



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:28 pm GMT

PDB ID : 4OHP  
Title : Human GKRP bound to AMG-3227 and S6P  
Authors : Jordan, S.R.; Chmait, S.  
Deposited on : 2014-01-17  
Resolution : 2.40 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

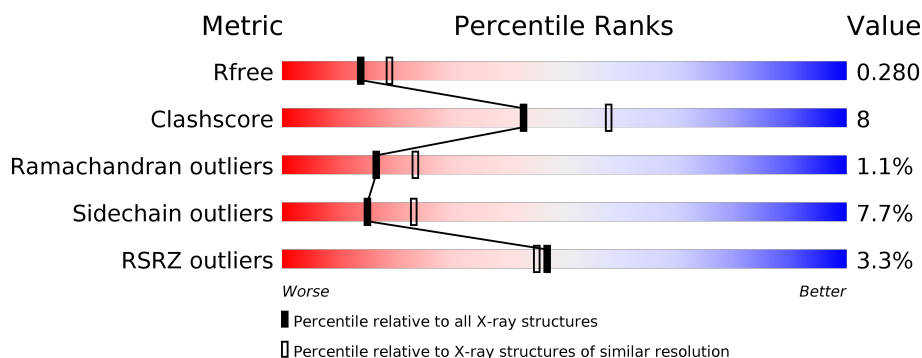
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	709	-	-	X	-
4	IOD	B	714	-	-	X	-
5	GOL	B	716	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9370 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:

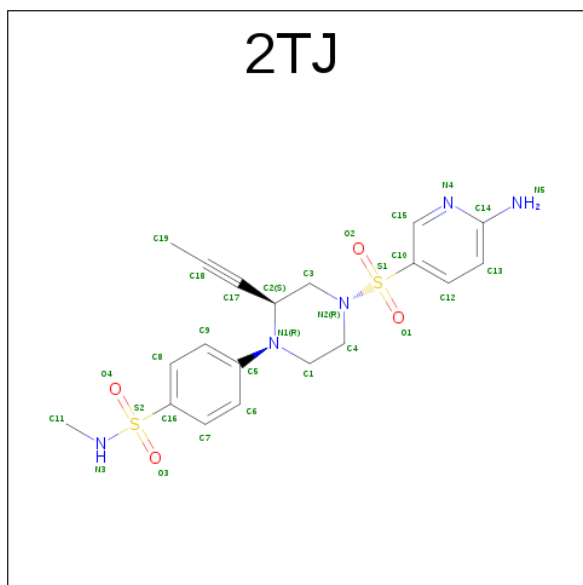
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q14397
A	-10	ALA	-	EXPRESSION TAG	UNP Q14397
A	-9	HIS	-	EXPRESSION TAG	UNP Q14397
A	-8	HIS	-	EXPRESSION TAG	UNP Q14397
A	-7	HIS	-	EXPRESSION TAG	UNP Q14397
A	-6	HIS	-	EXPRESSION TAG	UNP Q14397
A	-5	HIS	-	EXPRESSION TAG	UNP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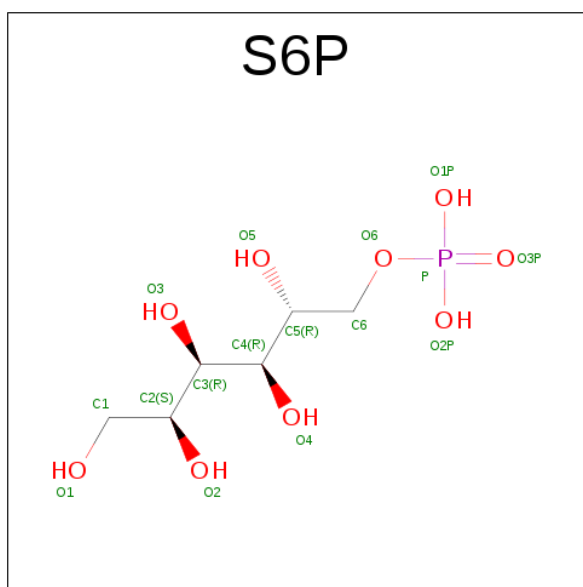
Chain	Residue	Modelled	Actual	Comment	Reference
B	626	GLY	-	EXPRESSION TAG	UNP Q14397

- Molecule 2 is 4-[(2S)-4-[(6-AMINOPYRIDIN-3-YL)SULFONYL]-2-(PROP-1-YN-1-YL)PIPERAZIN-1-YL]-N-METHYLBENZENESULFONAMIDE (three-letter code: 2TJ) (formula:  $C_{19}H_{23}N_5O_4S_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			30	19	5	4	2		
2	B	1	Total	C	N	O	S	0	0
			30	19	5	4	2		

