



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:46 PM GMT

PDB ID : 4PX5
Title : Human GKRP bound to AMG-0696 and Sorbitol-6-phosphate
Authors : Jordan, S.R.; Chmait, S.
Deposited on : 2014-03-21
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

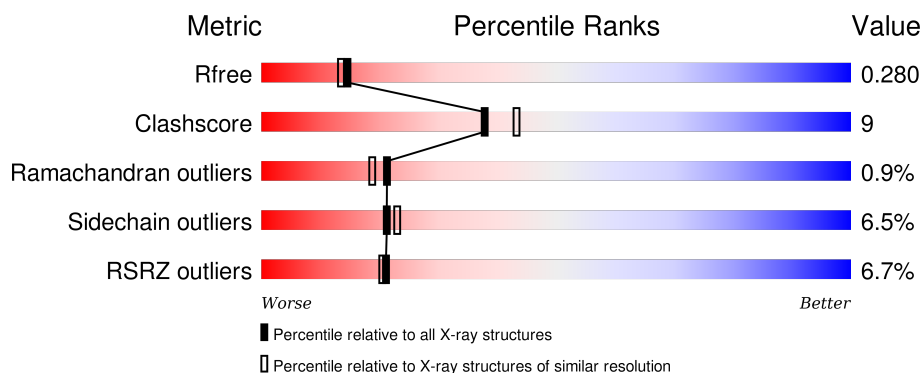
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 ≥ 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	<div> <div>5%</div> <div>71%</div> <div>18%</div> <div>8%</div> </div>
1	B	638	<div> <div>7%</div> <div>78%</div> <div>12%</div> <div>8%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IOD	A	716	-	-	X	-
4	IOD	B	713	-	-	X	-
5	GOL	A	718	-	-	-	X
6	SO4	A	719	-	-	-	X
6	SO4	B	723	-	-	X	-
6	SO4	B	724	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9380 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:

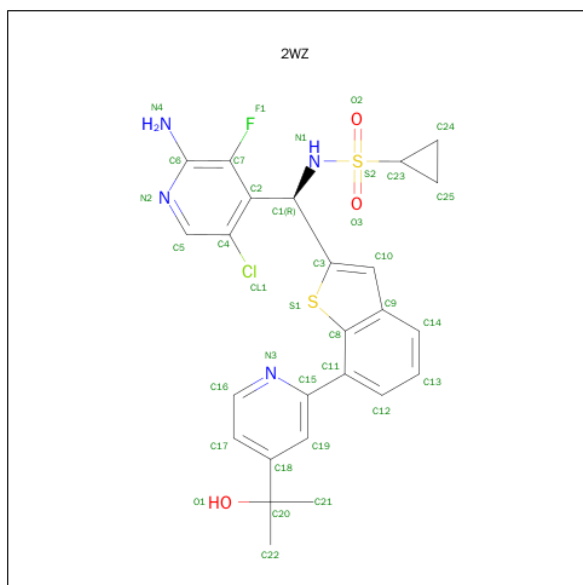
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q14397
A	-10	ALA	-	EXPRESSION TAG	UNP Q14397
A	-9	HIS	-	EXPRESSION TAG	UNP Q14397
A	-8	HIS	-	EXPRESSION TAG	UNP Q14397
A	-7	HIS	-	EXPRESSION TAG	UNP Q14397
A	-6	HIS	-	EXPRESSION TAG	UNP Q14397
A	-5	HIS	-	EXPRESSION TAG	UNP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

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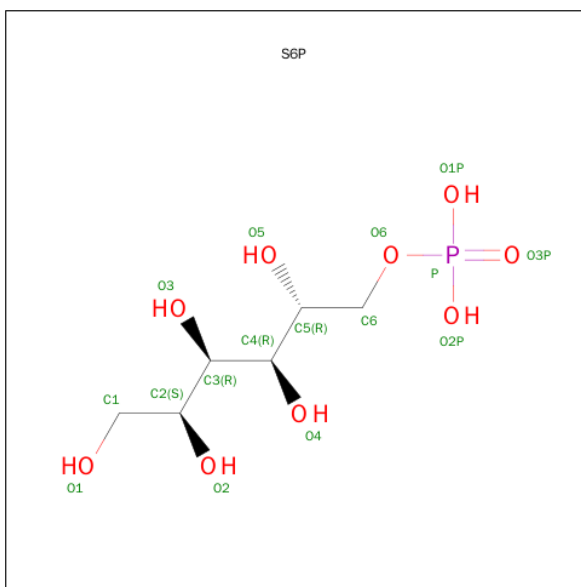
Chain	Residue	Modelled	Actual	Comment	Reference
B	626	GLY	-	EXPRESSION TAG	UNP Q14397

- Molecule 2 is N-[(R)-(2-AMINO-5-CHLORO-3-FLUOROPYRIDIN-4-YL){7-[4-(2-HYDROXYPROPAN-2-YL)PYRIDIN-2-YL]-1-BENZOTHIOPHEN-2-YL}METHYL]CYCLOPROPANESULFONAMIDE (three-letter code: 2WZ) (formula: C₂₅H₂₄ClFN₄O₃S₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	0
			36	25	1	1	4	3	2		
2	B	1	Total	C	Cl	F	N	O	S	0	0
			36	25	1	1	4	3	2		

- Molecule 3 is SUGAR (D-SORBITOL-6-PHOSPHATE) (three-letter code: S6P) (formula: C₆H₁₅O₉P).

