



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:32 PM GMT

PDB ID : 4LY9  
Title : Human GKRP complexed to AMG-1694 [(2R)-1,1,1-trifluoro-2-{4-[(2S)-2-{[(3S)-3-methylmorpholin-4-yl]methyl}-4-(thiophen-2-ylsulfonyl)piperazin-1-yl]phenyl}propan-2-ol] and sorbitol-6-phosphate  
Authors : Jordan, S.R.  
Deposited on : 2013-07-30  
Resolution : 2.35 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

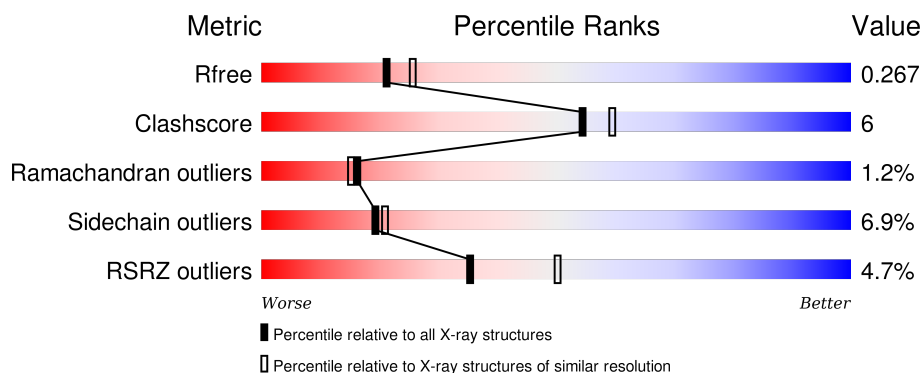
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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. 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	637	
1	B	637	

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
2	IOD	A	711	-	-	X	-
2	IOD	B	710	-	-	X	-
5	GOL	B	717	-	-	X	X
6	SO4	B	718	-	-	-	X
6	SO4	B	719	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9364 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
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			

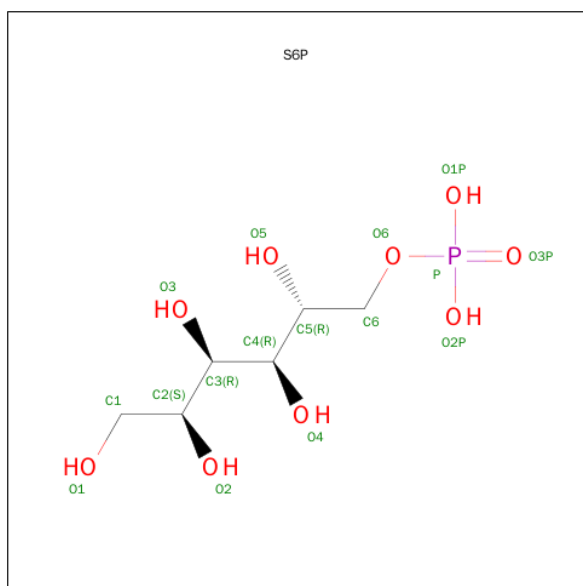
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q14397
A	-10	ALA	-	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	-11	MET	-	EXPRESSION TAG	UNP Q14397
B	-10	ALA	-	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 IODIDE ION (three-letter code: IOD) (formula: I).

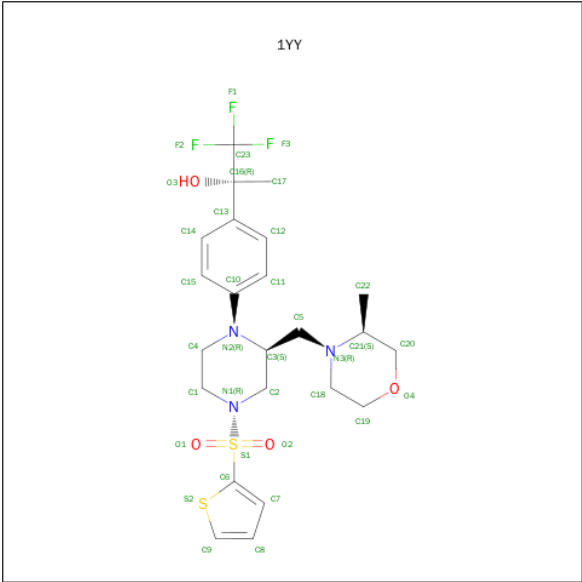
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	14	Total	I	0	0
			14	14		
2	A	12	Total	I	0	0
			12	12		

- Molecule 3 is SUGAR (D-SORBITOL-6-PHOSPHATE) (three-letter code: S6P) (formula: C<sub>6</sub>H<sub>15</sub>O<sub>9</sub>P).



