



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:46 PM GMT

PDB ID : 4PX2  
Title : Human GKRP bound to AMG2882 and Sorbitol-6-Phosphate  
Authors : Jordan, S.R.; Chmait, S.  
Deposited on : 2014-03-21  
Resolution : 2.15 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

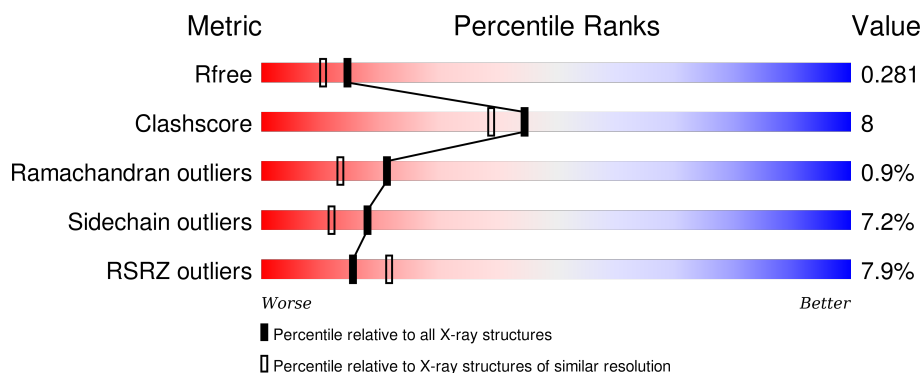
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	638	
1	B	638	

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
4	IOD	A	711	-	-	X	-
4	IOD	B	712	-	-	X	-
4	IOD	B	713	-	-	X	-
4	IOD	B	716	-	-	X	-
5	GOL	A	716	-	-	-	X
6	SO4	B	723	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9386 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 26 discrepancies between the modelled and reference sequences:

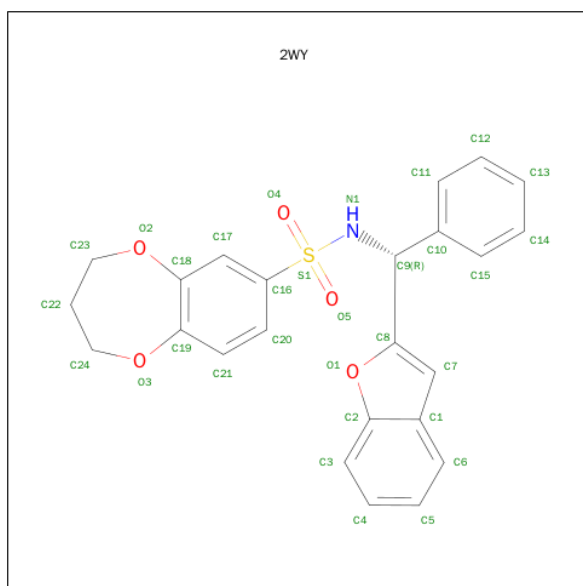
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	INITIATING METHIONINE	UNP Q14397
A	-10	ALA	-	EXPRESSION TAG	UNP Q14397
A	-9	HIS	-	EXPRESSION TAG	UNP Q14397
A	-8	HIS	-	EXPRESSION TAG	UNP Q14397
A	-7	HIS	-	EXPRESSION TAG	UNP Q14397
A	-6	HIS	-	EXPRESSION TAG	UNP Q14397
A	-5	HIS	-	EXPRESSION 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
A	626	GLY	-	EXPRESSION TAG	UNP Q14397
B	-11	MET	-	INITIATING METHIONINE	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

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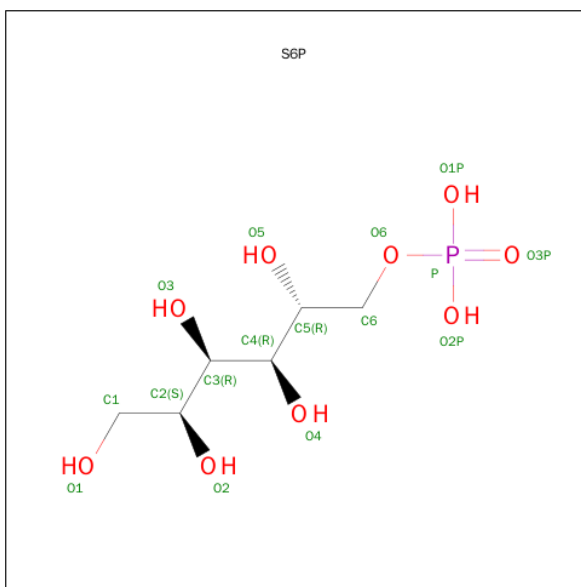
Chain	Residue	Modelled	Actual	Comment	Reference
B	626	GLY	-	EXPRESSION TAG	UNP Q14397

- Molecule 2 is N-[(R)-1-BENZOFURAN-2-YL(PHENYL)METHYL]-3,4-DIHYDRO-2H-1,5-BENZODIOXEPINE-7-SULFONAMIDE (three-letter code: 2WY) (formula:  $C_{24}H_{21}NO_5S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	24	1	5	1		
2	B	1	Total	C	N	O	S	0	0
			31	24	1	5	1		

- 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		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

