



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:42 AM GMT

PDB ID : 2Y2H  
Title : PENICILLIN-BINDING PROTEIN 1B (PBP-1B) IN COMPLEX WITH AN ALKYL BORONATE (ZA2)  
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 : 1.96 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

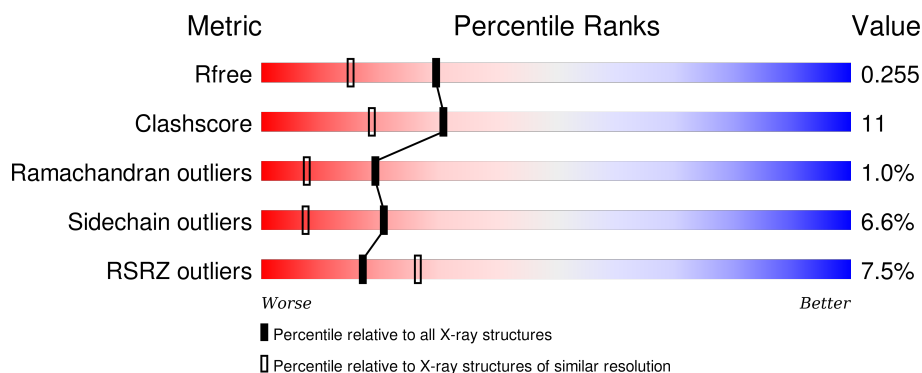
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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>6%</div> <div>76%</div> <div>16%</div> <div>5%</div> </div>
1	B	494	<div> <div>8%</div> <div>73%</div> <div>20%</div> <div>• • •</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
5	NA	A	1300	-	-	-	X
5	NA	B	1300	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7669 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.

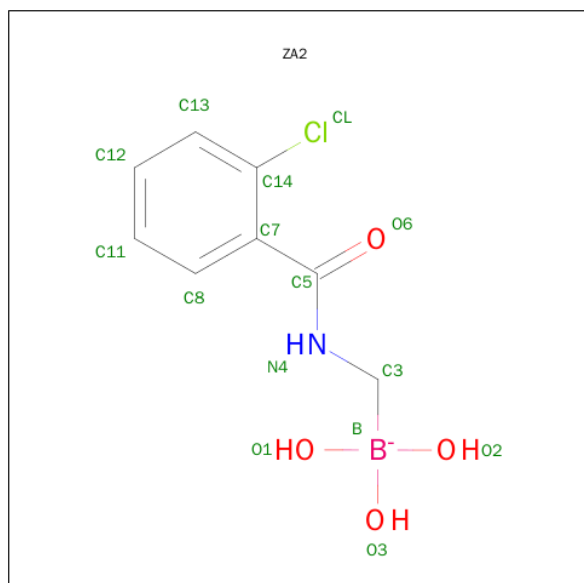
- Molecule 1 is a protein called PENICILLIN-BINDING PROTEIN 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3594	2249	609	721	15			
1	B	472	Total	C	N	O	S	0	1	0
			3639	2277	614	733	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-CHLOROPHENYL)CARBONYLAMINO]METHYL-TRIHYDROXY-BORON (three-letter code: ZA2) (formula: C<sub>8</sub>H<sub>10</sub>BClNO<sub>4</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	B	C	Cl	N	O	0	0
			14	1	8	1	1	3		
2	B	1	Total	B	C	Cl	N	O	0	0
			14	1	8	1	1	3		

- 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	8	Total	Cl	0	0
			8	8		
4	A	10	Total	Cl	0	0
			10	10		