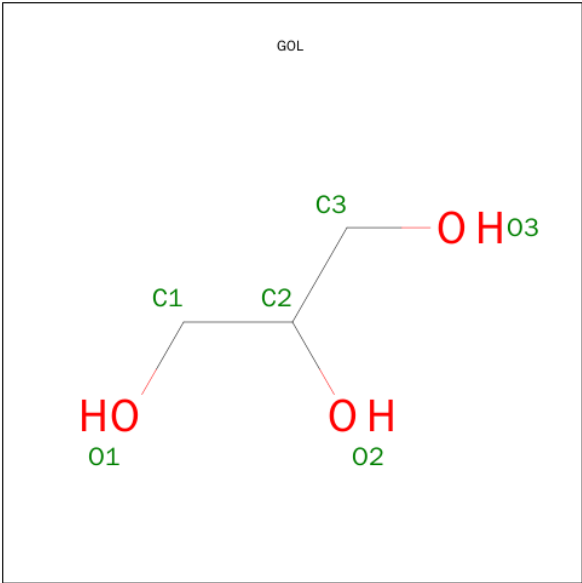
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is (2R)-1,1,1-TRIFLUORO-2-{4-[(2S)-2-[(3S)-3-METHYLMORPHOLIN-4-YL] METHYL}-4-(THIOPHEN-2-YLSULFONYL)PIPERAZIN-1-YL]PHENYL}PROPAN-2-O L (three-letter code: 1YY) (formula: C<sub>23</sub>H<sub>30</sub>F<sub>3</sub>N<sub>3</sub>O<sub>4</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			35	23	3	3	4	2		
4	B	1	Total	C	F	N	O	S	0	0
			35	23	3	3	4	2		

- 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		
5	B	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		

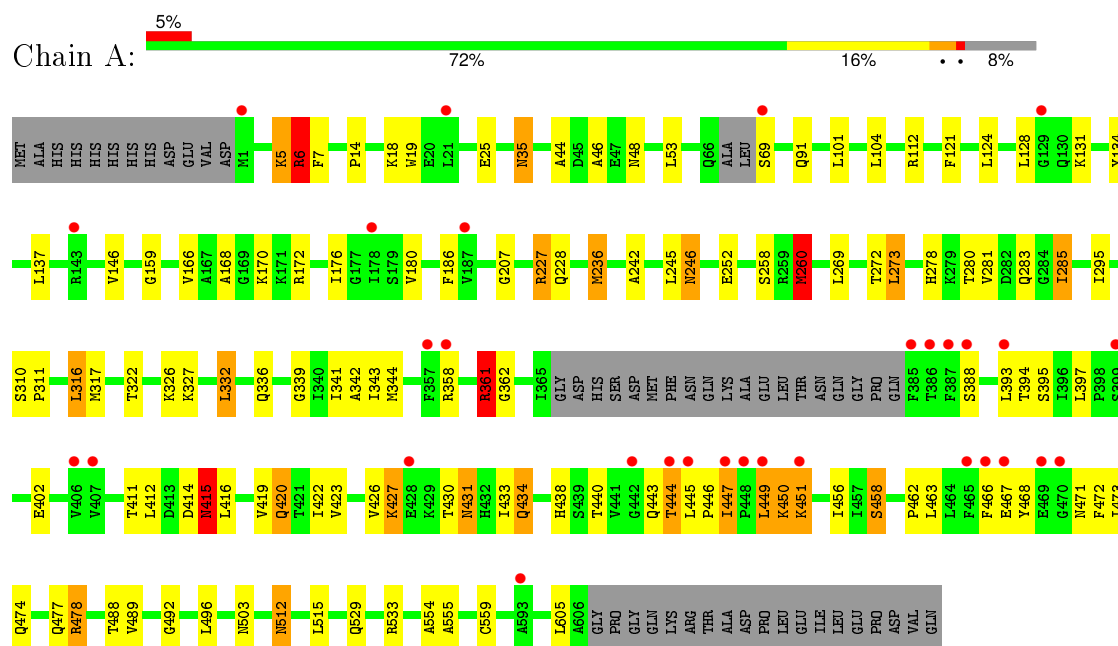
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	56	Total	O	0	0
			56	56		
7	B	83	Total	O	0	0
			83	83		

