



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:10 am BST

PDB ID : 2Y2Q
Title : PENICILLIN-BINDING PROTEIN 1B (PBP-1B) IN COMPLEX WITH AN ALKYL BORONATE (Z06)
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 : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

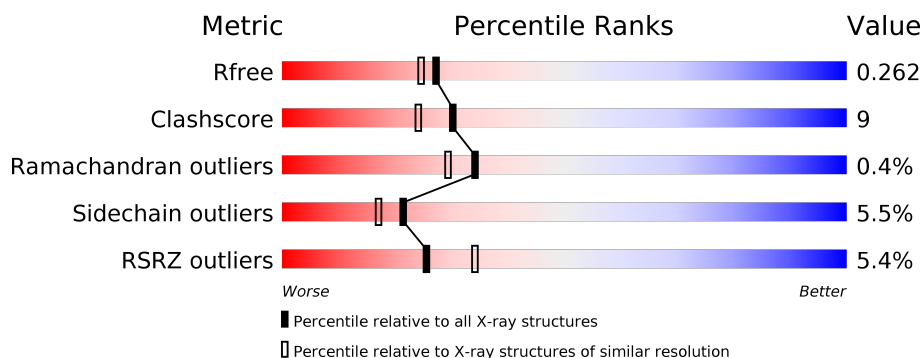
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 respectively. 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	 4% 73% 19% • 5%
1	B	494	 6% 81% 14% • •

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	A	1207	-	-	X	-
4	CL	A	1212	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7870 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.

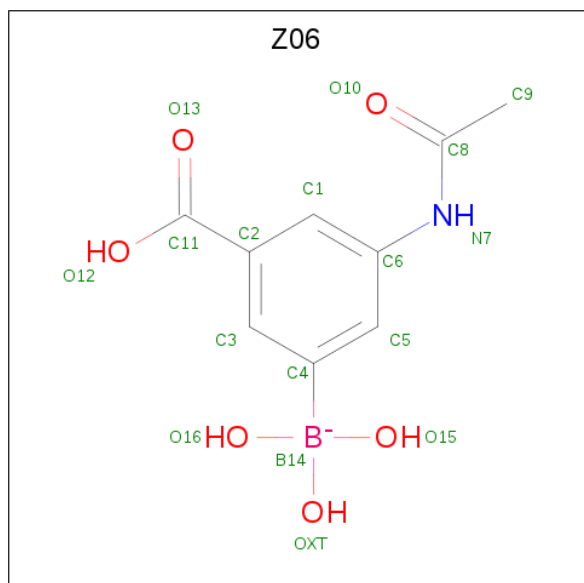
- Molecule 1 is a protein called PENICILLIN-BINDING PROTEIN 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	3	0
			3637	2279	619	724	15			
1	B	474	Total	C	N	O	S	0	0	0
			3654	2288	617	734	15			

There are 6 discrepancies between the modelled and reference sequences:

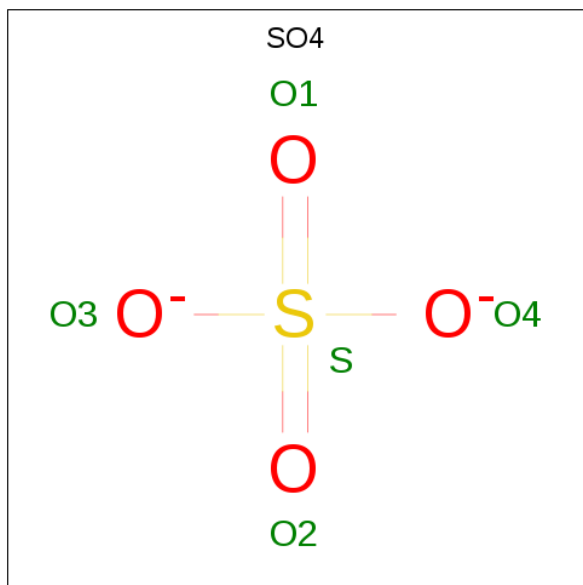
Chain	Residue	Modelled	Actual	Comment	Reference
A	656	GLY	ASN	engineered mutation	UNP Q7CRA4
A	686	GLN	ARG	engineered mutation	UNP Q7CRA4
A	687	GLN	ARG	engineered mutation	UNP Q7CRA4
B	656	GLY	ASN	engineered mutation	UNP Q7CRA4
B	686	GLN	ARG	engineered mutation	UNP Q7CRA4
B	687	GLN	ARG	engineered mutation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

