



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:42 AM GMT

PDB ID : 2Y2G  
Title : PENICILLIN-BINDING PROTEIN 1B (PBP-1B) IN COMPLEX WITH AN ALKYL BORONATE (A01)  
Authors : Contreras-Martel, C.; Amoroso, A.; Woon, E.C.; Zervosen, A.; Inglis, S.; Martins, A.; Verlaine, O.; Rydzik, A.; Job, V.; Luxen, A.; Joris, B.; Schofield, C.J.; Dessen, A.  
Deposited on : 2010-12-15  
Resolution : 2.05 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.

---

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

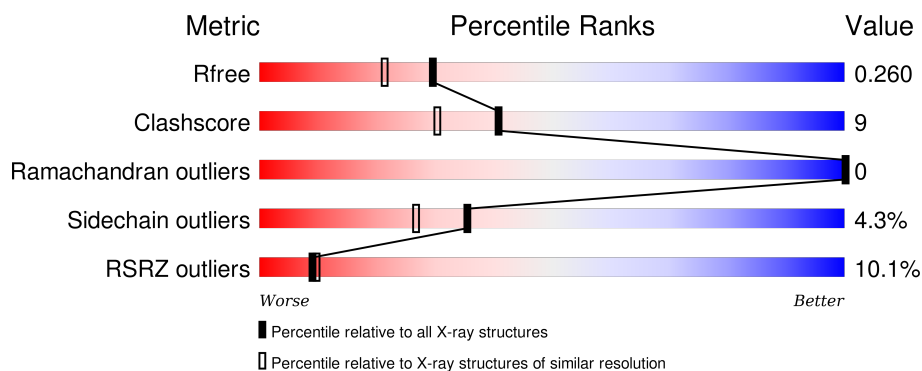
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	494	<div> <div>9%</div> <div>79% 14% • 6%</div> </div>
1	B	494	<div> <div>10%</div> <div>79% 14% • 6%</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	CL	B	1792	-	-	-	X
5	NA	A	1300	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7930 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.

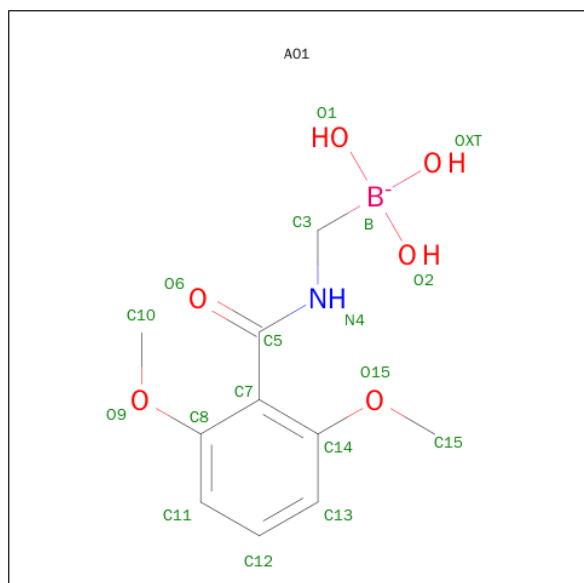
- Molecule 1 is a protein called PENICILLIN-BINDING PROTEIN 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	2	0
			3610	2260	614	721	15			
1	B	466	Total	C	N	O	S	0	1	0
			3603	2255	613	720	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	656	GLY	ASN	ENGINEERED MUTATION	UNP Q7CRA4
A	686	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4
A	687	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4
B	656	GLY	ASN	ENGINEERED MUTATION	UNP Q7CRA4
B	686	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4
B	687	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4

- Molecule 2 is [(2,6-DIMETHOXYPHENYL)CARBONYLAMINO]METHYL-TRIHYDROXY-BORON (three-letter code: A01) (formula: C<sub>10</sub>H<sub>15</sub>BN<sub>1</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	0	0
			17	1	10	1	5		
2	B	1	Total	B	C	N	O	0	0
			17	1	10	1	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	17	Total	Cl	0	0
			17	17		
4	A	13	Total	Cl	0	0
			13	13		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

