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

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	3494	0	3500	80	0
2	B	3438	0	3356	52	0
3	A	35	0	0	4	0
3	B	20	0	0	0	0
4	A	6	0	8	2	0
4	B	6	0	8	0	0
5	A	43	0	0	2	0
5	B	43	0	0	3	0
6	B	10	0	14	0	0
7	A	2	0	0	0	0
7	B	3	0	0	1	0
All	All	7100	0	6886	124	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 9.

All (124) 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:B:265:ARG:NH1	2:B:290:SER:O	2.13	0.82
1:A:540:ALA:HB3	1:A:552:TRP:HB2	1.63	0.79
1:A:567:LYS:NZ	1:A:590:GLU:OE2	2.12	0.78
1:A:503:ASP:OD2	1:A:526:TYR:OH	2.00	0.78
1:A:395:ARG:NH1	3:A:707:SO4:O1	2.17	0.78
2:B:272[A]:ARG:NH1	7:B:801:HOH:O	2.18	0.77
2:B:138:ARG:NH1	2:B:157:LEU:O	2.18	0.76
1:A:184:ILE:HD11	1:A:207:ARG:HH11	1.50	0.76
2:B:282:GLU:HB3	2:B:313:ARG:HH12	1.57	0.70
1:A:556:HIS:HA	1:A:596:SER:HA	1.75	0.69
1:A:238:ALA:HB2	1:A:417:ALA:HB1	1.74	0.68
1:A:519:THR:HG22	1:A:539:MET:HG2	1.78	0.66
1:A:327:CYS:HB3	1:A:362:MET:HE2	1.79	0.65
1:A:125:GLU:OE1	1:A:207:ARG:NH2	2.27	0.65
2:B:281:ASP:OD1	2:B:283:HIS:ND1	2.24	0.64
1:A:110:ARG:NH1	3:A:706:SO4:O3	2.25	0.64
1:A:278:PHE:HD1	1:A:398:GLY:HA2	1.62	0.64
1:A:322:ARG:NH1	1:A:352:ARG:NH1	2.45	0.63
2:B:297:PRO:HB2	2:B:299:ILE:HG22	1.80	0.63
2:B:304:PRO:HA	2:B:568:HIS:HB2	1.80	0.62
1:A:307:ASP:OD1	1:A:582:ARG:NH1	2.33	0.62
1:A:580:HIS:ND1	3:A:702:SO4:O1	2.33	0.61
1:A:431:MET:HG3	2:B:431:MET:HB2	1.82	0.61
2:B:336:GLN:HB2	2:B:340:LEU:HD12	1.83	0.60
1:A:563:TRP:NE1	1:A:590:GLU:OE1	2.35	0.60
2:B:322:ARG:NH2	2:B:352:ARG:O	2.35	0.60
1:A:276:TYR:CZ	1:A:284:GLY:HA3	2.37	0.60
2:B:291:LYS:NZ	2:B:297:PRO:HD3	2.18	0.59
1:A:521:SER:HB2	1:A:595:ARG:HG2	1.84	0.59
2:B:252:ASP:OD2	2:B:255:LEU:N	2.22	0.58
1:A:270:TYR:HD1	1:A:404:HIS:HB2	1.68	0.58
1:A:202:TYR:OH	1:A:220:ARG:NH2	2.37	0.58
1:A:613:ILE:HG12	2:B:453:ASP:OD2	2.04	0.58
1:A:320:ARG:NH2	2:B:246:GLN:OE1	2.32	0.58
1:A:184:ILE:HD11	1:A:207:ARG:NH1	2.19	0.56
1:A:275:VAL:HG22	1:A:400:VAL:HG22	1.87	0.56
1:A:500:GLN:HE22	1:A:536:VAL:HG21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:LEU:HB3	2:B:402:CYS:HB2	1.87	0.56
1:A:204:ILE:HB	1:A:215:ASP:HB2	1.89	0.55
2:B:292:ARG:HB3	2:B:295:LEU:HD13	1.87	0.55
2:B:108:ILE:HG23	2:B:352:ARG:NH1	2.22	0.55
1:A:188:ASN:O	2:B:236:LYS:NZ	2.39	0.55
1:A:190:VAL:HB	1:A:203:ALA:HB3	1.89	0.55
1:A:282:GLU:OE1	1:A:313:ARG:NH1	2.40	0.55