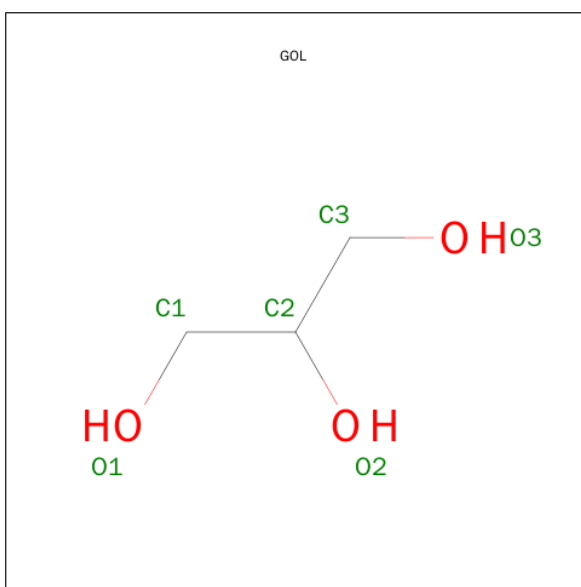


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

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

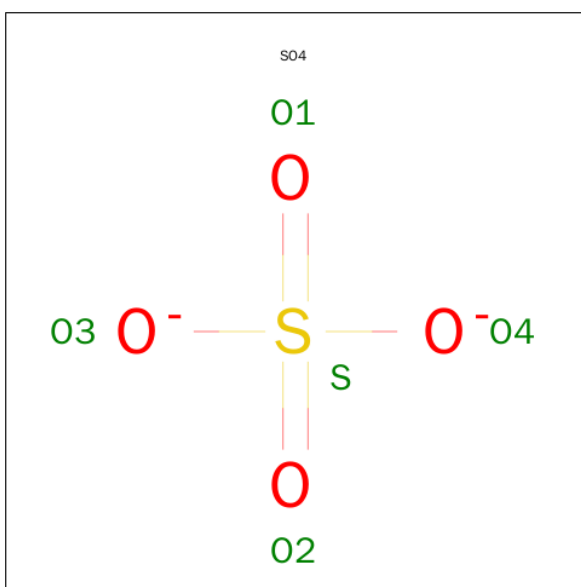
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	16	Total	I	0	0
			16	16		
4	A	15	Total	I	0	0
			15	15		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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: O₄S).



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

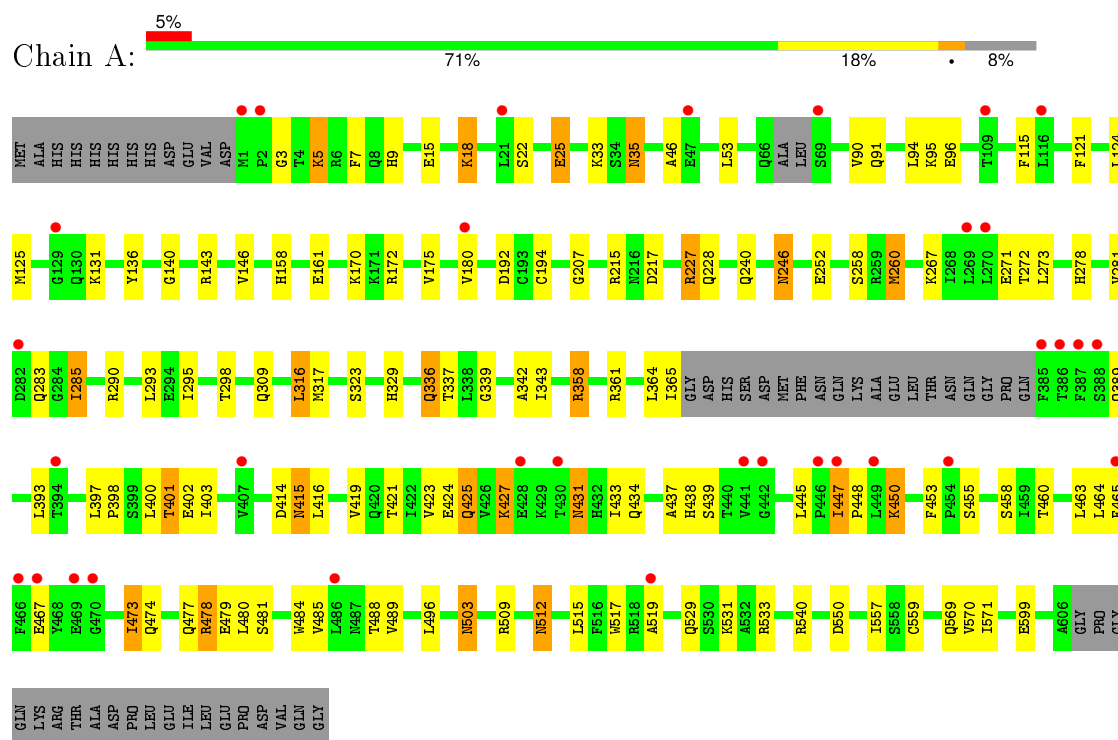
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	54	Total	O	0	0
			54	54		
7	B	73	Total	O	0	0
			73	73		