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

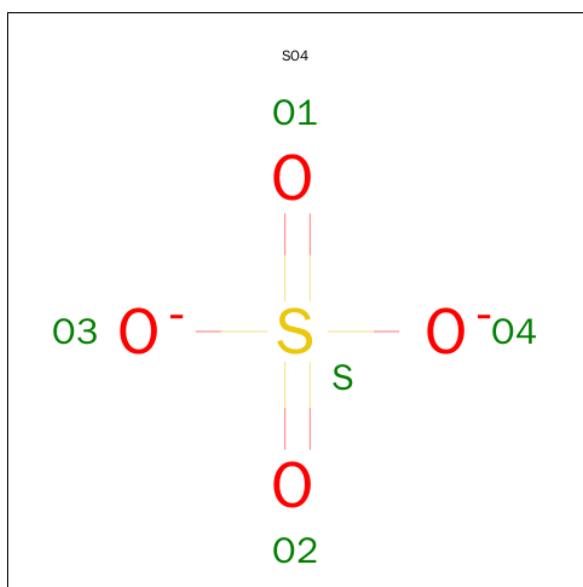
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	15	Total	I	0	0
			15	15		
4	A	13	Total	I	0	0
			13	13		

- 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		
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		

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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		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

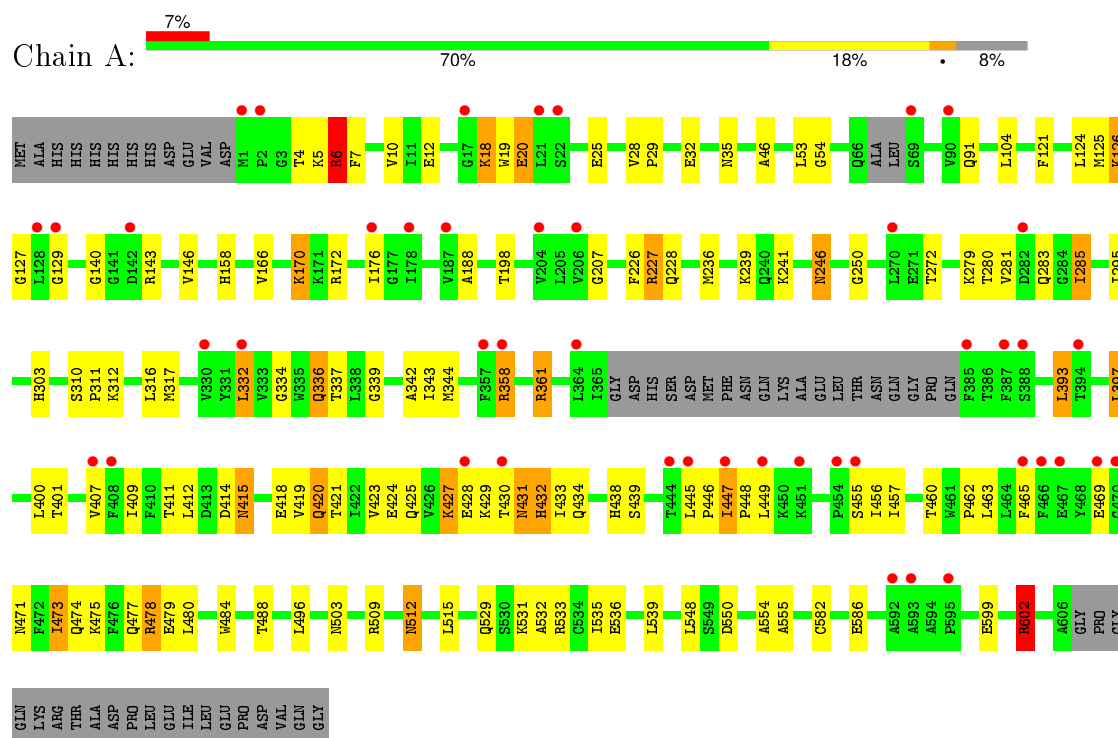
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	53	Total	O	0	0
			53	53		
7	B	98	Total	O	0	0
			98	98		



