W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:15 AM GMT

PDB ID	:	2PZI
Title	:	Crystal Structure of Protein kinase PknG from Mycobacterium tuberculosis in Complex with Tetrahydrobenzothiophene AX20017
Authors	:	Honnappa, S.; Steinmetz, M.O.
Deposited on	:	2007-05-18
Resolution	:	2.40 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

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.
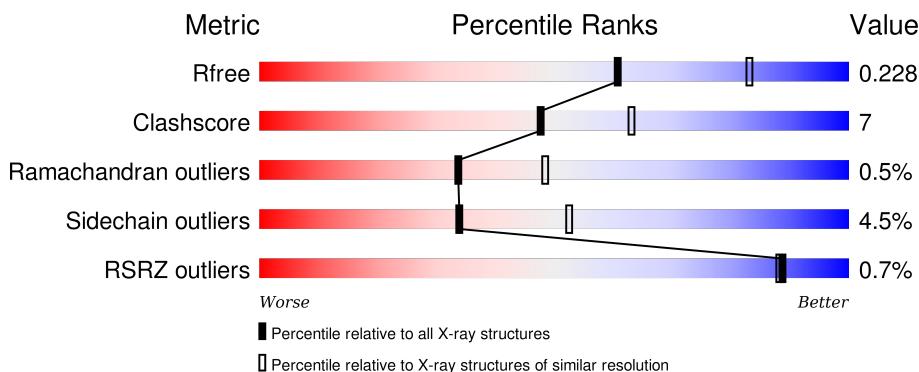
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 >=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 <=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	681	79% ... 15% · ·
1	B	681	% ... 80% ... 13% · 5%
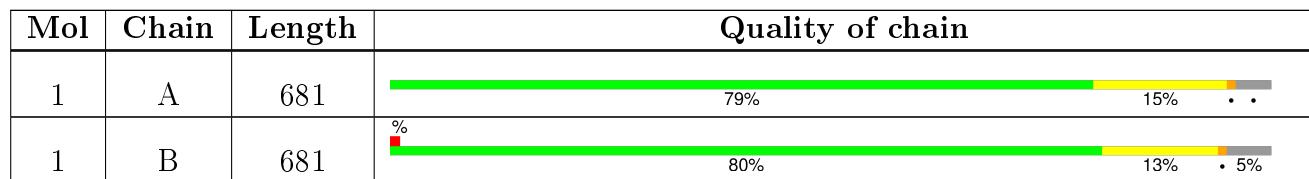
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	754	-	-	-	X
5	GOL	A	755	-	-	X	-
5	GOL	A	756	-	-	X	X
5	GOL	A	757	-	-	-	X
5	GOL	B	754	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10346 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 Probable serine/threonine-protein kinase pknG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total 5029	C 3184	N 885	O 946	S 14	0	0	0
1	B	644	Total 4946	C 3129	N 872	O 931	S 14	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	GLY	-	CLONING ARTIFACT	UNP P65728
A	70	SER	-	CLONING ARTIFACT	UNP P65728
A	71	HIS	-	CLONING ARTIFACT	UNP P65728
A	72	MET	-	CLONING ARTIFACT	UNP P65728
B	69	GLY	-	CLONING ARTIFACT	UNP P65728
B	70	SER	-	CLONING ARTIFACT	UNP P65728
B	71	HIS	-	CLONING ARTIFACT	UNP P65728
B	72	MET	-	CLONING ARTIFACT	UNP P65728

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cl 1	0	0

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Cd 1	0	0
3	A	1	Total 1	Cd 1	0	0

- Molecule 4 is 2-[(CYCLOPROPYLCARBONYL)AMINO]-4,5,6,7-TETRAHYDRO-1-BEN

ZOTHIOPHENE-3-CARBOXAMIDE (three-letter code: AXX) (formula: $C_{13}H_{16}N_2O_2S$).