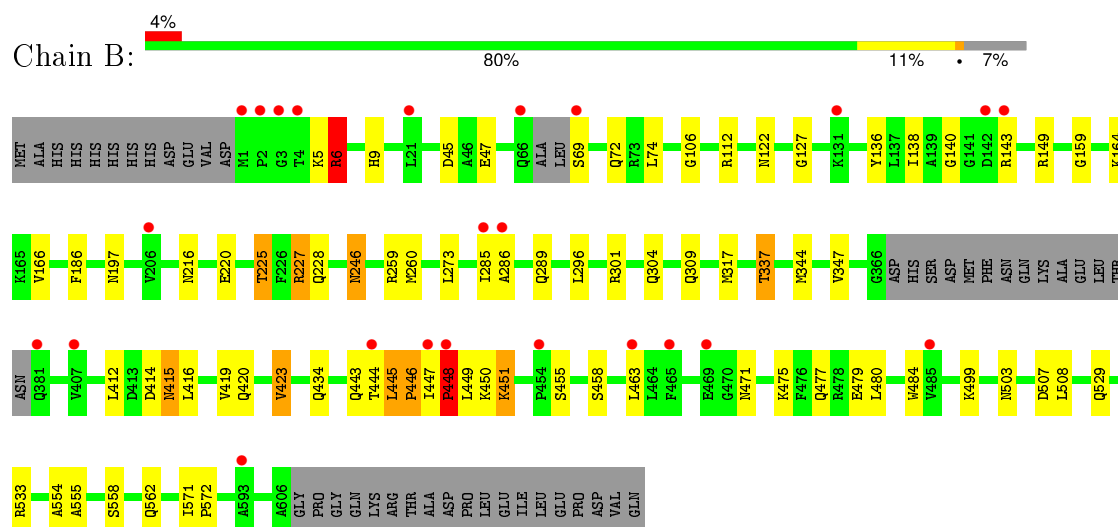
### 3 Residue-property plots [i](#)

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



- Molecule 1: Glucokinase regulatory protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.87Å 148.87Å 132.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.87 – 2.35 28.87 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.87-2.35) 98.9 (28.87-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.214 , 0.270 0.216 , 0.267	Depositor DCC
$R_{free}$ test set	3430 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.0	EDS
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 68444 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9364	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, IOD, 1YY, SO4, S6P

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	0.79	0/4603	0.90	9/6228 (0.1%)
1	B	0.82	0/4637	0.94	10/6274 (0.2%)
All	All	0.81	0/9240	0.92	19/12502 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ARG	NE-CZ-NH2	-17.17	111.71	120.30
1	B	259	ARG	NE-CZ-NH1	13.78	127.19	120.30
1	A	227	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	A	227	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	B	301	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	478	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	273	LEU	CA-CB-CG	6.73	130.79	115.30
1	A	260	MET	CG-SD-CE	-6.48	89.83	100.20
1	B	507	ASP	CB-CG-OD2	-6.00	112.91	118.30
1	B	507	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	45	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	478	ARG	NE-CZ-NH2	-5.51	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	6	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	236	MET	CG-SD-CE	5.26	108.62	100.20
1	B	273	LEU	CA-CB-CG	5.21	127.29	115.30
1	B	317	MET	CG-SD-CE	-5.21	91.86	100.20
1	B	6	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	227	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	451	LYS	Peptide
1	A	69	SER	Peptide
1	B	448	PRO	Peptide

## 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	4521	0	4618	77	0
1	B	4554	0	4647	41	0
2	A	12	0	0	5	0
2	B	14	0	0	4	0
3	A	16	0	13	1	0
3	B	16	0	13	0	0
4	A	35	0	30	1	0
4	B	35	0	30	0	0
5	A	6	0	8	2	0
5	B	6	0	8	4	0
6	B	10	0	0	0	0
7	A	56	0	0	1	0
7	B	83	0	0	1	0
All	All	9364	0	9367	118	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 6.

