Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 11:51 PM EST

PDB ID	:	4MSU
Title	:	Human GKRP bound to AMG-6861 and Sorbitol-6-phosphate
Authors	:	Ashton, K.S.; Andrews, K.L.; Bryan, M.C.; Chen, J.; Chen, K.; Chen, M.; Chmait, S.; Croghan, M.; Cupples, R.; Fotsch, C.; Helmering, J.; Jordan, S.R.; Kurzeja, R.J.; Michelsen, K.; Pennington, L.D.; Poon, S.F.; Sivits, G.; Van, G.; Vonderfecht, S.L.; Wahl, R.C.; Zhang, J.; Lloyd, D.J.; Hale, C.; St Jean, D.J.
Deposited on	:	2013-09-18
Resolution	:	2.50 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:

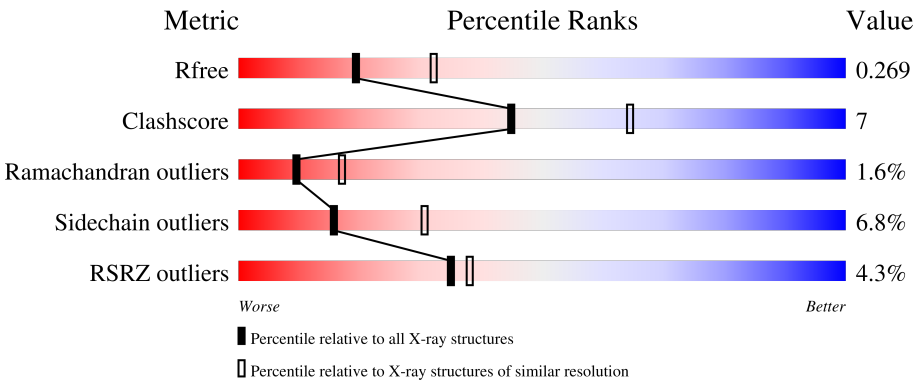
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	A	636	4% 72% 17% • 8%
1	B	636	4% 78% 12% • 7%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9262 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.

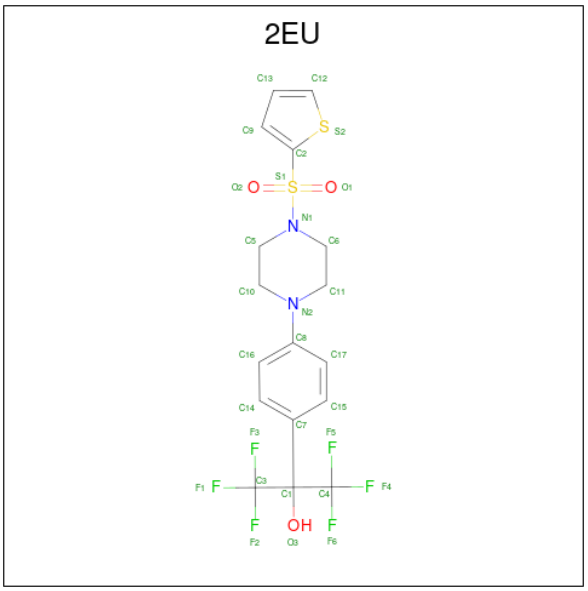
- Molecule 1 is a protein called Glucokinase regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	585	4521	2882	774	841	24	0	0	0
1	B	590	4554	2901	781	848	24	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

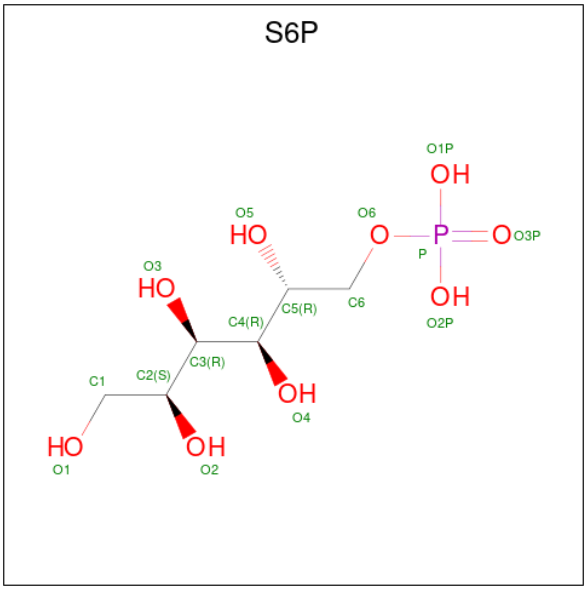
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP Q14397
A	-9	HIS	-	expression tag	UNP Q14397
A	-8	HIS	-	expression tag	UNP Q14397
A	-7	HIS	-	expression tag	UNP Q14397
A	-6	HIS	-	expression tag	UNP Q14397
A	-5	HIS	-	expression tag	UNP Q14397
A	-4	HIS	-	expression tag	UNP Q14397
A	-3	ASP	-	expression tag	UNP Q14397
A	-2	GLU	-	expression tag	UNP Q14397
A	-1	VAL	-	expression tag	UNP Q14397
A	0	ASP	-	expression tag	UNP Q14397
B	-10	MET	-	expression tag	UNP Q14397
B	-9	HIS	-	expression tag	UNP Q14397
B	-8	HIS	-	expression tag	UNP Q14397
B	-7	HIS	-	expression tag	UNP Q14397
B	-6	HIS	-	expression tag	UNP Q14397
B	-5	HIS	-	expression tag	UNP Q14397
B	-4	HIS	-	expression tag	UNP Q14397
B	-3	ASP	-	expression tag	UNP Q14397
B	-2	GLU	-	expression tag	UNP Q14397
B	-1	VAL	-	expression tag	UNP Q14397
B	0	ASP	-	expression tag	UNP Q14397

- Molecule 2 is 1,1,1,3,3,3-hexafluoro-2-{4-[4-(thiophen-2-ylsulfonyl)piperazin-1-yl]phenyl}propan-2-ol (three-letter code: 2EU) (formula: $C_{17}H_{16}F_6N_2O_3S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
2	A	1	30	17	6	2	3	2	0	0
			Total	C	F	N	O	S		
2	B	1	30	17	6	2	3	2	0	0

- Molecule 3 is D-SORBITOL-6-PHOSPHATE (three-letter code: S6P) (formula: $C_6H_{15}O_9P$).