1:A:557:THR:HG22	1:A:597:GLN:HG2	1.89	0.55
1:A:310:GLN:HG2	1:A:313:ARG:NH1	2.22	0.55
2:B:156:ILE:HG21	2:B:195:LYS:HE2	1.90	0.54
1:A:304:PRO:HA	1:A:568:HIS:HB2	1.89	0.54
1:A:117:PHE:HB3	1:A:325:VAL:HG21	1.89	0.53
1:A:208:ILE:HG13	1:A:210:VAL:H	1.73	0.53
1:A:134:SER:HA	1:A:334:VAL:HA	1.91	0.52
2:B:276:TYR:CZ	2:B:284:GLY:HA3	2.45	0.52
2:B:310:GLN:HG2	2:B:313:ARG:HH21	1.75	0.52
2:B:260:VAL:HG21	2:B:425:PHE:CD1	2.44	0.51
1:A:238:ALA:HB3	2:B:235:GLN:HE22	1.77	0.50
2:B:291:LYS:HZ2	2:B:297:PRO:HD3	1.75	0.49
1:A:272[B]:ARG:NE	4:A:708:GOL:O2	2.45	0.49
1:A:278:PHE:CD1	1:A:398:GLY:HA2	2.46	0.49
2:B:171:SER:HB3	2:B:192:ILE:HG12	1.94	0.49
1:A:289:GLU:HG2	1:A:299:ILE:HB	1.94	0.49
1:A:217:GLU:HG2	1:A:351:LEU:HD11	1.95	0.48
1:A:310:GLN:HG2	1:A:313:ARG:HH11	1.78	0.48
1:A:445:LEU:HD12	2:B:442:LYS:HG3	1.95	0.48
2:B:337:ASP:OD1	2:B:338:ASP:N	2.47	0.48
1:A:143:ILE:HD11	1:A:166:LEU:HD22	1.95	0.47
1:A:190:VAL:HG12	1:A:192:ILE:HG13	1.95	0.47
1:A:272[A]:ARG:NE	4:A:708:GOL:O2	2.47	0.47
2:B:272[A]:ARG:NH2	2:B:296:GLU:O	2.43	0.46
2:B:272[A]:ARG:NH1	2:B:295:LEU:HD23	2.31	0.46
1:A:534:ASP:O	1:A:556:HIS:ND1	2.48	0.46
1:A:109:GLN:HA	1:A:347:VAL:HG22	1.98	0.46
1:A:308:ILE:HG12	5:A:709:O6E:CBL	2.46	0.46
1:A:403:HIS:NE2	5:A:709:O6E:OAK	2.40	0.46
1:A:164:ARG:HG3	1:A:175:LEU:HD11	1.98	0.46
2:B:563:TRP:NE1	2:B:590:GLU:OE1	2.48	0.46
1:A:270:TYR:CD1	1:A:404:HIS:HB2	2.50	0.46
1:A:375:VAL:HG22	1:A:422:MET:HE1	1.96	0.46
1:A:279:HIS:NE2	1:A:285:GLU:OE1	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:GLY:HA3	1:A:553:PHE:HB2	1.98	0.45
2:B:119:CYS:SG	2:B:140:MET:HB2	2.56	0.45
1:A:272[B]:ARG:NH2	1:A:296:GLU:O	2.44	0.45
2:B:282:GLU:OE1	2:B:313:ARG:NH2	2.44	0.45
2:B:307:ASP:HA	5:B:707:O6E:OBQ	2.16	0.45
1:A:498:GLU:OE2	1:A:498:GLU:N	2.41	0.45
1:A:326:ASP:OD1	1:A:329:ALA:N	2.50	0.45
1:A:562:LYS:HB3	1:A:589:LEU:HD23	1.99	0.44
2:B:144:MET:HA	2:B:145:PRO:HD3	1.89	0.44
2:B:226:LEU:O	2:B:230:GLY:N	2.51	0.44
1:A:142:GLY:HA3	1:A:197:THR:HG23	1.99	0.44
1:A:569:HIS:HB2	1:A:572:ASP:HB2	1.99	0.43
1:A:257:CYS:O	1:A:260:VAL:HG12	2.18	0.43
2:B:316:PHE:HB3	2:B:374:ALA:HB2	1.99	0.43
2:B:483:PHE:HD1	2:B:550:LEU:HD22	1.83	0.43
2:B:272[A]:ARG:HH12	2:B:295:LEU:HD23	1.82	0.43
1:A:278:PHE:CE2	1:A:313:ARG:HD3	2.54	0.43
1:A:278:PHE:HE1	1:A:399:LEU:HG	1.84	0.43
1:A:322:ARG:O	1:A:371:LEU:HD12	2.19	0.43
2:B:322:ARG:NH1	5:B:707:O6E:OBA	2.47	0.43