- Molecule 2 is (3-acetamido-5-carboxy-phenyl)-trihydroxy-boron (three-letter code: Z06) (formula: C₉H₁₁BNO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	0	0
			16	1	9	1	5		
2	B	1	Total	B	C	N	O	0	0
			16	1	9	1	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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	12	Total	Cl	0	0
			12	12		
4	A	13	Total	Cl	0	0
			13	13		

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

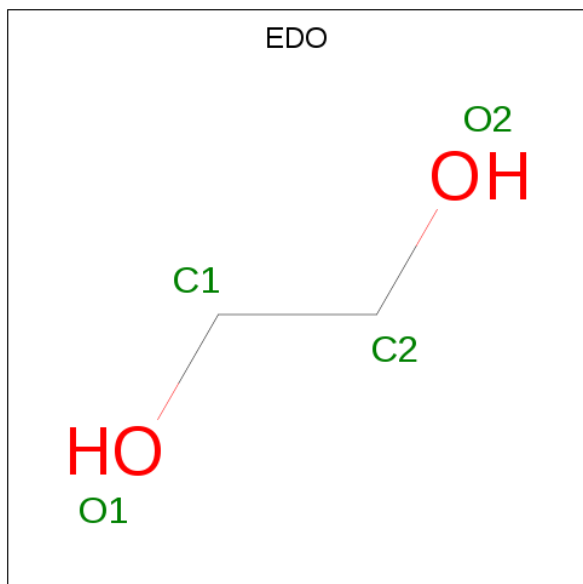
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		

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: $C_2H_6O_2$).



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

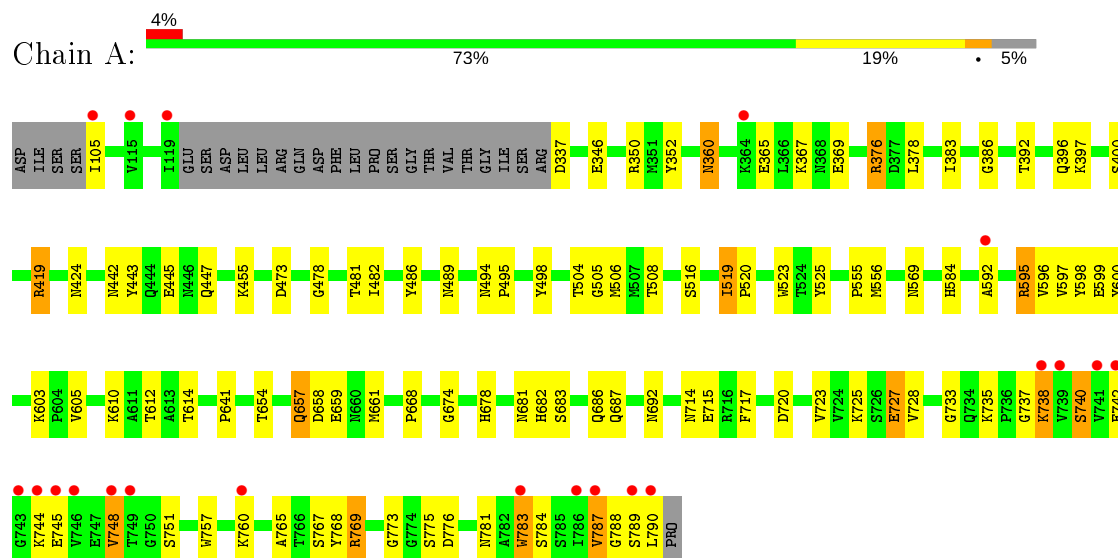
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	241	Total	O	0	0
			241	241		
7	B	264	Total	O	0	0
			264	264		