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



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

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

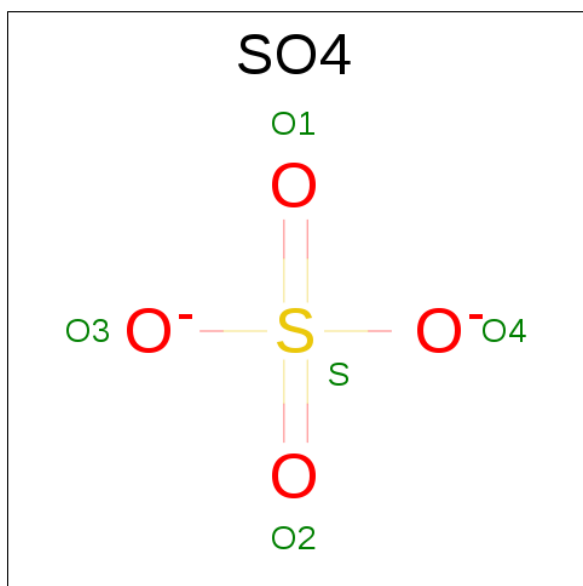
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	13	Total	I	0	0
			13	13		
4	A	11	Total	I	0	0
			11	11		

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



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

- Molecule 6 is SULFATE ION (three-letter code: SO<sub>4</sub>) (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		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

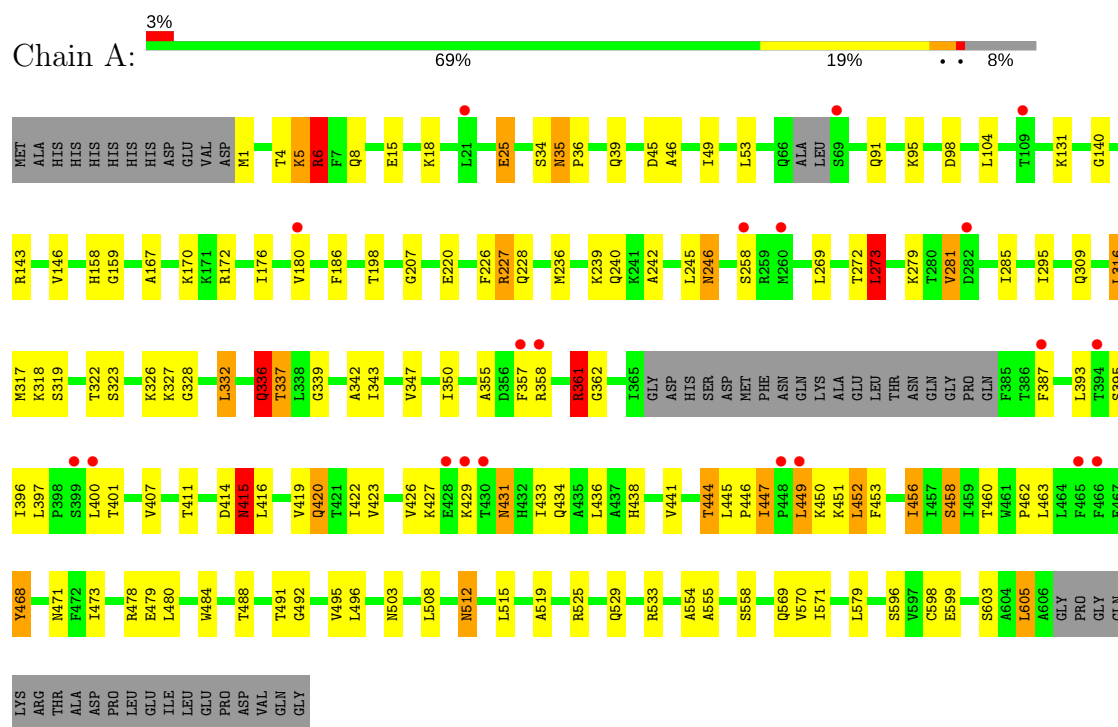
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	61	Total 61	O 61	0	0
7	B	97	Total 97	O 97	0	0