1:A:164:ARG:HB3	1:A:172:SER:HB3	2.00	0.43
2:B:301:LEU:HB3	2:B:562:LYS:HG2	2.00	0.43
1:A:143:ILE:HD13	1:A:157:LEU:HB2	2.00	0.42
1:A:164:ARG:NH2	3:A:705:SO4:O1	2.34	0.42
1:A:303:TYR:HB3	1:A:307:ASP:OD2	2.20	0.42
1:A:235:GLN:NE2	2:B:235:GLN:OE1	2.52	0.42
1:A:272[B]:ARG:NH2	1:A:295:LEU:HB3	2.35	0.42
1:A:293:ASP:OD1	1:A:294:ASP:N	2.52	0.42
1:A:535:ALA:O	1:A:555:SER:HA	2.19	0.42
2:B:95:SER:HB2	2:B:317:LYS:NZ	2.34	0.42
2:B:375:VAL:HG22	2:B:398:GLY:O	2.20	0.42
1:A:189:PRO:HD2	2:B:229:ALA:HA	2.02	0.42
1:A:369:ALA:HB3	1:A:404:HIS:HB3	2.01	0.42
1:A:188:ASN:HA	1:A:189:PRO:HA	1.90	0.41
1:A:322:ARG:HH11	1:A:322:ARG:HG2	1.84	0.41
1:A:272[A]:ARG:NH2	1:A:295:LEU:HB3	2.35	0.41
2:B:208:ILE:HD13	2:B:213:VAL:HG23	2.02	0.41
2:B:308:ILE:HG12	5:B:707:O6E:CBL	2.51	0.41
2:B:115:GLN:HE22	2:B:324:ILE:HA	1.85	0.41
2:B:566:ALA:N	2:B:582:ARG:NH1	2.69	0.41
2:B:156:ILE:O	2:B:161:THR:HG21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ASP:OD1	2:B:210:VAL:N	2.50	0.41
2:B:569:HIS:N	2:B:572:ASP:OD2	2.47	0.40
1:A:304:PRO:HD2	1:A:307:ASP:OD2	2.21	0.40
1:A:124:ASP:OD2	1:A:127:SER:OG	2.25	0.40
2:B:196:ASN:OD1	2:B:196:ASN: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	A	433/544 (80%)	405 (94%)	27 (6%)	1 (0%)	47	78
2	B	409/544 (75%)	385 (94%)	24 (6%)	0	100	100
All	All	842/1088 (77%)	790 (94%)	51 (6%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	594	SER

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	379/461 (82%)	371 (98%)	8 (2%)	53 76
2	B	364/447 (81%)	359 (99%)	5 (1%)	67 83
All	All	743/908 (82%)	730 (98%)	13 (2%)	59 80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	ILE
1	A	220	ARG
1	A	259	THR
1	A	316	PHE
1	A	414	LEU
1	A	476	VAL
1	A	519	THR
1	A	591	VAL
2	B	280	GLU
2	B	315	LEU
2	B	416	TYR
2	B	536	VAL
2	B	589	LEU

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

Mol	Chain	Res	Type
1	A	235	GLN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	705	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	702	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	B	702	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	705	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	707	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	A	708	-	5,5,5	0.37	0	5,5,5	0.30	0
6	PGE	B	706	-	9,9,9	0.66	0	8,8,8	1.50	0
3	SO4	B	704	-	4,4,4	0.14	0	6,6,6	0.05	0
5	O6E	A	709	1	36,46,46	3.09	13 (36%)	44,67,67	2.21	7 (15%)