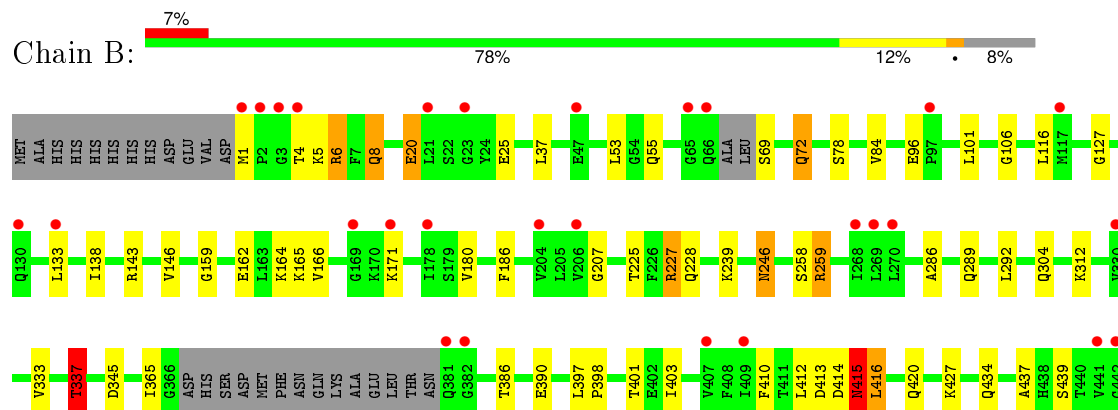
3 Residue-property plots

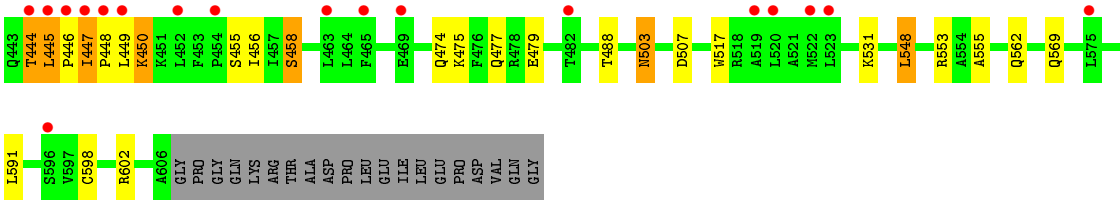
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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, α , β , γ	148.45Å 148.45Å 132.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.49 – 2.20 29.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.49-2.20) 99.8 (29.49-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.220 , 0.279 0.225 , 0.280	Depositor DCC
R_{free} test set	4161 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.7	EDS
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 83384 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9380	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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, 2WZ, IOD, 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	0.77	0/4603	0.88	7/6228 (0.1%)
1	B	0.77	0/4637	0.88	4/6274 (0.1%)
All	All	0.77	0/9240	0.88	11/12502 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ARG	NE-CZ-NH2	-11.48	114.56	120.30
1	B	259	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	A	540	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	A	227	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	478	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	A	550	ASP	CB-CG-OD1	6.15	123.84	118.30
1	B	507	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	217	ASP	CB-CG-OD1	-6.02	112.89	118.30
1	A	540	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	227	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	227	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	103	0
1	B	4554	0	4647	68	0
2	A	36	0	24	3	0
2	B	36	0	24	4	0
3	A	16	0	13	0	0
3	B	16	0	13	1	0
4	A	15	0	0	11	0
4	B	16	0	0	5	0
5	A	6	0	8	0	0
5	B	12	0	16	2	0
6	A	5	0	0	1	0
6	B	20	0	0	2	0
7	A	54	0	0	1	0
7	B	73	0	0	0	1
All	All	9380	0	9363	172	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 9.