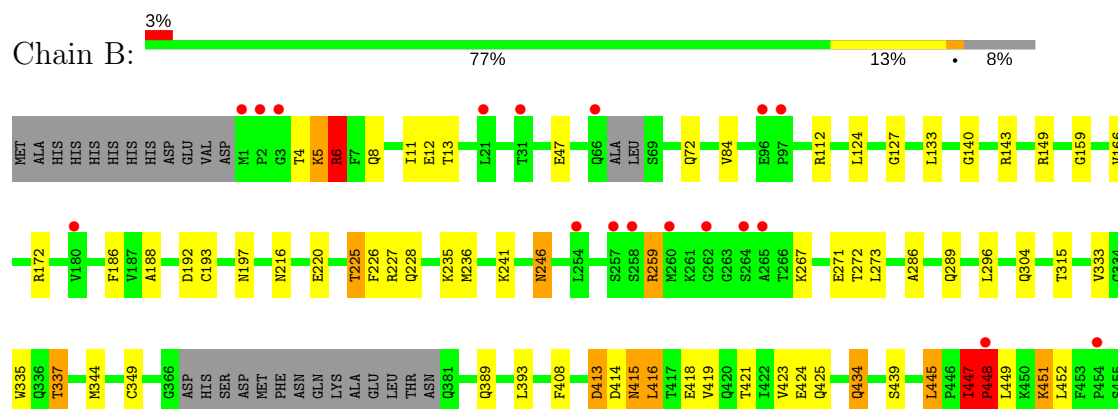
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glucokinase regulatory protein



- Molecule 1: Glucokinase regulatory protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.97Å 148.97Å 132.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.24 – 2.40 39.24 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.24-2.40) 94.4 (39.24-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.218 , 0.281 0.223 , 0.280	Depositor DCC
$R_{free}$ test set	3110 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.2	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9370	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, SO4, S6P, 2TJ

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	0.72	0/4603	0.86	9/6228 (0.1%)
1	B	0.74	0/4637	0.87	3/6274 (0.0%)
All	All	0.73	0/9240	0.86	12/12502 (0.1%)

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	2
All	All	0	4

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ARG	NE-CZ-NH2	-14.13	113.23	120.30
1	B	259	ARG	NE-CZ-NH1	10.41	125.50	120.30
1	A	478	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	227	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	A	227	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	361	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	6	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	A	429	LYS	CD-CE-NZ	5.81	125.07	111.70
1	A	478	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	273	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	6	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	449	LEU	CA-CB-CG	5.06	126.95	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	ALA	Peptide
1	A	468	TYR	Peptide
1	B	447	ILE	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	82	0
1	B	4554	0	4647	62	0
2	A	30	0	23	1	0
2	B	30	0	23	6	0
3	A	16	0	13	0	0
3	B	16	0	12	0	0
4	A	11	0	0	4	0
4	B	13	0	0	4	0
5	B	6	0	8	0	0
6	B	15	0	0	0	0
7	A	61	0	0	0	0
7	B	97	0	0	2	0
All	All	9370	0	9344	144	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 8.