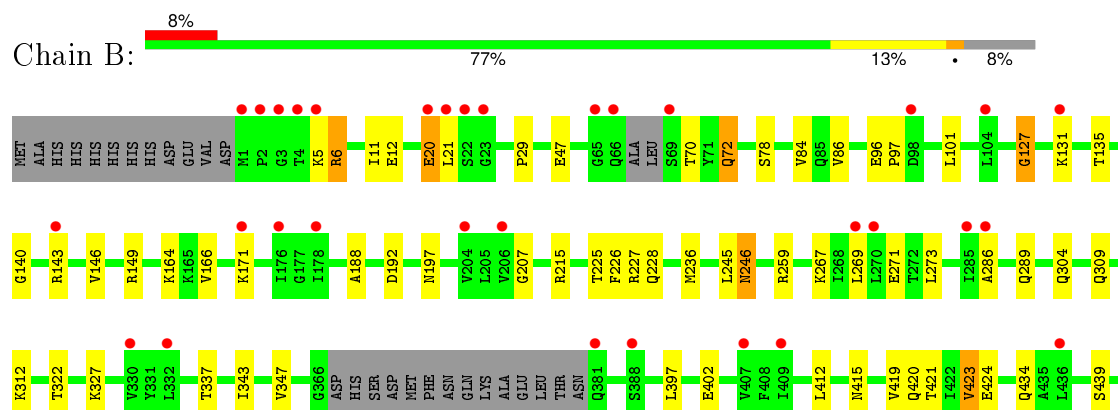
### 3 Residue-property plots

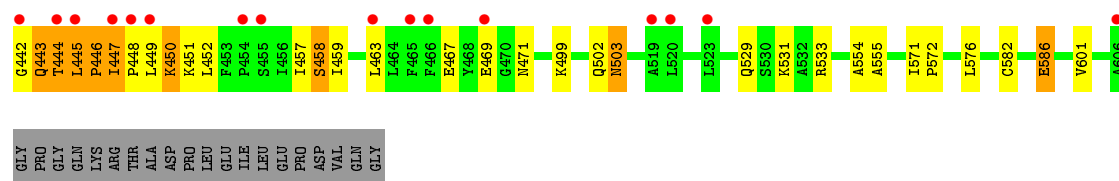
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



- Molecule 1: Glucokinase regulatory protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.16Å 148.16Å 131.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.00 – 2.15 27.62 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.3 (27.00-2.15) 98.4 (27.62-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.227 , 0.279 0.234 , 0.281	Depositor DCC
$R_{free}$ test set	4370 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.6	EDS
Estimated twinning fraction	0.028 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 87338 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, IOD, SO4, S6P, 2WY

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	0.81	1/4603 (0.0%)	0.91	10/6228 (0.2%)
1	B	0.81	0/4637	0.93	5/6274 (0.1%)
All	All	0.81	1/9240 (0.0%)	0.92	15/12502 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	GLU	CD-OE2	-5.33	1.19	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ARG	NE-CZ-NH2	-18.32	111.14	120.30
1	B	259	ARG	NE-CZ-NH1	14.87	127.74	120.30
1	A	227	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	A	227	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	361	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	A	602	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	550	ASP	CB-CG-OD1	6.42	124.08	118.30
1	B	192	ASP	CB-CG-OD1	6.26	123.93	118.30
1	B	586	GLU	OE1-CD-OE2	-6.04	116.06	123.30
1	A	361	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	344	MET	CG-SD-CE	5.73	109.37	100.20
1	A	6	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	358	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	478	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	259	ARG	CD-NE-CZ	5.09	130.73	123.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4521	0	4618	85	0
1	B	4554	0	4647	64	0
2	A	31	0	21	2	0
2	B	31	0	21	2	0
3	A	16	0	13	0	0
3	B	16	0	13	0	0
4	A	13	0	0	4	0
4	B	15	0	0	10	0
5	A	6	0	8	0	0
5	B	12	0	16	1	0
6	B	20	0	0	1	0
7	A	53	0	0	4	0
7	B	98	0	0	1	1
All	All	9386	0	9357	147	1

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 8.