All (172) 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:B:5:LYS:HB2	4:B:710:IOD:I	2.33	0.99
1:A:400:LEU:O	1:A:401:THR:OG1	1.81	0.98
1:A:431:ASN:HD22	1:A:431:ASN:H	1.10	0.95
1:A:228:GLN:HE22	1:B:228:GLN:HE22	1.17	0.92
1:A:439:SER:OG	1:A:460:THR:HG22	1.82	0.80
1:A:431:ASN:ND2	1:A:431:ASN:H	1.82	0.77
1:A:317:MET:HE2	1:A:496:LEU:HD11	1.71	0.72
1:A:18:LYS:HD3	4:A:717:IOD:I	2.61	0.70
2:A:701:2WZ:S1	2:A:701:2WZ:N3	2.64	0.70
1:B:146:VAL:O	1:B:146:VAL:HG12	1.93	0.68
1:B:447:ILE:HA	1:B:450:LYS:HD2	1.75	0.68
1:A:272:THR:HA	1:A:295:ILE:HG21	1.76	0.67
1:B:333:VAL:CG1	1:B:365:ILE:HD11	2.24	0.66
1:A:509:ARG:NH1	7:A:836:HOH:O	2.28	0.66
1:A:480:LEU:HD21	1:A:484:TRP:CH2	2.31	0.66
1:A:90:VAL:O	1:A:94:LEU:HG	1.96	0.66
1:A:309:GLN:NE2	1:A:458:SER:O	2.29	0.65
1:A:397:LEU:O	1:A:400:LEU:HD13	1.97	0.65
1:A:228:GLN:HE22	1:B:228:GLN:NE2	1.92	0.64
1:B:458:SER:HB3	4:B:713:IOD:I	2.68	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ILE:O	1:A:434:GLN:HG2	1.98	0.64
1:B:414:ASP:O	1:B:416:LEU:HD22	1.98	0.63
1:B:503:ASN:H	1:B:503:ASN:HD22	1.47	0.63
1:A:317:MET:CE	1:A:496:LEU:HD11	2.28	0.63
1:A:140:GLY:H	1:A:158:HIS:HE1	1.45	0.62
1:B:164:LYS:HG2	5:B:720:GOL:H32	1.80	0.62
1:A:398:PRO:HA	6:A:719:SO4:O3	2.00	0.61
1:B:447:ILE:HG22	1:B:450:LYS:CE	2.30	0.61
1:A:298:THR:HG21	1:A:473:ILE:HD11	1.82	0.60
1:A:419:VAL:O	1:A:423:VAL:HG23	2.02	0.60
1:A:9:HIS:CD2	1:A:9:HIS:H	2.19	0.59
1:A:146:VAL:O	1:A:146:VAL:HG12	2.03	0.59
1:A:15:GLU:H	1:A:18:LYS:HE3	1.68	0.59
1:B:259:ARG:NH2	1:B:345:ASP:OD1	2.35	0.58
1:A:46:ALA:HA	1:A:317:MET:HE1	1.85	0.58
1:A:337:THR:HG21	1:A:479:GLU:OE2	2.04	0.58
1:A:529:GLN:HE21	1:A:533:ARG:HE	1.50	0.58
1:B:337:THR:HG21	1:B:479:GLU:OE1	2.04	0.57
1:A:140:GLY:H	1:A:158:HIS:CE1	2.23	0.57
1:A:215:ARG:HG3	2:A:701:2WZ:C7	2.35	0.57
1:B:84:VAL:HG13	1:B:292:LEU:CD1	2.35	0.57
1:B:84:VAL:HG13	1:B:292:LEU:HD12	1.87	0.56
1:A:246:ASN:N	1:A:246:ASN:HD22	2.03	0.56
1:A:458:SER:CB	4:A:716:IOD:I	3.23	0.56
1:A:445:LEU:HG	4:A:716:IOD:I	2.76	0.56
1:A:358:ARG:NH1	1:A:358:ARG:O	2.39	0.56
1:B:517:TRP:CG	2:B:701:2WZ:H8	2.41	0.55
1:B:548:LEU:HD22	1:B:553:ARG:HG3	1.88	0.55
2:B:701:2WZ:N3	2:B:701:2WZ:S1	2.80	0.55
1:B:598:CYS:O	1:B:602:ARG:HG3	2.07	0.54
1:A:207:GLY:O	1:A:246:ASN:HA	2.07	0.54
1:B:415:ASN:HD22	1:B:415:ASN:C	2.10	0.54
1:A:445:LEU:HD11	4:A:716:IOD:I	2.77	0.54
1:A:447:ILE:HG22	1:A:450:LYS:HZ2	1.72	0.54
1:B:517:TRP:CD2	2:B:701:2WZ:H8	2.41	0.53
1:A:509:ARG:HH11	1:A:509:ARG:HB2	1.74	0.53
1:B:503:ASN:N	1:B:503:ASN:HD22	2.02	0.53
1:A:146:VAL:O	1:A:146:VAL:CG1	2.56	0.53
1:A:365:ILE:HD12	1:A:365:ILE:N	2.23	0.53
1:B:447:ILE:HG22	1:B:450:LYS:HD2	1.89	0.53
1:A:474:GLN:HA	1:A:477:GLN:HE21	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:GLY:O	4:B:716:IOD:I	2.96	0.53
1:B:444:THR:O	1:B:446:PRO:HD3	2.08	0.53
1:A:447:ILE:HG22	1:A:450:LYS:NZ	2.24	0.53
1:A:283:GLN:HB2	1:A:285:ILE:HG22	1.91	0.52
1:B:258:SER:OG	3:B:702:S6P:H11	2.08	0.52
1:B:333:VAL:CG1	1:B:365:ILE:CD1	2.87	0.52
1:A:509:ARG:NH1	1:A:509:ARG:HB2	2.24	0.52
1:A:458:SER:HB2	4:A:716:IOD:I	2.81	0.51
1:A:474:GLN:HG3	1:A:478:ARG:HH11	1.75	0.51
1:A:246:ASN:H	1:A:246:ASN:HD22	1.57	0.51
1:A:15:GLU:H	1:A:18:LYS:CE	2.24	0.51
1:B:146:VAL:O	1:B:146:VAL:CG1	2.58	0.51
1:A:336:GLN:NE2	1:A:414:ASP:OD1	2.44	0.51
1:A:458:SER:HB3	4:A:716:IOD:I	2.81	0.51
1:B:447:ILE:HD12	1:B:448:PRO:HD3	1.94	0.50
1:A:53:LEU:HD12	1:A:488:THR:HG23	1.93	0.50
1:B:412:LEU:HD12	1:B:439:SER:HB3	1.93	0.50
1:B:101:LEU:HD12	1:B:133:LEU:O	2.12	0.50
1:A:437:ALA:O	1:A:458:SER:HA	2.12	0.49
1:A:414:ASP:O	1:A:416:LEU:HD13	2.12	0.49
1:A:121:PHE:O	1:A:125:MET:HG3	2.13	0.49
1:B:246:ASN:HD22	1:B:246:ASN:N	2.11	0.49
1:A:278:HIS:O	1:A:281:VAL:HG22	2.13	0.49
1:B:225:THR:H	1:B:228:GLN:HE21	1.61	0.49
1:A:512:ASN:C	1:A:512:ASN:HD22	2.16	0.49