All (144) 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:504:HIS:HE1	2:B:701:2TJ:H1	1.10	1.13
1:B:504:HIS:CE1	2:B:701:2TJ:H1	1.95	1.00
1:B:504:HIS:CE1	2:B:701:2TJ:C11	2.48	0.96
1:B:504:HIS:HE1	2:B:701:2TJ:C11	1.80	0.95
1:A:447:ILE:HG22	1:A:450:LYS:N	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ASN:OD1	1:B:225:THR:HG21	1.85	0.75
1:A:336:GLN:NE2	1:A:414:ASP:OD1	2.20	0.75
1:B:532:ALA:O	1:B:536:GLU:HG3	1.88	0.73
1:A:228:GLN:HE22	1:B:228:GLN:HE22	1.38	0.70
1:A:317:MET:HE2	1:A:496:LEU:HD11	1.73	0.70
1:A:5:LYS:HB2	4:A:709:IOD:I	2.63	0.69
1:B:5:LYS:HB2	4:B:710:IOD:I	2.63	0.68
1:B:529:GLN:NE2	1:B:533:ARG:HE	1.95	0.64
1:B:419:VAL:O	1:B:423:VAL:HG12	1.98	0.64
1:B:445:LEU:HG	4:B:713:IOD:I	2.68	0.64
1:B:220:GLU:OE1	1:B:558:SER:OG	2.14	0.63
1:A:140:GLY:H	1:A:158:HIS:HE1	1.47	0.63
1:B:286:ALA:HA	1:B:289:GLN:HE21	1.64	0.62
1:B:389:GLN:OE1	1:B:421:THR:HG21	1.99	0.61
1:A:4:THR:O	1:A:8:GLN:HB2	2.00	0.61
1:B:414:ASP:O	1:B:416:LEU:HD13	2.00	0.61
1:A:447:ILE:HG22	1:A:449:LEU:C	2.21	0.60
1:A:416:LEU:O	1:A:420:GLN:HG2	2.03	0.59
1:A:419:VAL:O	1:A:423:VAL:HG23	2.03	0.58
1:B:140:GLY:O	1:B:149:ARG:NH2	2.36	0.58
1:A:236:MET:HE2	1:A:242:ALA:HB2	1.86	0.57
1:A:414:ASP:O	1:A:415:ASN:CB	2.53	0.56
1:A:480:LEU:HD21	1:A:484:TRP:CH2	2.40	0.56
1:A:6:ARG:HD3	1:A:555:ALA:O	2.05	0.56
1:A:343:ILE:HA	1:A:362:GLY:HA3	1.86	0.56
1:B:337:THR:HG21	1:B:479:GLU:OE1	2.07	0.55
1:B:315:THR:HG22	1:B:434:GLN:NE2	2.21	0.55
1:B:504:HIS:CE1	2:B:701:2TJ:H2	2.38	0.55
1:A:337:THR:HG21	1:A:479:GLU:OE2	2.07	0.55
4:A:711:IOD:I	4:B:714:IOD:I	3.65	0.54
1:B:508:LEU:C	1:B:508:LEU:HD12	2.28	0.54
1:B:389:GLN:HE21	1:B:418:GLU:HG3	1.73	0.54
1:B:159:GLY:HA2	1:B:186:PHE:CE1	2.43	0.54
1:A:444:THR:O	1:A:446:PRO:HD3	2.08	0.54
1:A:416:LEU:N	1:A:416:LEU:HD12	2.23	0.54
1:B:246:ASN:HD22	1:B:246:ASN:N	2.06	0.53
1:A:468:TYR:HB2	4:A:703:IOD:I	2.78	0.53
1:A:34:SER:H	2:A:701:2TJ:H1	1.74	0.53
1:A:456:ILE:HD13	1:A:458:SER:HB2	1.92	0.52
1:B:273:LEU:C	1:B:273:LEU:HD23	2.30	0.52
1:A:512:ASN:C	1:A:512:ASN:HD22	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:THR:O	1:B:8:GLN:HG3	2.10	0.51
1:A:318:LYS:O	1:A:322:THR:OG1	2.25	0.51
1:A:596:SER:OG	1:A:599:GLU:HG3	2.11	0.51
1:A:317:MET:SD	1:A:492:GLY:HA3	2.51	0.50
1:B:448:PRO:HD3	1:B:451:LYS:CG	2.41	0.50
1:A:491:THR:O	1:A:495:VAL:HG23	2.11	0.50
1:A:339:GLY:O	1:A:342:ALA:HB3	2.11	0.50
1:A:350:ILE:HA	1:A:355:ALA:O	2.12	0.49
1:A:91:GLN:HG2	1:A:281:VAL:HG13	1.94	0.49
1:B:267:LYS:NZ	1:B:271:GLU:OE1	2.45	0.49
1:A:449:LEU:O	1:A:451:LYS:N	2.44	0.49
1:B:447:ILE:HB	1:B:448:PRO:HD2	1.94	0.49
1:A:104:LEU:HD23	1:A:176:ILE:HB	1.93	0.49
1:A:46:ALA:HA	1:A:317:MET:HE1	1.95	0.49
1:A:332:LEU:HB3	1:A:342:ALA:HB1	1.93	0.49
1:A:6:ARG:HD2	1:A:554:ALA:O	2.13	0.49
1:B:529:GLN:HE21	1:B:533:ARG:HE	1.59	0.48
1:A:53:LEU:HD12	1:A:488:THR:HG23	1.95	0.48
1:A:46:ALA:HA	1:A:317:MET:CE	2.43	0.48
1:A:395:SER:HB2	1:A:396:ILE:HD12	1.94	0.48
1:B:259:ARG:HD3	7:B:864:HOH:O	2.12	0.48
1:B:246:ASN:HD22	1:B:246:ASN:H	1.62	0.47
1:A:220:GLU:OE1	1:A:558:SER:OG	2.31	0.47
1:A:273:LEU:HD23	1:A:273:LEU:C	2.35	0.47
1:A:140:GLY:N	1:A:158:HIS:HE1	2.12	0.47
1:A:272:THR:HA	1:A:295:ILE:HG21	1.95	0.47
1:A:433:ILE:HD12	1:A:453:PHE:CE1	2.50	0.47
1:A:15:GLU:H	1:A:18:LYS:HE2	1.79	0.47