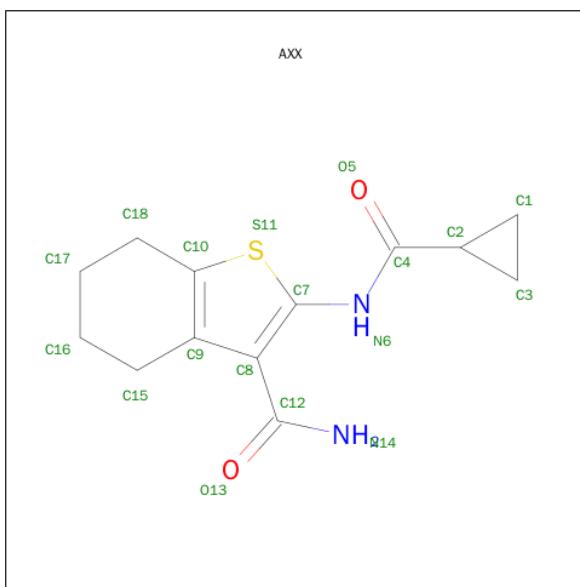
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			18	13	2	2	1		
4	A	1	Total	C	N	O	S	0	0
			18	13	2	2	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
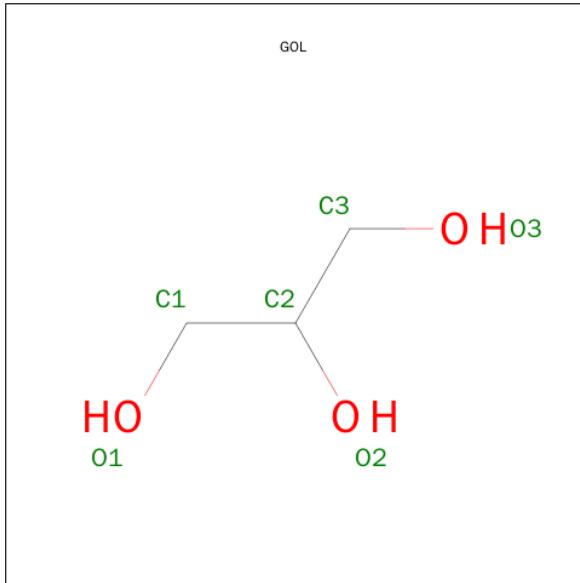
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	151	Total 151	O 151	0	0
6	B	145	Total 145	O 145	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 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: Probable serine/threonine-protein kinase pknG
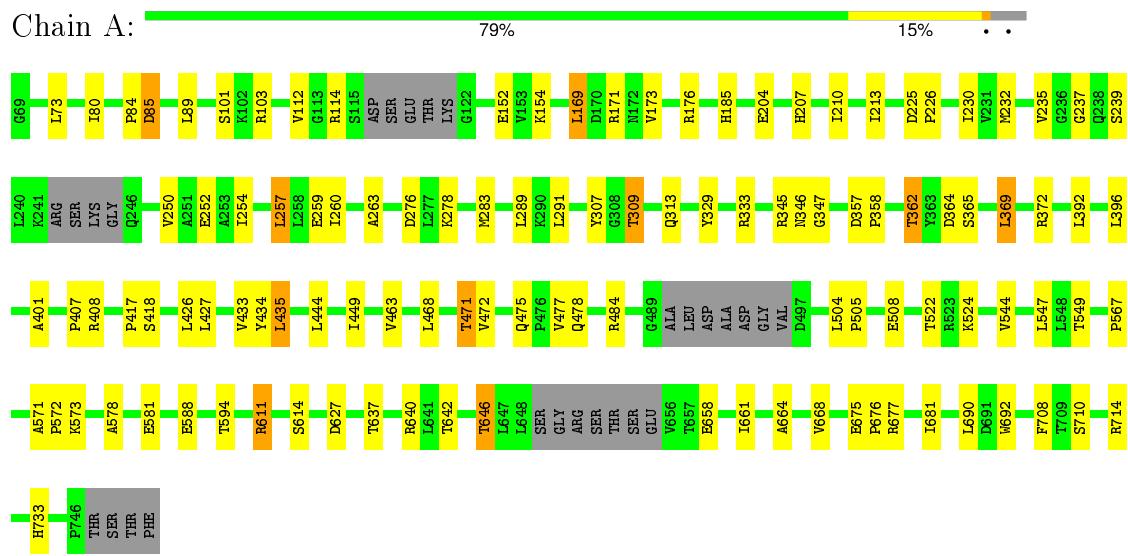
• Molecule 1: Probable serine/threonine-protein kinase pknG
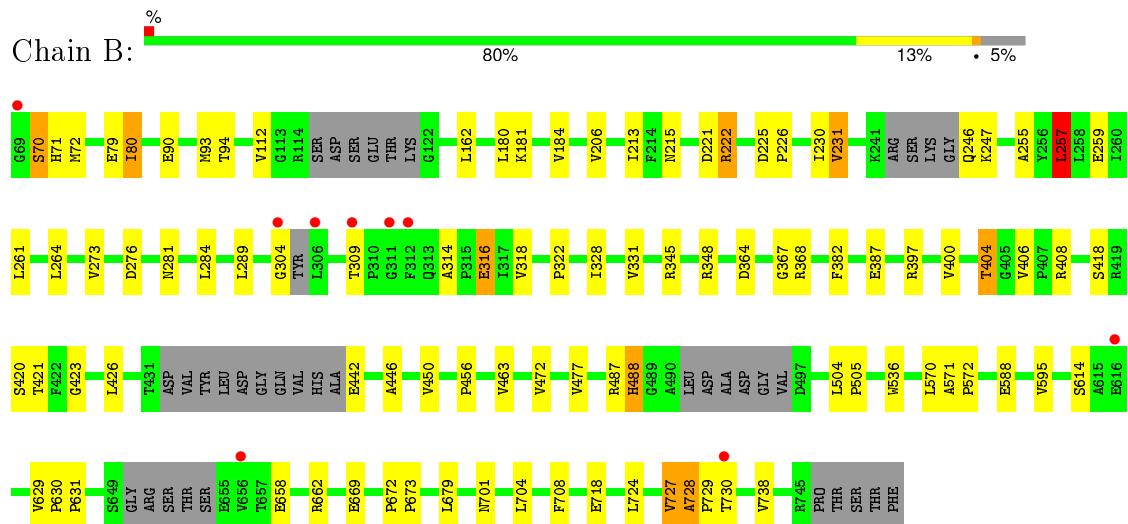
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	122.55Å 122.55Å 243.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	106.00 – 2.40 48.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (106.00-2.40) 99.9 (48.92-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.84 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.183 , 0.233 0.179 , 0.228	Depositor DCC
R_{free} test set	4045 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	56.9	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.0	EDS