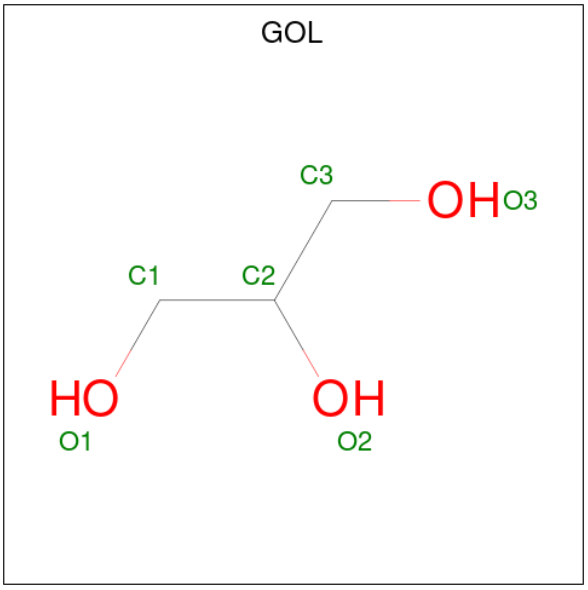


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	16	6	9	1	0	0
			Total	C	O	P		
3	B	1	16	6	9	1	0	0

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

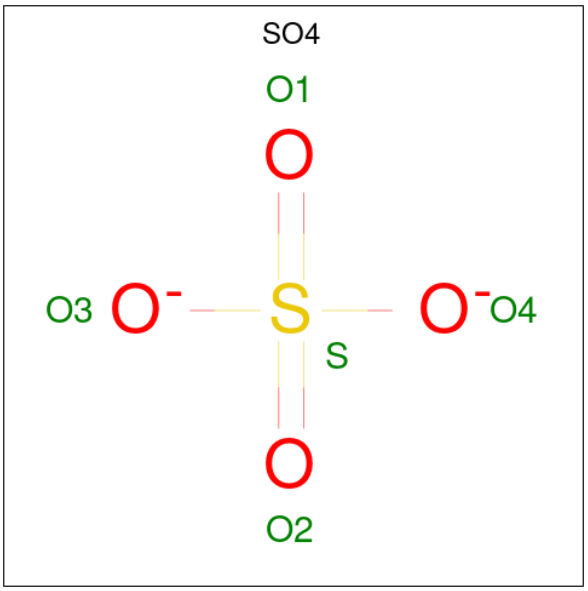
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
4	A	11	11	11	0	0
			Total	I		
4	B	12	12	12	0	0

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



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is water.

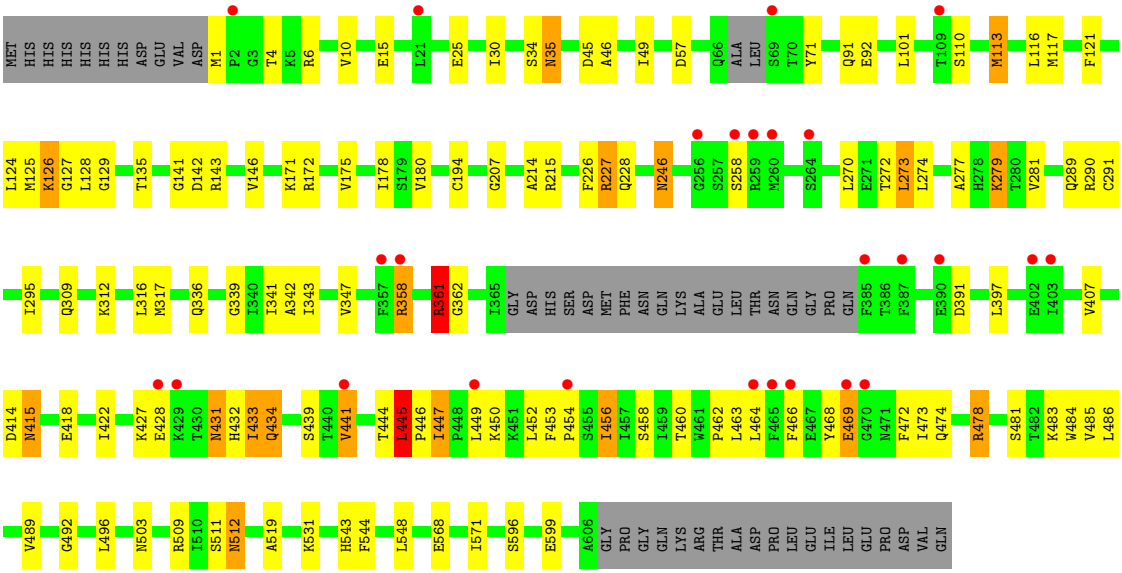
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	25	Total O 25 25	0	0
7	B	31	Total O 31 31	0	0

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.

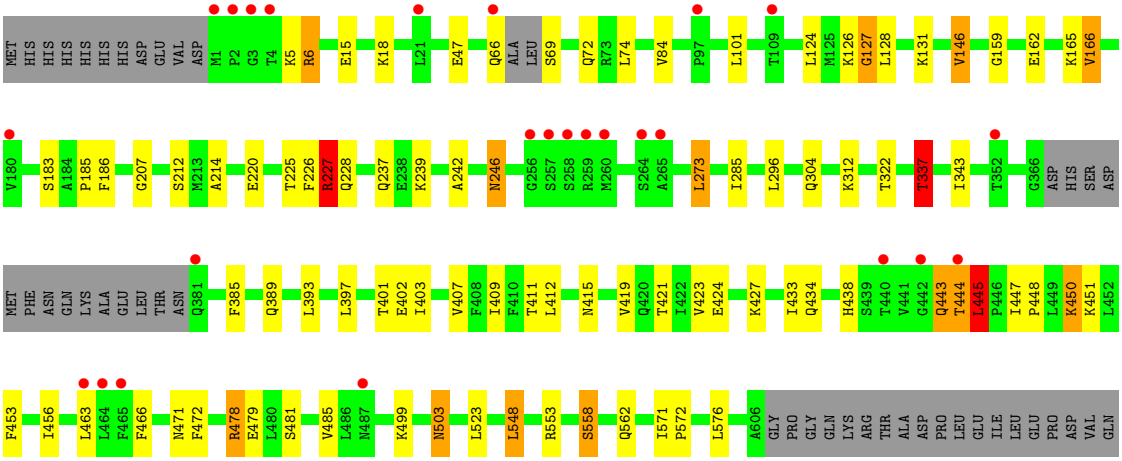
- Molecule 1: Glucokinase regulatory protein

Chain A:



- Molecule 1: Glucokinase regulatory protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	148.43Å 148.43Å 132.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.86 – 2.50 37.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (37.86-2.50) 98.1 (37.86-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.212 , 0.271 0.214 , 0.269	Depositor DCC
R_{free} test set	2837 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	60.3	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.030 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9262	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: IOD, S6P, GOL, SO4, 2EU