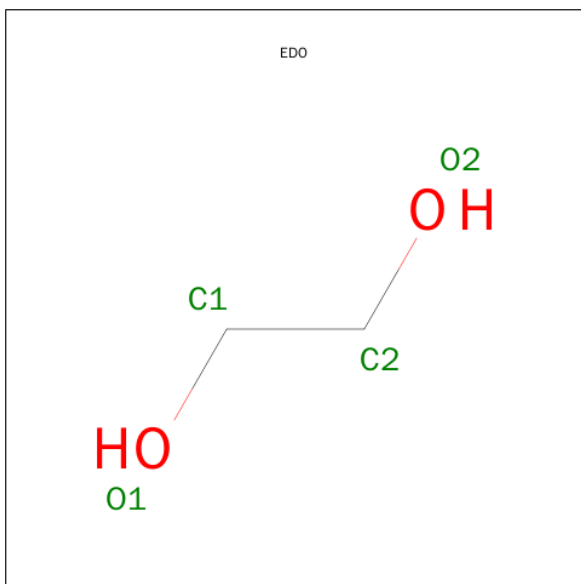
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

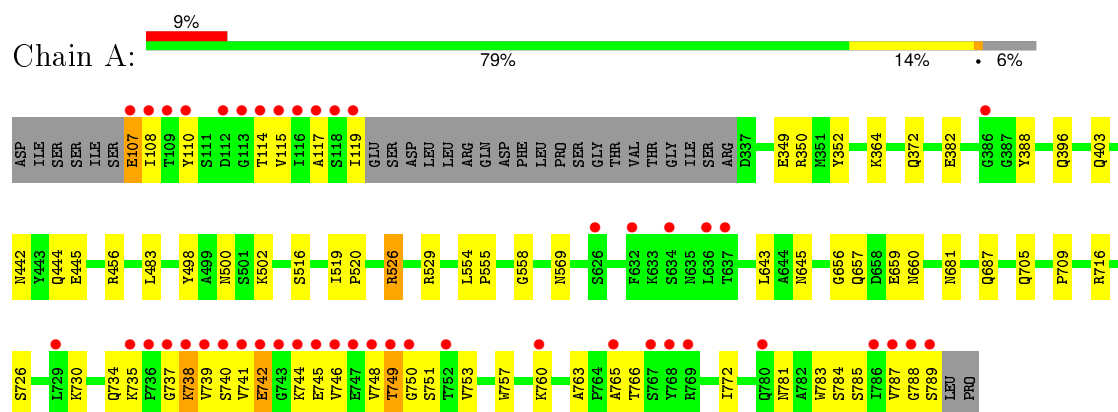
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	318	Total	O	0	0
			318	318		
7	B	307	Total	O	0	0
			307	307		

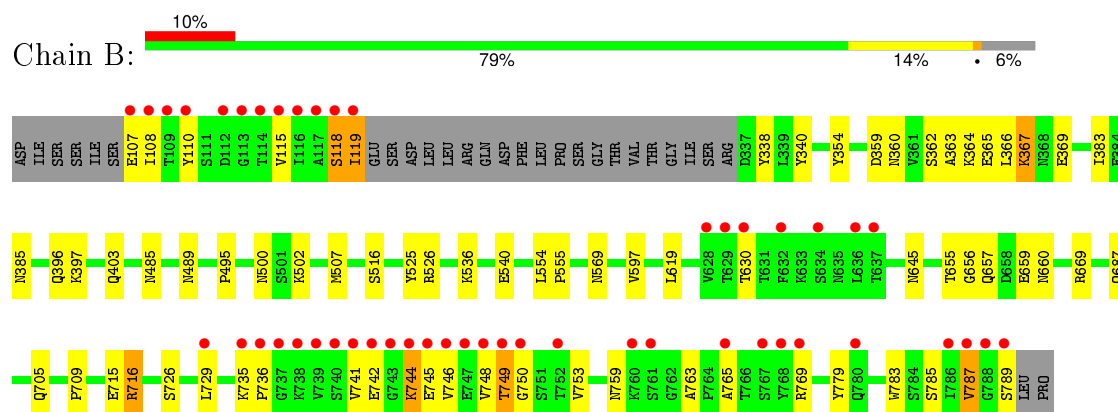
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: PENICILLIN-BINDING PROTEIN 1B