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.47$, $<L^2> = 0.30$	Xtriage
Outliers	0 of 80540 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10346	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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, AXX, CL, CD

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	0.52	0/5135	0.67	4/6999 (0.1%)
1	B	0.57	2/5046 (0.0%)	0.65	3/6872 (0.0%)
All	All	0.55	2/10181 (0.0%)	0.66	7/13871 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	GLY	C-O	11.03	1.41	1.23
1	B	304	GLY	CA-C	5.40	1.60	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	THR	CA-CB-CG2	-6.97	102.64	112.40
1	B	257	LEU	CA-CB-CG	-6.95	99.32	115.30
1	A	257	LEU	CA-CB-CG	-6.23	100.96	115.30
1	B	304	GLY	CA-C-O	-6.18	109.48	120.60
1	A	611	ARG	NE-CZ-NH1	-5.91	117.34	120.30
1	A	369	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	89	LEU	CA-CB-CG	5.20	127.25	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	5029	0	5023	85	0
1	B	4946	0	4947	62	0
2	A	1	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	18	0	16	2	0
4	B	18	0	16	1	0
5	A	24	0	32	28	0
5	B	12	0	16	4	0
6	A	151	0	0	6	0
6	B	145	0	0	4	0
All	All	10346	0	10050	149	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 7.