All (147) 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:429:LYS:NZ	7:A:849:HOH:O	1.61	1.28
1:B:458:SER:HB3	4:B:713:IOD:I	2.37	0.94
1:A:337:THR:HG21	1:A:479:GLU:OE2	1.67	0.94
1:A:400:LEU:O	1:A:401:THR:OG1	1.92	0.87
1:B:20:GLU:HG2	1:B:21:LEU:HD22	1.64	0.80
1:A:6:ARG:HD3	1:A:555:ALA:O	1.82	0.78
1:A:4:THR:O	4:A:711:IOD:I	2.76	0.72
1:A:602:ARG:HH11	1:A:602:ARG:HG3	1.58	0.69
1:A:228:GLN:HE22	1:B:228:GLN:HE22	1.37	0.69
1:B:469:GLU:HG2	4:B:716:IOD:I	2.63	0.69
1:A:439:SER:OG	1:A:460:THR:HG22	1.91	0.69
1:A:393:LEU:O	1:A:397:LEU:HB3	1.93	0.68
1:B:140:GLY:O	1:B:149:ARG:NH2	2.27	0.68
1:A:532:ALA:O	1:A:536:GLU:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:GLN:HA	1:A:477:GLN:HE21	1.58	0.67
1:A:317:MET:HE2	1:A:496:LEU:HD11	1.77	0.66
1:A:336:GLN:NE2	1:A:414:ASP:OD1	2.29	0.66
1:A:140:GLY:H	1:A:158:HIS:HE1	1.42	0.65
1:A:433:ILE:O	1:A:434:GLN:HG2	1.98	0.63
1:A:474:GLN:O	1:A:478:ARG:HD3	1.98	0.62
1:B:502:GLN:NE2	4:B:717:IOD:I	3.01	0.62
1:B:72:GLN:CD	1:B:78:SER:HG	2.02	0.62
1:A:415:ASN:HD22	1:A:418:GLU:H	1.46	0.62
1:B:445:LEU:HG	4:B:713:IOD:I	2.70	0.61
1:B:448:PRO:O	1:B:451:LYS:HB2	2.01	0.60
1:A:283:GLN:HB2	1:A:285:ILE:HG22	1.84	0.60
1:B:6:ARG:HD2	1:B:554:ALA:O	2.02	0.59
1:A:146:VAL:HG12	1:A:146:VAL:O	2.03	0.59
1:B:146:VAL:O	1:B:146:VAL:HG12	2.01	0.59
1:A:582:CYS:HB2	1:A:586:GLU:OE2	2.02	0.58
1:A:339:GLY:O	1:A:342:ALA:HB3	2.04	0.58
1:A:246:ASN:H	1:A:246:ASN:HD22	1.50	0.58
1:A:19:TRP:O	1:A:20:GLU:CB	2.52	0.58
1:A:480:LEU:HD21	1:A:484:TRP:CH2	2.39	0.57
1:A:46:ALA:HA	1:A:317:MET:HE1	1.87	0.57
1:A:246:ASN:N	1:A:246:ASN:HD22	2.03	0.56
1:B:286:ALA:HA	1:B:289:GLN:HE21	1.70	0.56
1:B:6:ARG:HD3	1:B:555:ALA:O	2.05	0.56
1:B:127:GLY:O	4:B:716:IOD:I	2.94	0.55
1:A:317:MET:CE	1:A:496:LEU:HD11	2.36	0.55
1:A:529:GLN:HE22	1:A:533:ARG:HH21	1.54	0.55
1:A:312:LYS:HB3	1:A:457:ILE:HG12	1.88	0.55
1:B:419:VAL:O	1:B:423:VAL:HG12	2.05	0.55
1:B:531:LYS:HE2	4:B:712:IOD:I	2.76	0.55
1:B:5:LYS:HB2	4:B:710:IOD:I	2.77	0.55
1:B:529:GLN:HE21	1:B:533:ARG:HE	1.53	0.55
1:B:503:ASN:HD22	1:B:503:ASN:H	1.56	0.54
1:A:512:ASN:ND2	1:A:515:LEU:H	2.03	0.54
1:B:225:THR:H	1:B:228:GLN:HE21	1.54	0.54
1:A:420:GLN:HB3	1:A:449:LEU:HG	1.90	0.54
1:A:198:THR:HG21	1:A:236:MET:HE1	1.90	0.54
1:B:164:LYS:HE2	5:B:719:GOL:H12	1.89	0.54
1:A:228:GLN:HE22	1:B:228:GLN:NE2	2.04	0.54
1:B:146:VAL:HG13	1:B:343:ILE:CG2	2.38	0.53
1:B:442:GLY:O	1:B:443:GLN:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:VAL:HG13	1:B:343:ILE:HG21	1.91	0.53
1:A:431:ASN:HD22	1:A:431:ASN:H	1.56	0.52
1:A:6:ARG:HD2	1:A:554:ALA:O	2.10	0.52
1:A:602:ARG:HH11	1:A:602:ARG:CG	2.21	0.51
1:A:46:ALA:HA	1:A:317:MET:CE	2.39	0.51
1:A:447:ILE:N	1:A:448:PRO:HD2	2.25	0.51
1:B:420:GLN:HA	1:B:423:VAL:HG13	1.92	0.51
1:A:104:LEU:HD23	1:A:176:ILE:HB	1.93	0.51
1:A:419:VAL:O	1:A:423:VAL:HG23	2.11	0.50
1:A:53:LEU:HD12	1:A:488:THR:HG23	1.93	0.50
1:B:309:GLN:NE2	1:B:458:SER:O	2.45	0.50
1:A:146:VAL:HG13	1:A:343:ILE:CG2	2.40	0.50
1:A:473:ILE:HD13	1:A:473:ILE:O	2.12	0.50
1:A:397:LEU:O	1:A:397:LEU:HD22	2.12	0.50
1:A:397:LEU:O	1:A:400:LEU:HD13	2.12	0.50
1:A:29:PRO:HG2	2:A:701:2WY:C11	2.42	0.50
1:A:280:THR:HB	1:A:285:ILE:O	2.12	0.50
1:A:4:THR:HA	4:A:711:IOD:I	2.82	0.50
1:B:447:ILE:HG22	1:B:450:LYS:CE	2.41	0.50