#### • Molecule 1: PENICILLIN-BINDING PROTEIN 1B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.53Å 97.53Å 149.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.05 48.76 – 2.05	Depositor EDS
% Data completeness (in resolution range)	90.3 (48.74-2.05) 90.4 (48.76-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.6.0095	Depositor
R, $R_{free}$	0.222 , 0.260 0.223 , 0.260	Depositor DCC
$R_{free}$ test set	4088 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.9	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 81301 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 96.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.6408e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SO4, A01, EDO, CL

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	0.48	0/3686	0.51	0/5001
1	B	0.47	0/3676	0.51	0/4989
All	All	0.47	0/7362	0.51	0/9990

There are no bond length outliers.

There are no bond angle outliers.

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	3610	0	3486	57	0
1	B	3603	0	3470	64	0
2	A	17	0	13	3	0
2	B	17	0	13	3	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	13	0	0	2	0
4	B	17	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	8	0	12	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	0	12	3	0
7	A	318	0	0	6	0
7	B	307	0	0	16	0
All	All	7930	0	7006	123	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 9.

All (123) 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:442:ASN:ND2	1:A:445:GLU:HG2	1.69	1.05
1:A:526[B]:ARG:HD3	7:A:2176:HOH:O	1.65	0.97
1:B:729:LEU:HD11	1:B:736:PRO:HA	1.47	0.96
1:B:687:GLN:HB2	7:B:2242:HOH:O	1.68	0.92
1:B:741:VAL:O	1:B:742:GLU:HG2	1.73	0.88
1:A:645:ASN:O	1:A:716:ARG:NH2	2.09	0.85
1:B:107:GLU:HG3	1:B:115:VAL:HG13	1.61	0.82
1:A:730[A]:LYS:HG3	1:A:753:VAL:HG13	1.62	0.78
1:B:107:GLU:HG3	1:B:115:VAL:CG1	2.13	0.77
1:A:502:LYS:HE2	7:A:2126:HOH:O	1.85	0.77
1:A:442:ASN:ND2	1:A:445:GLU:CG	2.47	0.76
1:B:107:GLU:HA	7:B:2001:HOH:O	1.86	0.75
1:B:742:GLU:O	1:B:742:GLU:HG3	1.87	0.74
1:B:500:ASN:HB2	7:B:2111:HOH:O	1.86	0.74
1:B:110:TYR:CG	1:B:396:GLN:HB2	2.23	0.73
1:A:687:GLN:HB2	7:A:2255:HOH:O	1.88	0.73
1:B:365:GLU:HB3	7:B:2020:HOH:O	1.89	0.72
1:B:525:TYR:CD2	1:B:526[B]:ARG:NH1	2.59	0.69
1:B:107:GLU:CG	1:B:115:VAL:HG13	2.24	0.68
1:B:645:ASN:O	1:B:716:ARG:NH2	2.26	0.67
1:B:119:ILE:HG23	1:B:340:TYR:OH	1.94	0.66
1:B:741:VAL:O	1:B:742:GLU:CG	2.44	0.64