All (149) 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)
5:A:757:GOL:H2	1:B:477:VAL:HB	1.49	0.92
1:A:475:GLN:HB2	5:A:755:GOL:H31	1.54	0.89
1:B:404:THR:HG21	1:B:408:ARG:HH21	1.40	0.87
1:A:594:THR:HG21	5:A:756:GOL:H11	1.55	0.87
1:A:84:PRO:O	1:A:85:ASP:HB2	1.74	0.86
1:A:637:THR:HG21	1:A:675:GLU:HG2	1.57	0.86
1:A:573:LYS:HE2	5:A:756:GOL:H12	1.64	0.78
1:B:80:ILE:HD11	1:B:284:LEU:HD21	1.66	0.78
1:A:475:GLN:HG3	1:B:420:SER:HB2	1.66	0.78
1:A:477:VAL:HB	5:A:755:GOL:H32	1.66	0.77
1:A:477:VAL:N	5:A:755:GOL:H32	1.99	0.77
1:B:273:VAL:HG11	1:B:322:PRO:HB2	1.66	0.76
1:A:477:VAL:HB	5:A:755:GOL:H12	1.67	0.75
1:A:154:LYS:HE3	1:A:169:LEU:HD22	1.69	0.74
1:A:235:VAL:HB	1:A:283:MET:HE1	1.69	0.74
1:A:581:GLU:CD	1:A:611:ARG:HH12	1.92	0.73
1:A:103:ARG:O	1:A:114:ARG:NH1	2.21	0.73
1:A:477:VAL:H	5:A:755:GOL:H32	1.52	0.73
1:A:235:VAL:HG12	1:A:283:MET:CE	2.18	0.73
1:B:418:SER:HB2	5:B:754:GOL:H11	1.71	0.72
1:B:728:ALA:N	1:B:729:PRO:HD3	2.06	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:PRO:O	1:A:362:THR:HG23	1.91	0.70
1:B:669:GLU:HG3	1:B:704:LEU:HD23	1.72	0.70
1:A:417:PRO:HB3	5:A:754:GOL:H11	1.74	0.69
1:A:235:VAL:HG12	1:A:283:MET:HE3	1.73	0.69
1:A:642:THR:O	1:A:646:THR:HG23	1.92	0.69
1:A:475:GLN:CB	5:A:755:GOL:H31	2.23	0.68
1:A:478:GLN:HB2	5:A:755:GOL:H11	1.77	0.67
1:A:594:THR:HG21	5:A:756:GOL:C1	2.22	0.67
1:A:463:VAL:HG23	6:A:897:HOH:O	1.94	0.66
1:A:581:GLU:OE2	1:A:611:ARG:NH1	2.29	0.65
1:B:328:ILE:HD13	1:B:382:PHE:O	1.96	0.65
1:A:276:ASP:OD1	1:A:309:THR:HG23	1.96	0.65
1:B:504:LEU:HB3	1:B:505:PRO:HD3	1.79	0.65
1:A:235:VAL:CG1	1:A:283:MET:CE	2.75	0.64
1:A:84:PRO:O	1:A:85:ASP:CB	2.47	0.63
1:B:463:VAL:HG23	6:B:788:HOH:O	1.97	0.63
1:A:364:ASP:HB3	5:A:756:GOL:H2	1.79	0.63
1:A:477:VAL:CB	5:A:755:GOL:H12	2.30	0.62
1:A:477:VAL:CB	5:A:755:GOL:H32	2.29	0.62
1:B:364:ASP:O	1:B:368:ARG:HG3	2.00	0.62
1:B:404:THR:HG21	1:B:408:ARG:NH2	2.13	0.61
1:B:71:HIS:HB2	1:B:80:ILE:O	2.00	0.61
1:B:276:ASP:O	1:B:281:ASN:ND2	2.33	0.61
1:B:662:ARG:NH2	1:B:701:ASN:O	2.34	0.60
1:A:152:GLU:OE2	1:A:171:ARG:NH1	2.34	0.59
1:A:276:ASP:OD1	1:A:309:THR:CG2	2.51	0.59
