



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2014 – 06:01 PM GMT

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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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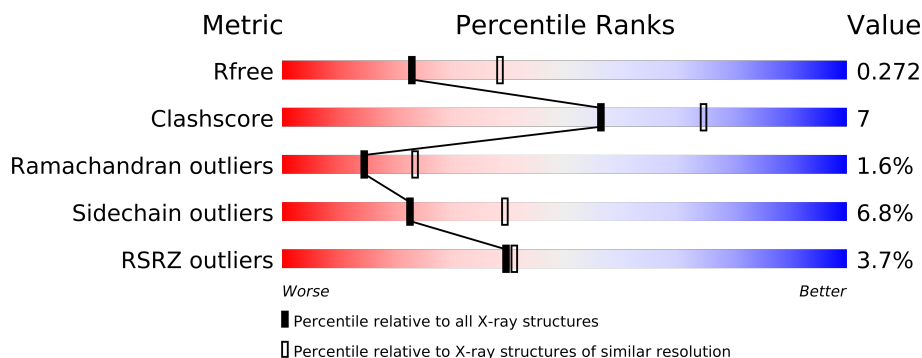
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : trunk22714  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk22714

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	636	
1	B	636	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	IOD	B	712	-	X
5	GOL	A	714	-	X
6	SO4	B	715	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9262 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

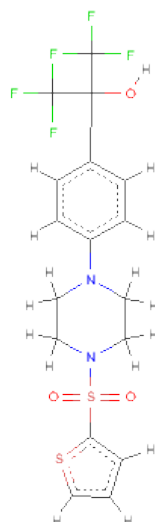
- Molecule 1 is a protein called Glucokinase regulatory protein.

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

There are 22 discrepancies between the modelled and reference sequences:

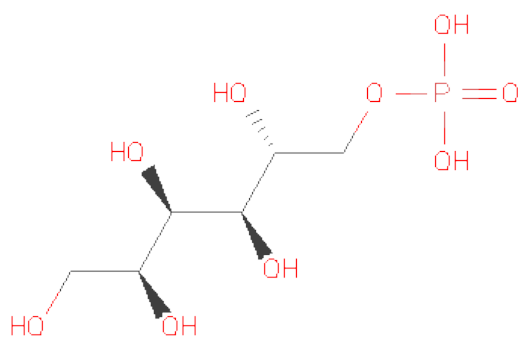
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP Q14397
A	-9	HIS	-	EXPRESSION TAG	UNP Q14397
A	-8	HIS	-	EXPRESSION TAG	UNP Q14397
A	-7	HIS	-	EXPRESSION TAG	UNP Q14397
A	-6	HIS	-	EXPRESSION TAG	UNP Q14397
A	-5	HIS	-	EXPRESSION TAG	UNP Q14397
A	-4	HIS	-	EXPRESSION TAG	UNP 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<sub>17</sub>H<sub>16</sub>F<sub>6</sub>N<sub>2</sub>O<sub>3</sub>S<sub>2</sub>).



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

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



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

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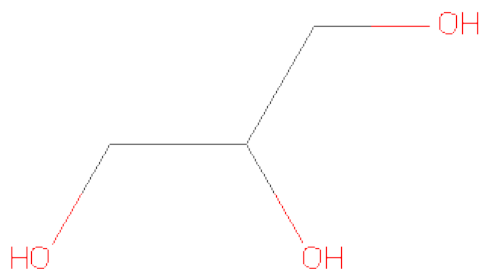
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 7 is water.