1:A:529:GLN:HE21	1:A:533:ARG:HE	1.62	0.47
1:B:6:ARG:HD3	1:B:555:ALA:O	2.15	0.47
1:A:433:ILE:O	1:A:434:GLN:HG2	2.16	0.46
1:A:512:ASN:ND2	1:A:515:LEU:H	2.13	0.46
1:B:124:LEU:HD23	1:B:124:LEU:O	2.15	0.46
1:A:246:ASN:N	1:A:246:ASN:HD22	2.13	0.46
1:A:180:VAL:HG11	1:A:258:SER:HB2	1.98	0.45
1:B:333:VAL:O	1:B:408:PHE:HA	2.16	0.45
2:B:701:2TJ:H25	2:B:701:2TJ:H8	1.97	0.45
1:B:272:THR:HG21	1:B:296:LEU:HG	1.98	0.45
1:B:286:ALA:HA	1:B:289:GLN:NE2	2.30	0.45
1:B:6:ARG:HD2	1:B:554:ALA:O	2.17	0.45
1:A:508:LEU:HD13	1:A:515:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:LEU:HD21	1:B:484:TRP:CH2	2.52	0.45
1:A:579:LEU:HD11	1:A:605:LEU:HD13	1.98	0.45
1:A:146:VAL:HG22	1:A:343:ILE:HG21	2.00	0.44
1:A:323:SER:O	1:A:328:GLY:N	2.46	0.44
1:B:389:GLN:NE2	1:B:418:GLU:HG3	2.32	0.44
1:B:335:TRP:CH2	1:B:419:VAL:HG22	2.53	0.44
1:A:358:ARG:HH21	1:A:361:ARG:HE	1.66	0.44
1:A:146:VAL:O	1:A:146:VAL:CG1	2.66	0.44
1:A:146:VAL:O	1:A:347:VAL:HG21	2.18	0.44
1:A:207:GLY:O	1:A:246:ASN:HA	2.18	0.44
1:A:393:LEU:O	1:A:397:LEU:HB3	2.17	0.44
1:B:112:ARG:HD3	1:B:344:MET:HG2	2.00	0.43
1:B:349:CYS:SG	1:B:490:SER:HB2	2.58	0.43
1:B:413:ASP:N	1:B:413:ASP:OD1	2.49	0.43
1:B:449:LEU:HA	1:B:452:LEU:HD12	2.01	0.43
1:B:529:GLN:HE22	1:B:533:ARG:HH21	1.66	0.43
1:A:146:VAL:HG22	1:A:343:ILE:CG2	2.49	0.43
1:A:246:ASN:H	1:A:246:ASN:HD22	1.66	0.43
1:A:95:LYS:HE3	1:A:281:VAL:HG12	2.00	0.43
1:A:447:ILE:O	1:A:450:LYS:HB2	2.18	0.43
1:A:451:LYS:N	1:A:452:LEU:HB2	2.33	0.43
1:A:569:GLN:O	1:A:570:VAL:C	2.56	0.42
1:B:193:CYS:HA	4:B:714:IOD:I	2.90	0.42
1:A:309:GLN:HA	1:A:309:GLN:HE21	1.84	0.42
1:A:5:LYS:CB	4:A:709:IOD:I	3.35	0.42
1:A:519:ALA:HB2	1:A:571:ILE:HD11	2.01	0.42
1:B:188:ALA:HB2	1:B:226:PHE:CD2	2.54	0.42
1:B:473:ILE:O	1:B:477:GLN:HG3	2.19	0.42
1:A:411:THR:HG22	1:A:438:HIS:HB2	2.02	0.41
1:B:315:THR:HG22	1:B:434:GLN:HE21	1.84	0.41
1:A:35:ASN:HD22	1:A:35:ASN:C	2.24	0.41
1:A:400:LEU:C	1:A:401:THR:HG1	2.23	0.41
1:B:469:GLU:HG2	7:B:803:HOH:O	2.21	0.41
1:B:571:ILE:HB	1:B:572:PRO:HD3	2.01	0.41
1:A:25:GLU:OE2	1:A:525:ARG:NH2	2.33	0.41
1:A:449:LEU:C	1:A:451:LYS:N	2.74	0.41
1:B:421:THR:O	1:B:424:GLU:HB2	2.21	0.41
1:B:393:LEU:HD22	1:B:425:GLN:NE2	2.35	0.41
1:B:448:PRO:HD3	1:B:451:LYS:CB	2.50	0.41
1:B:548:LEU:HA	1:B:548:LEU:HD23	1.88	0.41
1:A:228:GLN:HE22	1:B:228:GLN:NE2	2.11	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASP:OD1	1:A:45:ASP:C	2.60	0.41
1:B:12:GLU:OE2	1:B:13:THR:N	2.54	0.41
1:B:172:ARG:HD2	1:B:172:ARG:HA	1.93	0.41
1:A:316:LEU:HD21	1:A:407:VAL:CG2	2.51	0.40
1:A:422:ILE:O	1:A:426:VAL:HG23	2.20	0.40
1:A:146:VAL:HG13	1:A:146:VAL:O	2.21	0.40
1:A:245:LEU:HD22	1:A:269:LEU:HD21	2.03	0.40
1:A:36:PRO:O	1:A:39:GLN:HG2	2.21	0.40
1:B:509:ARG:NH1	1:B:565:HIS:O	2.51	0.40
1:A:309:GLN:OE1	1:A:458:SER:O	2.39	0.40
1:B:469:GLU:H	1:B:469:GLU:HG2	1.80	0.40
1:A:159:GLY:HA2	1:A:186:PHE:CE1	2.57	0.40
1:A:387:PHE:CD2	1:A:396:ILE:HD11	2.57	0.40
1:A:49:ILE:HB	1:A:317:MET:HE1	2.04	0.40
1:B:236:MET:HE2	1:B:236:MET:HB3	1.96	0.40
1:B:571:ILE:N	1:B:572:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	579/638 (91%)	536 (93%)	34 (6%)	9 (2%)	11	15
1	B	584/638 (92%)	563 (96%)	17 (3%)	4 (1%)	25	37
All	All	1163/1276 (91%)	1099 (94%)	51 (4%)	13 (1%)	17	23