1:A:254:ILE:HG23	1:A:392:LEU:HG	1.84	0.59
1:A:345:ARG:O	1:A:346:ASN:HB2	2.03	0.59
5:A:757:GOL:C2	1:B:477:VAL:HB	2.28	0.58
1:A:504:LEU:HB3	1:A:505:PRO:HD3	1.85	0.58
1:B:727:VAL:C	1:B:729:PRO:HD3	2.23	0.58
1:A:477:VAL:HB	5:A:755:GOL:C3	2.33	0.58
1:B:221:ASP:O	1:B:222:ARG:HB2	2.05	0.57
1:A:435:LEU:HD12	6:A:884:HOH:O	2.04	0.57
1:B:215:ASN:HB3	1:B:231:VAL:HG13	1.85	0.57
1:A:237:GLY:H	1:A:283:MET:HE3	1.71	0.56
1:A:477:VAL:CA	5:A:755:GOL:H32	2.36	0.55
1:B:418:SER:H	5:B:754:GOL:H11	1.71	0.55
1:B:367:GLY:HA3	6:B:844:HOH:O	2.07	0.55
1:A:484:ARG:NH2	6:A:802:HOH:O	2.40	0.55
1:A:477:VAL:HB	5:A:755:GOL:C1	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:THR:CG2	1:B:408:ARG:HH21	2.15	0.54
5:A:755:GOL:HO2	1:B:420:SER:HG	1.55	0.54
1:B:72:MET:HG3	1:B:79:GLU:OE2	2.08	0.54
1:A:449:ILE:HD13	1:A:578:ALA:HB1	1.89	0.53
1:A:80:ILE:HD11	1:A:252:GLU:HG2	1.91	0.53
1:A:664:ALA:O	1:A:668:VAL:HG23	2.09	0.52
1:A:278:LYS:NZ	1:A:309:THR:HG21	2.24	0.52
1:A:401:ALA:HB2	1:A:408:ARG:HG2	1.90	0.52
1:B:314:ALA:HB1	1:B:316:GLU:OE2	2.09	0.52
1:A:73:LEU:HD22	1:A:259:GLU:HG3	1.90	0.52
1:B:80:ILE:CD1	1:B:284:LEU:HD21	2.37	0.51
1:A:207:HIS:HB3	1:A:210:ILE:HD12	1.93	0.51
1:A:571:ALA:HB3	1:A:572:PRO:HD3	1.92	0.51
1:B:487:ARG:O	1:B:488:HIS:HB2	2.12	0.49
1:B:658:GLU:OE2	1:B:662:ARG:NH1	2.45	0.49
4:B:752:AXX:S11	4:B:752:AXX:O5	2.70	0.49
1:A:417:PRO:CB	5:A:754:GOL:H11	2.42	0.49
1:B:701:ASN:HD22	1:B:701:ASN:H	1.60	0.49
1:A:468:LEU:O	1:A:471:THR:HG22	2.12	0.49
1:B:423:GLY:HA2	1:B:426:LEU:HD13	1.95	0.48
1:A:658:GLU:HB2	1:A:692:TRP:CH2	2.49	0.48
1:A:213:ILE:HD12	1:A:230:ILE:HD11	1.95	0.48
1:A:418:SER:N	5:A:754:GOL:H12	2.29	0.48
1:B:571:ALA:HB3	1:B:572:PRO:HD3	1.95	0.47
1:A:185:HIS:HD2	6:A:907:HOH:O	1.98	0.47
1:A:235:VAL:CB	1:A:283:MET:HE1	2.42	0.47
1:A:346:ASN:HB3	1:A:347:GLY:H	1.55	0.47
1:A:477:VAL:H	5:A:755:GOL:C3	2.23	0.47
1:B:418:SER:HB2	5:B:754:GOL:C1	2.42	0.47
1:B:588:GLU:HG2	6:B:873:HOH:O	2.15	0.47
1:B:255:ALA:O	1:B:259:GLU:HG2	2.15	0.47
1:B:387:GLU:HB2	6:B:776:HOH:O	2.13	0.47
1:B:727:VAL:O	1:B:727:VAL:HG13	2.15	0.47
1:B:213:ILE:HD12	1:B:230:ILE:HD11	1.97	0.46