3	SO4	A	703	-	4,4,4	0.14	0	6,6,6	0.05	0
5	O6E	B	707	2	36,46,46	3.01	13 (36%)	44,67,67	2.18	7 (15%)
4	GOL	B	701	-	5,5,5	0.39	0	5,5,5	0.26	0
3	SO4	A	704	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	701	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	A	706	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	703	-	4,4,4	0.14	0	6,6,6	0.05	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
6	PGE	B	706	-	-	1/7/7/7	-
5	O6E	A	709	1	-	5/21/74/74	0/4/4/4
5	O6E	B	707	2	-	5/21/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	701	-	-	2/4/4/4	-
4	GOL	A	708	-	-	2/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	709	O6E	CAO-CAV	12.89	1.45	1.35
5	B	707	O6E	CAO-CAV	12.21	1.45	1.35
5	A	709	O6E	CAP-CBL	7.51	1.58	1.40
5	B	707	O6E	CAP-CBL	7.40	1.57	1.40
5	B	707	O6E	CAT-CBD	-4.50	1.43	1.53
5	A	709	O6E	CAT-CBD	-4.42	1.43	1.53
5	A	709	O6E	CAY-CAQ	4.41	1.58	1.41
5	B	707	O6E	CAY-CAQ	4.34	1.58	1.41
5	A	709	O6E	CBO-CAO	3.25	1.53	1.41
5	B	707	O6E	CBO-CAO	3.20	1.53	1.41
5	B	707	O6E	CAV-CBB	-3.16	1.40	1.45
5	A	709	O6E	CAV-CBB	-2.92	1.41	1.45
5	B	707	O6E	CAB-CBI	2.84	1.55	1.47
5	A	709	O6E	CAB-CBI	2.83	1.55	1.47
5	B	707	O6E	CBL-CBH	-2.79	1.39	1.45
5	B	707	O6E	CAV-NAE	-2.72	1.32	1.38
5	A	709	O6E	CBL-CBH	-2.69	1.40	1.45
5	A	709	O6E	CAA-CBB	2.67	1.58	1.51
5	A	709	O6E	CAW-CBC	-2.63	1.40	1.45
5	B	707	O6E	CAW-CBC	-2.61	1.40	1.45
5	A	709	O6E	CAV-NAE	-2.59	1.33	1.38
5	A	709	O6E	CBI-CBM	-2.54	1.40	1.47
5	B	707	O6E	CAA-CBB	2.53	1.57	1.51
5	B	707	O6E	CBI-CBM	-2.53	1.40	1.47
5	A	709	O6E	CAW-NAJ	-2.21	1.34	1.37
5	B	707	O6E	CAW-NAJ	-2.09	1.34	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	707	O6E	CBD-CAX-NBP	10.29	117.14	108.27
5	A	709	O6E	CBD-CAX-NBP	10.23	117.09	108.27
5	B	707	O6E	OBQ-CAX-CBD	-6.86	120.72	126.17
5	A	709	O6E	OBQ-CAX-CBD	-6.45	121.05	126.17
5	A	709	O6E	CAW-CAP-CBL	-2.83	121.16	128.08
5	A	709	O6E	CAR-CBH-CBL	2.62	129.09	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	709	O6E	OBQ-CAX-NBP	-2.54	121.86	124.94
5	A	709	O6E	CBI-CBM-NAJ	2.50	109.02	106.19
5	B	707	O6E	CAS-CBC-CAW	2.38	127.14	124.17
5	B	707	O6E	OBQ-CAX-NBP	-2.32	122.14	124.94
5	B	707	O6E	CBI-CBM-NAJ	2.32	108.81	106.19
5	B	707	O6E	CAR-CBH-CBL	2.30	128.61	125.06
5	B	707	O6E	CAW-CAP-CBL	-2.11	122.92	128.08
5	A	709	O6E	CAS-CBC-CAW	2.05	126.73	124.17

There are no chirality outliers.