1:A:512:ASN:ND2	1:A:515:LEU:H	2.11	0.48
1:A:393:LEU:O	1:A:397:LEU:HB3	2.14	0.48
1:A:427:LYS:HE3	1:A:427:LYS:HA	1.95	0.48
1:A:124:LEU:HD23	1:A:124:LEU:C	2.34	0.48
1:A:18:LYS:HD2	1:A:22:SER:HB3	1.96	0.48
1:A:298:THR:HG21	1:A:473:ILE:CD1	2.44	0.48
1:A:339:GLY:O	1:A:342:ALA:HB3	2.13	0.48
1:A:329:HIS:HB3	1:A:358:ARG:NH1	2.28	0.48
1:A:35:ASN:C	1:A:35:ASN:HD22	2.18	0.48
1:A:91:GLN:HG2	1:A:281:VAL:HG13	1.95	0.47
1:A:9:HIS:HD2	1:A:9:HIS:H	1.61	0.47
1:A:95:LYS:HE3	1:A:281:VAL:HG12	1.97	0.47
1:B:25:GLU:HA	1:B:25:GLU:OE2	2.14	0.47
1:A:438:HIS:HB3	1:A:478:ARG:HE	1.80	0.47
1:B:239:LYS:HB2	6:B:723:SO4:O4	2.15	0.47
1:B:162:GLU:OE1	1:B:165:LYS:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:LYS:HE3	4:B:712:IOD:I	2.85	0.46
1:A:15:GLU:O	1:A:18:LYS:HG3	2.15	0.46
1:B:180:VAL:HG11	1:B:258:SER:HB2	1.97	0.46
1:A:46:ALA:HA	1:A:317:MET:CE	2.44	0.46
1:B:333:VAL:HG13	1:B:365:ILE:HD11	1.94	0.46
1:A:447:ILE:N	1:A:448:PRO:HD2	2.30	0.46
1:B:447:ILE:HG22	1:B:450:LYS:CD	2.46	0.46
1:B:286:ALA:HA	1:B:289:GLN:NE2	2.31	0.46
1:A:25:GLU:OE2	1:A:25:GLU:HA	2.16	0.46
1:A:96:GLU:HG3	1:A:96:GLU:O	2.16	0.45
1:B:569:GLN:HG2	1:B:591:LEU:HD21	1.98	0.45
1:A:175:VAL:HG21	1:A:194:CYS:SG	2.57	0.45
1:B:447:ILE:N	1:B:448:PRO:HD2	2.31	0.45
1:B:503:ASN:ND2	1:B:503:ASN:N	2.65	0.45
1:B:401:THR:HG22	1:B:403:ILE:HG12	1.99	0.45
1:A:3:GLY:O	1:A:7:PHE:HD2	1.99	0.45
1:A:316:LEU:HD13	1:A:489:VAL:HG21	1.99	0.44
1:B:4:THR:O	1:B:8:GLN:HB2	2.17	0.44
1:A:474:GLN:CG	1:A:478:ARG:HH11	2.30	0.44
1:B:414:ASP:O	1:B:416:LEU:N	2.51	0.44
1:A:5:LYS:HG3	4:A:709:IOD:I	2.88	0.44
1:B:164:LYS:HE3	5:B:720:GOL:H12	2.00	0.44
1:B:401:THR:HG22	1:B:403:ILE:H	1.81	0.44
1:B:447:ILE:CA	1:B:450:LYS:HD2	2.46	0.44
1:B:420:GLN:HB3	1:B:449:LEU:HG	2.00	0.44
1:B:6:ARG:HD3	1:B:555:ALA:O	2.17	0.44
1:A:424:GLU:O	1:A:427:LYS:HB2	2.17	0.43
1:A:481:SER:O	1:A:485:VAL:HG23	2.19	0.43
1:A:529:GLN:NE2	1:A:533:ARG:HE	2.16	0.43
1:A:337:THR:CG2	1:A:479:GLU:HG2	2.48	0.43
1:A:273:LEU:C	1:A:273:LEU:HD23	2.40	0.43
1:A:252:GLU:OE1	1:A:260:MET:HB2	2.18	0.42
1:A:323:SER:HB2	1:A:403:ILE:O	2.19	0.42
1:B:239:LYS:HG3	6:B:723:SO4:O1	2.20	0.42
1:A:421:THR:O	1:A:425:GLN:NE2	2.53	0.42
1:A:33:LYS:HG2	4:A:710:IOD:I	2.90	0.42
2:B:701:2WZ:C3	2:B:701:2WZ:H9	2.50	0.42
1:B:207:GLY:O	1:B:246:ASN:HA	2.20	0.42
1:A:480:LEU:CD2	1:A:484:TRP:CH2	3.00	0.42
1:A:517:TRP:CE2	2:A:701:2WZ:H8	2.55	0.42
1:B:397:LEU:N	1:B:398:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:PHE:O	1:B:437:ALA:HA	2.19	0.42
1:A:15:GLU:HB2	1:A:18:LYS:HG2	2.01	0.41
1:B:333:VAL:HG12	1:B:365:ILE:HD12	2.02	0.41
1:A:433:ILE:HD12	1:A:453:PHE:CE1	2.55	0.41
1:A:115:PHE:HD1	1:A:136:TYR:CE1	2.38	0.41
1:B:446:PRO:O	1:B:450:LYS:HB3	2.21	0.41
1:A:474:GLN:CG	1:A:478:ARG:NH1	2.83	0.41
1:B:474:GLN:HA	1:B:477:GLN:OE1	2.20	0.41
1:B:475:LYS:HE2	1:B:479:GLU:OE1	2.20	0.41
1:B:246:ASN:HD22	1:B:246:ASN:H	1.67	0.41
1:A:364:LEU:C	1:A:365:ILE:HD12	2.41	0.41
1:A:503:ASN:H	1:A:503:ASN:HD22	1.69	0.41
1:B:445:LEU:HG	4:B:713:IOD:I	2.91	0.41
1:B:106:GLY:O	1:B:138:ILE:HA	2.21	0.41
1:A:180:VAL:HG11	1:A:258:SER:HB2	2.03	0.41
1:A:267:LYS:O	1:A:271:GLU:HB2	2.21	0.41
1:B:37:LEU:HD13	1:B:55:GLN:HG2	2.02	0.41
1:A:519:ALA:HB2	1:A:571:ILE:HD11	2.03	0.41
1:A:400:LEU:HD12	1:A:400:LEU:N	2.36	0.41
1:A:445:LEU:CD1	4:A:716:IOD:I	3.38	0.41
1:A:146:VAL:HG13	1:A:343:ILE:CG2	2.50	0.41
1:A:531:LYS:HE2	4:A:711:IOD:I	2.91	0.40
1:A:569:GLN:O	1:A:570:VAL:C	2.58	0.40
1:A:445:LEU:CG	4:A:716:IOD:I	3.39	0.40
1:B:159:GLY:HA2	1:B:186:PHE:CE1	2.56	0.40
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.86	0.40
1:B:72:GLN:HG2	1:B:78:SER:OG	2.21	0.40
1:B:312:LYS:HD3	1:B:455:SER:O	2.21	0.40
1:B:53:LEU:HD12	1:B:488:THR:HG23	2.03	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:860:HOH:O	7:B:864:HOH:O[5_555]	1.67	0.53