All (118) 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:458:SER:OG	2:A:712:IOD:I	2.47	1.03
1:B:216:ASN:OD1	1:B:225:THR:HG21	1.81	0.78
1:B:508:LEU:C	1:B:508:LEU:HD12	2.11	0.71
1:B:122:ASN:HD22	5:B:717:GOL:H31	1.56	0.70
1:B:122:ASN:HD22	5:B:717:GOL:C3	2.05	0.70
1:A:245:LEU:HD13	1:A:269:LEU:HD21	1.73	0.68
1:A:317:MET:HE2	1:A:496:LEU:HD11	1.76	0.67
1:B:447:ILE:HB	1:B:448:PRO:HD2	1.77	0.66
1:B:337:THR:HG21	1:B:479:GLU:OE1	1.96	0.66
1:A:447:ILE:HG22	1:A:449:LEU:C	2.18	0.64
1:B:6:ARG:HD3	1:B:555:ALA:O	1.97	0.64
1:A:7:PHE:HB2	5:A:715:GOL:H32	1.80	0.63
1:A:468:TYR:HB2	2:A:701:IOD:I	2.68	0.63
1:A:6:ARG:HD3	1:A:555:ALA:O	2.00	0.62
1:A:474:GLN:HA	1:A:477:GLN:HE21	1.64	0.61
1:B:419:VAL:O	1:B:423:VAL:HG12	2.01	0.61
1:A:447:ILE:HG22	1:A:450:LYS:N	2.15	0.61
1:B:6:ARG:HD2	1:B:554:ALA:O	2.01	0.59
1:A:411:THR:HG21	1:A:478:ARG:NH2	2.17	0.59
1:A:6:ARG:HD2	1:A:554:ALA:O	2.03	0.58
1:B:74:LEU:HD21	1:B:296:LEU:HD22	1.84	0.58
1:A:433:ILE:O	1:A:434:GLN:O	2.22	0.58
1:A:236:MET:HE2	1:A:242:ALA:HB2	1.85	0.57
1:B:480:LEU:HD21	1:B:484:TRP:CH2	2.40	0.57
1:A:245:LEU:HD13	1:A:269:LEU:CD2	2.35	0.56
1:A:411:THR:CG2	1:A:478:ARG:NH2	2.69	0.55
1:A:104:LEU:HD23	1:A:176:ILE:HB	1.89	0.55
1:A:412:LEU:HD12	1:A:443:GLN:HB3	1.89	0.55
1:A:444:THR:O	1:A:446:PRO:HD3	2.06	0.54
1:A:207:GLY:O	1:A:246:ASN:HA	2.07	0.54
1:A:44:ALA:HB1	1:A:48:ASN:HB3	1.89	0.54
1:A:246:ASN:N	1:A:246:ASN:HD22	2.06	0.53
1:B:309:GLN:HA	1:B:309:GLN:HE21	1.74	0.53
1:A:430:THR:HG22	1:A:431:ASN:N	2.24	0.53
1:A:339:GLY:O	1:A:342:ALA:HB3	2.09	0.53
1:B:112:ARG:HD3	1:B:344:MET:HG2	1.89	0.53
1:A:5:LYS:HB3	2:A:707:IOD:I	2.79	0.53
1:A:512:ASN:C	1:A:512:ASN:HD22	2.12	0.53
1:A:228:GLN:HE22	1:B:228:GLN:HE22	1.56	0.52
1:B:286:ALA:HA	1:B:289:GLN:HE21	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:O	1:A:397:LEU:HB3	2.10	0.52
1:B:420:GLN:HA	1:B:423:VAL:CG1	2.40	0.52
1:A:416:LEU:N	1:A:416:LEU:HD12	2.25	0.51
1:B:246:ASN:HD22	1:B:246:ASN:N	2.07	0.51
1:B:159:GLY:HA2	1:B:186:PHE:CE1	2.46	0.51
1:A:317:MET:SD	1:A:492:GLY:HA3	2.51	0.51
1:A:431:ASN:HD22	1:A:431:ASN:H	1.57	0.51
1:A:447:ILE:HG23	1:A:449:LEU:HD23	1.92	0.51
1:A:18:LYS:HE3	2:A:711:IOD:I	2.81	0.51
1:A:236:MET:HB2	1:A:242:ALA:HB3	1.94	0.50
1:B:220:GLU:OE1	1:B:558:SER:OG	2.27	0.49
1:A:449:LEU:C	1:A:451:LYS:H	2.16	0.49
1:A:316:LEU:HD13	1:A:489:VAL:HG21	1.95	0.49
1:B:414:ASP:O	1:B:416:LEU:N	2.46	0.49
1:A:159:GLY:HA2	1:A:186:PHE:CE1	2.48	0.49
1:B:122:ASN:HD22	5:B:717:GOL:H32	1.77	0.49
1:A:332:LEU:HB3	1:A:342:ALA:HB1	1.95	0.48
1:B:458:SER:HB3	2:B:710:IOD:I	2.84	0.48
1:A:53:LEU:HD12	1:A:488:THR:HG23	1.94	0.48
1:A:46:ALA:HA	1:A:317:MET:CE	2.43	0.48
1:B:140:GLY:O	1:B:149:ARG:NH2	2.46	0.48