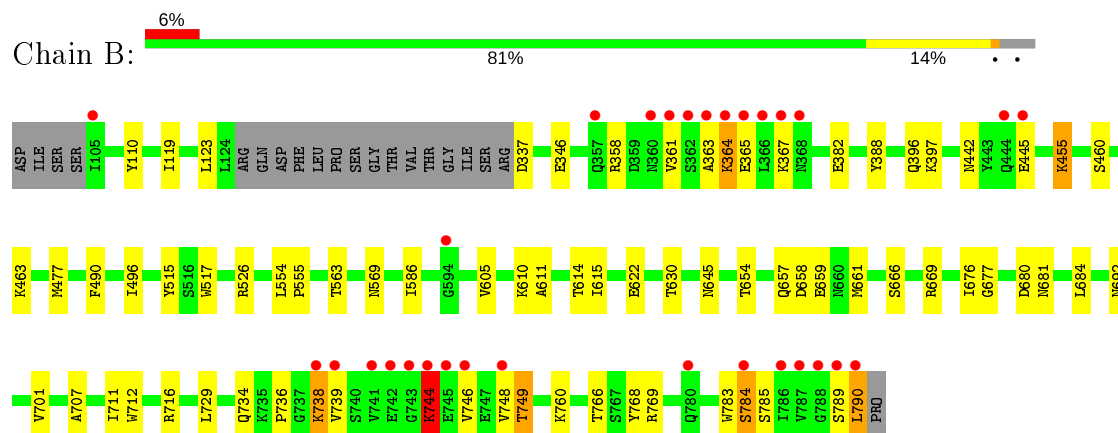
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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, α , β , γ	96.15Å 101.81Å 145.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.64 – 2.15 45.64 – 2.15	Depositor EDS
% Data completeness (in resolution range)	93.5 (45.64-2.15) 93.5 (45.64-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.6.0095	Depositor
R, R_{free}	0.203 , 0.262 0.204 , 0.262	Depositor DCC
R_{free} test set	3744 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7870	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: NA, SO4, Z06, 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	0.46	1/3719 (0.0%)	0.55	0/5045
1	B	0.46	1/3727 (0.0%)	0.54	0/5059
All	All	0.46	2/7446 (0.0%)	0.55	0/10104

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	783	TRP	CZ3-CH2	7.06	1.51	1.40
1	B	744	LYS	CD-CE	6.79	1.68	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	666	SER	Peptide