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	LYS
1	A	336	GLN

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Mol	Chain	Res	Type
1	A	415	ASN
1	A	462	PRO
1	B	415	ASN
1	B	448	PRO
1	A	337	THR
1	A	456	ILE
1	A	431	ASN
1	A	452	LEU
1	A	447	ILE
1	B	127	GLY
1	B	456	ILE

### 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%)	453 (91%)	45 (9%)	11	16
1	B	501/542 (92%)	469 (94%)	32 (6%)	20	32
All	All	999/1084 (92%)	922 (92%)	77 (8%)	15	23

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LYS
1	A	6	ARG
1	A	25	GLU
1	A	35	ASN
1	A	98	ASP
1	A	131	LYS
1	A	143	ARG
1	A	170	LYS
1	A	172	ARG
1	A	198	THR
1	A	226	PHE

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Mol	Chain	Res	Type
1	A	227	ARG
1	A	239	LYS
1	A	240	GLN
1	A	246	ASN
1	A	273	LEU
1	A	279	LYS
1	A	281	VAL
1	A	285	ILE
1	A	316	LEU
1	A	319	SER
1	A	327	LYS
1	A	332	LEU
1	A	336	GLN
1	A	357	PHE
1	A	361	ARG
1	A	415	ASN
1	A	420	GLN
1	A	427	LYS
1	A	431	ASN
1	A	436	LEU
1	A	441	VAL
1	A	444	THR
1	A	445	LEU
1	A	458	SER
1	A	460	THR
1	A	463	LEU
1	A	471	ASN
1	A	473	ILE
1	A	503	ASN
1	A	512	ASN
1	A	598	CYS
1	A	603	SER
1	A	605	LEU
1	B	5	LYS
1	B	6	ARG
1	B	11	ILE
1	B	47	GLU
1	B	72	GLN
1	B	84	VAL
1	B	133	LEU
1	B	143	ARG
1	B	166	VAL

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Mol	Chain	Res	Type
1	B	192	ASP
1	B	197	ASN
1	B	225	THR
1	B	227	ARG
1	B	235	LYS
1	B	241	LYS
1	B	246	ASN
1	B	304	GLN
1	B	337	THR
1	B	413	ASP
1	B	415	ASN
1	B	416	LEU
1	B	434	GLN
1	B	439	SER
1	B	445	LEU
1	B	447	ILE
1	B	451	LYS
1	B	463	LEU
1	B	469	GLU
1	B	471	ASN
1	B	499	LYS
1	B	503	ASN
1	B	603	SER

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	55	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	309	GLN
1	A	415	ASN
1	A	471	ASN
1	A	503	ASN
1	A	512	ASN
1	A	529	GLN