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%)	541 (93%)	32 (6%)	6 (1%)	19	16
1	B	584/638 (92%)	554 (95%)	26 (4%)	4 (1%)	26	25
All	All	1163/1276 (91%)	1095 (94%)	58 (5%)	10 (1%)	21	19

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	402	GLU
1	B	20	GLU
1	B	415	ASN
1	A	389	GLN
1	A	415	ASN
1	A	336	GLN
1	B	337	THR
1	A	401	THR
1	A	260	MET
1	B	456	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%)	462 (93%)	36 (7%)	18	18
1	B	501/542 (92%)	472 (94%)	29 (6%)	25	28
All	All	999/1084 (92%)	934 (94%)	65 (6%)	21	23

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	18	LYS
1	A	25	GLU
1	A	35	ASN
1	A	131	LYS
1	A	143	ARG
1	A	161	GLU
1	A	170	LYS
1	A	172	ARG
1	A	192	ASP
1	A	227	ARG
1	A	240	GLN
1	A	246	ASN
1	A	285	ILE
1	A	290	ARG
1	A	293	LEU
1	A	316	LEU
1	A	358	ARG
1	A	361	ARG
1	A	415	ASN
1	A	425	GLN
1	A	427	LYS
1	A	431	ASN
1	A	447	ILE
1	A	450	LYS
1	A	455	SER
1	A	463	LEU
1	A	464	LEU
1	A	465	PHE
1	A	467	GLU
1	A	473	ILE
1	A	503	ASN
1	A	512	ASN
1	A	557	ILE
1	A	559	CYS
1	A	599	GLU
1	B	1	MET
1	B	6	ARG
1	B	8	GLN
1	B	20	GLU
1	B	69	SER
1	B	72	GLN

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Mol	Chain	Res	Type
1	B	96	GLU
1	B	143	ARG
1	B	166	VAL
1	B	171	LYS
1	B	227	ARG
1	B	246	ASN
1	B	304	GLN
1	B	337	THR
1	B	386	THR
1	B	390	GLU
1	B	413	ASP
1	B	415	ASN
1	B	416	LEU
1	B	427	LYS
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	503	ASN
1	B	548	LEU
1	B	562	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	35	ASN
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	420	GLN
1	A	425	GLN
1	A	431	ASN
1	A	432	HIS
1	A	477	GLN
1	A	503	ASN