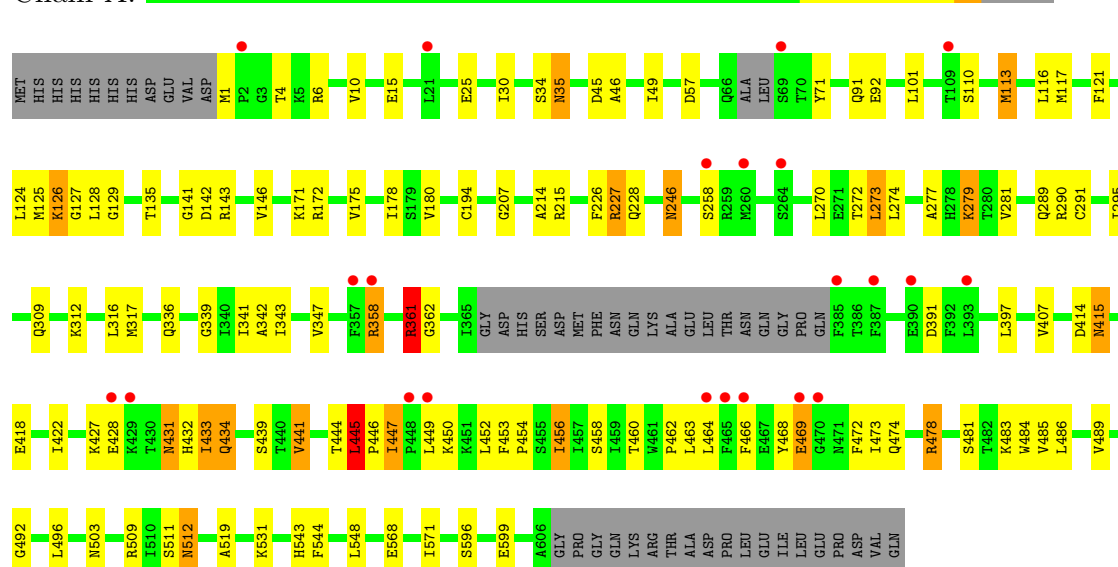
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	25	Total	O	0	0
			25	25		
7	B	31	Total	O	0	0
			31	31		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

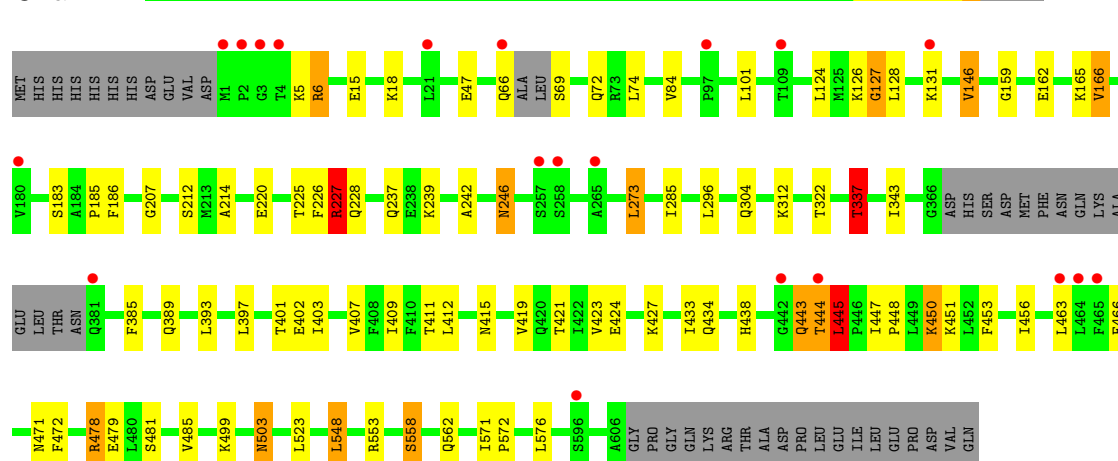
#### • Molecule 1: Glucokinase regulatory protein

Chain A:



#### • Molecule 1: Glucokinase regulatory protein

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.212 , 0.271 0.216 , 0.272	Depositor DCC
$R_{free}$ test set	2837 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.3	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 34.0	EDS
Estimated twinning fraction	0.030 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 55949 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9262	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, IOD, SO4, S6P, 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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4521	0	4618	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4554	0	4647	49	0
2	A	30	0	0	1	0
2	B	30	0	0	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	9299	121	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (121) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:HD23	1:A:273:LEU:C	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	Distance(Å)	Clash(Å)
1:B:183:SER:O	1:B:185:PRO:HD3	2.08	0.54
1:B:412:LEU:HB2	1:B:443:GLN:OE1	2.07	0.54
1:A:207:GLY:O	1:A:246:ASN:HA	2.06	0.54
1:B:407:VAL:HG12	1:B:409:ILE:HD11	1.90	0.54
1:B:225:THR:H	1:B:228:GLN:HE21	1.56	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:418:GLU:O	1:A:422:ILE:HD12	2.12	0.50
1:A:175:VAL:HG21	1:A:194:CYS:SG	2.52	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:O	1:B:146:VAL:HG13	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:433:ILE:O	1:A:434:GLN:CG	2.58	0.47
1:A:279:LYS:HD3	1:A:291:CYS:SG	2.54	0.47
1:B:127:GLY:O	1:B:128:LEU:HD23	2.15	0.47
1:B:466:PHE:HB2	4:B:703:IOD:I	2.85	0.46
1:B:427:LYS:O	1:B:427:LYS:HD2	2.15	0.46
1:B:159:GLY:HA2	1:B:186:PHE:CE1	2.51	0.46
1:A:361:ARG:HH11	1:A:361:ARG:CG	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
1:B:214:ALA:O	1:B:227:ARG:HD3	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:127:GLY:HA3	1:A:469:GLU:HG3	1.98	0.45
1:A:35:ASN:HD22	1:A:35:ASN:C	2.20	0.45
1:B:407:VAL:HG12	1:B:409:ILE:CD1	2.45	0.45
1:A:358:ARG:NH2	1:A:361:ARG:HD3	2.31	0.45
1:B:343:ILE:HD13	1:B:385:PHE:HB2	1.98	0.45
1:A:246:ASN:N	1:A:246:ASN:HD22	2.14	0.45
1:A:113:MET:HE1	1:A:483:LYS:HD2	1.99	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:433:ILE:O	1:A:434:GLN:CB	2.64	0.44
1:A:317:MET:SD	1:A:492:GLY:HA3	2.57	0.44
1:A:431:ASN:O	1:A:433:ILE:N	2.50	0.44
1:A:46:ALA:HA	1:A:317:MET:CE	2.47	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:N	1:B:503:ASN:HD22	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:B:401:THR:HG22	1:B:403:ILE:H	1.83	0.43
1:A:116:LEU:HA	1:A:116:LEU:HD23	1.81	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:HD22	1:A:431:ASN:H	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:N	1:A:431:ASN:HD22	2.17	0.42
1:B:445:LEU:HD13	1:B:450:LYS:HB3	2.02	0.42
1:A:447:ILE:HG22	1:A:450:LYS:N	2.35	0.42
1:A:274:LEU:O	1:A:277:ALA:N	2.53	0.42
1:B:15:GLU:HB2	1:B:18:LYS:HG3	2.02	0.41
1:A:519:ALA:HB2	1:A:571:ILE:HD11	2.02	0.41
1:B:433:ILE:HD12	1:B:453:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:ND2	1:A:431:ASN:H	2.19	0.41
1:A:512:ASN:C	1:A:512:ASN:HD22	2.24	0.41
1:A:509:ARG:HG2	1:A:511:SER:OG	2.20	0.41
1:B:237:GLN:HA	1:B:242:ALA:O	2.21	0.41
1:A:341:ILE:HG22	1:A:486:LEU:HD12	2.02	0.41
1:A:110:SER:HB3	1:A:178:ILE:CG2	2.51	0.41
1:B:6:ARG:HG2	1:B:6:ARG:H	1.74	0.41
1:B:523:LEU:HA	1:B:523:LEU:HD23	1.86	0.40
1:A:543:HIS:O	1:A:544:PHE:C	2.60	0.40
1:A:45:ASP:OD1	1:A:45:ASP:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	579/636 (91%)	515 (89%)	49 (8%)	15 (3%)	8	11
1	B	584/636 (92%)	544 (93%)	36 (6%)	4 (1%)	30	50
All	All	1163/1272 (91%)	1059 (91%)	85 (7%)	19 (2%)	14	23

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLN
1	A	456	ILE
1	B	445	LEU
1	A	391	ASP
1	A	432	HIS
1	A	433	ILE
1	A	441	VAL

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Mol	Chain	Res	Type
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 ⓘ

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%)	21	36
1	B	501/542 (92%)	469 (94%)	32 (6%)	25	43
All	All	999/1084 (92%)	931 (93%)	68 (7%)	22	39

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
1	A	128	LEU
1	A	142	ASP
1	A	143	ARG
1	A	171	LYS
1	A	172	ARG
1	A	226	PHE

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Mol	Chain	Res	Type
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
1	B	273	LEU
1	B	285	ILE
1	B	304	GLN
1	B	322	THR
1	B	337	THR
1	B	402	GLU

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Mol	Chain	Res	Type
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

Some 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
1	B	196	ASN
1	B	197	ASN
1	B	216	ASN
1	B	228	GLN
1	B	246	ASN
1	B	289	GLN