All (15) torsion outliers are listed below:

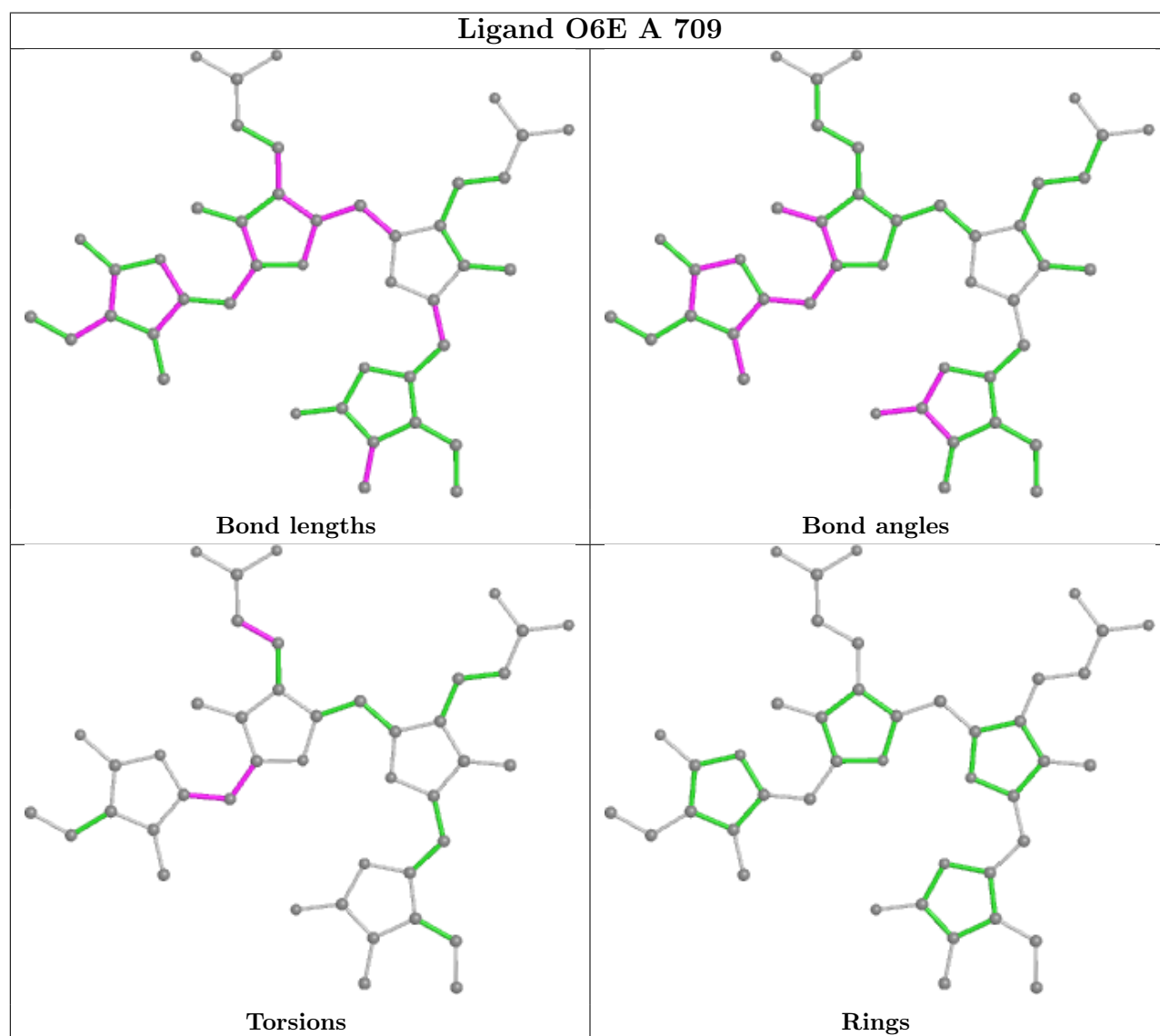
Mol	Chain	Res	Type	Atoms
4	A	708	GOL	O1-C1-C2-C3
5	A	709	O6E	CAW-CAP-CBL-NAE
5	A	709	O6E	CBL-CAP-CAW-CBC
5	B	707	O6E	CBB-CAA-CAF-CAL
5	B	707	O6E	CAW-CAP-CBL-NAE
5	B	707	O6E	CAW-CAP-CBL-CBH
5	A	709	O6E	CAW-CAP-CBL-CBH
5	A	709	O6E	CBL-CAP-CAW-NAJ
5	A	709	O6E	CBB-CAA-CAF-CAL
4	B	701	GOL	O1-C1-C2-C3
4	A	708	GOL	O1-C1-C2-O2
5	B	707	O6E	CBL-CAP-CAW-NAJ
5	B	707	O6E	CBL-CAP-CAW-CBC
4	B	701	GOL	O1-C1-C2-O2
6	B	706	PGE	O2-C3-C4-O3

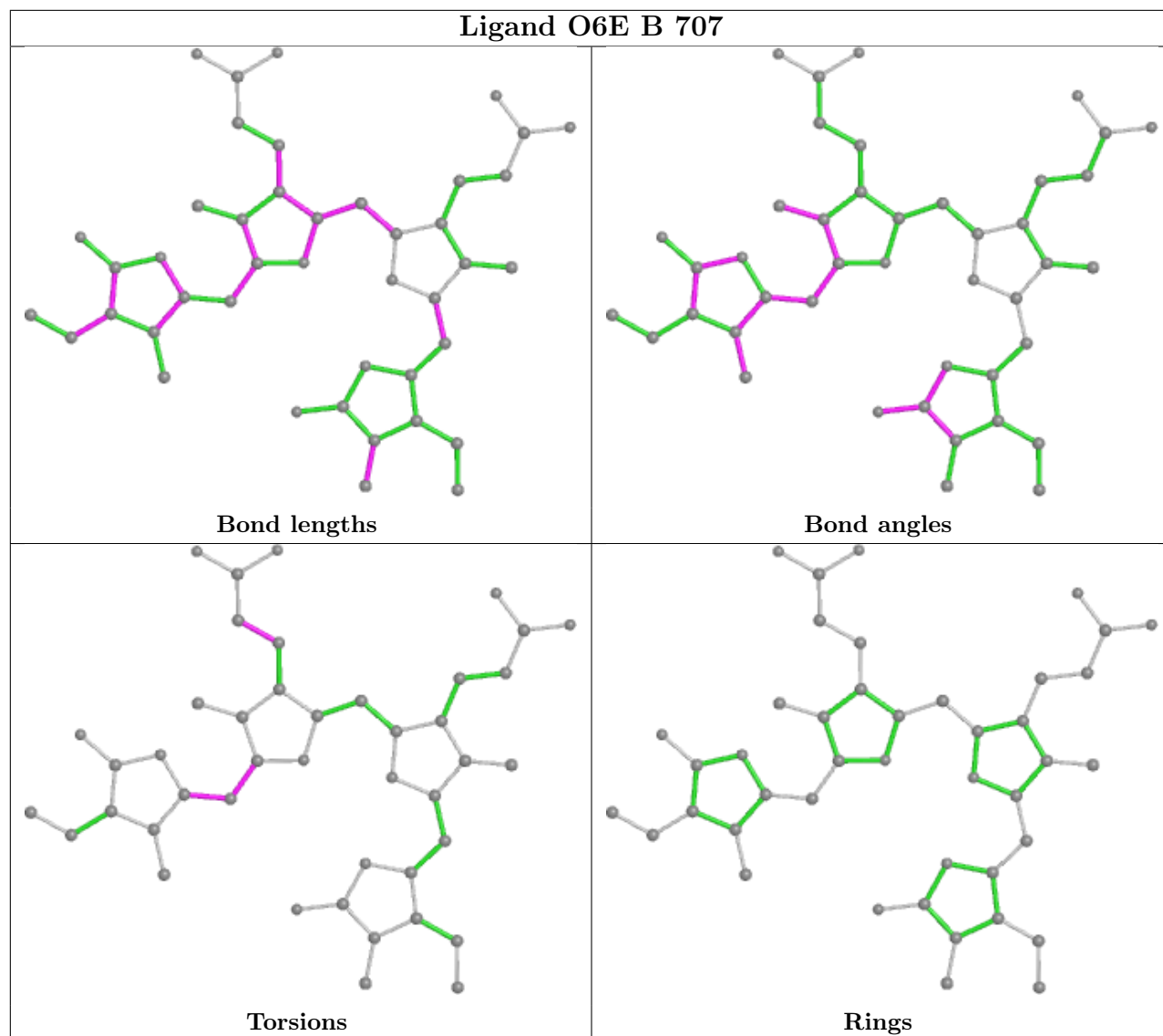
There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	705	SO4	1	0
3	A	702	SO4	1	0
3	A	707	SO4	1	0
4	A	708	GOL	2	0
5	A	709	O6E	2	0
5	B	707	O6E	3	0
3	A	706	SO4	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	448/544 (82%)	0.57	57 (12%) 3 4	51, 81, 248, 318	0
2	B	426/544 (78%)	0.39	32 (7%) 14 16	58, 80, 207, 290	0
All	All	874/1088 (80%)	0.48	89 (10%) 6 8	51, 81, 229, 318	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	453	ASP	9.7