1:B:451:LYS:HE3	1:B:451:LYS:HA	1.97	0.47
1:A:416:LEU:O	1:A:420:GLN:HG3	2.14	0.47
1:A:146:VAL:O	1:A:146:VAL:CG1	2.62	0.47
1:A:252:GLU:OE1	1:A:260:MET:HB2	2.14	0.47
1:A:283:GLN:HB2	1:A:285:ILE:HG22	1.96	0.47
1:A:414:ASP:O	1:A:415:ASN:CB	2.63	0.47
1:A:272:THR:HA	1:A:295:ILE:HG21	1.96	0.46
1:B:529:GLN:HE22	1:B:533:ARG:HH21	1.63	0.46
1:B:448:PRO:HA	1:B:451:LYS:H	1.80	0.46
1:A:512:ASN:ND2	1:A:515:LEU:H	2.14	0.46
1:A:180:VAL:HG11	1:A:258:SER:HB2	1.98	0.46
1:A:101:LEU:HD21	1:A:166:VAL:HG13	1.97	0.46
1:B:309:GLN:HA	1:B:309:GLN:NE2	2.30	0.46
1:A:280:THR:HB	1:A:285:ILE:HG23	1.97	0.46
1:B:136:TYR:HD1	5:B:717:GOL:H12	1.81	0.46
1:B:225:THR:H	1:B:228:GLN:HE21	1.64	0.46
1:A:422:ILE:O	1:A:426:VAL:HG23	2.16	0.45
1:A:419:VAL:O	1:A:423:VAL:HG23	2.17	0.45
1:A:46:ALA:HA	1:A:317:MET:HE1	1.99	0.45
1:A:18:LYS:HD2	2:A:711:IOD:I	2.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LYS:HA	1:A:430:THR:O	2.17	0.44
1:A:529:GLN:HE21	1:A:533:ARG:HE	1.65	0.44
1:A:361:ARG:HH11	1:A:361:ARG:CG	2.30	0.44
1:A:35:ASN:HD22	1:A:35:ASN:C	2.21	0.44
1:A:529:GLN:HE22	1:A:533:ARG:HH21	1.66	0.44
1:A:7:PHE:HB2	5:A:715:GOL:C3	2.46	0.43
1:A:91:GLN:HG2	1:A:281:VAL:HG13	2.00	0.43
1:B:529:GLN:NE2	1:B:533:ARG:HE	2.17	0.43
1:A:278:HIS:O	1:A:281:VAL:HG22	2.19	0.43
1:A:14:PRO:HG2	1:A:19:TRP:CD2	2.52	0.43
1:B:412:LEU:HD12	1:B:443:GLN:HB3	1.98	0.43
1:B:475:LYS:HE2	1:B:479:GLU:OE1	2.19	0.43
1:A:124:LEU:O	1:A:128:LEU:HG	2.19	0.43
1:B:477:GLN:NE2	7:B:831:HOH:O	2.52	0.43
1:B:106:GLY:O	1:B:138:ILE:HA	2.19	0.43
1:B:571:ILE:HB	1:B:572:PRO:HD3	2.00	0.43
1:A:310:SER:HB2	1:A:311:PRO:HD3	2.01	0.43
1:A:228:GLN:HE22	1:B:228:GLN:NE2	2.15	0.42
1:A:447:ILE:O	1:A:450:LYS:HB2	2.19	0.42
1:A:283:GLN:CB	1:A:285:ILE:HG22	2.49	0.42
1:B:5:LYS:HB2	2:B:708:IOD:I	2.89	0.42
1:A:414:ASP:O	1:A:415:ASN:HB2	2.19	0.42
1:A:121:PHE:HB3	1:A:134:TYR:CE2	2.55	0.42
1:B:444:THR:O	1:B:446:PRO:HD3	2.20	0.42
3:A:713:S6P:O1P	7:A:825:HOH:O	2.21	0.41
1:A:466:PHE:O	1:A:466:PHE:CD1	2.73	0.41
1:B:164:LYS:HG2	2:B:712:IOD:I	2.91	0.41
4:A:714:1YY:H30	4:A:714:1YY:H25	1.81	0.41
1:B:480:LEU:CD2	1:B:484:TRP:CH2	3.03	0.41
1:A:317:MET:CE	1:A:496:LEU:HD11	2.46	0.41
1:B:445:LEU:HG	2:B:710:IOD:I	2.91	0.41
1:A:112:ARG:HD3	1:A:344:MET:HG2	2.02	0.41
1:A:438:HIS:CG	1:A:478:ARG:HG2	2.56	0.41
1:A:343:ILE:HA	1:A:362:GLY:HA3	2.02	0.41
1:A:246:ASN:H	1:A:246:ASN:HD22	1.69	0.40
1:A:124:LEU:HD12	1:A:472:PHE:CD2	2.56	0.40
1:A:137:LEU:HD23	1:A:137:LEU:HA	1.88	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	579/637 (91%)	537 (93%)	33 (6%)	9 (2%)	12	10
1	B	584/637 (92%)	562 (96%)	17 (3%)	5 (1%)	21	22
All	All	1163/1274 (91%)	1099 (94%)	50 (4%)	14 (1%)	16	15