1:A:236:MET:CE	1:A:241:LYS:HB3	2.42	0.49
1:B:246:ASN:N	1:B:246:ASN:HD22	2.09	0.49
1:A:91:GLN:HG2	1:A:281:VAL:HG13	1.95	0.49
1:B:458:SER:CB	4:B:713:IOD:I	3.23	0.49
1:B:444:THR:O	1:B:446:PRO:HD3	2.13	0.49
1:A:7:PHE:HB2	4:A:711:IOD:I	2.83	0.49
1:B:529:GLN:HE22	1:B:533:ARG:HH21	1.60	0.49
1:B:412:LEU:CD1	1:B:439:SER:HB3	2.43	0.48
1:A:121:PHE:O	1:A:125:MET:HG3	2.14	0.48
1:A:332:LEU:HD12	1:A:407:VAL:HB	1.94	0.48
1:B:236:MET:HG2	6:B:722:SO4:O3	2.13	0.48
1:A:207:GLY:O	1:A:246:ASN:HA	2.14	0.48
1:B:421:THR:O	1:B:424:GLU:HB2	2.13	0.48
1:A:475:LYS:HE2	1:A:479:GLU:OE2	2.14	0.47
1:A:18:LYS:HE2	7:A:850:HOH:O	2.14	0.47
1:A:126:LYS:O	1:A:129:GLY:N	2.38	0.47
1:B:207:GLY:O	1:B:246:ASN:HA	2.15	0.47
1:A:334:GLY:HA2	1:A:409:ILE:O	2.14	0.47
1:A:54:GLY:O	1:A:303:HIS:NE2	2.48	0.47
1:A:170:LYS:HD2	1:A:170:LYS:N	2.30	0.47
1:B:309:GLN:HG3	1:B:459:ILE:HD13	1.96	0.47
1:A:18:LYS:CE	7:A:850:HOH:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:ILE:HB	1:B:572:PRO:HD3	1.97	0.46
1:A:412:LEU:N	1:A:412:LEU:HD23	2.30	0.46
1:B:246:ASN:HD22	1:B:246:ASN:H	1.64	0.46
1:B:267:LYS:NZ	1:B:271:GLU:OE1	2.49	0.46
1:A:91:GLN:HG2	1:A:281:VAL:CG1	2.46	0.46
1:B:582:CYS:HB2	1:B:586:GLU:OE1	2.16	0.45
1:A:512:ASN:C	1:A:512:ASN:HD22	2.19	0.45
1:A:124:LEU:HD23	1:A:124:LEU:C	2.37	0.45
1:A:535:ILE:O	1:A:539:LEU:HG	2.17	0.44
1:A:427:LYS:O	1:A:427:LYS:HE2	2.17	0.44
1:A:509:ARG:NH1	7:A:841:HOH:O	2.43	0.44
1:B:529:GLN:NE2	1:B:533:ARG:HE	2.15	0.44
1:A:430:THR:HG22	1:A:432:HIS:H	1.81	0.44
1:B:245:LEU:HG	1:B:269:LEU:HD21	1.98	0.44
1:A:283:GLN:CB	1:A:285:ILE:HG22	2.48	0.44
1:B:11:ILE:HG22	1:B:12:GLU:N	2.33	0.44
1:A:10:VAL:HB	1:A:531:LYS:HE3	2.00	0.44
1:B:72:GLN:CG	1:B:78:SER:OG	2.66	0.44
1:B:503:ASN:ND2	1:B:503:ASN:H	2.16	0.44
1:B:503:ASN:HD22	1:B:503:ASN:N	2.14	0.44
1:B:449:LEU:HA	1:B:452:LEU:HD12	1.99	0.43
1:A:400:LEU:C	1:A:401:THR:HG1	2.08	0.43
1:A:250:GLY:HA2	4:A:705:IOD:I	2.88	0.43
1:A:188:ALA:HB2	1:A:226:PHE:CD2	2.53	0.43
1:B:86:VAL:HG12	1:B:273:LEU:HD21	2.00	0.43
1:B:215:ARG:HG3	2:B:701:2WY:C11	2.48	0.43
1:A:146:VAL:HG13	1:A:343:ILE:HG21	1.99	0.43
1:B:503:ASN:ND2	1:B:503:ASN:N	2.66	0.43
1:B:447:ILE:N	1:B:448:PRO:HD2	2.34	0.42
1:A:272:THR:HA	1:A:295:ILE:HG21	2.00	0.42
1:B:412:LEU:HD12	1:B:443:GLN:HB3	2.01	0.42
1:A:310:SER:HB2	1:A:311:PRO:HD3	2.01	0.42
1:B:447:ILE:HG22	1:B:450:LYS:HE3	2.02	0.42
1:B:101:LEU:HD11	1:B:135:THR:HG22	2.02	0.42
1:B:531:LYS:CE	4:B:712:IOD:I	3.38	0.42
1:A:146:VAL:CG1	1:A:146:VAL:O	2.66	0.42
1:A:28:VAL:HG22	2:A:701:2WY:C4	2.49	0.42
1:B:312:LYS:HB3	1:B:457:ILE:HG12	2.01	0.42
1:B:572:PRO:O	1:B:576:LEU:HG	2.20	0.41
1:B:188:ALA:HB2	1:B:226:PHE:CD2	2.55	0.41
1:B:96:GLU:N	1:B:97:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:THR:HG22	1:A:432:HIS:N	2.35	0.41
1:B:29:PRO:HG2	2:B:701:2WY:C11	2.51	0.41
1:B:601:VAL:HG21	4:B:704:IOD:I	2.91	0.41
1:A:400:LEU:HD12	1:A:400:LEU:N	2.35	0.41
1:B:322:THR:HB	7:B:826:HOH:O	2.20	0.41
1:A:400:LEU:C	1:A:401:THR:OG1	2.57	0.41
1:A:438:HIS:CG	1:A:478:ARG:HG2	2.56	0.40
1:A:421:THR:O	1:A:424:GLU:HB2	2.21	0.40
1:A:548:LEU:HD23	1:A:548:LEU:HA	1.89	0.40
1:B:286:ALA:HA	1:B:289:GLN:NE2	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:891:HOH:O	7:B:895:HOH:O[6_554]	1.55	0.65