1:A:278:LYS:CE	1:A:309:THR:HG21	2.46	0.46
1:B:679:LEU:HB2	1:B:724:LEU:HD21	1.96	0.46
1:A:254:ILE:HG21	1:A:396:LEU:HB2	1.96	0.46
1:A:594:THR:CG2	5:A:756:GOL:H11	2.39	0.46
4:A:753:AXX:H141	4:A:753:AXX:C15	2.28	0.46
1:B:257:LEU:HD22	1:B:331:VAL:HG13	1.98	0.46
1:B:261:LEU:HD23	1:B:264:LEU:HD12	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ALA:O	1:B:450:VAL:HG23	2.17	0.45
1:A:313:GLN:HB3	6:A:809:HOH:O	2.16	0.45
1:B:630:PRO:HA	1:B:631:PRO:HD3	1.88	0.45
1:B:487:ARG:O	1:B:488:HIS:CB	2.64	0.45
1:B:426:LEU:O	1:B:442:GLU:HB3	2.17	0.45
1:B:397:ARG:NH1	5:B:753:GOL:O1	2.37	0.45
1:B:669:GLU:HG3	1:B:704:LEU:CD2	2.45	0.45
1:A:508:GLU:OE1	1:A:524:LYS:HE2	2.17	0.45
1:A:260:ILE:O	1:A:263:ALA:HB3	2.16	0.45
1:B:400:VAL:O	1:B:404:THR:HB	2.17	0.44
1:A:407:PRO:C	1:A:408:ARG:HD2	2.38	0.44
1:B:225:ASP:HA	1:B:226:PRO:HD3	1.88	0.44
1:B:728:ALA:N	1:B:729:PRO:CD	2.78	0.43
1:B:246:GLN:CG	1:B:247:LYS:H	2.31	0.43
1:A:213:ILE:HD13	1:A:232:MET:HG2	1.99	0.43
1:B:162:LEU:HB2	1:B:181:LYS:HE2	1.99	0.43
1:A:676:PRO:O	1:A:677:ARG:HB2	2.19	0.43
1:A:477:VAL:HB	5:A:755:GOL:C2	2.48	0.43
1:B:456:PRO:HB3	1:B:536:TRP:CH2	2.53	0.43
1:A:478:GLN:N	5:A:755:GOL:C1	2.82	0.43
1:A:594:THR:HG23	5:A:756:GOL:H32	2.01	0.43
1:A:426:LEU:HD11	1:A:444:LEU:HB2	2.01	0.43
1:B:404:THR:HG23	1:B:406:VAL:H	1.84	0.43
1:A:235:VAL:O	4:A:753:AXX:H2	2.19	0.42
1:B:718:GLU:OE1	1:B:727:VAL:HG23	2.19	0.42
1:A:407:PRO:O	1:A:408:ARG:HD2	2.19	0.42
1:B:261:LEU:HD23	1:B:261:LEU:HA	1.84	0.42
1:B:629:VAL:HA	1:B:630:PRO:HD3	1.87	0.42
1:A:173:VAL:HB	1:A:176:ARG:HG2	2.00	0.42
1:A:365:SER:HB2	1:A:567:PRO:O	2.18	0.42
1:A:627:ASP:HA	1:A:640:ARG:HH12	1.85	0.42
1:B:718:GLU:HA	1:B:718:GLU:OE1	2.18	0.42
1:A:434:TYR:O	1:A:733:HIS:HE1	2.02	0.42
1:A:329:TYR:O	1:A:333:ARG:HG2	2.20	0.41
1:B:180:LEU:HA	1:B:230:ILE:O	2.20	0.41
1:A:658:GLU:HB2	1:A:692:TRP:CZ2	2.55	0.41
1:B:672:PRO:HA	1:B:673:PRO:HD2	1.95	0.41
1:A:690:LEU:CD1	1:A:714:ARG:HG3	2.50	0.41
1:A:478:GLN:N	5:A:755:GOL:H12	2.35	0.41
1:B:420:SER:OG	1:B:421:THR:N	2.54	0.41
1:A:544:VAL:O	1:A:547:LEU:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:751:CL:CL	6:A:880:HOH:O	2.60	0.40