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	ASN
1	A	434	GLN
1	B	415	ASN
1	B	448	PRO
1	A	326	LYS
1	A	456	ILE
1	B	127	GLY
1	A	260	MET
1	A	336	GLN
1	B	446	PRO
1	A	168	ALA
1	B	260	MET
1	A	462	PRO
1	A	447	ILE

### 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%)	458 (92%)	40 (8%)	15	16
1	B	501/542 (92%)	472 (94%)	29 (6%)	25	29
All	All	999/1084 (92%)	930 (93%)	69 (7%)	19	21

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	6	ARG
1	A	25	GLU
1	A	35	ASN
1	A	131	LYS
1	A	170	LYS
1	A	172	ARG
1	A	227	ARG
1	A	246	ASN
1	A	273	LEU
1	A	285	ILE
1	A	316	LEU
1	A	322	THR
1	A	327	LYS
1	A	332	LEU
1	A	341	ILE
1	A	358	ARG
1	A	361	ARG
1	A	388	SER
1	A	394	THR
1	A	395	SER
1	A	402	GLU
1	A	415	ASN
1	A	420	GLN
1	A	427	LYS
1	A	431	ASN
1	A	440	THR
1	A	444	THR
1	A	445	LEU
1	A	449	LEU
1	A	450	LYS
1	A	458	SER
1	A	463	LEU
1	A	467	GLU
1	A	471	ASN

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Mol	Chain	Res	Type
1	A	473	ILE
1	A	503	ASN
1	A	512	ASN
1	A	559	CYS
1	A	605	LEU
1	B	6	ARG
1	B	9	HIS
1	B	47	GLU
1	B	69	SER
1	B	72	GLN
1	B	143	ARG
1	B	166	VAL
1	B	197	ASN
1	B	225	THR
1	B	227	ARG
1	B	246	ASN
1	B	285	ILE
1	B	304	GLN
1	B	337	THR
1	B	347	VAL
1	B	415	ASN
1	B	423	VAL
1	B	434	GLN
1	B	445	LEU
1	B	448	PRO
1	B	449	LEU
1	B	450	LYS
1	B	451	LYS
1	B	455	SER
1	B	463	LEU
1	B	471	ASN
1	B	499	LYS
1	B	503	ASN
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	9	HIS
1	A	35	ASN
1	A	91	GLN
1	A	123	GLN

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Mol	Chain	Res	Type
1	A	190	GLN
1	A	196	ASN
1	A	246	ASN
1	A	309	GLN
1	A	415	ASN
1	A	431	ASN
1	A	471	ASN
1	A	477	GLN
1	A	503	ASN
1	A	512	ASN
1	A	529	GLN
1	B	9	HIS
1	B	39	GLN
1	B	48	ASN
1	B	55	GLN
1	B	196	ASN
1	B	197	ASN
1	B	228	GLN
1	B	246	ASN
1	B	289	GLN
1	B	309	GLN
1	B	384	GLN
1	B	389	GLN
1	B	425	GLN
1	B	431	ASN
1	B	434	GLN
1	B	471	ASN
1	B	474	GLN
1	B	503	ASN
1	B	529	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 26 are monoatomic - leaving 8 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$
3	S6P	A	713	-	15,15,15	1.19	2 (13%)	18,21,21	1.49	3 (16%)
4	1YY	A	714	-	36,38,38	1.81	7 (19%)	44,58,58	2.73	14 (31%)
5	GOL	A	715	-	5,5,5	0.74	0	5,5,5	0.87	0
3	S6P	B	715	-	15,15,15	1.30	2 (13%)	18,21,21	1.12	0
4	1YY	B	716	-	36,38,38	1.60	7 (19%)	44,58,58	2.18	9 (20%)
5	GOL	B	717	-	5,5,5	0.56	0	5,5,5	0.75	0
6	SO4	B	718	-	4,4,4	0.99	0	6,6,6	0.48	0
6	SO4	B	719	-	4,4,4	1.11	0	6,6,6	0.91	1 (16%)