1:B:397:LYS:HE3	7:B:2033:HOH:O	1.98	0.63
1:B:110:TYR:CD2	1:B:396:GLN:HB2	2.34	0.62
1:A:526[B]:ARG:NH1	1:A:529:ARG:HG3	2.14	0.61
1:B:526[B]:ARG:HD3	7:B:2139:HOH:O	1.99	0.61
1:A:554:LEU:N	1:A:555:PRO:HD2	2.16	0.61
1:B:489:ASN:HD22	1:B:495:PRO:HA	1.67	0.60
1:B:749:THR:HG23	1:B:750:GLY:N	2.17	0.60
1:B:716:ARG:HD3	7:B:2271:HOH:O	2.02	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:GLU:HG2	7:B:2023:HOH:O	2.02	0.59
1:B:362:SER:OG	1:B:365:GLU:HG3	2.01	0.59
1:B:729:LEU:CD1	1:B:736:PRO:HA	2.25	0.59
2:B:1000:A01:H12	7:B:2244:HOH:O	2.01	0.58
1:A:749:THR:HG23	1:A:750:GLY:N	2.18	0.58
1:A:352:TYR:OH	1:A:372:GLN:HG2	2.03	0.58
1:A:526[B]:ARG:HH11	1:A:529:ARG:HG3	1.69	0.57
1:A:735:LYS:HB2	1:A:765:ALA:HA	1.87	0.57
1:B:502:LYS:HE2	7:B:2117:HOH:O	2.05	0.56
1:B:526[B]:ARG:CD	7:B:2139:HOH:O	2.53	0.56
1:B:779:TYR:O	1:B:783:TRP:HD1	1.89	0.56
1:B:110:TYR:CD1	1:B:396:GLN:HB2	2.41	0.56
1:A:783:TRP:O	1:A:787:VAL:HB	2.06	0.55
1:B:359:ASP:O	1:B:360:ASN:HB2	2.06	0.55
1:A:656:GLY:O	2:A:1000:A01:H151	2.07	0.55
1:A:738:LYS:HA	1:A:746:VAL:O	2.08	0.54
1:A:705:GLN:HE22	6:A:1401:EDO:H22	1.73	0.54
1:B:363:ALA:O	1:B:367:LYS:HD2	2.07	0.54
1:A:657:GLN:HB2	1:A:659:GLU:CD	2.28	0.53
1:B:554:LEU:N	1:B:555:PRO:HD2	2.23	0.53
1:B:107:GLU:CA	7:B:2001:HOH:O	2.50	0.53
1:B:118:SER:C	1:B:119:ILE:HG12	2.28	0.53
1:A:785:SER:O	1:A:788:GLY:N	2.41	0.53
1:A:705:GLN:OE1	6:A:1401:EDO:H11	2.09	0.53
1:A:781:ASN:O	1:A:784:SER:HB3	2.09	0.52
1:A:110:TYR:CG	1:A:396:GLN:HB2	2.45	0.52
1:B:354:TYR:CG	1:B:597:VAL:HG13	2.46	0.51
1:A:442:ASN:HD21	1:A:445:GLU:HG2	1.71	0.51
1:B:729:LEU:HD21	1:B:736:PRO:HB3	1.93	0.51
1:B:735:LYS:HD2	1:B:763:ALA:O	2.10	0.51
1:B:657:GLN:HB2	1:B:659:GLU:CD	2.32	0.51
1:B:769:ARG:HA	1:B:779:TYR:CE1	2.46	0.50
1:A:730[A]:LYS:HD2	1:A:751:SER:OG	2.11	0.50
1:B:655:THR:HG21	1:B:660:ASN:HD22	1.76	0.50
1:A:456:ARG:HD2	1:A:660:ASN:OD1	2.12	0.49
1:B:759:ASN:HB2	4:B:1203:CL:CL	2.49	0.49
1:A:108:ILE:HD12	1:A:119:ILE:HD11	1.92	0.49
1:A:403:GLN:NE2	7:A:2037:HOH:O	2.42	0.49
1:B:619:LEU:HD23	6:B:1400:EDO:H11	1.94	0.49
1:B:705:GLN:HE22	6:B:1401:EDO:H22	1.77	0.48
1:A:108:ILE:CD1	1:A:119:ILE:HD11	2.44	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ILE:CG2	1:B:340:TYR:OH	2.62	0.48
1:A:554:LEU:N	1:A:555:PRO:CD	2.75	0.48
1:B:656:GLY:O	2:B:1000:A01:H151	2.13	0.48
1:A:442:ASN:HD22	1:A:445:GLU:CG	2.25	0.48
1:A:498:TYR:OH	2:A:1000:A01:H103	2.14	0.47