- 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 1	Na 1	0	0

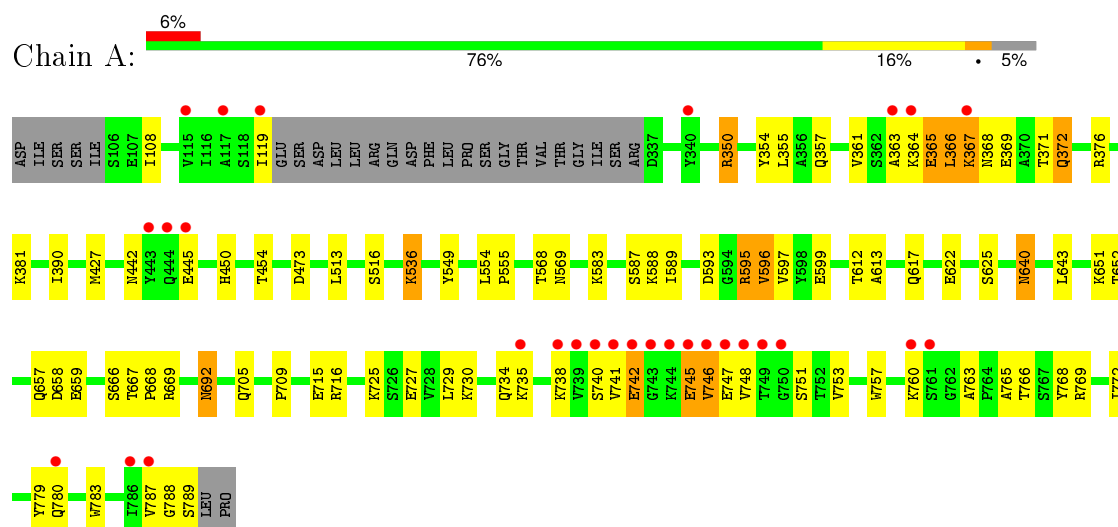
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	167	Total 167	O 167	0	0
6	B	211	Total 211	O 211	0	0

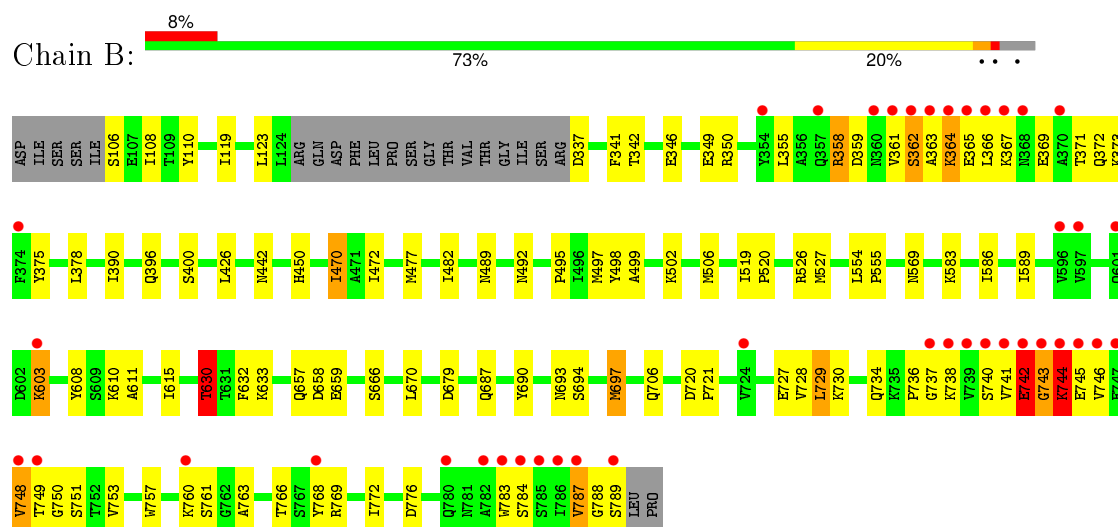
### 3 Residue-property plots

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: 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, $\alpha$ , $\beta$ , $\gamma$	95.99Å 100.48Å 143.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 1.96 48.00 – 1.96	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.00-1.96) 94.8 (48.00-1.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.6.0095	Depositor
R, $R_{free}$	0.212 , 0.254 0.213 , 0.255	Depositor DCC
$R_{free}$ test set	9459 reflections (11.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.6	EDS
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 94827 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7669	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ZA2, SO4, 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	0.64	0/3667	0.66	0/4977
1	B	0.71	0/3715	0.72	2/5042 (0.0%)
All	All	0.67	0/7382	0.69	2/10019 (0.0%)

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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	697	MET	CG-SD-CE	6.16	110.06	100.20
1	B	630	THR	CB-CA-C	-5.11	97.81	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	666	SER	Peptide
1	B	630	THR	Mainchain
1	B	666	SER	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	3594	0	3459	67	0
1	B	3639	0	3502	86	0
2	A	14	0	9	1	0
2	B	14	0	9	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	10	0	0	1	0
4	B	8	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	167	0	0	6	0
6	B	211	0	0	8	0
All	All	7669	0	6979	155	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 11.