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
3	S6P	A	713	-	-	0/20/20/20	0/0/0/0
4	1YY	A	714	-	-	0/29/59/59	0/4/4/4
5	GOL	A	715	-	-	0/4/4/4	0/0/0/0
3	S6P	B	715	-	-	0/20/20/20	0/0/0/0
4	1YY	B	716	-	-	0/29/59/59	0/4/4/4
5	GOL	B	717	-	-	0/4/4/4	0/0/0/0
6	SO4	B	718	-	-	0/0/0/0	0/0/0/0
6	SO4	B	719	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	714	1YY	C3-N2	-5.16	1.42	1.47
3	A	713	S6P	C2-C3	-2.94	1.47	1.53
4	A	714	1YY	C1-N1	-2.94	1.44	1.47
4	B	716	1YY	C3-N2	-2.81	1.44	1.47
3	B	715	S6P	C2-C3	-2.67	1.48	1.53
4	A	714	1YY	C6-S2	-2.60	1.67	1.72
4	B	716	1YY	C6-S1	-2.20	1.73	1.76
4	B	716	1YY	C1-N1	-2.16	1.45	1.47
4	A	714	1YY	C16-C13	-2.07	1.50	1.53
3	A	713	S6P	P-O3P	2.30	1.58	1.51
4	B	716	1YY	C18-N3	2.36	1.52	1.47
4	A	714	1YY	C2-C3	2.59	1.57	1.51
3	B	715	S6P	P-O3P	2.81	1.60	1.51
4	B	716	1YY	O2-S1	3.83	1.48	1.43
4	B	716	1YY	S1-N1	3.94	1.69	1.63
4	B	716	1YY	O1-S1	4.01	1.48	1.43
4	A	714	1YY	O1-S1	4.30	1.49	1.43
4	A	714	1YY	O2-S1	4.59	1.49	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	714	1YY	C1-N1-C2	-10.54	103.39	112.64
4	B	716	1YY	C1-N1-C2	-9.47	104.32	112.64
4	A	714	1YY	C8-C9-S2	-6.61	105.91	113.23
4	B	716	1YY	C1-N1-S1	-4.04	109.35	117.12
4	B	716	1YY	C8-C9-S2	-3.81	109.01	113.23
4	A	714	1YY	C17-C16-C13	-3.69	104.34	110.70
4	A	714	1YY	C1-N1-S1	-3.24	110.87	117.12
4	A	714	1YY	C2-N1-S1	-3.08	111.63	117.35
3	A	713	S6P	O2P-P-O3P	-3.08	100.68	110.58
4	B	716	1YY	O1-S1-O2	-2.34	115.44	119.47
4	B	716	1YY	C19-O4-C20	-2.29	106.40	109.95
4	A	714	1YY	C14-C13-C16	-2.23	119.01	121.51
6	B	719	SO4	O2-S-O1	-2.05	103.00	109.50
4	B	716	1YY	O1-S1-C6	2.05	111.30	107.39
4	B	716	1YY	C1-C4-N2	2.09	113.14	110.45
4	A	714	1YY	F3-C23-F1	2.16	114.55	107.56
4	A	714	1YY	O3-C16-C23	2.24	109.74	106.21
4	B	716	1YY	C18-N3-C21	2.24	115.69	110.54
4	A	714	1YY	C6-S1-N1	2.28	111.27	106.70
3	A	713	S6P	O2P-P-O1P	2.43	116.65	107.38
4	A	714	1YY	O1-S1-N1	2.72	109.37	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	713	S6P	O6-P-O3P	2.91	114.55	107.14
4	A	714	1YY	C23-C16-C13	3.54	114.52	109.53
4	A	714	1YY	C4-C1-N1	3.92	112.20	109.02
4	A	714	1YY	C19-O4-C20	3.96	116.10	109.95
4	B	716	1YY	C4-C1-N1	5.40	113.41	109.02
4	A	714	1YY	C1-C4-N2	6.23	118.44	110.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	713	S6P	1	0
4	A	714	1YY	1	0
5	A	715	GOL	2	0
5	B	717	GOL	4	0