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	0.68	0/4603	0.85	4/6228 (0.1%)
1	B	0.71	0/4637	0.83	2/6274 (0.0%)
All	All	0.69	0/9240	0.84	6/12502 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	478	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	361	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	113	MET	CG-SD-CE	5.20	108.52	100.20
1	B	443	GLN	N-CA-C	-5.13	97.15	111.00
1	A	361	ARG	CG-CD-NE	5.05	122.40	111.80
1	B	227	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4521	0	4618	73	0
1	B	4554	0	4647	49	0
2	A	30	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	30	0	15	0	0
3	A	16	0	13	0	0
3	B	16	0	13	0	0
4	A	11	0	0	2	0
4	B	12	0	0	2	0
5	A	6	0	8	1	0
6	B	10	0	0	0	0
7	A	25	0	0	0	0
7	B	31	0	0	0	0
All	All	9262	0	9330	121	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 (121) 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:450:LYS:HA	1:A:452:LEU:HD12	1.63	0.80
1:B:220:GLU:OE1	1:B:558:SER:OG	2.02	0.77
1:A:15:GLU:OE2	4:A:711:IOD:I	2.76	0.73
1:A:433:ILE:O	1:A:434:GLN:HG3	1.90	0.72
1:A:474:GLN:O	1:A:478:ARG:HD3	1.90	0.71
1:B:419:VAL:O	1:B:423:VAL:HG23	1.90	0.71
1:A:336:GLN:NE2	1:A:414:ASP:OD1	2.27	0.68
1:A:468:TYR:HB2	4:A:703:IOD:I	2.66	0.66
1:A:596:SER:OG	1:A:599:GLU:HG3	1.96	0.65
1:B:445:LEU:O	1:B:450:LYS:NZ	2.27	0.65
1:A:101:LEU:HD11	1:A:135:THR:HG22	1.80	0.63
1:A:273:LEU:C	1:A:273:LEU:HD23	2.20	0.62
1:A:531:LYS:HE2	5:A:714:GOL:H12	1.80	0.62
1:B:312:LYS:NZ	1:B:456:ILE:O	2.33	0.62
1:A:309:GLN:NE2	1:A:458:SER:O	2.33	0.61
1:A:272:THR:HA	1:A:295:ILE:HG21	1.82	0.60
1:A:415:ASN:HD22	1:A:418:GLU:H	1.49	0.58
1:B:101:LEU:HD21	1:B:166:VAL:CG1	2.33	0.58
1:A:126:LYS:O	1:A:129:GLY:N	2.33	0.58
1:A:146:VAL:O	1:A:347:VAL:HG21	2.04	0.57
1:A:317:MET:HE2	1:A:496:LEU:HD11	1.87	0.57
1:B:444:THR:O	1:B:445:LEU:CB	2.53	0.57
1:A:444:THR:O	1:A:445:LEU:CB	2.53	0.55
1:A:215:ARG:HG3	2:A:701:2EU:S2	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:SER:O	1:B:185:PRO:HD3	2.08	0.54
1:A:207:GLY:O	1:A:246:ASN:HA	2.06	0.54
1:B:412:LEU:HB2	1:B:443:GLN:OE1	2.07	0.54
1:B:225:THR:H	1:B:228:GLN:HE21	1.56	0.54
1:B:407:VAL:HG12	1:B:409:ILE:HD11	1.90	0.54
1:B:444:THR:O	1:B:445:LEU:HB2	2.08	0.53
1:A:453:PHE:HB2	1:A:456:ILE:HG23	1.91	0.53
1:B:572:PRO:O	1:B:576:LEU:HG	2.08	0.53
1:A:447:ILE:HG23	1:A:449:LEU:HB3	1.91	0.53
1:B:438:HIS:CG	1:B:478:ARG:HG2	2.44	0.53
1:B:389:GLN:OE1	1:B:421:THR:HG21	2.09	0.52
1:A:277:ALA:O	1:A:281:VAL:HG23	2.09	0.52
1:B:5:LYS:HB2	4:B:710:IOD:I	2.80	0.52
1:A:49:ILE:HB	1:A:317:MET:HE1	1.92	0.51
1:A:339:GLY:O	1:A:342:ALA:HB3	2.10	0.51
1:A:343:ILE:HA	1:A:362:GLY:HA3	1.92	0.51
1:A:228:GLN:HE22	1:B:228:GLN:HE22	1.59	0.51
1:A:444:THR:O	1:A:445:LEU:HB2	2.10	0.50
1:A:175:VAL:HG21	1:A:194:CYS:SG	2.52	0.50
1:A:418:GLU:O	1:A:422:ILE:HD12	2.12	0.50
1:A:481:SER:O	1:A:485:VAL:HG23	2.11	0.50
1:A:10:VAL:HB	1:A:531:LYS:HE3	1.93	0.50
1:A:121:PHE:O	1:A:125:MET:HG3	2.12	0.49
1:B:146:VAL:HG13	1:B:146:VAL:O	2.12	0.49
1:B:571:ILE:HB	1:B:572:PRO:HD3	1.93	0.49
1:B:101:LEU:HD21	1:B:166:VAL:HG13	1.94	0.49
1:B:337:THR:HG21	1:B:479:GLU:OE1	2.12	0.48
1:A:180:VAL:HG11	1:A:258:SER:HB2	1.95	0.48
1:B:162:GLU:OE1	1:B:165:LYS:NZ	2.37	0.48
1:B:503:ASN:HD22	1:B:503:ASN:H	1.61	0.48
1:A:316:LEU:HD11	1:A:407:VAL:HG21	1.95	0.48
1:B:225:THR:H	1:B:228:GLN:NE2	2.11	0.48
1:A:279:LYS:HD3	1:A:291:CYS:SG	2.54	0.47
1:A:433:ILE:O	1:A:434:GLN:CG	2.58	0.47
1:B:127:GLY:O	1:B:128:LEU:HD23	2.15	0.47
1:B:427:LYS:HD2	1:B:427:LYS:O	2.15	0.46
1:B:466:PHE:HB2	4:B:703:IOD:I	2.85	0.46
1:B:159:GLY:HA2	1:B:186:PHE:CE1	2.51	0.46
1:A:361:ARG:CG	1:A:361:ARG:HH11	2.29	0.46
1:A:433:ILE:HD12	1:A:453:PHE:CE1	2.50	0.46
1:B:124:LEU:HD12	1:B:472:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ALA:O	1:B:227:ARG:HD3	2.16	0.46
1:A:91:GLN:O	1:A:92:GLU:C	2.53	0.46
1:A:124:LEU:HD12	1:A:472:PHE:CD2	2.51	0.45
1:A:35:ASN:C	1:A:35:ASN:HD22	2.20	0.45
1:A:127:GLY:HA3	1:A:469:GLU:HG3	1.98	0.45
1:A:358:ARG:NH2	1:A:361:ARG:HD3	2.31	0.45
1:B:407:VAL:HG12	1:B:409:ILE:CD1	2.45	0.45
1:B:343:ILE:HD13	1:B:385:PHE:HB2	1.98	0.45
1:A:113:MET:HE1	1:A:483:LYS:HD2	1.99	0.45
1:A:246:ASN:N	1:A:246:ASN:HD22	2.14	0.45
1:A:146:VAL:O	1:A:146:VAL:CG1	2.64	0.45
1:A:46:ALA:HA	1:A:317:MET:HE2	1.99	0.45
1:A:117:MET:HE1	1:A:270:LEU:HD12	1.98	0.45
1:A:509:ARG:NH2	1:A:568:GLU:OE2	2.50	0.45
1:A:317:MET:SD	1:A:492:GLY:HA3	2.57	0.44
1:A:433:ILE:O	1:A:434:GLN:CB	2.64	0.44
1:A:46:ALA:HA	1:A:317:MET:CE	2.47	0.44
1:A:431:ASN:O	1:A:433:ILE:N	2.50	0.44
1:B:74:LEU:HD21	1:B:296:LEU:HD22	1.99	0.44
1:B:481:SER:O	1:B:485:VAL:HG23	2.17	0.44
1:B:421:THR:O	1:B:424:GLU:HB2	2.17	0.44
1:A:596:SER:OG	1:A:599:GLU:CG	2.64	0.44
1:B:503:ASN:HD22	1:B:503:ASN:N	2.16	0.44
1:A:30:ILE:HD11	1:A:71:TYR:CD2	2.53	0.43
1:A:290:ARG:CZ	1:A:290:ARG:HB3	2.47	0.43
1:B:393:LEU:CD2	1:B:397:LEU:HD22	2.48	0.43
1:A:101:LEU:HD11	1:A:135:THR:CG2	2.48	0.43
1:B:411:THR:HG22	1:B:438:HIS:HB2	1.99	0.43
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.81	0.43
1:B:401:THR:HG22	1:B:403:ILE:H	1.83	0.43
1:B:66:GLN:O	1:B:69:SER:OG	2.35	0.42
1:B:207:GLY:O	1:B:246:ASN:HA	2.18	0.42
1:A:431:ASN:H	1:A:431:ASN:HD22	1.66	0.42
1:A:316:LEU:HD11	1:A:407:VAL:CG2	2.49	0.42
1:B:273:LEU:C	1:B:273:LEU:HD23	2.40	0.42
1:B:548:LEU:HD13	1:B:553:ARG:CZ	2.50	0.42
1:A:431:ASN:HD22	1:A:431:ASN:N	2.17	0.42
1:B:445:LEU:HD13	1:B:450:LYS:HB3	2.02	0.42
1:A:274:LEU:O	1:A:277:ALA:N	2.53	0.42
1:A:447:ILE:HG22	1:A:450:LYS:N	2.35	0.42
1:A:519:ALA:HB2	1:A:571:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:GLU:HB2	1:B:18:LYS:HG3	2.02	0.41
1:B:433:ILE:HD12	1:B:453:PHE:CE1	2.56	0.41
1:B:447:ILE:N	1:B:448:PRO:HD2	2.35	0.41
1:A:57:ASP:OD2	1:A:484:TRP:CD1	2.72	0.41
1:A:214:ALA:O	1:A:227:ARG:HD3	2.21	0.41
1:A:431:ASN:H	1:A:431:ASN:ND2	2.19	0.41
1:A:512:ASN:HD22	1:A:512:ASN:C	2.24	0.41
1:A:110:SER:HB3	1:A:178:ILE:CG2	2.51	0.41
1:A:341:ILE:HG22	1:A:486:LEU:HD12	2.02	0.41
1:A:509:ARG:HG2	1:A:511:SER:OG	2.20	0.41
1:B:6:ARG:H	1:B:6:ARG:HG2	1.74	0.41
1:B:237:GLN:HA	1:B:242:ALA:O	2.21	0.41
1:B:523:LEU:HD23	1:B:523:LEU:HA	1.86	0.40
1:A:45:ASP:OD1	1:A:45:ASP:C	2.60	0.40
1:A:543:HIS:O	1:A:544:PHE:C	2.60	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	579/636 (91%)	515 (89%)	49 (8%)	15 (3%)	5 8
1	B	584/636 (92%)	544 (93%)	36 (6%)	4 (1%)	22 39
All	All	1163/1272 (91%)	1059 (91%)	85 (7%)	19 (2%)	9 17