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
2	2EU	A	701	-	32,32,32	1.71	6 (18%)	49,51,51	2.75	14 (28%)
3	S6P	A	702	-	15,15,15	1.40	3 (20%)	21,21,21	1.73	6 (28%)
5	GOL	A	714	-	5,5,5	0.22	0	5,5,5	1.52	1 (20%)
2	2EU	B	701	-	32,32,32	1.78	5 (15%)	49,51,51	3.12	13 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	S6P	B	702	-	15,15,15	1.54	3 (20%)	21,21,21	1.32	3 (14%)
6	SO4	B	715	-	4,4,4	0.62	0	6,6,6	0.27	0
6	SO4	B	716	-	4,4,4	0.71	0	6,6,6	0.67	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
2	2EU	A	701	-	-	0/34/50/50	0/3/3/3
3	S6P	A	702	-	-	0/20/20/20	0/0/0/0
5	GOL	A	714	-	-	0/4/4/4	0/0/0/0
2	2EU	B	701	-	-	0/34/50/50	0/3/3/3
3	S6P	B	702	-	-	0/20/20/20	0/0/0/0
6	SO4	B	715	-	-	0/0/0/0	0/0/0/0
6	SO4	B	716	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	2EU	O2-S1	5.98	1.51	1.43
2	A	701	2EU	O2-S1	5.19	1.50	1.43
2	A	701	2EU	O1-S1	5.09	1.50	1.43
2	B	701	2EU	S1-N1	4.57	1.70	1.63
2	B	701	2EU	O1-S1	3.45	1.47	1.43
2	A	701	2EU	S1-N1	3.19	1.68	1.63
3	B	702	S6P	P-O3P	3.02	1.61	1.51
3	A	702	S6P	C6-C5	2.89	1.56	1.51
3	B	702	S6P	C6-C5	2.77	1.56	1.51
2	B	701	2EU	C9-C2	-2.53	1.32	1.38
2	B	701	2EU	O3-C1	-2.34	1.36	1.42
3	B	702	S6P	P-O6	-2.27	1.52	1.60
3	A	702	S6P	P-O1P	2.25	1.62	1.54
3	A	702	S6P	P-O6	-2.21	1.52	1.60
2	A	701	2EU	C9-C2	-2.07	1.33	1.38
2	A	701	2EU	C13-C9	-2.06	1.33	1.39
2	A	701	2EU	C2-S2	-2.06	1.68	1.72