## 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, 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	585/637 (91%)	0.23	31 (5%) 30 45	23, 45, 80, 128	0
1	B	590/637 (92%)	0.10	24 (4%) 41 55	21, 40, 70, 121	0
All	All	1175/1274 (92%)	0.16	55 (4%) 35 50	21, 42, 77, 128	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	LEU	12.4
1	B	448	PRO	8.6
1	A	465	PHE	5.7
1	A	357	PHE	4.8
1	A	466	PHE	4.7
1	B	1	MET	4.6
1	B	4	THR	4.1
1	A	387	PHE	4.1
1	B	2	PRO	4.1
1	B	381	GLN	3.9
1	A	385	PHE	3.8
1	B	465	PHE	3.8
1	A	448	PRO	3.6
1	B	447	ILE	3.4
1	A	21	LEU	3.3
1	A	407	VAL	3.3
1	B	469	GLU	3.3
1	B	285	ILE	3.3
1	B	69	SER	3.2
1	A	593	ALA	3.0
1	A	69	SER	3.0
1	B	21	LEU	3.0
1	B	286	ALA	2.8
1	A	358	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	442	GLY	2.7
1	A	399	SER	2.6
1	B	206	VAL	2.6
1	A	469	GLU	2.6
1	A	467	GLU	2.6
1	B	463	LEU	2.6
1	B	131	LYS	2.5
1	A	129	GLY	2.5
1	A	451	LYS	2.5
1	A	447	ILE	2.5
1	B	444	THR	2.5
1	A	386	THR	2.4
1	B	66	GLN	2.4
1	A	388	SER	2.4
1	A	445	LEU	2.4
1	B	593	ALA	2.3
1	A	143	ARG	2.2
1	B	142	ASP	2.2
1	B	143	ARG	2.2
1	A	444	THR	2.2
1	A	470	GLY	2.2
1	A	178	ILE	2.1
1	B	407	VAL	2.1
1	B	485	VAL	2.1
1	A	428	GLU	2.1
1	A	393	LEU	2.0
1	B	454	PRO	2.0
1	A	406	VAL	2.0
1	B	3	GLY	2.0
1	A	1	MET	2.0
1	A	187	VAL	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	B	717	6/6	0.88	0.21	6.03	48,52,54,55	0
6	SO4	B	718	5/5	0.79	0.19	4.97	57,57,65,80	5
6	SO4	B	719	5/5	0.78	0.23	2.47	63,65,68,95	0
4	1YY	A	714	35/35	0.97	0.12	-0.23	28,32,36,37	0
5	GOL	A	715	6/6	0.90	0.13	-0.24	44,48,50,54	0
3	S6P	A	713	16/16	0.99	0.14	-0.32	24,27,30,31	0
4	1YY	B	716	35/35	0.97	0.11	-0.47	25,29,35,36	0
3	S6P	B	715	16/16	0.98	0.13	-0.50	20,23,26,26	0
2	IOD	B	708	1/1	0.98	0.13	-1.37	78,78,78,78	1
2	IOD	A	705	1/1	0.96	0.09	-1.44	46,46,46,46	1
2	IOD	A	701	1/1	0.93	0.04	-1.60	70,70,70,70	0
2	IOD	A	710	1/1	0.95	0.04	-1.60	62,62,62,62	1
2	IOD	A	712	1/1	0.93	0.06	-1.72	63,63,63,63	1
2	IOD	B	710	1/1	0.92	0.06	-2.15	78,78,78,78	1
2	IOD	A	707	1/1	0.94	0.06	-2.25	82,82,82,82	1
2	IOD	B	701	1/1	0.95	0.06	-2.52	53,53,53,53	0
2	IOD	A	702	1/1	0.99	0.05	-3.22	50,50,50,50	0
2	IOD	B	702	1/1	0.99	0.04	-3.80	49,49,49,49	0
2	IOD	B	705	1/1	0.98	0.03	-	68,68,68,68	0
2	IOD	B	707	1/1	0.98	0.07	-	70,70,70,70	1
2	IOD	B	711	1/1	0.95	0.16	-	81,81,81,81	1
2	IOD	B	706	1/1	0.95	0.05	-	47,47,47,47	1
2	IOD	A	711	1/1	0.81	0.13	-	82,82,82,82	1
2	IOD	A	703	1/1	1.00	0.05	-	39,39,39,39	1
2	IOD	B	712	1/1	0.97	0.09	-	75,75,75,75	1
2	IOD	B	703	1/1	0.99	0.07	-	39,39,39,39	1
2	IOD	B	709	1/1	0.86	0.07	-	74,74,74,74	1
2	IOD	B	713	1/1	0.97	0.03	-	78,78,78,78	1
2	IOD	A	706	1/1	0.98	0.04	-	53,53,53,53	1
2	IOD	B	704	1/1	0.97	0.06	-	51,51,51,51	0
2	IOD	A	704	1/1	0.95	0.04	-	72,72,72,72	1
2	IOD	B	714	1/1	0.78	0.15	-	85,85,85,85	1
2	IOD	A	709	1/1	0.97	0.07	-	78,78,78,78	1
2	IOD	A	708	1/1	0.76	0.09	-	82,82,82,82	1



## 6.5 Other polymers [i](#)

There are no such residues in this entry.