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Mol	Chain	Res	Type
1	A	512	ASN
1	A	529	GLN
1	B	48	ASN
1	B	55	GLN
1	B	196	ASN
1	B	228	GLN
1	B	246	ASN
1	B	289	GLN
1	B	384	GLN
1	B	389	GLN
1	B	415	ASN
1	B	431	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 43 ligands modelled in this entry, 31 are monoatomic - leaving 12 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	2WZ	A	701	-	30,40,40	1.77	4 (13%)	35,62,62	2.04	8 (22%)
3	S6P	A	702	-	15,15,15	1.50	1 (6%)	18,21,21	1.57	4 (22%)
5	GOL	A	718	-	5,5,5	0.41	0	5,5,5	0.58	0
6	SO4	A	719	-	4,4,4	0.49	0	6,6,6	0.76	0
2	2WZ	B	701	-	30,40,40	2.05	5 (16%)	35,62,62	1.82	9 (25%)
3	S6P	B	702	-	15,15,15	1.10	2 (13%)	18,21,21	1.50	3 (16%)
5	GOL	B	719	-	5,5,5	0.15	0	5,5,5	0.83	0
5	GOL	B	720	-	5,5,5	0.19	0	5,5,5	0.92	0
6	SO4	B	721	-	4,4,4	0.54	0	6,6,6	0.25	0
6	SO4	B	722	-	4,4,4	0.22	0	6,6,6	0.41	0
6	SO4	B	723	-	4,4,4	0.66	0	6,6,6	0.41	0
6	SO4	B	724	-	4,4,4	0.64	0	6,6,6	0.26	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	2WZ	A	701	-	-	0/23/31/31	0/4/5/5
3	S6P	A	702	-	-	0/20/20/20	0/0/0/0
5	GOL	A	718	-	-	0/4/4/4	0/0/0/0
6	SO4	A	719	-	-	0/0/0/0	0/0/0/0
2	2WZ	B	701	-	-	0/23/31/31	0/4/5/5
3	S6P	B	702	-	-	0/20/20/20	0/0/0/0
5	GOL	B	719	-	-	0/4/4/4	0/0/0/0
5	GOL	B	720	-	-	0/4/4/4	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
6	SO4	B	724	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	2WZ	C3-S1	-5.40	1.64	1.74
2	A	701	2WZ	C11-C15	-4.72	1.41	1.49
2	B	701	2WZ	C11-C15	-4.69	1.41	1.49
2	A	701	2WZ	C21-C20	-3.20	1.49	1.53
3	B	702	S6P	C2-C3	-2.57	1.48	1.53
3	B	702	S6P	P-O2P	2.09	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	2WZ	O2-S2	2.17	1.46	1.43
2	B	701	2WZ	S2-N1	2.25	1.66	1.60
2	B	701	2WZ	O2-S2	3.83	1.48	1.43
3	A	702	S6P	P-O3P	3.93	1.64	1.51
2	A	701	2WZ	O3-S2	5.64	1.50	1.43
2	B	701	2WZ	O3-S2	5.69	1.50	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	2WZ	O2-S2-O3	-7.25	107.43	119.34
2	B	701	2WZ	O2-S2-O3	-4.32	112.24	119.34
2	B	701	2WZ	C4-C5-N2	-4.13	119.55	123.03
2	A	701	2WZ	C5-C4-C2	-3.89	117.87	120.39
2	A	701	2WZ	C16-C17-C18	-3.31	116.81	119.54
2	A	701	2WZ	C19-C15-N3	-3.07	117.98	122.02
2	B	701	2WZ	C19-C15-N3	-2.76	118.38	122.02
2	B	701	2WZ	C16-C17-C18	-2.69	117.32	119.54
3	A	702	S6P	O6-P-O3P	-2.58	100.57	107.14
3	A	702	S6P	C5-C4-C3	-2.53	108.35	112.47
3	A	702	S6P	C2-C3-C4	-2.43	108.52	112.47
3	B	702	S6P	O2P-P-O3P	-2.38	102.93	110.58
2	B	701	2WZ	F1-C7-C6	-2.36	116.36	119.11
2	A	701	2WZ	C24-C25-C23	-2.24	57.93	59.99
2	A	701	2WZ	C1-N1-S2	-2.02	117.83	122.25
2	B	701	2WZ	C16-N3-C15	2.11	120.11	117.20
2	B	701	2WZ	F1-C7-C2	2.31	123.44	120.36
3	B	702	S6P	O1P-P-O3P	2.42	118.35	110.58
2	B	701	2WZ	O1-C20-C21	2.52	111.57	106.79
2	A	701	2WZ	C24-C23-C25	2.71	62.33	60.03
2	A	701	2WZ	C16-N3-C15	2.86	121.15	117.20
3	B	702	S6P	O6-P-O3P	3.55	116.18	107.14
3	A	702	S6P	O2P-P-O6	3.61	116.95	106.56
2	B	701	2WZ	C5-N2-C6	3.96	123.47	118.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	2WZ	3	0
6	A	719	SO4	1	0
2	B	701	2WZ	4	0
3	B	702	S6P	1	0
5	B	720	GOL	2	0
6	B	723	SO4	2	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, 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	585/638 (91%)	0.17	33 (5%)	28 27	34, 56, 90, 127	0
1	B	590/638 (92%)	0.17	46 (7%)	16 15	34, 56, 83, 126	0
All	All	1175/1276 (92%)	0.17	79 (6%)	21 20	34, 56, 88, 127	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	8.2
1	A	465	PHE	7.2
1	B	4	THR	6.3
1	B	2	PRO	6.1
1	A	1	MET	4.9