1	A	473	MET	6.7
1	A	472	ILE	6.7
1	A	475	LEU	5.8
1	A	611	GLN	5.7
1	A	615	ARG	5.7
2	B	483	PHE	5.4
1	A	613	ILE	5.0
1	A	500	GLN	4.8
2	B	451	LEU	4.6
1	A	517	LEU	4.4
1	A	494	VAL	4.4
2	B	454	MET	4.3
1	A	442	LYS	4.2
1	A	447	THR	4.2
1	A	555	SER	4.2
1	A	536	VAL	4.1
1	A	496	PRO	4.0
1	A	493	GLY	3.9
1	A	612	LEU	3.9
2	B	539	MET	3.7
2	B	604	MET	3.7
2	B	609	SER	3.7
1	A	527	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	607	ILE	3.5
1	A	439	MET	3.5
1	A	446	ARG	3.5
1	A	539	MET	3.5
1	A	614	LEU	3.4
2	B	541	VAL	3.4
2	B	553	PHE	3.4
1	A	609	SER	3.4
1	A	508	LEU	3.3
2	B	607	ILE	3.2
1	A	610	LEU	3.2
2	B	542	ALA	3.2
2	B	534	ASP	3.1
2	B	522	LEU	3.1
1	A	551	PHE	3.0
1	A	509	LEU	3.0
1	A	531	ALA	3.0
2	B	444	VAL	3.0
1	A	518	SER	3.0
2	B	448	GLN	3.0
2	B	452	CYS	3.0
1	A	616	ASP	2.9
1	A	474	ASP	2.9
1	A	552	TRP	2.9
1	A	604	MET	2.9
1	A	101	ILE	2.9
1	A	471	SER	2.8
1	A	530	ALA	2.8
2	B	608	HIS	2.7
1	A	478	CYS	2.7
1	A	504	VAL	2.6