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Mol	Chain	Res	Type
1	B	9	HIS
1	B	39	GLN
1	B	48	ASN
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	415	ASN
1	B	425	GLN
1	B	431	ASN
1	B	434	GLN
1	B	471	ASN
1	B	503	ASN
1	B	504	HIS
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 32 ligands modelled in this entry, 24 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
2	2TJ	A	701	-	30,32,32	2.78	9 (30%)	41,47,47	2.00	12 (29%)
3	S6P	A	702	-	15,15,15	1.39	2 (13%)	20,21,21	1.51	3 (15%)
2	2TJ	B	701	-	30,32,32	2.55	7 (23%)	41,47,47	2.48	14 (34%)
3	S6P	B	702	-	15,15,15	1.75	4 (26%)	20,21,21	1.30	4 (20%)
5	GOL	B	716	-	5,5,5	0.36	0	5,5,5	0.82	0
6	SO4	B	717	-	4,4,4	0.69	0	6,6,6	0.39	0
6	SO4	B	718	-	4,4,4	0.42	0	6,6,6	0.85	0
6	SO4	B	719	-	4,4,4	0.22	0	6,6,6	0.78	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	2TJ	A	701	-	-	0/25/41/41	0/3/3/3
3	S6P	A	702	-	-	0/20/20/20	0/0/0/0
2	2TJ	B	701	-	-	0/25/41/41	0/3/3/3
3	S6P	B	702	-	-	0/20/20/20	0/0/0/0
5	GOL	B	716	-	-	0/4/4/4	0/0/0/0
6	SO4	B	717	-	-	0/0/0/0	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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	2TJ	C3-N2	-4.55	1.43	1.47
3	B	702	S6P	C2-C3	-3.80	1.46	1.53
2	A	701	2TJ	C16-S2	-3.77	1.71	1.76
2	A	701	2TJ	C10-S1	-3.46	1.71	1.76
2	B	701	2TJ	C16-S2	-3.39	1.71	1.76
3	B	702	S6P	O3-C3	-3.23	1.35	1.43
3	A	702	S6P	C2-C3	-2.88	1.47	1.53
3	B	702	S6P	C4-C3	-2.49	1.48	1.53
2	A	701	2TJ	C4-N2	-2.05	1.45	1.47
3	A	702	S6P	P-O2P	2.13	1.63	1.54
2	B	701	2TJ	C19-C18	2.15	1.51	1.47
2	A	701	2TJ	C2-C17	2.70	1.50	1.48
3	B	702	S6P	P-O3P	2.89	1.60	1.50
2	B	701	2TJ	C15-C10	3.43	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	2TJ	O2-S1	3.79	1.48	1.43
2	A	701	2TJ	O1-S1	4.04	1.48	1.43
2	B	701	2TJ	O2-S1	4.98	1.49	1.43
2	A	701	2TJ	C11-N3	5.50	1.52	1.46
2	A	701	2TJ	O3-S2	5.51	1.49	1.43
2	B	701	2TJ	O3-S2	5.58	1.49	1.43
2	B	701	2TJ	O4-S2	8.55	1.52	1.43
2	A	701	2TJ	O4-S2	9.38	1.53	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	2TJ	C4-N2-C3	-5.72	107.82	112.69
2	B	701	2TJ	C4-N2-S1	-4.82	107.95	117.06
2	B	701	2TJ	O3-S2-N3	-4.29	102.27	107.11
2	A	701	2TJ	O4-S2-O3	-4.10	114.31	119.55
2	B	701	2TJ	O3-S2-C16	-4.02	102.99	107.95
2	A	701	2TJ	C3-N2-S1	-4.02	109.70	117.22
2	B	701	2TJ	O4-S2-O3	-3.88	114.59	119.55
2	A	701	2TJ	C4-N2-S1	-3.80	109.88	117.06
2	A	701	2TJ	C4-N2-C3	-3.74	109.50	112.69
2	A	701	2TJ	O2-S1-O1	-3.61	113.38	119.46
2	B	701	2TJ	C3-N2-S1	-3.59	110.50	117.22
3	A	702	S6P	C5-C4-C3	-3.32	107.11	112.46
3	A	702	S6P	O2-C2-C3	-2.91	101.88	109.09
2	A	701	2TJ	C10-C15-N4	-2.89	119.20	123.16
2	B	701	2TJ	O2-S1-O1	-2.80	114.75	119.46
3	B	702	S6P	O3-C3-C4	-2.42	103.68	109.46
2	B	701	2TJ	O1-S1-C10	-2.39	104.89	108.00
3	B	702	S6P	O2-C2-C1	-2.25	104.00	109.21
2	A	701	2TJ	O3-S2-C16	-2.24	105.19	107.95
3	B	702	S6P	C1-C2-C3	-2.10	107.72	112.41
2	A	701	2TJ	O4-S2-N3	2.07	109.45	107.11
3	B	702	S6P	O2P-P-O6	2.13	112.39	106.73
2	B	701	2TJ	O2-S1-C10	2.27	110.96	108.00
2	A	701	2TJ	C1-N1-C2	2.41	117.63	110.91