## 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	579/638 (91%)	540 (93%)	31 (5%)	8 (1%)	14	7
1	B	584/638 (92%)	554 (95%)	27 (5%)	3 (0%)	34	26
All	All	1163/1276 (91%)	1094 (94%)	58 (5%)	11 (1%)	21	13

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	B	443	GLN
1	A	456	ILE

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Mol	Chain	Res	Type
1	B	127	GLY
1	A	127	GLY
1	A	336	GLN
1	A	469	GLU
1	A	446	PRO
1	A	432	HIS
1	A	462	PRO
1	B	446	PRO

### 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%)	458 (92%)	40 (8%)	15	9
1	B	501/542 (92%)	469 (94%)	32 (6%)	22	15
All	All	999/1084 (92%)	927 (93%)	72 (7%)	18	12

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	6	ARG
1	A	12	GLU
1	A	18	LYS
1	A	25	GLU
1	A	35	ASN
1	A	126	LYS
1	A	143	ARG
1	A	166	VAL
1	A	170	LYS
1	A	172	ARG
1	A	227	ARG
1	A	239	LYS
1	A	246	ASN
1	A	279	LYS

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Mol	Chain	Res	Type
1	A	285	ILE
1	A	316	LEU
1	A	332	LEU
1	A	358	ARG
1	A	361	ARG
1	A	393	LEU
1	A	397	LEU
1	A	411	THR
1	A	415	ASN
1	A	420	GLN
1	A	425	GLN
1	A	427	LYS
1	A	428	GLU
1	A	431	ASN
1	A	445	LEU
1	A	447	ILE
1	A	455	SER
1	A	463	LEU
1	A	465	PHE
1	A	471	ASN
1	A	473	ILE
1	A	503	ASN
1	A	512	ASN
1	A	599	GLU
1	A	602	ARG
1	B	6	ARG
1	B	20	GLU
1	B	47	GLU
1	B	70	THR
1	B	72	GLN
1	B	84	VAL
1	B	131	LYS
1	B	143	ARG
1	B	166	VAL
1	B	171	LYS
1	B	197	ASN
1	B	227	ARG
1	B	246	ASN
1	B	304	GLN
1	B	327	LYS
1	B	337	THR
1	B	347	VAL

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Mol	Chain	Res	Type
1	B	397	LEU
1	B	402	GLU
1	B	415	ASN
1	B	423	VAL
1	B	434	GLN
1	B	444	THR
1	B	445	LEU
1	B	447	ILE
1	B	450	LYS
1	B	458	SER
1	B	463	LEU
1	B	467	GLU
1	B	471	ASN
1	B	499	LYS
1	B	503	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) 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
1	A	158	HIS
1	A	190	GLN
1	A	196	ASN
1	A	246	ASN
1	A	289	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	8	GLN
1	B	9	HIS
1	B	39	GLN
1	B	48	ASN
1	B	130	GLN
1	B	197	ASN
1	B	228	GLN

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Mol	Chain	Res	Type
1	B	246	ASN
1	B	289	GLN
1	B	389	GLN
1	B	415	ASN
1	B	431	ASN
1	B	434	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 28 are monoatomic - leaving 11 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	2WY	A	701	-	30,35,35	2.53	11 (36%)	39,50,50	2.48	15 (38%)
3	S6P	A	702	-	15,15,15	1.08	1 (6%)	18,21,21	2.04	3 (16%)
5	GOL	A	716	-	5,5,5	0.38	0	5,5,5	1.70	2 (40%)
2	2WY	B	701	-	30,35,35	2.50	8 (26%)	39,50,50	2.92	14 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	S6P	B	702	-	15,15,15	2.01	4 (26%)	18,21,21	1.16	1 (5%)
5	GOL	B	718	-	5,5,5	0.66	0	5,5,5	0.90	0
5	GOL	B	719	-	5,5,5	0.52	0	5,5,5	0.18	0
6	SO4	B	720	-	4,4,4	0.80	0	6,6,6	0.52	0
6	SO4	B	721	-	4,4,4	0.26	0	6,6,6	0.92	1 (16%)
6	SO4	B	722	-	4,4,4	0.92	0	6,6,6	0.37	0
6	SO4	B	723	-	4,4,4	0.59	0	6,6,6	0.33	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	2WY	A	701	-	-	0/15/27/27	0/3/5/5
3	S6P	A	702	-	-	0/20/20/20	0/0/0/0
5	GOL	A	716	-	-	0/4/4/4	0/0/0/0
2	2WY	B	701	-	-	0/15/27/27	0/3/5/5
3	S6P	B	702	-	-	0/20/20/20	0/0/0/0
5	GOL	B	718	-	-	0/4/4/4	0/0/0/0
5	GOL	B	719	-	-	0/4/4/4	0/0/0/0
6	SO4	B	720	-	-	0/0/0/0	0/0/0/0
6	SO4	B	721	-	-	0/0/0/0	0/0/0/0
6	SO4	B	722	-	-	0/0/0/0	0/0/0/0
6	SO4	B	723	-	-	0/0/0/0	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	S6P	C2-C3	-3.54	1.46	1.53
2	A	701	2WY	C7-C8	-3.09	1.32	1.39
3	A	702	S6P	C2-C3	-2.97	1.47	1.53
3	B	702	S6P	P-O1P	-2.44	1.45	1.54
2	B	701	2WY	C7-C8	-2.44	1.33	1.39
2	A	701	2WY	C10-C9	2.06	1.55	1.52
2	B	701	2WY	O2-C23	2.25	1.49	1.44
2	B	701	2WY	C22-C24	2.29	1.56	1.51
2	B	701	2WY	C22-C23	2.40	1.57	1.51
2	A	701	2WY	C22-C24	2.46	1.57	1.51
2	A	701	2WY	C22-C23	2.47	1.57	1.51
2	A	701	2WY	O3-C24	2.48	1.49	1.44
2	A	701	2WY	C20-C16	2.53	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	2WY	S1-N1	2.64	1.66	1.61
3	B	702	S6P	C6-C5	2.73	1.55	1.51
2	A	701	2WY	C11-C10	3.14	1.44	1.39
2	A	701	2WY	C16-S1	3.40	1.81	1.76
3	B	702	S6P	P-O3P	4.28	1.65	1.51
2	A	701	2WY	O5-S1	5.32	1.49	1.43
2	B	701	2WY	O4-S1	5.38	1.49	1.43
2	A	701	2WY	S1-N1	5.75	1.71	1.61
2	B	701	2WY	O5-S1	6.47	1.50	1.43
2	A	701	2WY	O4-S1	6.74	1.50	1.43
2	B	701	2WY	C16-S1	7.91	1.88	1.76