1:A:677:ARG:O	1:A:681:ILE:HG12	2.21	0.40
1:A:225:ASP:HA	1:A:226:PRO:HD3	1.96	0.40
1:A:357:ASP:HA	1:A:358:PRO:HD3	1.86	0.40
1:B:570:LEU:HD22	1:B:595:VAL:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	644/681 (95%)	624 (97%)	19 (3%)	1 (0%)	52	69
1	B	630/681 (92%)	604 (96%)	21 (3%)	5 (1%)	24	35
All	All	1274/1362 (94%)	1228 (96%)	40 (3%)	6 (0%)	34	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	ASP
1	B	488	HIS
1	B	70	SER
1	B	222	ARG
1	B	727	VAL
1	B	728	ALA

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	537/559 (96%)	510 (95%)	27 (5%)	30	48
1	B	528/559 (94%)	507 (96%)	21 (4%)	38	58
All	All	1065/1118 (95%)	1017 (96%)	48 (4%)	34	52

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	SER
1	A	112	VAL
1	A	169	LEU
1	A	204	GLU
1	A	239	SER
1	A	250	VAL
1	A	257	LEU
1	A	289	LEU
1	A	291	LEU
1	A	307	TYR
1	A	309	THR
1	A	362	THR
1	A	369	LEU
1	A	372	ARG
1	A	427	LEU
1	A	433	VAL
1	A	435	LEU
1	A	471	THR
1	A	472	VAL
1	A	522	THR
1	A	549	THR
1	A	588	GLU
1	A	614	SER
1	A	646	THR
1	A	661	ILE
1	A	708	PHE
1	A	710	SER
1	B	70	SER
1	B	80	ILE
1	B	90	GLU
1	B	93	MET
1	B	94	THR
1	B	112	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	184	VAL
1	B	206	VAL
1	B	231	VAL
1	B	257	LEU
1	B	289	LEU
1	B	316	GLU
1	B	318	VAL
1	B	345	ARG
1	B	348	ARG
1	B	404	THR
1	B	472	VAL
1	B	614	SER
1	B	708	PHE
1	B	730	THR
1	B	738	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	733	HIS
1	B	107	ASN
1	B	172	ASN
1	B	701	ASN
1	B	711	HIS

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 11 ligands modelled in this entry, 3 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	#$|Z| > 2$
4	AXX	A	753	-	18,20,20	0.99	1 (5%)	17,29,29	3.08	5 (29%)
5	GOL	A	754	-	5,5,5	0.38	0	5,5,5	0.78	0
5	GOL	A	755	-	5,5,5	1.03	1 (20%)	5,5,5	1.53	1 (20%)
5	GOL	A	756	-	5,5,5	0.44	0	5,5,5	0.53	0
5	GOL	A	757	-	5,5,5	0.88	0	5,5,5	0.95	0
4	AXX	B	752	-	18,20,20	1.04	1 (5%)	17,29,29	2.51	4 (23%)
5	GOL	B	753	-	5,5,5	0.35	0	5,5,5	0.47	0
5	GOL	B	754	-	5,5,5	0.37	0	5,5,5	0.49	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