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	2EU	O1-S1-N1	11.68	118.47	106.70
2	B	701	2EU	C13-C12-S2	-9.20	103.27	113.18
2	A	701	2EU	C13-C12-S2	-8.23	104.32	113.18
2	B	701	2EU	C6-N1-S1	-8.12	102.57	116.98
2	B	701	2EU	C12-S2-C2	6.42	94.74	91.91
2	A	701	2EU	C12-S2-C2	6.08	94.59	91.91
2	A	701	2EU	C11-C6-N1	6.01	113.83	109.04
2	A	701	2EU	C10-C5-N1	5.95	113.78	109.04
2	A	701	2EU	C6-N1-S1	-5.86	106.59	116.98
2	B	701	2EU	C6-N1-C5	-5.40	105.48	112.13
2	A	701	2EU	C11-N2-C10	5.33	122.64	111.66
2	B	701	2EU	C11-C6-N1	5.26	113.23	109.04
2	A	701	2EU	O1-S1-N1	4.97	111.71	106.70
2	B	701	2EU	O2-S1-O1	-4.67	111.09	119.41
2	A	701	2EU	C6-N1-C5	-3.77	107.50	112.13
3	A	702	S6P	O6-P-O3P	3.70	118.00	106.72
3	A	702	S6P	C5-C4-C3	-3.58	106.66	112.44
2	A	701	2EU	O2-S1-N1	3.57	110.30	106.70
2	B	701	2EU	C10-C5-N1	3.52	111.85	109.04
2	A	701	2EU	F4-C4-C1	-3.24	105.22	111.90
2	A	701	2EU	C5-N1-S1	-2.96	111.72	116.98
2	A	701	2EU	O2-S1-O1	-2.96	114.13	119.41
2	A	701	2EU	C6-C11-N2	2.94	116.34	110.67
2	A	701	2EU	F2-C3-C1	-2.87	105.97	111.90
3	B	702	S6P	O1P-P-O6	2.85	114.85	106.67
2	B	701	2EU	C11-N2-C10	2.82	117.47	111.66
3	B	702	S6P	P-O6-C6	-2.56	112.10	118.63
3	A	702	S6P	O2-C2-C3	-2.49	102.78	109.04
3	A	702	S6P	O2-C2-C1	-2.38	103.65	109.22
5	A	714	GOL	O1-C1-C2	-2.35	99.92	110.37
3	A	702	S6P	C2-C3-C4	2.24	116.06	112.44
2	B	701	2EU	C9-C13-C12	2.23	120.61	114.07
2	B	701	2EU	F4-C4-C1	-2.19	107.39	111.90
3	B	702	S6P	O5-C5-C4	-2.18	103.55	109.04
2	B	701	2EU	F2-C3-C1	-2.18	107.40	111.90
2	B	701	2EU	C4-C1-C3	2.04	112.11	110.43
3	A	702	S6P	O5-C5-C4	-2.02	103.96	109.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	585/636 (91%)	0.05	22 (3%)	38 40	39, 65, 109, 154	0
1	B	590/636 (92%)	-0.07	20 (3%)	43 44	39, 60, 91, 135	0
All	All	1175/1272 (92%)	-0.01	42 (3%)	39 42	39, 62, 103, 154	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	PHE	6.7
1	A	449	LEU	5.0
1	B	2	PRO	4.5
1	B	1	MET	4.5
1	B	21	LEU	4.3
1	A	21	LEU	4.2
1	A	385	PHE	3.7
1	A	260	MET	3.4
1	A	357	PHE	3.4
1	A	390	GLU	3.3
1	B	463	LEU	3.3
1	B	66	GLN	3.2
1	A	2	PRO	3.1
1	B	465	PHE	3.1
1	A	466	PHE	3.0
1	A	470	GLY	3.0
1	A	469	GLU	2.9
1	B	3	GLY	2.6
1	B	4	THR	2.6
1	B	265	ALA	2.5
1	A	429	LYS	2.5
1	B	381	GLN	2.5
1	A	264	SER	2.5
1	B	442	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	464	LEU	2.5
1	A	69	SER	2.4
1	B	257	SER	2.4
1	A	258	SER	2.3
1	A	109	THR	2.3
1	A	428	GLU	2.3
1	A	387	PHE	2.3
1	B	258	SER	2.2
1	B	109	THR	2.2
1	B	97	PRO	2.2
1	A	358	ARG	2.2
1	B	596	SER	2.2
1	B	180	VAL	2.1
1	B	444	THR	2.1
1	A	393	LEU	2.1
1	B	131	LYS	2.1
1	A	464	LEU	2.1
1	A	448	PRO	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	714	6/6	0.21	3.11	59,60,61,62	0
4	IOD	B	712	1/1	0.14	2.32	90,90,90,90	1
6	SO4	B	715	5/5	0.22	2.08	89,93,99,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	B	716	5/5	0.19	1.77	91,93,99,117	0
3	S6P	B	702	16/16	0.27	1.02	35,40,47,47	0
4	IOD	A	710	1/1	0.13	0.58	96,96,96,96	1
3	S6P	A	702	16/16	0.19	0.04	33,44,53,53	0
4	IOD	B	711	1/1	0.13	-0.34	111,111,111,111	1
2	2EU	A	701	30/30	0.12	-0.62	40,51,60,73	0
4	IOD	A	708	1/1	0.08	-0.68	102,102,102,102	1
2	2EU	B	701	30/30	0.12	-0.80	35,49,60,74	0
4	IOD	A	713	1/1	0.12	-0.97	98,98,98,98	1
4	IOD	A	712	1/1	0.06	-1.03	94,94,94,94	1
4	IOD	B	710	1/1	0.16	-1.12	113,113,113,113	1
4	IOD	B	708	1/1	0.08	-1.28	95,95,95,95	1
4	IOD	A	709	1/1	0.08	-1.29	96,96,96,96	1
4	IOD	A	711	1/1	0.07	-1.37	94,94,94,94	1
4	IOD	A	707	1/1	0.04	-1.44	97,97,97,97	1
4	IOD	B	714	1/1	0.12	-1.51	91,91,91,91	1
4	IOD	A	704	1/1	0.06	-1.58	79,79,79,79	0
4	IOD	A	703	1/1	0.06	-1.76	105,105,105,105	0
4	IOD	B	713	1/1	0.05	-1.89	89,89,89,89	1
4	IOD	B	706	1/1	0.05	-2.11	78,78,78,78	0
4	IOD	B	703	1/1	0.06	-2.92	85,85,85,85	0
4	IOD	A	706	1/1	0.07	-3.12	106,106,106,106	0
4	IOD	B	707	1/1	0.06	-3.22	99,99,99,99	0
4	IOD	B	704	1/1	0.05	-3.39	71,71,71,71	0
4	IOD	B	709	1/1	0.09	-5.36	117,117,117,117	1
4	IOD	B	705	1/1	0.03	-5.70	75,75,75,75	1
4	IOD	A	705	1/1	0.04	-6.25	70,70,70,70	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.