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	2WY	O4-S1-O5	-6.91	110.37	119.54
2	B	701	2WY	O4-S1-O5	-6.57	110.83	119.54
3	A	702	S6P	C5-C4-C3	-5.46	103.59	112.47
3	A	702	S6P	O1-C1-C2	-3.94	102.54	111.10
2	A	701	2WY	C13-C12-C11	-3.79	114.63	120.19
2	B	701	2WY	C13-C12-C11	-3.66	114.83	120.19
2	B	701	2WY	C20-C16-C17	-3.52	116.44	120.52
2	B	701	2WY	C14-C15-C10	-3.44	116.09	120.64
2	A	701	2WY	C10-C9-N1	-3.23	105.13	111.47
2	A	701	2WY	C24-O3-C19	-3.14	110.95	115.83
2	A	701	2WY	C14-C15-C10	-2.40	117.46	120.64
5	A	716	GOL	O2-C2-C1	-2.29	98.13	108.65
2	A	701	2WY	C5-C6-C1	-2.23	116.86	120.44
6	B	721	SO4	O2-S-O1	-2.18	102.59	109.50
2	B	701	2WY	O3-C19-C21	-2.10	112.39	117.25
2	A	701	2WY	O3-C19-C18	2.01	125.97	123.27
2	A	701	2WY	C6-C1-C2	2.04	122.75	119.92
2	A	701	2WY	C23-O2-C18	2.06	119.04	115.83
2	B	701	2WY	C23-O2-C18	2.15	119.18	115.83
3	B	702	S6P	O2P-P-O6	2.15	112.76	106.56
2	A	701	2WY	C13-C14-C15	2.18	123.38	120.19
2	B	701	2WY	C15-C10-C11	2.41	121.38	118.31
5	A	716	GOL	O2-C2-C3	2.49	120.05	108.65
2	B	701	2WY	C7-C1-C2	2.55	108.50	106.27
2	A	701	2WY	C12-C11-C10	2.67	124.17	120.64
2	A	701	2WY	O2-C18-C19	3.10	127.42	123.27
2	A	701	2WY	C5-C4-C3	3.10	124.96	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	2WY	C17-C16-S1	3.60	123.11	119.09
2	B	701	2WY	C21-C20-C16	3.91	123.80	119.48
2	B	701	2WY	O3-C19-C18	4.08	128.75	123.27
3	A	702	S6P	O6-P-O3P	4.41	118.37	107.14
2	A	701	2WY	O2-C23-C22	4.98	120.15	112.75
2	B	701	2WY	O3-C24-C22	6.42	122.29	112.75
2	A	701	2WY	O4-S1-C16	6.45	116.12	107.96
2	B	701	2WY	O5-S1-C16	6.96	116.77	107.96
2	B	701	2WY	O2-C23-C22	7.80	124.34	112.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	2WY	2	0
2	B	701	2WY	2	0
5	B	719	GOL	1	0
6	B	722	SO4	1	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	585/638 (91%)	0.40	45 (7%)	16 22	26, 48, 81, 109	0
1	B	590/638 (92%)	0.35	48 (8%)	15 21	25, 45, 74, 109	0
All	All	1175/1276 (92%)	0.38	93 (7%)	15 22	25, 46, 79, 109	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	PRO	7.6
1	A	465	PHE	7.2
1	A	357	PHE	6.6
1	B	454	PRO	6.1
1	B	1	MET	6.1
1	B	21	LEU	6.0
1	B	22	SER	5.9
1	A	454	PRO	5.7
1	A	21	LEU	5.4
1	A	69	SER	5.4
1	B	465	PHE	5.3
1	B	65	GLY	5.0
1	B	3	GLY	4.8
1	B	4	THR	4.6
1	A	470	GLY	4.5
1	A	2	PRO	4.5
1	A	469	GLU	4.4
1	A	445	LEU	4.3
1	B	381	GLN	4.3
1	A	447	ILE	4.2
1	A	1	MET	4.1
1	B	407	VAL	3.9
1	A	387	PHE	3.9
1	A	407	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	22	SER	3.7
1	B	447	ILE	3.6
1	A	455	SER	3.6
1	B	66	GLN	3.4
1	A	444	THR	3.3
1	A	385	PHE	3.2
1	A	466	PHE	3.2
1	A	270	LEU	3.2
1	A	428	GLU	3.1
1	A	129	GLY	3.1
1	B	143	ARG	3.1
1	A	451	LYS	3.0
1	B	69	SER	3.0
1	A	330	VAL	3.0
1	A	449	LEU	3.0
1	B	442	GLY	2.9
1	B	286	ALA	2.9
1	A	394	THR	2.9