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLN
1	A	456	ILE
1	B	445	LEU

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Mol	Chain	Res	Type
1	A	391	ASP
1	A	432	HIS
1	A	433	ILE
1	A	441	VAL
1	A	462	PRO
1	A	469	GLU
1	B	127	GLY
1	B	548	LEU
1	A	141	GLY
1	A	446	PRO
1	A	548	LEU
1	A	428	GLU
1	A	445	LEU
1	A	447	ILE
1	A	454	PRO
1	B	337	THR

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	A	498/542 (92%)	462 (93%)	36 (7%)	14 28
1	B	501/542 (92%)	469 (94%)	32 (6%)	17 33
All	All	999/1084 (92%)	931 (93%)	68 (7%)	16 30

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	THR
1	A	6	ARG
1	A	25	GLU
1	A	34	SER
1	A	35	ASN
1	A	126	LYS

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Mol	Chain	Res	Type
1	A	128	LEU
1	A	142	ASP
1	A	143	ARG
1	A	171	LYS
1	A	172	ARG
1	A	226	PHE
1	A	227	ARG
1	A	246	ASN
1	A	273	LEU
1	A	279	LYS
1	A	289	GLN
1	A	312	LYS
1	A	358	ARG
1	A	361	ARG
1	A	397	LEU
1	A	415	ASN
1	A	427	LYS
1	A	431	ASN
1	A	439	SER
1	A	441	VAL
1	A	445	LEU
1	A	460	THR
1	A	463	LEU
1	A	464	LEU
1	A	466	PHE
1	A	473	ILE
1	A	489	VAL
1	A	503	ASN
1	A	512	ASN
1	B	6	ARG
1	B	47	GLU
1	B	72	GLN
1	B	84	VAL
1	B	126	LYS
1	B	131	LYS
1	B	146	VAL
1	B	166	VAL
1	B	212	SER
1	B	226	PHE
1	B	227	ARG
1	B	239	LYS
1	B	246	ASN

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Mol	Chain	Res	Type
1	B	273	LEU
1	B	285	ILE
1	B	304	GLN
1	B	322	THR
1	B	337	THR
1	B	402	GLU
1	B	415	ASN
1	B	434	GLN
1	B	444	THR
1	B	445	LEU
1	B	450	LYS
1	B	451	LYS
1	B	463	LEU
1	B	471	ASN
1	B	478	ARG
1	B	499	LYS
1	B	503	ASN
1	B	558	SER
1	B	562	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	39	GLN
1	A	123	GLN
1	A	130	GLN
1	A	190	GLN
1	A	196	ASN
1	A	246	ASN
1	A	336	GLN
1	A	415	ASN
1	A	431	ASN
1	A	471	ASN
1	A	503	ASN
1	A	512	ASN
1	A	529	GLN
1	B	8	GLN
1	B	39	GLN
1	B	48	ASN
1	B	55	GLN
1	B	130	GLN

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Mol	Chain	Res	Type
1	B	196	ASN
1	B	197	ASN
1	B	216	ASN
1	B	228	GLN
1	B	246	ASN
1	B	289	GLN
1	B	304	GLN
1	B	309	GLN
1	B	381	GLN
1	B	415	ASN
1	B	431	ASN
1	B	443	GLN
1	B	471	ASN
1	B	503	ASN
1	B	529	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 30 ligands modelled in this entry, 23 are monoatomic - leaving 7 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	SO4	B	716	-	4,4,4	0.51	0	6,6,6	0.60	0
2	2EU	B	701	-	31,32,32	1.93	5 (16%)	46,51,51	3.43	11 (23%)
2	2EU	A	701	-	31,32,32	1.90	6 (19%)	46,51,51	2.97	16 (34%)
3	S6P	B	702	-	15,15,15	1.65	3 (20%)	21,21,21	1.32	3 (14%)
6	SO4	B	715	-	4,4,4	0.49	0	6,6,6	0.34	0
5	GOL	A	714	-	5,5,5	0.26	0	5,5,5	1.47	1 (20%)
3	S6P	A	702	-	15,15,15	1.45	3 (20%)	21,21,21	1.79	6 (28%)