All (155) 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:706:GLN:HG3	6:B:2182:HOH:O	1.44	1.14
1:B:495:PRO:HB2	1:B:497:MET:HE2	1.27	1.14
1:A:427:MET:HE2	1:A:568:THR:HG22	1.15	1.14
1:B:495:PRO:HB2	1:B:497:MET:CE	1.86	1.04
1:A:427:MET:CE	1:A:568:THR:HG22	1.89	1.02
1:B:527:MET:HE3	1:B:772:ILE:HG23	1.45	0.98
1:B:527:MET:CE	1:B:772:ILE:HG23	2.03	0.88
1:A:427:MET:HE3	1:A:569:ASN:HA	1.59	0.84
1:B:743:GLY:O	1:B:744:LYS:HB2	1.76	0.83
1:B:450:HIS:HE1	1:B:679:ASP:OD1	1.66	0.77
1:A:569:ASN:HD21	1:A:583:LYS:H	1.30	0.76
1:A:108:ILE:HG13	1:A:119:ILE:HD11	1.66	0.76
1:B:742:GLU:O	1:B:743:GLY:O	2.04	0.75
2:B:1000:ZA2:CL	6:B:2064:HOH:O	2.42	0.73
1:A:427:MET:HE2	1:A:568:THR:CG2	2.09	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:THR:O	1:B:346:GLU:HG2	1.90	0.72
1:B:495:PRO:CB	1:B:497:MET:HE2	2.15	0.71
1:B:470:ILE:HD13	1:B:608:TYR:HE2	1.56	0.70
1:B:757:TRP:NE1	1:B:763:ALA:HB2	2.06	0.70
2:A:1000:ZA2:CL	6:A:2042:HOH:O	2.46	0.70
1:B:741:VAL:C	1:B:742:GLU:HG3	2.12	0.70
1:A:569:ASN:ND2	1:A:583:LYS:H	1.89	0.69
1:A:727:GLU:HG3	6:A:2157:HOH:O	1.92	0.68
1:B:730:LYS:HG2	1:B:753:VAL:CG1	2.24	0.67
1:B:603:LYS:HE2	6:B:2117:HOH:O	1.95	0.67
1:B:363:ALA:HA	1:B:366:LEU:HB2	1.77	0.67
1:B:489:ASN:HD22	1:B:495:PRO:HA	1.60	0.67
1:B:630:THR:HG22	1:B:632:PHE:H	1.61	0.66
1:B:400:SER:HB2	6:B:2018:HOH:O	1.95	0.66
1:B:497:MET:HE1	1:B:502:LYS:HA	1.79	0.65
1:A:741:VAL:C	1:A:742:GLU:HG2	2.16	0.65
1:B:495:PRO:CB	1:B:497:MET:CE	2.72	0.64
1:B:730:LYS:HG2	1:B:753:VAL:HG13	1.78	0.64
1:B:527:MET:HE3	1:B:772:ILE:CG2	2.25	0.62
1:B:527:MET:CE	1:B:772:ILE:HD12	2.29	0.62
1:B:787:VAL:O	1:B:789:SER:N	2.27	0.62
1:A:365:GLU:O	1:A:368:ASN:HB3	2.00	0.61
1:B:749:THR:HG22	1:B:750:GLY:N	2.15	0.61
1:B:729:LEU:HD11	1:B:736:PRO:HB3	1.82	0.60
1:A:390:ILE:HD13	1:A:589:ILE:HG23	1.84	0.60
1:B:737:GLY:O	1:B:748:VAL:HG23	2.02	0.60
1:A:372:GLN:O	1:A:376:ARG:HG3	2.03	0.59
1:B:554:LEU:N	1:B:555:PRO:HD2	2.17	0.59
1:A:640:ASN:HD22	1:A:640:ASN:C	2.05	0.59
1:B:693:ASN:O	1:B:697:MET:HG3	2.03	0.58
1:A:692:ASN:HD22	1:A:692:ASN:H	1.51	0.57
1:B:657:GLN:HB2	1:B:659:GLU:OE2	2.05	0.57
1:A:427:MET:HE3	1:A:569:ASN:CA	2.34	0.56
1:B:657:GLN:HB2	1:B:659:GLU:CD	2.26	0.56
1:A:589:ILE:HG22	1:A:597:VAL:CG1	2.37	0.55
1:A:760:LYS:HB2	4:A:1203:CL:CL	2.44	0.55
1:B:630:THR:HG23	1:B:694:SER:OG	2.07	0.55
1:A:740:SER:HA	1:A:745:GLU:HA	1.89	0.55
1:A:569:ASN:ND2	6:A:2081:HOH:O	2.40	0.54