1	A	595	PRO	2.9
1	B	388	SER	2.9
1	B	463	LEU	2.9
1	B	176	ILE	2.8
1	B	455	SER	2.8
1	B	270	LEU	2.8
1	A	142	ASP	2.8
1	A	17	GLY	2.7
1	A	176	ILE	2.7
1	A	358	ARG	2.7
1	B	206	VAL	2.7
1	B	444	THR	2.7
1	B	448	PRO	2.7
1	A	430	THR	2.7
1	B	445	LEU	2.6
1	B	469	GLU	2.6
1	A	332	LEU	2.5
1	B	332	LEU	2.5
1	A	388	SER	2.5
1	B	409	ILE	2.5
1	A	128	LEU	2.4
1	A	178	ILE	2.4
1	B	520	LEU	2.4
1	B	204	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	449	LEU	2.3
1	A	467	GLU	2.3
1	A	408	PHE	2.3
1	B	20	GLU	2.3
1	B	519	ALA	2.3
1	B	171	LYS	2.3
1	A	90	VAL	2.2
1	A	187	VAL	2.2
1	B	5	LYS	2.2
1	B	523	LEU	2.2
1	B	131	LYS	2.2
1	A	206	VAL	2.2
1	B	466	PHE	2.2
1	A	364	LEU	2.1
1	A	592	ALA	2.1
1	B	330	VAL	2.1
1	B	178	ILE	2.1
1	B	606	ALA	2.1
1	B	104	LEU	2.1
1	A	593	ALA	2.1
1	A	282	ASP	2.1
1	B	98	ASP	2.1
1	B	23	GLY	2.1
1	B	285	ILE	2.0
1	A	204	VAL	2.0
1	B	269	LEU	2.0
1	B	436	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	A	716	6/6	0.83	0.20	3.04	38,50,55,62	0
6	SO4	B	723	5/5	0.86	0.18	2.71	76,80,90,91	0
2	2WY	B	701	31/31	0.88	0.18	1.39	42,56,65,65	0
5	GOL	B	719	6/6	0.86	0.15	1.21	41,43,50,58	0
2	2WY	A	701	31/31	0.89	0.16	1.13	37,48,54,57	0
5	GOL	B	718	6/6	0.89	0.13	0.78	40,55,60,64	0
3	S6P	A	702	16/16	0.99	0.15	0.04	25,28,31,33	0
3	S6P	B	702	16/16	0.98	0.14	-0.05	25,28,33,33	0
4	IOD	A	711	1/1	0.88	0.11	-0.70	90,90,90,90	1
4	IOD	B	713	1/1	0.90	0.10	-0.74	80,80,80,80	1
4	IOD	B	715	1/1	0.74	0.10	-1.13	90,90,90,90	1
4	IOD	B	710	1/1	0.94	0.16	-1.15	91,91,91,91	1
4	IOD	A	714	1/1	0.95	0.06	-1.28	65,65,65,65	1
4	IOD	A	709	1/1	0.97	0.11	-1.37	87,87,87,87	1
4	IOD	B	703	1/1	0.96	0.07	-1.58	53,53,53,53	0
4	IOD	A	703	1/1	0.94	0.05	-2.14	61,61,61,61	0
4	IOD	A	704	1/1	0.98	0.04	-3.21	60,60,60,60	0
4	IOD	B	704	1/1	0.99	0.05	-3.88	53,53,53,53	0
4	IOD	B	705	1/1	0.99	0.04	-9.79	48,48,48,48	1
4	IOD	B	706	1/1	0.96	0.07	-	48,48,48,48	1
6	SO4	B	720	5/5	0.93	0.14	-	65,67,73,90	0
4	IOD	A	705	1/1	0.99	0.06	-	42,42,42,42	1
6	SO4	B	722	5/5	0.88	0.25	-	53,69,75,87	0
4	IOD	A	708	1/1	0.94	0.06	-	73,73,73,73	1
6	SO4	B	721	5/5	0.97	0.10	-	40,44,46,52	5
4	IOD	A	712	1/1	0.95	0.10	-	66,66,66,66	1
4	IOD	B	716	1/1	0.91	0.14	-	92,92,92,92	1
4	IOD	A	707	1/1	0.94	0.08	-	51,51,51,51	1
4	IOD	B	714	1/1	0.93	0.09	-	61,61,61,61	1
4	IOD	B	708	1/1	0.95	0.05	-	57,57,57,57	1
4	IOD	B	711	1/1	0.98	0.03	-	62,62,62,62	1
4	IOD	A	713	1/1	0.92	0.04	-	62,62,62,62	1
4	IOD	B	707	1/1	0.95	0.04	-	72,72,72,72	0
4	IOD	B	717	1/1	0.98	0.08	-	86,86,86,86	1
4	IOD	B	709	1/1	0.94	0.05	-	74,74,74,74	1
4	IOD	B	712	1/1	0.83	0.21	-	89,89,89,89	1
4	IOD	A	715	1/1	0.69	0.13	-	85,85,85,85	1
4	IOD	A	710	1/1	0.99	0.05	-	53,53,53,53	1
4	IOD	A	706	1/1	0.98	0.03	-	77,77,77,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.