4	AXX	A	753	-	-	0/6/21/21	0/2/3/3
5	GOL	A	754	-	-	0/4/4/4	0/0/0/0
5	GOL	A	755	-	-	0/4/4/4	0/0/0/0
5	GOL	A	756	-	-	0/4/4/4	0/0/0/0
5	GOL	A	757	-	-	0/4/4/4	0/0/0/0
4	AXX	B	752	-	-	0/6/21/21	0/2/3/3
5	GOL	B	753	-	-	0/4/4/4	0/0/0/0
5	GOL	B	754	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	755	GOL	O2-C2	-2.06	1.37	1.43
4	B	752	AXX	C8-C7	2.53	1.47	1.41
4	A	753	AXX	C8-C7	2.79	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	753	AXX	C3-C2-C4	-10.11	107.61	117.26
4	B	752	AXX	C1-C2-C4	-7.13	110.45	117.26
4	B	752	AXX	C3-C2-C4	-4.95	112.53	117.26
4	A	753	AXX	C1-C2-C4	-4.75	112.72	117.26
4	A	753	AXX	C17-C18-C10	-4.37	106.12	113.48
4	B	752	AXX	C17-C18-C10	-4.26	106.31	113.48
4	A	753	AXX	O13-C12-C8	-2.66	116.19	119.60
4	A	753	AXX	C8-C9-C10	-2.30	111.21	113.61
4	B	752	AXX	O13-C12-C8	-2.23	116.73	119.60
5	A	755	GOL	O3-C3-C2	2.06	120.17	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	753	AXX	2	0
5	A	754	GOL	3	0
5	A	755	GOL	17	0
5	A	756	GOL	6	0
5	A	757	GOL	2	0
4	B	752	AXX	1	0
5	B	753	GOL	1	0
5	B	754	GOL	3	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(Å²)	Q<0.9
1	A	654/681 (96%)	-0.31	0	100	100	26, 44, 66, 84	0
1	B	644/681 (94%)	-0.23	9 (1%)	78	77	27, 46, 67, 91	0
All	All	1298/1362 (95%)	-0.27	9 (0%)	89	88	26, 45, 66, 91	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	69	GLY	5.2
1	B	311	GLY	2.7
1	B	306	LEU	2.6
1	B	309	THR	2.5
1	B	616	GLU	2.3
1	B	304	GLY	2.3
1	B	730	THR	2.1
1	B	656	VAL	2.1
1	B	312	PHE	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(Å²)	Q<0.9
5	GOL	A	757	6/6	0.89	0.32	10.47	45,56,69,74	0
5	GOL	A	756	6/6	0.86	0.25	6.82	80,83,85,90	0
5	GOL	A	754	6/6	0.83	0.23	4.89	57,62,76,81	0
5	GOL	B	754	6/6	0.77	0.22	2.72	62,70,77,86	0
5	GOL	A	755	6/6	0.92	0.22	1.85	51,52,70,73	0
3	CD	A	752	1/1	0.99	0.15	1.46	53,53,53,53	0
2	CL	A	751	1/1	0.98	0.14	0.47	66,66,66,66	0
3	CD	B	751	1/1	0.99	0.15	0.39	70,70,70,70	0
5	GOL	B	753	6/6	0.94	0.13	-0.43	56,70,75,78	0
4	AXX	A	753	18/18	0.99	0.11	-0.48	33,46,53,57	0
4	AXX	B	752	18/18	0.98	0.10	-0.66	33,45,49,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.