1:B:720:ASP:CG	1:B:721:PRO:HD2	2.28	0.54
1:B:470:ILE:CD1	1:B:608:TYR:HE2	2.20	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:THR:CG2	1:B:694:SER:OG	2.56	0.54
1:B:364:LYS:HG3	1:B:365:GLU:N	2.23	0.54
1:A:730:LYS:HE2	1:A:753:VAL:HG13	1.89	0.54
1:A:596:VAL:HG21	1:A:599:GLU:HB2	1.91	0.53
1:B:749:THR:CG2	1:B:750:GLY:N	2.71	0.53
1:B:730:LYS:CG	1:B:753:VAL:HG13	2.37	0.53
1:B:364:LYS:HG3	1:B:365:GLU:H	1.72	0.53
1:A:589:ILE:HB	1:A:597:VAL:HG13	1.91	0.52
1:A:363:ALA:HA	1:A:366:LEU:HB2	1.91	0.52
1:B:108:ILE:CD1	1:B:119:ILE:HD11	2.39	0.52
1:B:611:ALA:O	1:B:615:ILE:HG13	2.10	0.52
1:B:527:MET:HE1	1:B:772:ILE:HD12	1.91	0.52
1:A:746:VAL:HG13	1:A:747:GLU:N	2.25	0.52
1:A:768:TYR:CE1	1:A:783:TRP:CD1	2.99	0.51
1:B:390:ILE:HG12	1:B:589:ILE:HD12	1.91	0.51
1:B:729:LEU:CD1	1:B:736:PRO:HB3	2.40	0.51
1:A:735:LYS:HB2	1:A:765:ALA:HA	1.93	0.51
1:B:337:ASP:O	1:B:341:PHE:CD2	2.64	0.50
1:A:369:GLU:HB2	6:A:2004:HOH:O	2.11	0.50
1:A:427:MET:CE	1:A:569:ASN:HA	2.36	0.50
1:A:657:GLN:O	1:A:658:ASP:HB2	2.10	0.50
1:B:569:ASN:ND2	1:B:583:LYS:H	2.10	0.50
1:A:730:LYS:HE3	1:A:751:SER:HB3	1.94	0.49
1:A:372:GLN:O	1:A:376:ARG:CG	2.60	0.49
1:A:364:LYS:O	1:A:367:LYS:HB2	2.13	0.49
1:B:361:VAL:HG12	1:B:366:LEU:HG	1.95	0.49
1:A:554:LEU:N	1:A:555:PRO:HD2	2.28	0.49
1:B:749:THR:CG2	6:B:2199:HOH:O	2.61	0.48
1:B:657:GLN:O	1:B:658:ASP:HB2	2.12	0.48
1:B:470:ILE:CD1	1:B:608:TYR:CE2	2.96	0.48
1:A:667:THR:HB	1:A:668:PRO:CD	2.44	0.48
1:B:730:LYS:HG2	1:B:753:VAL:HG11	1.96	0.48
1:A:657:GLN:HB2	1:A:659:GLU:OE2	2.13	0.48
1:A:730:LYS:HE2	1:A:753:VAL:CG1	2.43	0.48
1:B:768:TYR:CE1	1:B:783:TRP:CD1	3.02	0.48
1:B:769:ARG:NH2	1:B:776:ASP:OD1	2.47	0.48
1:B:337:ASP:O	1:B:341:PHE:HD2	1.96	0.48
1:B:569:ASN:HD21	1:B:583:LYS:H	1.62	0.48
1:A:746:VAL:CG1	1:A:747:GLU:N	2.77	0.48
1:B:359:ASP:OD2	1:B:375:TYR:OH	2.24	0.48
1:B:492:ASN:C	1:B:492:ASN:OD1	2.52	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:VAL:CG1	1:A:366:LEU:HD13	2.44	0.47
1:A:657:GLN:HB2	1:A:659:GLU:CD	2.35	0.47
1:B:610:LYS:HD2	6:B:2113:HOH:O	2.14	0.47
1:A:536:LYS:HG3	1:A:549:TYR:CE1	2.50	0.47
1:A:669:ARG:NH2	1:A:715:GLU:OE2	2.46	0.47
1:B:527:MET:HB2	1:B:527:MET:HE2	1.66	0.47
1:B:358:ARG:HE	1:B:358:ARG:HB3	1.37	0.47
1:B:757:TRP:CE2	1:B:763:ALA:HB2	2.50	0.46
1:A:427:MET:CE	1:A:568:THR:C	2.83	0.46
1:A:354:TYR:CG	1:A:597:VAL:HG23	2.50	0.46
1:B:355:LEU:HD13	1:B:378:LEU:HG	1.98	0.46
1:B:603:LYS:HB3	1:B:603:LYS:HE3	1.36	0.46