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	2EU	B	701	-	-	2/34/50/50	0/3/3/3
2	2EU	A	701	-	-	0/34/50/50	0/3/3/3
3	S6P	B	702	-	-	2/20/20/20	-
5	GOL	A	714	-	-	3/4/4/4	-
3	S6P	A	702	-	-	2/20/20/20	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	2EU	O2-S1	6.83	1.51	1.43
2	A	701	2EU	O2-S1	5.94	1.50	1.43
2	A	701	2EU	O1-S1	5.83	1.50	1.43
2	B	701	2EU	S1-N1	4.88	1.70	1.63
2	B	701	2EU	O1-S1	3.96	1.47	1.43
2	A	701	2EU	S1-N1	3.41	1.68	1.63
3	B	702	S6P	P-O3P	3.30	1.61	1.50
3	A	702	S6P	C6-C5	3.16	1.56	1.51
3	B	702	S6P	C6-C5	3.02	1.56	1.51
3	B	702	S6P	P-O6	-2.48	1.52	1.60
3	A	702	S6P	P-O6	-2.41	1.52	1.60
2	B	701	2EU	O3-C1	-2.18	1.36	1.41
2	A	701	2EU	C3-C1	-2.18	1.50	1.54
2	B	701	2EU	C3-C1	-2.16	1.50	1.54
2	A	701	2EU	C2-S2	-2.15	1.68	1.72
2	A	701	2EU	C13-C9	-2.13	1.33	1.39
3	A	702	S6P	P-O1P	2.08	1.62	1.54

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	2EU	O1-S1-N1	12.92	118.47	106.69
2	B	701	2EU	C13-C12-S2	-11.97	103.27	112.98
2	A	701	2EU	C13-C12-S2	-10.67	104.32	112.98
2	B	701	2EU	C6-N1-S1	-7.97	102.57	117.05
2	A	701	2EU	C11-C6-N1	6.43	113.83	108.91
2	A	701	2EU	C10-C5-N1	6.37	113.78	108.91
2	B	701	2EU	C6-N1-C5	-6.04	105.48	112.17
2	A	701	2EU	C6-N1-S1	-5.76	106.59	117.05
2	B	701	2EU	C11-C6-N1	5.65	113.23	108.91
2	A	701	2EU	O1-S1-N1	5.51	111.71	106.69
2	B	701	2EU	O2-S1-O1	-5.20	111.09	119.52
2	A	701	2EU	C11-N2-C10	5.04	122.64	111.52
2	A	701	2EU	C6-N1-C5	-4.22	107.50	112.17
3	A	702	S6P	O6-P-O3P	4.11	118.00	106.47
2	A	701	2EU	O2-S1-N1	3.96	110.30	106.69
2	B	701	2EU	C10-C5-N1	3.84	111.85	108.91
3	A	702	S6P	C5-C4-C3	-3.71	106.66	112.47
2	A	701	2EU	F4-C4-C1	-3.47	105.22	111.85
2	A	701	2EU	O2-S1-O1	-3.33	114.13	119.52
2	A	701	2EU	F2-C3-C1	-3.08	105.97	111.85
3	B	702	S6P	O1P-P-O6	3.05	114.85	106.73
2	A	701	2EU	C5-N1-S1	-2.93	111.72	117.05
2	A	701	2EU	C6-C11-N2	2.90	116.34	110.70
2	B	701	2EU	C11-N2-C10	2.70	117.47	111.52
3	A	702	S6P	O2-C2-C3	-2.60	102.78	109.10
2	B	701	2EU	C9-C13-C12	2.48	120.61	113.74
3	A	702	S6P	O2-C2-C1	-2.34	103.65	109.14
2	B	701	2EU	F4-C4-C1	-2.34	107.39	111.85
2	B	701	2EU	F2-C3-C1	-2.33	107.40	111.85
3	A	702	S6P	C2-C3-C4	2.30	116.06	112.47
3	B	702	S6P	O5-C5-C4	-2.28	103.55	109.10
3	B	702	S6P	P-O6-C6	-2.25	112.10	118.30
2	A	701	2EU	C9-C13-C12	2.17	119.74	113.74
5	A	714	GOL	O1-C1-C2	-2.14	99.92	110.20
3	A	702	S6P	O5-C5-C4	-2.11	103.96	109.10
2	A	701	2EU	F3-C3-C1	-2.07	107.90	111.85
2	A	701	2EU	C2-S1-N1	2.03	110.57	106.81

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	714	GOL	C1-C2-C3-O3
2	B	701	2EU	C5-N1-S1-O1
5	A	714	GOL	O2-C2-C3-O3
3	B	702	S6P	O1-C1-C2-O2
2	B	701	2EU	C5-N1-S1-C2
5	A	714	GOL	O1-C1-C2-O2
3	A	702	S6P	O1-C1-C2-C3
3	A	702	S6P	O1-C1-C2-O2
3	B	702	S6P	C6-O6-P-O3P

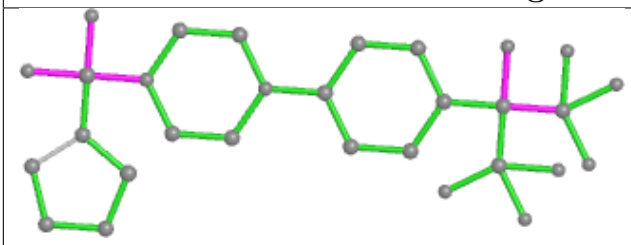
There are no ring outliers.

2 monomers are involved in 2 short contacts:

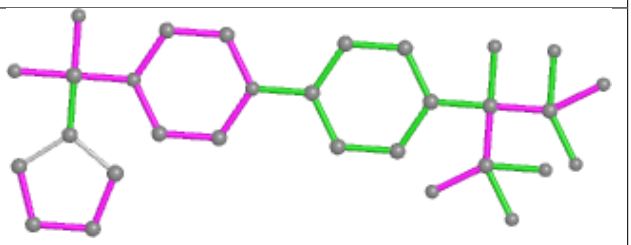
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	2EU	1	0
5	A	714	GOL	1	0

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.