1:A:107:GLU:HG3	1:A:115:VAL:HG13	1.96	0.47
1:A:110:TYR:CD2	1:A:396:GLN:HB2	2.49	0.47
1:A:741:VAL:C	1:A:742:GLU:HG3	2.35	0.47
1:B:525:TYR:CE2	1:B:526[B]:ARG:NH1	2.82	0.46
1:A:110:TYR:HB3	4:A:1216:CL:CL	2.53	0.46
1:B:687:GLN:HG2	7:B:2246:HOH:O	2.16	0.46
1:B:525:TYR:HD2	1:B:526[B]:ARG:HH11	1.63	0.46
1:B:741:VAL:C	1:B:742:GLU:HG2	2.36	0.46
1:B:525:TYR:HD2	1:B:526[B]:ARG:NH1	2.09	0.45
1:A:382:GLU:HG3	1:A:388:TYR:CE1	2.50	0.45
1:A:107:GLU:HB2	1:A:117:ALA:O	2.17	0.45
1:A:498:TYR:CZ	2:A:1000:A01:H103	2.52	0.45
1:B:779:TYR:O	1:B:783:TRP:CD1	2.70	0.44
1:A:738:LYS:HD2	1:A:745:GLU:OE2	2.17	0.44
1:A:350:ARG:HA	1:A:350:ARG:HD3	1.78	0.44
1:A:739:VAL:CG1	1:A:740:SER:N	2.80	0.44
1:A:114:THR:HG21	1:A:396:GLN:OE1	2.18	0.44
1:A:519:ILE:N	1:A:520:PRO:CD	2.81	0.44
1:B:338:TYR:HB2	4:B:1213:CL:CL	2.55	0.44
1:B:403:GLN:NE2	7:B:2038:HOH:O	2.34	0.44
1:A:737:GLY:O	1:A:748:VAL:HG23	2.17	0.43
1:B:705:GLN:O	1:B:709:PRO:HA	2.18	0.43
1:B:783:TRP:O	1:B:787:VAL:HB	2.17	0.43
1:B:669:ARG:NH2	1:B:715:GLU:OE2	2.51	0.43
1:B:108:ILE:HD11	1:B:119:ILE:CD1	2.49	0.43
1:A:643:LEU:HD13	1:A:705:GLN:HG3	2.00	0.43
1:A:483:LEU:HD23	1:A:772:ILE:HB	2.01	0.42
1:B:536:LYS:O	1:B:540:GLU:HG3	2.18	0.42
1:B:107:GLU:HG3	1:B:115:VAL:HG11	1.96	0.42
1:A:500:ASN:HB2	7:A:2121:HOH:O	2.19	0.42
1:B:729:LEU:HD13	1:B:748:VAL:HG12	2.01	0.42
1:A:760:LYS:HB2	4:A:1203:CL:CL	2.57	0.42
2:B:1000:A01:C12	7:B:2244:HOH:O	2.66	0.42
1:A:757:TRP:NE1	1:A:763:ALA:HB2	2.35	0.41
1:A:734:GLN:OE1	1:A:766:THR:HA	2.19	0.41
1:B:735:LYS:HB2	1:B:765:ALA:HA	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:GLN:O	1:A:709:PRO:HA	2.20	0.41
1:B:705:GLN:OE1	6:B:1401:EDO:H11	2.21	0.41
1:A:110:TYR:CD1	1:A:396:GLN:HB2	2.56	0.41
1:A:526[A]:ARG:NE	7:A:2149:HOH:O	2.53	0.41
1:A:657:GLN:HB2	1:A:659:GLU:OE2	2.20	0.41
1:B:744:LYS:O	1:B:746:VAL:HG23	2.21	0.41
1:A:787:VAL:O	1:A:787:VAL:CG1	2.69	0.41
1:B:118:SER:HA	7:B:2001:HOH:O	2.21	0.40
1:A:741:VAL:O	1:A:742:GLU:HG3	2.21	0.40
1:A:554:LEU:HD12	1:A:558:GLY:O	2.22	0.40
1:B:485:ASN:HB3	1:B:507:MET:HE3	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	464/494 (94%)	450 (97%)	14 (3%)	0	100	100
1	B	463/494 (94%)	442 (96%)	21 (4%)	0	100	100
All	All	927/988 (94%)	892 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	384/408 (94%)	369 (96%)	15 (4%)	39	30
1	B	382/408 (94%)	363 (95%)	19 (5%)	30	20
All	All	766/816 (94%)	732 (96%)	34 (4%)	35	26