1:B:527:MET:HE3	1:B:772:ILE:HD12	1.98	0.46
1:B:586:ILE:HG21	1:B:589:ILE:HD11	1.98	0.46
1:B:497:MET:CE	1:B:502:LYS:HG2	2.46	0.46
1:A:450:HIS:CD2	1:A:454:THR:HG21	2.51	0.46
1:A:769:ARG:HD2	1:A:779:TYR:CE2	2.51	0.45
1:A:354:TYR:CD1	1:A:597:VAL:HG23	2.51	0.45
1:A:640:ASN:ND2	1:A:643:LEU:H	2.15	0.45
1:B:749:THR:HG22	6:B:2199:HOH:O	2.14	0.45
1:A:692:ASN:H	1:A:692:ASN:ND2	2.14	0.45
1:B:450:HIS:CE1	1:B:679:ASP:OD1	2.57	0.45
1:B:482:ILE:CG2	1:B:506:MET:HB3	2.47	0.45
1:A:622:GLU:HA	1:A:625:SER:HB2	1.99	0.45
1:B:744:LYS:O	1:B:746:VAL:HG23	2.17	0.45
1:A:757:TRP:NE1	1:A:763:ALA:HB2	2.32	0.44
1:A:734:GLN:OE1	1:A:766:THR:HA	2.17	0.44
1:B:757:TRP:HE1	1:B:763:ALA:HB2	1.82	0.44
1:A:760:LYS:HA	1:A:760:LYS:HD3	1.55	0.44
1:B:738:LYS:HA	1:B:746:VAL:O	2.18	0.44
1:B:734:GLN:OE1	1:B:766:THR:HA	2.18	0.44
1:A:364:LYS:HD2	1:A:364:LYS:HA	1.90	0.43
1:B:350:ARG:HA	1:B:350:ARG:HD3	1.74	0.43
1:B:110:TYR:CG	1:B:396:GLN:HB2	2.54	0.43
1:A:787:VAL:O	1:A:789:SER:N	2.51	0.43
1:A:729:LEU:HD13	1:A:748:VAL:HG12	2.01	0.43
1:B:470:ILE:N	1:B:470:ILE:HD13	2.33	0.43
1:B:554:LEU:N	1:B:555:PRO:CD	2.81	0.43
1:B:687:GLN:HB2	6:B:2169:HOH:O	2.18	0.43
1:A:368:ASN:ND2	1:A:371:THR:H	2.17	0.42
1:A:473:ASP:HA	1:A:612:THR:OG1	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:HH11	1:A:350:ARG:HG3	1.84	0.42
1:B:362:SER:O	1:B:366:LEU:N	2.51	0.42
1:A:613:ALA:O	1:A:617:GLN:HG3	2.20	0.42
1:B:519:ILE:N	1:B:520:PRO:CD	2.82	0.42
1:B:472:ILE:HG13	1:B:477:MET:HG2	2.00	0.42
1:B:498:TYR:O	1:B:499:ALA:HB3	2.20	0.42
1:A:445:GLU:HB2	6:A:2018:HOH:O	2.20	0.42
1:A:361:VAL:HG11	1:A:366:LEU:HD13	2.03	0.41
1:A:716:ARG:NH1	6:A:2149:HOH:O	2.47	0.41
1:B:741:VAL:O	1:B:741:VAL:HG12	2.20	0.41
1:A:651:LYS:HG3	1:A:652:THR:N	2.35	0.41
1:A:390:ILE:CD1	1:A:589:ILE:HG23	2.50	0.41
1:B:687:GLN:OE1	1:B:690:TYR:CD2	2.73	0.41
1:A:593:ASP:OD1	1:A:595:ARG:HG2	2.21	0.41
1:B:426:LEU:HD11	1:B:670:LEU:HD13	2.02	0.40
1:A:705:GLN:NE2	1:A:709:PRO:O	2.53	0.40
1:A:554:LEU:N	1:A:555:PRO:CD	2.85	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	463/494 (94%)	445 (96%)	16 (4%)	2 (0%)	39	27
1	B	469/494 (95%)	445 (95%)	17 (4%)	7 (2%)	13	3
All	All	932/988 (94%)	890 (96%)	33 (4%)	9 (1%)	19	8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	788	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	743	GLY
1	B	740	SER
1	B	744	LYS
1	B	788	GLY
1	A	442	ASN
1	B	742	GLU
1	B	442	ASN
1	B	787	VAL