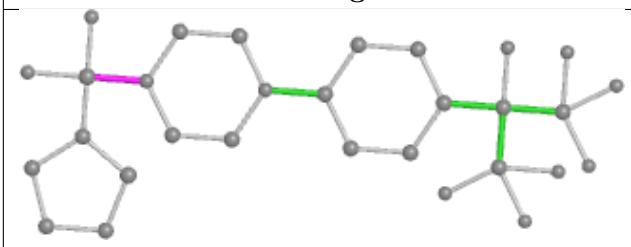
Ligand 2EU B 701



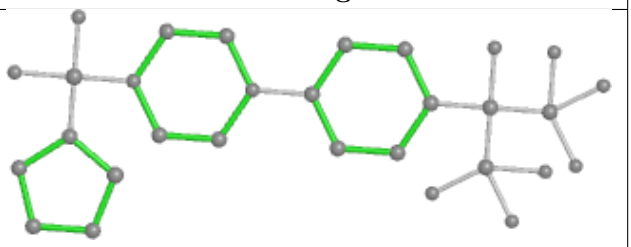
Bond lengths



Bond angles

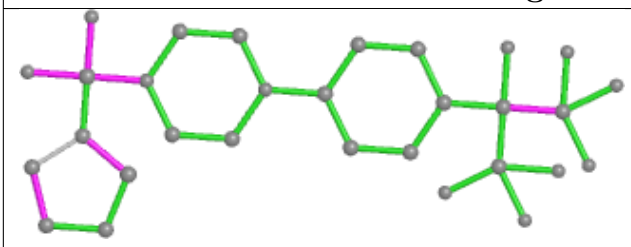


Torsions

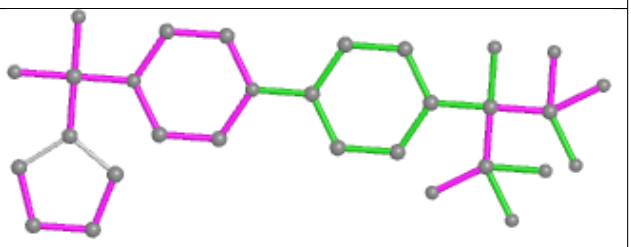


Rings

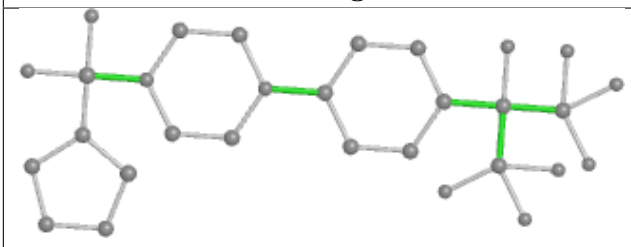
Ligand 2EU A 701



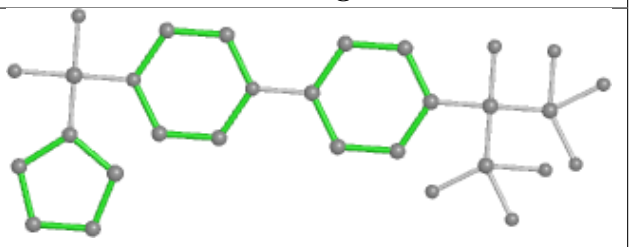
Bond lengths



Bond angles

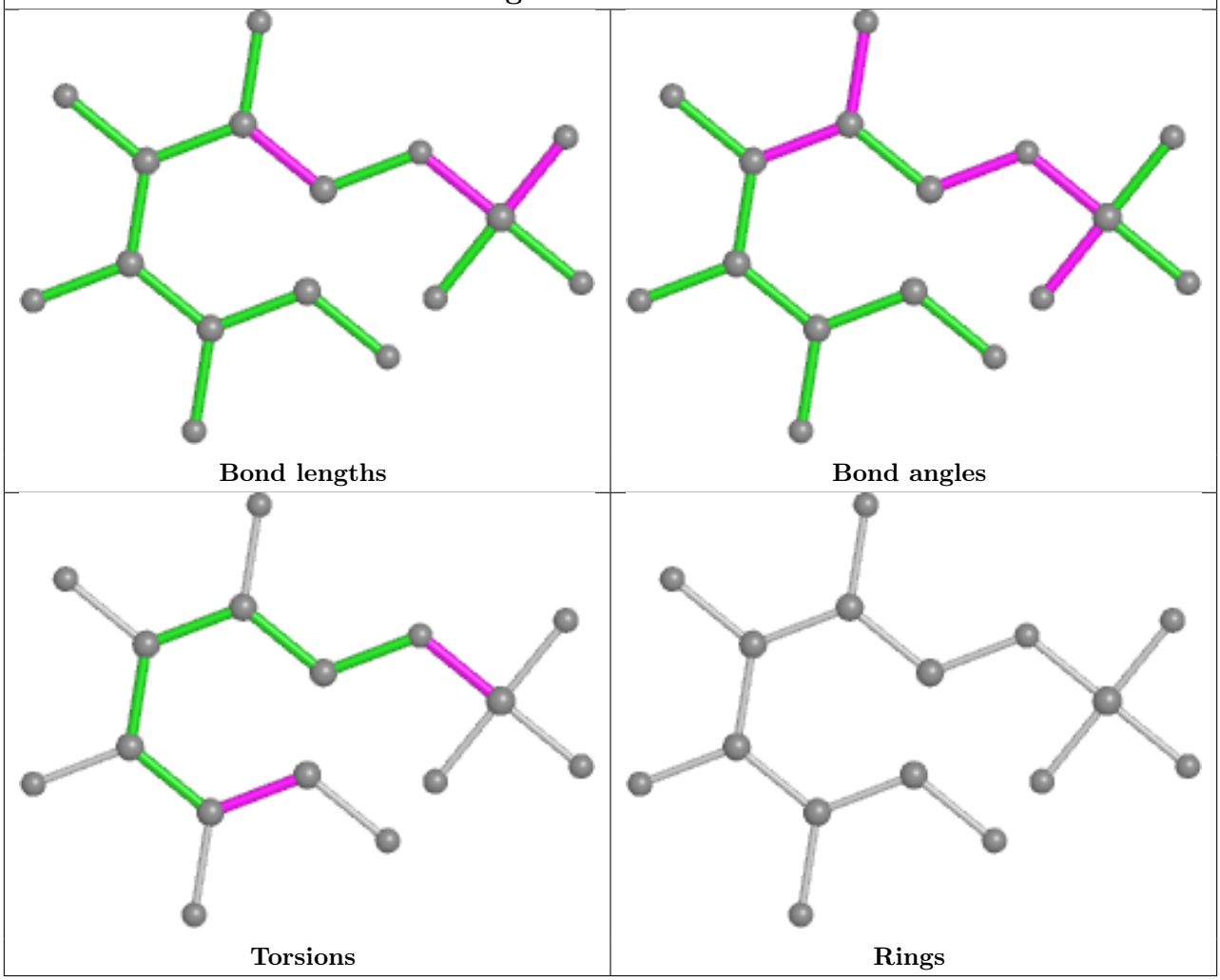


Torsions

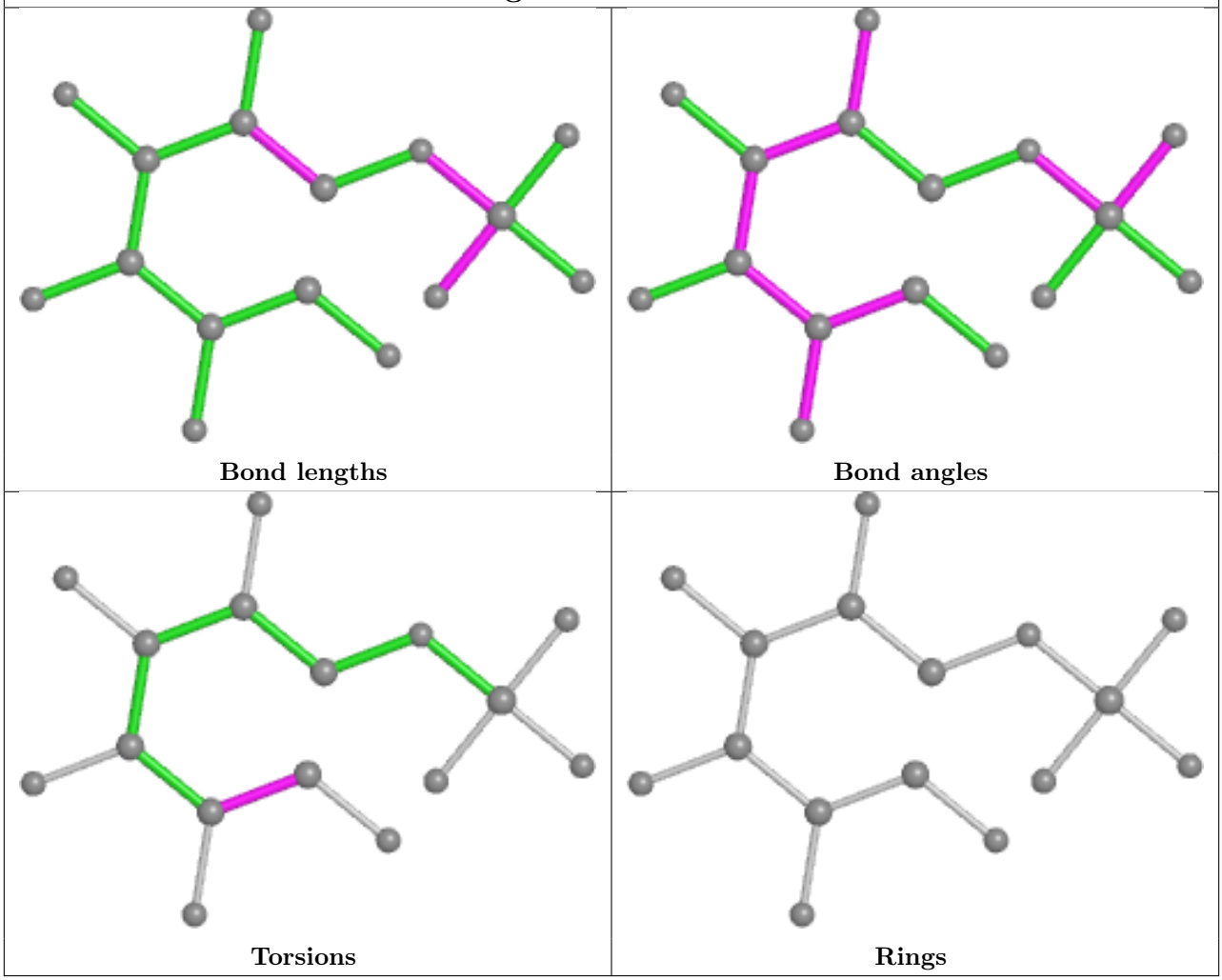


Rings

Ligand S6P B 702



Ligand S6P A 702



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	585/636 (91%)	0.03	26 (4%)	34	37	39, 65, 109, 154	0
1	B	590/636 (92%)	-0.04	25 (4%)	36	39	39, 60, 91, 134	0
All	All	1175/1272 (92%)	-0.00	51 (4%)	35	38	39, 62, 103, 154	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	PHE	6.8
1	B	2	PRO	5.0
1	B	21	LEU	4.9
1	A	449	LEU	4.6
1	B	1	MET	4.1
1	A	469	GLU	3.9
1	A	21	LEU	3.9
1	A	357	PHE	3.7
1	B	66	GLN	3.6
1	A	2	PRO	3.6
1	B	3	GLY	3.6
1	A	260	MET	3.5
1	A	390	GLU	3.5
1	B	257	SER	3.5
1	A	466	PHE	3.4
1	A	470	GLY	3.4
1	B	260	MET	3.2
1	A	385	PHE	3.1
1	B	265	ALA	3.0
1	B	258	SER	2.9
1	B	463	LEU	2.9
1	B	109	THR	2.7
1	B	465	PHE	2.6
1	A	429	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	381	GLN	2.6
1	A	464	LEU	2.5
1	A	109	THR	2.5
1	B	442	GLY	2.5
1	B	259	ARG	2.5
1	A	454	PRO	2.5
1	B	4	THR	2.5
1	B	256	GLY	2.4
1	A	258	SER	2.4
1	B	264	SER	2.3
1	A	264	SER	2.3
1	B	352	THR	2.3
1	B	97	PRO	2.3
1	A	256	GLY	2.2
1	A	69	SER	2.2
1	A	428	GLU	2.2
1	B	180	VAL	2.2
1	A	403	ILE	2.1
1	A	441	VAL	2.1
1	B	464	LEU	2.1
1	A	387	PHE	2.1
1	B	487	ASN	2.1