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	GLU
1	A	349	GLU
1	A	364	LYS
1	A	444	GLN
1	A	516	SER
1	A	526[A]	ARG
1	A	526[B]	ARG
1	A	569	ASN
1	A	681	ASN
1	A	726	SER
1	A	738	LYS
1	A	742	GLU
1	A	744	LYS
1	A	749	THR
1	A	789	SER
1	B	118	SER
1	B	119	ILE
1	B	364	LYS
1	B	366	LEU
1	B	367	LYS
1	B	383	ILE
1	B	385	ASN
1	B	516	SER
1	B	569	ASN
1	B	630	THR
1	B	716	ARG
1	B	726	SER
1	B	744	LYS
1	B	745	GLU
1	B	749	THR
1	B	753	VAL
1	B	785	SER
1	B	787	VAL
1	B	789	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	489	ASN
1	A	692	ASN
1	B	448	ASN
1	B	489	ASN
1	B	657	GLN
1	B	692	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 40 ligands modelled in this entry, 32 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	A01	A	1000	1,5	14,17,18	0.77	1 (7%)	16,22,25	1.85	5 (31%)
3	SO4	A	1100	-	4,4,4	0.61	0	6,6,6	0.34	0
6	EDO	A	1400	-	3,3,3	0.48	0	2,2,2	0.52	0
6	EDO	A	1401	-	3,3,3	0.50	0	2,2,2	0.50	0
2	A01	B	1000	1,5	14,17,18	0.66	0	16,22,25	1.76	5 (31%)
3	SO4	B	1100	-	4,4,4	0.66	0	6,6,6	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	B	1400	-	3,3,3	0.44	0	2,2,2	0.55	0
6	EDO	B	1401	-	3,3,3	0.53	0	2,2,2	0.53	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	A01	A	1000	1,5	-	0/10/13/14	0/1/1/1
3	SO4	A	1100	-	-	0/0/0/0	0/0/0/0
6	EDO	A	1400	-	-	0/1/1/1	0/0/0/0
6	EDO	A	1401	-	-	0/1/1/1	0/0/0/0
2	A01	B	1000	1,5	-	0/10/13/14	0/1/1/1
3	SO4	B	1100	-	-	0/0/0/0	0/0/0/0
6	EDO	B	1400	-	-	0/1/1/1	0/0/0/0
6	EDO	B	1401	-	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	A01	C7-C5	2.13	1.54	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	A01	O15-C14-C13	-3.78	117.99	124.35
2	B	1000	A01	O15-C14-C13	-3.33	118.74	124.35
2	A	1000	A01	O9-C8-C11	-2.63	119.92	124.35
2	B	1000	A01	O9-C8-C11	-2.02	120.95	124.35
2	B	1000	A01	O9-C8-C7	2.29	119.34	115.78
2	A	1000	A01	O9-C8-C7	2.74	120.05	115.78
2	A	1000	A01	C10-O9-C8	3.05	122.17	117.54
2	B	1000	A01	C10-O9-C8	3.25	122.46	117.54
2	B	1000	A01	O15-C14-C7	3.62	121.40	115.78
2	A	1000	A01	O15-C14-C7	3.68	121.50	115.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	A01	3	0