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	3637	0	3527	81	0
1	B	3654	0	3525	53	0
2	A	16	0	9	3	0
2	B	16	0	9	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	13	0	0	6	0
4	B	12	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
6	A	4	0	6	0	0
7	A	241	0	0	25	1
7	B	264	0	0	11	1
All	All	7870	0	7076	134	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (134) 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:445:GLU:HG3	7:B:2049:HOH:O	1.42	1.20
1:A:419:ARG:HH11	1:A:419:ARG:HG3	1.30	0.96
1:A:419:ARG:HD3	7:A:2047:HOH:O	1.78	0.84
1:A:592:ALA:HB3	4:A:1206:CL:CL	2.15	0.83
1:A:768:TYR:CE1	1:A:783:TRP:CD1	2.68	0.81
1:A:489:ASN:HD22	1:A:495:PRO:HA	1.44	0.80
1:A:556:MET:HB3	2:A:1000:Z06:H7	1.45	0.80
1:A:738:LYS:HB3	7:A:2219:HOH:O	1.82	0.80
1:A:346:GLU:HG3	4:A:1212:CL:CL	2.23	0.76
1:B:363:ALA:HB2	7:B:2021:HOH:O	1.84	0.76
1:A:365:GLU:HG2	7:A:2023:HOH:O	1.87	0.75
1:A:725:LYS:HE3	7:A:2214:HOH:O	1.87	0.74
1:B:645:ASN:O	1:B:716:ARG:NH2	2.21	0.73
1:B:396:GLN:HG2	7:B:2031:HOH:O	1.89	0.71
1:A:498:TYR:OH	7:A:2085:HOH:O	2.09	0.70
1:A:776:ASP:HB2	4:A:1207:CL:CL	2.28	0.70
1:A:419:ARG:HG3	1:A:419:ARG:NH1	2.07	0.70
1:A:350:ARG:HD3	7:A:2013:HOH:O	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:GLU:OE1	7:A:2215:HOH:O	2.08	0.69
1:A:737:GLY:O	1:A:748:VAL:HG23	1.93	0.69
1:A:455[A]:LYS:NZ	7:A:2066:HOH:O	2.26	0.68
1:A:442:ASN:HD22	1:A:445:GLU:HG2	1.56	0.68
1:B:442:ASN:ND2	1:B:445:GLU:HG2	2.08	0.67
1:B:749:THR:HG22	1:B:790:LEU:HD22	1.76	0.67
1:B:657:GLN:HB2	1:B:659:GLU:OE1	1.95	0.66
1:A:508:THR:HG23	7:A:2092:HOH:O	1.96	0.64
1:A:768:TYR:CD1	1:A:783:TRP:NE1	2.65	0.64
1:B:768:TYR:CE1	1:B:783:TRP:CD1	2.86	0.63
1:A:442:ASN:ND2	1:A:445:GLU:HG2	2.13	0.63
1:B:442:ASN:HD22	1:B:445:GLU:HG2	1.64	0.62
1:B:654:THR:HG23	1:B:661:MET:SD	2.39	0.62
1:A:346:GLU:CG	4:A:1212:CL:CL	2.85	0.61
1:A:687:GLN:HB2	7:A:2193:HOH:O	1.98	0.61
1:A:556:MET:HB3	2:A:1000:Z06:N7	2.15	0.61
1:A:686:GLN:HG3	7:A:2189:HOH:O	2.00	0.60
1:B:361:VAL:CG1	1:B:365:GLU:HB2	2.31	0.60
1:B:622:GLU:CG	7:B:2171:HOH:O	2.50	0.58
1:B:692:ASN:HD22	1:B:692:ASN:H	1.51	0.58
1:A:481:THR:HG22	1:A:482:ILE:N	2.20	0.57
1:B:364:LYS:CE	1:B:364:LYS:HA	2.34	0.57
1:B:397:LYS:HE3	7:B:2033:HOH:O	2.04	0.56
1:A:605:VAL:CG2	7:A:2142:HOH:O	2.53	0.56
1:B:657:GLN:O	1:B:658:ASP:HB2	2.04	0.56
1:A:740:SER:HA	1:A:745:GLU:HA	1.88	0.54
1:B:669:ARG:HD3	7:B:2200:HOH:O	2.07	0.53
1:A:481:THR:CG2	1:A:482:ILE:N	2.71	0.53
1:A:654:THR:HG23	1:A:661:MET:SD	2.49	0.52
1:B:396:GLN:CG	7:B:2031:HOH:O	2.51	0.52
1:A:692:ASN:HD22	1:A:692:ASN:H	1.57	0.52
1:A:443:TYR:O	1:A:447:GLN:NE2	2.41	0.52
1:A:728:VAL:HG11	1:A:733:GLY:O	2.09	0.52
1:A:657:GLN:O	1:A:658:ASP:HB2	2.09	0.52