1	A	358	ARG	2.1
1	B	444	THR	2.0
1	A	259	ARG	2.0
1	A	402	GLU	2.0
1	B	440	THR	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,

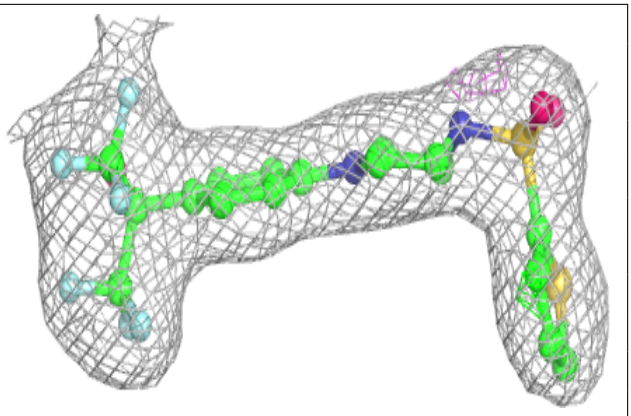
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

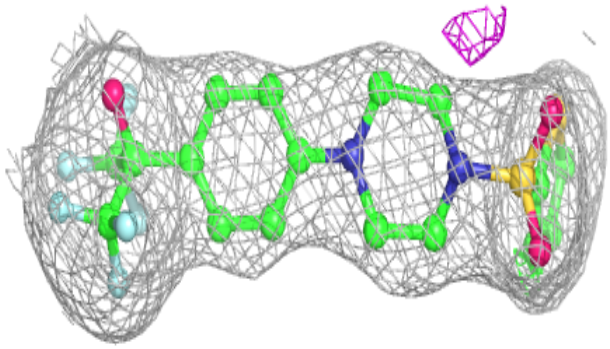
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	IOD	A	713	1/1	0.72	0.10	98,98,98,98	1
4	IOD	B	710	1/1	0.80	0.19	113,113,113,113	1
4	IOD	B	712	1/1	0.85	0.15	90,90,90,90	1
4	IOD	A	710	1/1	0.86	0.14	96,96,96,96	1
6	SO4	B	716	5/5	0.87	0.21	91,93,99,117	0
4	IOD	A	708	1/1	0.89	0.09	102,102,102,102	1
4	IOD	A	703	1/1	0.89	0.06	105,105,105,105	0
4	IOD	B	714	1/1	0.91	0.13	91,91,91,91	1
6	SO4	B	715	5/5	0.92	0.24	89,93,99,108	0
5	GOL	A	714	6/6	0.93	0.18	59,60,61,62	0
4	IOD	B	713	1/1	0.93	0.05	89,89,89,89	1
4	IOD	A	709	1/1	0.93	0.08	96,96,96,96	1
4	IOD	A	712	1/1	0.94	0.06	94,94,94,94	1
4	IOD	B	711	1/1	0.94	0.17	111,111,111,111	1
4	IOD	A	707	1/1	0.94	0.05	97,97,97,97	1
4	IOD	B	709	1/1	0.94	0.13	117,117,117,117	1
4	IOD	B	708	1/1	0.95	0.07	95,95,95,95	1
4	IOD	A	706	1/1	0.96	0.07	106,106,106,106	0
4	IOD	B	703	1/1	0.96	0.05	85,85,85,85	0
4	IOD	A	711	1/1	0.97	0.10	94,94,94,94	1
4	IOD	B	707	1/1	0.97	0.06	99,99,99,99	0
2	2EU	A	701	30/30	0.97	0.13	40,51,60,73	0
2	2EU	B	701	30/30	0.97	0.12	35,49,60,74	0
3	S6P	B	702	16/16	0.98	0.29	35,40,47,47	0
3	S6P	A	702	16/16	0.98	0.20	33,44,53,53	0
4	IOD	A	704	1/1	0.99	0.07	79,79,79,79	0
4	IOD	B	704	1/1	0.99	0.05	71,71,71,71	0
4	IOD	B	705	1/1	0.99	0.04	75,75,75,75	1
4	IOD	B	706	1/1	0.99	0.05	78,78,78,78	0
4	IOD	A	705	1/1	0.99	0.05	70,70,70,70	1