2	B	701	2TJ	O4-S2-C16	2.49	111.03	107.95
2	A	701	2TJ	C10-S1-N2	2.70	110.60	107.31
2	B	701	2TJ	O4-S2-N3	2.83	110.31	107.11
3	A	702	S6P	O2P-P-O6	2.87	114.37	106.73
2	A	701	2TJ	O2-S1-N2	3.52	110.02	106.69
2	B	701	2TJ	C10-S1-N2	3.62	111.71	107.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	2TJ	C16-S2-N3	3.75	112.43	107.53
2	B	701	2TJ	C1-C4-N2	5.63	113.34	108.94
2	B	701	2TJ	C16-S2-N3	5.96	115.32	107.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	2TJ	1	0
2	B	701	2TJ	6	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%)	-0.01	20 (3%) 46 44	29, 50, 86, 123	0
1	B	590/638 (92%)	-0.09	19 (3%) 48 46	24, 44, 73, 116	0
All	All	1175/1276 (92%)	-0.05	39 (3%) 47 45	24, 47, 81, 123	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	LEU	7.2
1	A	430	THR	4.9
1	B	2	PRO	4.2
1	B	1	MET	4.1
1	A	387	PHE	3.3
1	A	466	PHE	2.9
1	B	258	SER	2.9
1	B	260	MET	2.9
1	B	66	GLN	2.9
1	B	21	LEU	2.7
1	B	257	SER	2.7
1	A	357	PHE	2.7
1	A	399	SER	2.6
1	B	265	ALA	2.6
1	B	180	VAL	2.6
1	B	593	ALA	2.5
1	B	454	PRO	2.5
1	A	428	GLU	2.5
1	A	282	ASP	2.5
1	A	465	PHE	2.4
1	A	358	ARG	2.4
1	A	109	THR	2.4
1	A	400	LEU	2.4
1	B	264	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	21	LEU	2.3
1	A	69	SER	2.3
1	A	258	SER	2.2
1	B	254	LEU	2.2
1	B	96	GLU	2.2
1	A	394	THR	2.2
1	B	31	THR	2.2
1	A	260	MET	2.1
1	B	3	GLY	2.1
1	A	429	LYS	2.1
1	A	448	PRO	2.1
1	B	97	PRO	2.0
1	B	262	GLY	2.0
1	A	180	VAL	2.0
1	B	448	PRO	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	B	716	6/6	0.90	0.19	3.50	41,56,59,62	0
2	2TJ	A	701	30/30	0.98	0.13	-0.03	28,33,44,52	0
3	S6P	A	702	16/16	0.98	0.20	-0.05	27,31,34,35	0
3	S6P	B	702	16/16	0.99	0.21	-0.13	22,24,31,32	0
2	2TJ	B	701	30/30	0.97	0.14	-0.20	28,31,40,50	0
4	IOD	B	710	1/1	0.97	0.12	-1.40	90,90,90,90	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	IOD	B	713	1/1	0.94	0.05	-2.02	75,75,75,75	1
4	IOD	B	704	1/1	1.00	0.05	-2.08	54,54,54,54	0
4	IOD	A	703	1/1	0.90	0.06	-2.10	80,80,80,80	0
4	IOD	B	703	1/1	0.94	0.10	-2.15	52,52,52,52	0
4	IOD	A	709	1/1	0.97	0.10	-2.16	85,85,85,85	1
4	IOD	B	715	1/1	0.86	0.10	-2.26	89,89,89,89	1
4	IOD	A	713	1/1	0.93	0.06	-2.65	64,64,64,64	1
4	IOD	A	704	1/1	0.98	0.06	-2.70	61,61,61,61	0
4	IOD	A	711	1/1	0.86	0.08	-2.87	77,77,77,77	1
4	IOD	B	705	1/1	0.98	0.06	-2.93	56,56,56,56	0
4	IOD	A	707	1/1	0.95	0.04	-3.41	68,68,68,68	1
6	SO4	B	719	5/5	0.97	0.13	-	37,40,43,44	5
4	IOD	B	712	1/1	0.95	0.05	-	58,58,58,58	1
4	IOD	A	706	1/1	0.97	0.05	-	82,82,82,82	0
4	IOD	A	710	1/1	0.97	0.05	-	63,63,63,63	1
4	IOD	A	708	1/1	0.94	0.05	-	83,83,83,83	1
6	SO4	B	718	5/5	0.92	0.32	-	57,64,81,97	0
4	IOD	B	709	1/1	0.92	0.07	-	80,80,80,80	1
4	IOD	B	714	1/1	0.96	0.05	-	76,76,76,76	1
4	IOD	B	708	1/1	0.94	0.05	-	61,61,61,61	1
4	IOD	A	712	1/1	0.97	0.05	-	68,68,68,68	1
4	IOD	B	711	1/1	0.90	0.10	-	96,96,96,96	1
4	IOD	A	705	1/1	0.99	0.06	-	52,52,52,52	1
4	IOD	B	706	1/1	0.98	0.06	-	62,62,62,62	0
4	IOD	B	707	1/1	0.99	0.04	-	72,72,72,72	0
6	SO4	B	717	5/5	0.82	0.17	-	67,67,80,95	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.