2	B	519	THR	2.6
1	A	495	ALA	2.6
2	B	517	LEU	2.6
1	A	541	VAL	2.6
1	A	608	HIS	2.5
1	A	602	ALA	2.5
2	B	550	LEU	2.5
1	A	528	GLY	2.5
2	B	491	PRO	2.5
1	A	501	ILE	2.4
1	A	550	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	542	ALA	2.4
2	B	484	LEU	2.4
2	B	595	ARG	2.3
2	B	99	GLN	2.3
2	B	610	LEU	2.3
2	B	447	THR	2.3
1	A	503	ASP	2.3
2	B	490	TYR	2.3
1	A	222	GLU	2.3
1	A	476	VAL	2.3
1	A	534	ASP	2.2
1	A	448	GLN	2.2
1	A	553	PHE	2.2
2	B	455	LEU	2.2
1	A	482	ALA	2.2
2	B	599	TRP	2.2
1	A	532	LEU	2.2
1	A	492	LEU	2.1
1	A	157	LEU	2.0
2	B	551	PHE	2.0
2	B	96	VAL	2.0
1	A	549	PHE	2.0
2	B	492	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.

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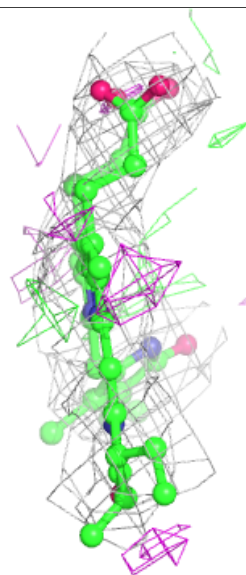
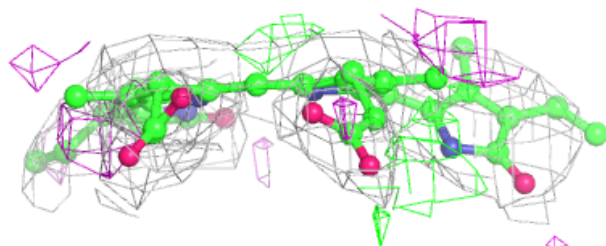
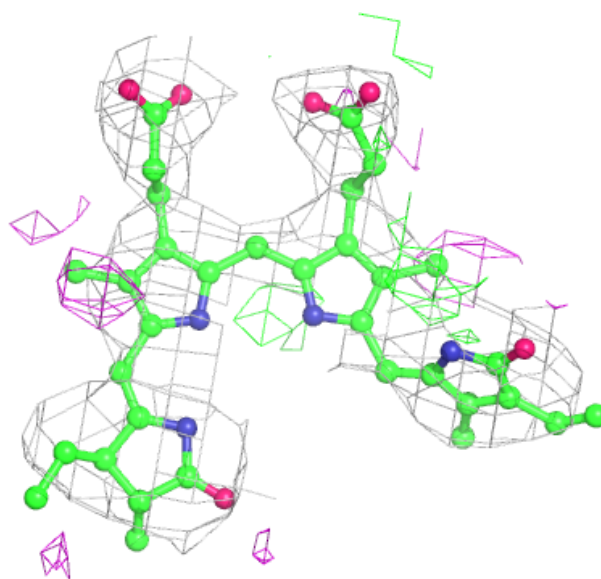
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	707	5/5	0.26	0.66	323,323,324,324	0
3	SO4	A	705	5/5	0.55	0.21	226,226,226,227	0