6	A	1401	EDO	2	0
2	B	1000	A01	3	0
6	B	1400	EDO	1	0
6	B	1401	EDO	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, 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	466/494 (94%)	0.47	46 (9%) <b>9</b> <b>10</b>	25, 42, 85, 134	0
1	B	466/494 (94%)	0.49	48 (10%) <b>9</b> <b>9</b>	24, 42, 86, 145	0
All	All	932/988 (94%)	0.48	94 (10%) <b>9</b> <b>10</b>	24, 42, 86, 145	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	787	VAL	7.6
1	A	744	LYS	7.1
1	B	117	ALA	6.7
1	A	787	VAL	6.7
1	A	117	ALA	6.2
1	B	746	VAL	6.1
1	B	744	LYS	6.0
1	A	738	LYS	6.0
1	A	746	VAL	5.7
1	B	739	VAL	5.6
1	A	739	VAL	5.2
1	A	115	VAL	5.0
1	B	748	VAL	5.0
1	A	737	GLY	4.8
1	B	118	SER	4.7
1	B	114	THR	4.6
1	B	119	ILE	4.6
1	B	738	LYS	4.6
1	B	737	GLY	4.5
1	B	736	PRO	4.5
1	A	119	ILE	4.4
1	A	740	SER	4.4
1	B	116	ILE	4.3
1	B	115	VAL	4.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	743	GLY	4.2
1	A	736	PRO	4.2
1	A	745	GLU	4.0
1	A	748	VAL	4.0
1	B	789	SER	3.9
1	A	786	ILE	3.9
1	A	742	GLU	3.8
1	B	750	GLY	3.8
1	A	780	GLN	3.8
1	A	743	GLY	3.7
1	B	108	ILE	3.7
1	B	113	GLY	3.6
1	B	110	TYR	3.6
1	A	735	LYS	3.6
1	B	786	ILE	3.5
1	B	780	GLN	3.5
1	B	741	VAL	3.5
1	A	108	ILE	3.5
1	A	113	GLY	3.4
1	A	741	VAL	3.4
1	A	788	GLY	3.3
1	B	745	GLU	3.2
1	A	118	SER	3.1
1	B	107	GLU	3.1
1	A	116	ILE	3.1
1	A	107	GLU	3.0
1	B	742	GLU	3.0
1	B	109	THR	2.9
1	B	735	LYS	2.9
1	B	729	LEU	2.9
1	A	112	ASP	2.9
1	B	747	GLU	2.8
1	B	740	SER	2.8
1	A	789	SER	2.8
1	A	749	THR	2.7
1	B	769	ARG	2.7
1	A	114	THR	2.7
1	A	750	GLY	2.7
1	A	110	TYR	2.6
1	A	747	GLU	2.6
1	A	769	ARG	2.6
1	A	636	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	760	LYS	2.5
1	A	109	THR	2.5
1	B	749	THR	2.5
1	A	386	GLY	2.4
1	A	729	LEU	2.4
1	B	632	PHE	2.4
1	A	767	SER	2.4
1	B	767	SER	2.4
1	A	637	THR	2.3
1	B	637	THR	2.3
1	B	112	ASP	2.3
1	B	788	GLY	2.3
1	B	761	SER	2.2
1	B	636	LEU	2.2
1	A	632	PHE	2.2
1	B	768	TYR	2.2
1	B	765	ALA	2.2
1	B	628	VAL	2.2
1	B	629	THR	2.2
1	A	765	ALA	2.2
1	B	760	LYS	2.2
1	A	626	SER	2.1
1	B	634	SER	2.1