1	A	385	PHE	4.5
1	B	381	GLN	4.0
1	A	470	GLY	3.8
1	B	449	LEU	3.8
1	B	442	GLY	3.7
1	A	387	PHE	3.4
1	B	448	PRO	3.4
1	A	466	PHE	3.4
1	A	469	GLU	3.4
1	A	447	ILE	3.4
1	B	21	LEU	3.3
1	B	447	ILE	3.3
1	A	386	THR	3.2
1	B	270	LEU	3.1
1	A	394	THR	3.1
1	A	407	VAL	3.1
1	B	523	LEU	3.0
1	A	2	PRO	3.0
1	B	444	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	409	ILE	3.0
1	B	169	GLY	2.9
1	B	407	VAL	2.9
1	A	449	LEU	2.9
1	A	21	LEU	2.9
1	B	452	LEU	2.9
1	A	441	VAL	2.9
1	A	69	SER	2.8
1	B	519	ALA	2.7
1	A	388	SER	2.6
1	A	270	LEU	2.6
1	B	268	ILE	2.6
1	B	465	PHE	2.6
1	A	129	GLY	2.6
1	A	442	GLY	2.5
1	B	97	PRO	2.5
1	B	441	VAL	2.5
1	B	206	VAL	2.5
1	A	47	GLU	2.5
1	B	66	GLN	2.4
1	A	467	GLU	2.4
1	B	204	VAL	2.4
1	B	482	THR	2.4
1	B	469	GLU	2.4
1	A	116	LEU	2.4
1	B	3	GLY	2.4
1	B	65	GLY	2.4
1	A	446	PRO	2.3
1	B	133	LEU	2.3
1	B	117	MET	2.2
1	B	463	LEU	2.2
1	B	520	LEU	2.2
1	B	522	MET	2.2
1	A	180	VAL	2.2
1	B	171	LYS	2.2
1	B	178	ILE	2.1
1	B	330	VAL	2.1
1	A	519	ALA	2.1
1	A	454	PRO	2.1
1	A	282	ASP	2.1
1	A	269	LEU	2.1
1	B	269	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	382	GLY	2.1
1	B	596	SER	2.1
1	A	430	THR	2.1
1	A	428	GLU	2.1
1	B	575	LEU	2.1
1	B	446	PRO	2.1
1	B	454	PRO	2.1
1	B	47	GLU	2.0
1	B	130	GLN	2.0
1	A	109	THR	2.0
1	A	486	LEU	2.0
1	B	445	LEU	2.0
1	B	23	GLY	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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	A	718	6/6	0.83	0.24	2.91	50,60,64,80	0
6	SO4	B	724	5/5	0.85	0.20	2.69	69,78,90,95	5
6	SO4	A	719	5/5	0.95	0.26	2.04	48,54,63,75	5
5	GOL	B	720	6/6	0.90	0.13	0.56	53,57,58,78	0
3	S6P	A	702	16/16	0.99	0.20	0.52	31,37,43,44	0
5	GOL	B	719	6/6	0.93	0.14	0.49	55,61,66,71	0
3	S6P	B	702	16/16	0.98	0.15	0.01	33,38,43,47	0
2	2WZ	A	701	36/36	0.97	0.11	-0.45	33,38,44,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	IOD	B	715	1/1	0.82	0.12	-0.56	98,98,98,98	1
2	2WZ	B	701	36/36	0.97	0.10	-0.59	35,43,50,54	0
4	IOD	B	710	1/1	0.96	0.12	-1.42	92,92,92,92	1
4	IOD	A	714	1/1	0.96	0.05	-1.66	74,74,74,74	1
4	IOD	A	709	1/1	0.94	0.07	-1.77	96,96,96,96	1
4	IOD	B	713	1/1	0.93	0.06	-1.85	88,88,88,88	1
4	IOD	B	704	1/1	0.99	0.08	-2.01	65,65,65,65	0
4	IOD	A	703	1/1	0.89	0.06	-2.08	80,80,80,80	0
4	IOD	A	716	1/1	0.95	0.04	-2.13	86,86,86,86	1
4	IOD	B	703	1/1	0.94	0.07	-2.60	63,63,63,63	0
4	IOD	A	704	1/1	0.98	0.06	-2.92	62,62,62,62	0
4	IOD	B	717	1/1	0.87	0.09	-	94,94,94,94	1
4	IOD	A	708	1/1	0.92	0.10	-	88,88,88,88	1
4	IOD	A	707	1/1	0.96	0.05	-	64,64,64,64	1
4	IOD	A	717	1/1	0.80	0.07	-	81,81,81,81	1
4	IOD	B	707	1/1	0.91	0.05	-	89,89,89,89	1
4	IOD	A	713	1/1	0.93	0.04	-	69,69,69,69	1
4	IOD	B	708	1/1	0.97	0.04	-	73,73,73,73	1
6	SO4	B	721	5/5	0.86	0.16	-	74,74,84,91	5
4	IOD	A	705	1/1	0.99	0.04	-	56,56,56,56	1
4	IOD	B	714	1/1	0.96	0.07	-	83,83,83,83	1
4	IOD	A	712	1/1	0.92	0.06	-	78,78,78,78	1
6	SO4	B	722	5/5	0.95	0.10	-	51,54,57,59	5
4	IOD	A	706	1/1	0.93	0.06	-	92,92,92,92	0
4	IOD	B	711	1/1	0.91	0.14	-	96,96,96,96	1
4	IOD	A	715	1/1	0.76	0.08	-	100,100,100,100	1
6	SO4	B	723	5/5	0.87	0.28	-	51,57,71,73	5
4	IOD	B	712	1/1	0.76	0.10	-	88,88,88,88	1
4	IOD	A	711	1/1	0.81	0.12	-	79,79,79,79	1
4	IOD	B	718	1/1	0.89	0.05	-	80,80,80,80	1
4	IOD	B	709	1/1	0.91	0.06	-	88,88,88,88	1
4	IOD	B	716	1/1	0.93	0.17	-	96,96,96,96	1
4	IOD	B	706	1/1	0.95	0.06	-	63,63,63,63	1
4	IOD	A	710	1/1	0.95	0.23	-	89,89,89,89	1
4	IOD	B	705	1/1	0.98	0.03	-	67,67,67,67	1

6.5 Other polymers

There are no such residues in this entry.