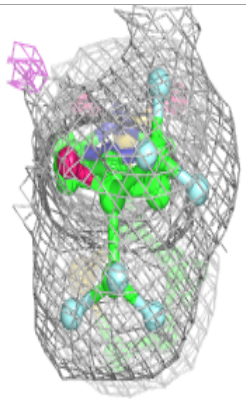
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2EU A 701:

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

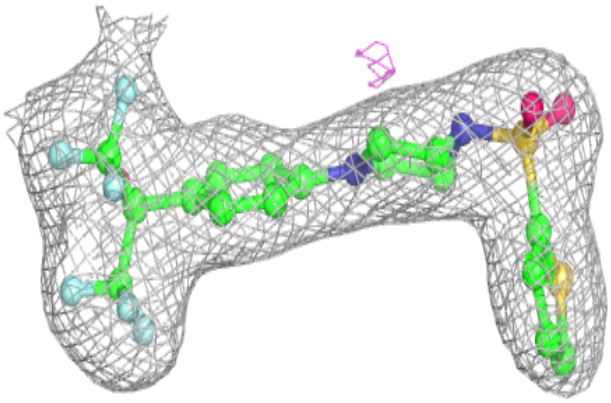


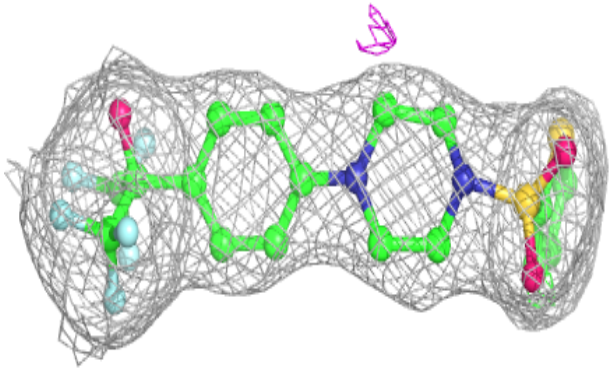


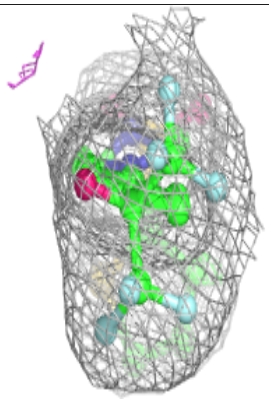


Electron density around 2EU B 701:

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

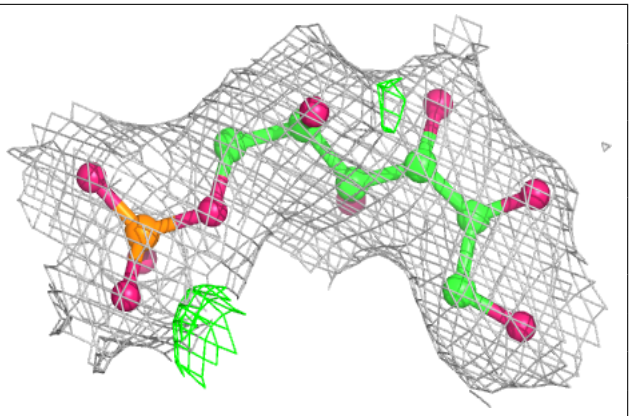


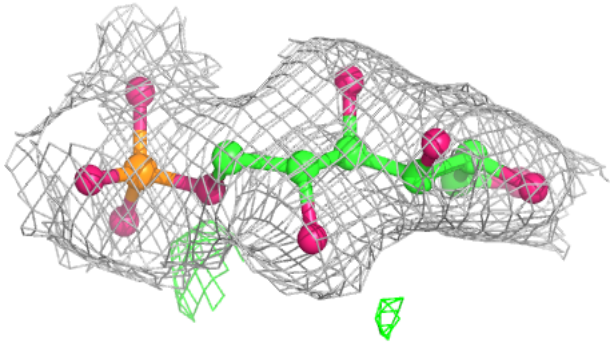


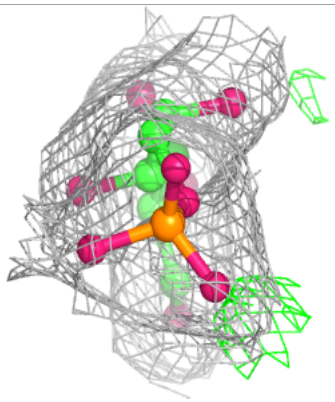


Electron density around S6P B 702:

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

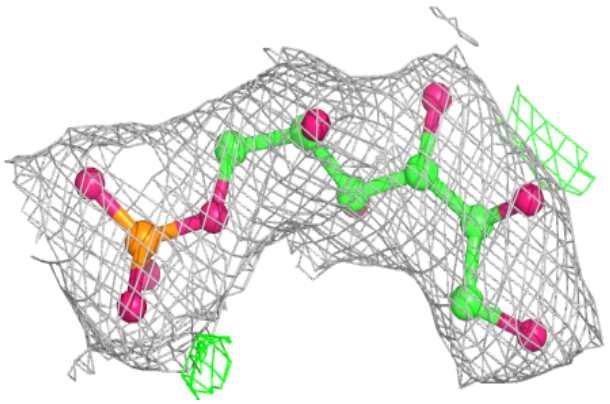


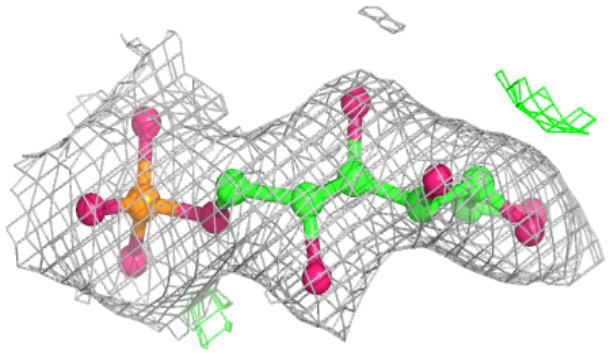


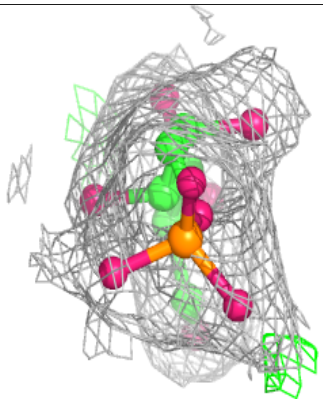


Electron density around S6P A 702:

$2mF_o$-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.