### 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	382/408 (94%)	358 (94%)	24 (6%)	22	8
1	B	388/408 (95%)	360 (93%)	28 (7%)	18	6
All	All	770/816 (94%)	718 (93%)	52 (7%)	21	7

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	ARG
1	A	355	LEU
1	A	357	GLN
1	A	365	GLU
1	A	366	LEU
1	A	367	LYS
1	A	372	GLN
1	A	381	LYS
1	A	513	LEU
1	A	516	SER
1	A	536	LYS
1	A	587	SER
1	A	588	LYS
1	A	595	ARG
1	A	596	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	640	ASN
1	A	692	ASN
1	A	725	LYS
1	A	738	LYS
1	A	742	GLU
1	A	745	GLU
1	A	746	VAL
1	A	772	ILE
1	A	780	GLN
1	B	106	SER
1	B	123	LEU
1	B	349	GLU
1	B	358	ARG
1	B	362	SER
1	B	364	LYS
1	B	367	LYS
1	B	369	GLU
1	B	371	THR
1	B	372	GLN
1	B	373	LYS
1	B	470	ILE
1	B	526	ARG
1	B	603	LYS
1	B	630	THR
1	B	633	LYS
1	B	727[A]	GLU
1	B	727[B]	GLU
1	B	728	VAL
1	B	729	LEU
1	B	742	GLU
1	B	744	LYS
1	B	745	GLU
1	B	748	VAL
1	B	751	SER
1	B	760	LYS
1	B	761	SER
1	B	784	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	357	GLN
1	A	368	ASN
1	A	385	ASN
1	A	429	ASN
1	A	569	ASN
1	A	606	GLN
1	A	640	ASN
1	A	692	ASN
1	B	403	GLN
1	B	424	ASN
1	B	429	ASN
1	B	448	ASN
1	B	450	HIS
1	B	489	ASN
1	B	569	ASN
1	B	681	ASN