3	SO4	A	706	5/5	0.72	0.20	189,190,190,191	0
3	SO4	A	703	5/5	0.74	0.13	171,171,172,173	0
3	SO4	A	704	5/5	0.78	0.17	199,199,200,200	0
3	SO4	B	705	5/5	0.80	0.16	206,207,207,207	0
4	GOL	A	708	6/6	0.80	0.53	108,109,113,114	0
6	PGE	B	706	10/10	0.83	0.30	64,70,74,76	0
3	SO4	B	704	5/5	0.84	0.19	169,169,170,170	0
3	SO4	A	701	5/5	0.84	0.29	186,188,189,189	0
4	GOL	B	701	6/6	0.85	0.36	54,60,65,68	0
3	SO4	B	703	5/5	0.87	0.32	173,173,174,175	0
3	SO4	B	702	5/5	0.90	0.24	128,129,131,134	0
5	O6E	A	709	43/43	0.93	0.28	44,58,79,84	0
5	O6E	B	707	43/43	0.94	0.31	32,57,76,86	0
3	SO4	A	702	5/5	0.97	0.11	58,59,65,68	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.

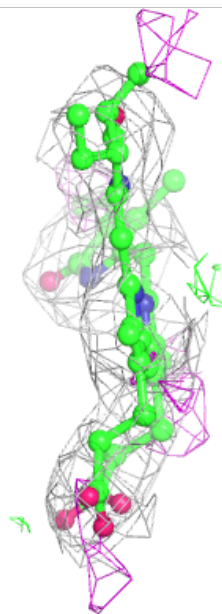
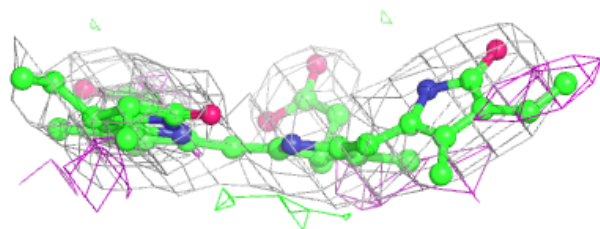
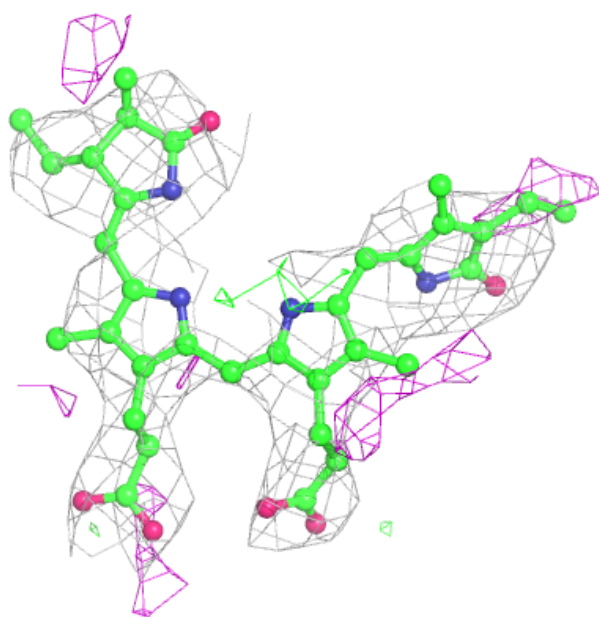
Electron density around O6E A 709:

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



Electron density around O6E B 707:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.