1	B	752	THR	2.0
1	A	752	THR	2.0
1	A	768	TYR	2.0
1	B	630	THR	2.0
1	A	634	SER	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
4	CL	B	1792	1/1	0.94	0.28	10.94	40,40,40,40	1
5	NA	A	1300	1/1	0.96	0.28	2.90	40,40,40,40	0
6	EDO	B	1401	4/4	0.88	0.14	1.72	39,55,59,61	0
5	NA	B	1300	1/1	0.97	0.22	1.26	37,37,37,37	0
4	CL	B	1791	1/1	1.00	0.23	0.30	29,29,29,29	0
4	CL	B	1224	1/1	0.99	0.13	0.25	59,59,59,59	0
6	EDO	B	1400	4/4	0.96	0.13	0.18	38,49,54,60	0
2	A01	B	1000	17/18	0.94	0.15	0.02	43,65,90,101	0
6	EDO	A	1401	4/4	0.88	0.12	-0.01	53,57,59,70	0
6	EDO	A	1400	4/4	0.95	0.11	-0.03	42,45,49,52	0
4	CL	B	1213	1/1	0.99	0.12	-0.09	53,53,53,53	0
4	CL	A	1216	1/1	0.84	0.19	-0.22	67,67,67,67	0
4	CL	B	1216	1/1	0.88	0.18	-0.28	69,69,69,69	0
2	A01	A	1000	17/18	0.94	0.12	-0.63	35,59,84,105	0
4	CL	A	1201	1/1	0.96	0.09	-0.73	47,47,47,47	0
4	CL	B	1234	1/1	0.93	0.11	-1.01	56,56,56,56	0
4	CL	A	1211	1/1	0.99	0.10	-1.03	40,40,40,40	0
4	CL	B	1211	1/1	1.00	0.10	-1.34	44,44,44,44	0
3	SO4	A	1100	5/5	0.99	0.09	-1.55	38,41,45,57	0
4	CL	A	1213	1/1	0.98	0.08	-1.79	60,60,60,60	0
3	SO4	B	1100	5/5	0.98	0.07	-3.49	42,44,52,54	0
4	CL	A	1214	1/1	0.92	0.09	-	64,64,64,64	0
4	CL	A	1208	1/1	0.90	0.28	-	73,73,73,73	0
4	CL	B	1235	1/1	0.94	0.29	-	60,60,60,60	0
4	CL	B	1202	1/1	0.95	0.19	-	62,62,62,62	0
4	CL	B	1208	1/1	0.78	0.21	-	71,71,71,71	0
4	CL	A	1200	1/1	0.97	0.07	-	51,51,51,51	0
4	CL	B	1203	1/1	0.88	0.29	-	76,76,76,76	0
4	CL	B	1201	1/1	0.98	0.09	-	48,48,48,48	0
4	CL	A	1204	1/1	0.80	0.32	-	77,77,77,77	0
4	CL	A	1229	1/1	0.99	0.05	-	59,59,59,59	0
4	CL	B	1200	1/1	0.96	0.09	-	47,47,47,47	0
4	CL	A	1203	1/1	0.85	0.22	-	75,75,75,75	0
4	CL	B	1206	1/1	0.82	0.33	-	78,78,78,78	0
4	CL	A	1206	1/1	0.94	0.13	-	56,56,56,56	0
4	CL	A	1202	1/1	0.93	0.26	-	64,64,64,64	0
4	CL	B	1212	1/1	0.99	0.08	-	43,43,43,43	0
4	CL	B	1229	1/1	0.98	0.07	-	55,55,55,55	0
4	CL	B	1214	1/1	0.96	0.12	-	57,57,57,57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	A	1212	1/1	0.98	0.07	-	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.