### 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 24 ligands modelled in this entry, 20 are monoatomic - leaving 4 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	ZA2	A	1000	1,5	11,14,15	0.95	0	14,18,21	1.16	1 (7%)
3	SO4	A	1100	-	4,4,4	0.53	0	6,6,6	0.35	0
2	ZA2	B	1000	1,5	11,14,15	1.06	1 (9%)	14,18,21	1.33	3 (21%)
3	SO4	B	1100	-	4,4,4	0.74	0	6,6,6	0.52	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	ZA2	A	1000	1,5	-	0/6/9/10	0/1/1/1
3	SO4	A	1100	-	-	0/0/0/0	0/0/0/0
2	ZA2	B	1000	1,5	-	0/6/9/10	0/1/1/1
3	SO4	B	1100	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	ZA2	C5-N4	2.30	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	ZA2	C7-C14-CL	-2.39	117.31	120.97
2	B	1000	ZA2	C14-C7-C5	-2.11	119.73	122.70
2	B	1000	ZA2	C3-N4-C5	2.85	129.94	121.83
2	A	1000	ZA2	C3-N4-C5	2.93	130.16	121.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	ZA2	1	0
2	B	1000	ZA2	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	467/494 (94%)	0.37	29 (6%) 24 34	25, 40, 76, 112	0
1	B	472/494 (95%)	0.62	41 (8%) 13 20	21, 36, 81, 121	0
All	All	939/988 (95%)	0.49	70 (7%) 17 26	21, 38, 80, 121	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	363	ALA	9.7
1	B	746	VAL	7.5
1	B	741	VAL	7.0
1	B	739	VAL	6.5
1	B	364	LYS	6.1
1	A	739	VAL	6.0
1	B	744	LYS	6.0
1	B	362	SER	5.9
1	B	742	GLU	5.8
1	A	748	VAL	5.8
1	B	787	VAL	5.6
1	B	366	LEU	5.3
1	B	748	VAL	5.2
1	B	743	GLY	5.0
1	B	367	LYS	4.8
1	A	744	LYS	4.4
1	B	786	ILE	4.3
1	B	365	GLU	4.3
1	B	760	LYS	4.3
1	B	740	SER	4.3
1	A	746	VAL	4.2
1	B	783	TRP	4.1
1	B	747	GLU	4.1
1	B	749	THR	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	787	VAL	4.1
1	A	743	GLY	4.0
1	A	363	ALA	3.9
1	B	738	LYS	3.6
1	B	368	ASN	3.5
1	A	741	VAL	3.5
1	A	119	ILE	3.5
1	B	768	TYR	3.4
1	A	115	VAL	3.3
1	B	737	GLY	3.3
1	B	361	VAL	3.2
1	A	742	GLU	3.2
1	B	780	GLN	3.2
1	A	364	LYS	3.1
1	A	750	GLY	3.1
1	A	761	SER	3.0
1	B	360	ASN	2.9
1	B	745	GLU	2.9
1	B	784	SER	2.8
1	A	780	GLN	2.7
1	A	760	LYS	2.6
1	B	785	SER	2.6
1	B	370	ALA	2.5
1	B	789	SER	2.5
1	A	749	THR	2.5
1	B	596	VAL	2.5
1	A	340	TYR	2.5
1	B	357	GLN	2.5
1	A	740	SER	2.4
1	A	367	LYS	2.4
1	A	786	ILE	2.4
1	B	597	VAL	2.4
1	A	747	GLU	2.4
1	B	782	ALA	2.4
1	B	354	TYR	2.3
1	B	724	VAL	2.2
1	B	374	PHE	2.2
1	B	603	LYS	2.2
1	A	745	GLU	2.2
1	A	735	LYS	2.2
1	A	445	GLU	2.1
1	B	601	GLN	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	444	GLN	2.1
1	A	117	ALA	2.0
1	A	443	TYR	2.0
1	A	738	LYS	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	NA	A	1300	1/1	0.99	0.18	2.71	30,30,30,30	0
5	NA	B	1300	1/1	0.98	0.21	2.39	26,26,26,26	0
2	ZA2	B	1000	14/15	0.85	0.16	1.37	31,48,70,90	0
2	ZA2	A	1000	14/15	0.92	0.15	1.32	38,58,80,108	0
4	CL	A	1791	1/1	0.99	0.19	0.88	31,31,31,31	0
4	CL	A	1792	1/1	0.79	0.14	0.56	61,61,61,61	0
4	CL	A	1213	1/1	0.97	0.15	0.39	58,58,58,58	0
4	CL	A	1216	1/1	0.94	0.12	-0.05	54,54,54,54	0
3	SO4	A	1100	5/5	0.98	0.08	-0.80	38,45,46,48	0
4	CL	B	1208	1/1	0.86	0.17	-1.06	61,61,61,61	0
4	CL	B	1213	1/1	0.99	0.07	-1.41	46,46,46,46	0
3	SO4	B	1100	5/5	0.99	0.08	-1.55	37,37,44,46	0
4	CL	B	1206	1/1	0.96	0.06	-1.91	57,57,57,57	0
4	CL	B	1201	1/1	0.98	0.07	-2.77	39,39,39,39	0
4	CL	B	1211	1/1	0.99	0.09	-2.84	33,33,33,33	0
4	CL	A	1211	1/1	0.98	0.07	-2.93	43,43,43,43	0
4	CL	A	1212	1/1	0.98	0.08	-	43,43,43,43	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	B	1202	1/1	0.93	0.26	-	58,58,58,58	0
4	CL	A	1203	1/1	0.89	0.11	-	65,65,65,65	0
4	CL	A	1200	1/1	0.98	0.09	-	42,42,42,42	0
4	CL	A	1202	1/1	0.94	0.11	-	55,55,55,55	0
4	CL	B	1212	1/1	0.97	0.08	-	46,46,46,46	0
4	CL	A	1201	1/1	0.96	0.06	-	50,50,50,50	0
4	CL	B	1200	1/1	0.91	0.09	-	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.