1:A:605:VAL:HG21	7:A:2142:HOH:O	2.10	0.51
1:A:489:ASN:ND2	1:A:495:PRO:HA	2.21	0.51
1:A:525:TYR:HB2	1:A:555:PRO:HG3	1.93	0.51
1:A:720:ASP:O	1:A:723:VAL:HG23	2.10	0.51
1:A:683:SER:OG	7:A:2187:HOH:O	2.19	0.50
1:A:715:GLU:CD	1:A:715:GLU:H	2.14	0.50
1:B:455:LYS:HD3	1:B:563:THR:HG23	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ARG:HG3	7:B:2019:HOH:O	2.11	0.50
1:B:729:LEU:HG	1:B:736:PRO:HG3	1.93	0.50
1:A:443:TYR:HE1	7:A:2059:HOH:O	1.94	0.50
1:A:369:GLU:HB2	7:A:2019:HOH:O	2.10	0.50
1:B:659:GLU:HG2	1:B:681:ASN:O	2.12	0.50
1:A:478:GLY:HA3	1:A:757:TRP:CE2	2.47	0.50
1:B:661:MET:HB2	1:B:676:ILE:HG13	1.94	0.49
1:B:734:GLN:OE1	1:B:766:THR:HA	2.13	0.49
1:B:738:LYS:HG2	7:B:2245:HOH:O	2.12	0.49
1:B:744:LYS:CB	1:B:744:LYS:HZ3	2.26	0.49
1:B:661:MET:HB2	1:B:676:ILE:CG1	2.43	0.49
1:A:775:SER:HB2	4:A:1207:CL:CL	2.50	0.49
1:A:735:LYS:HB2	1:A:765:ALA:HA	1.94	0.49
1:A:692:ASN:H	1:A:692:ASN:ND2	2.11	0.48
1:A:769:ARG:NH1	7:A:2228:HOH:O	2.45	0.48
1:B:744:LYS:CB	1:B:744:LYS:NZ	2.76	0.48
1:B:605:VAL:HG21	7:B:2128:HOH:O	2.13	0.48
1:A:735:LYS:HE2	4:A:1208:CL:CL	2.51	0.47
1:A:486:TYR:HE2	1:A:506:MET:HG2	1.80	0.47
1:B:739:VAL:CG2	1:B:748:VAL:HG21	2.45	0.47
1:A:678:HIS:CG	1:A:682:HIS:CE1	3.02	0.47
1:A:519:ILE:HB	1:A:520:PRO:HD3	1.97	0.47
1:A:668:PRO:HD3	1:A:717:PHE:CE2	2.49	0.47
1:A:396:GLN:O	1:A:400:SER:HB2	2.15	0.47
1:A:787:VAL:CG1	1:A:788:GLY:N	2.78	0.47
1:B:701:VAL:HG22	1:B:712:TRP:CZ2	2.50	0.46
1:B:397:LYS:HE2	1:B:707:ALA:O	2.15	0.46
1:B:783:TRP:O	1:B:784:SER:C	2.53	0.46
1:B:610:LYS:O	1:B:614:THR:HG23	2.15	0.46
1:A:504:THR:OG1	1:A:505:GLY:N	2.48	0.45
1:A:787:VAL:HG12	1:A:788:GLY:N	2.31	0.45
1:A:376[B]:ARG:NH1	7:A:2026:HOH:O	2.48	0.45
1:A:596:VAL:HG11	1:A:599:GLU:HB2	1.98	0.45
1:A:605:VAL:HG23	7:A:2142:HOH:O	2.17	0.45
1:A:378:LEU:O	1:A:378:LEU:HG	2.17	0.45
1:A:392:THR:O	7:A:2031:HOH:O	2.20	0.45
1:B:361:VAL:HG13	1:B:365:GLU:HB2	1.99	0.45
1:B:460:SER:O	1:B:463:LYS:HG3	2.17	0.45
1:A:473:ASP:HA	1:A:612:THR:OG1	2.17	0.44
1:B:346:GLU:HG2	1:B:586:ILE:CG1	2.47	0.44
1:B:611:ALA:O	1:B:615:ILE:HG13	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:GLU:HG3	7:B:2171:HOH:O	2.14	0.43
1:A:595[A]:ARG:HE	1:A:595[A]:ARG:HB3	1.46	0.43
1:B:677:GLY:HA2	1:B:684:LEU:HD11	2.01	0.43
1:A:455[B]:LYS:HE2	7:A:2066:HOH:O	2.18	0.43
1:A:603:LYS:O	1:A:605:VAL:HG23	2.18	0.43
1:A:769:ARG:HG3	7:A:2229:HOH:O	2.18	0.43
1:A:654:THR:H	2:A:1000:Z06:H15	1.64	0.43
1:B:680:ASP:C	1:B:680:ASP:OD1	2.57	0.43
1:A:523:TRP:CG	1:A:773:GLY:HA3	2.53	0.43
1:B:119:ILE:HD13	1:B:119:ILE:N	2.33	0.42
1:B:364:LYS:HE2	1:B:364:LYS:HA	1.99	0.42
1:B:110:TYR:CG	1:B:396:GLN:HB2	2.53	0.42
1:A:641:PRO:HD2	7:A:2167:HOH:O	2.19	0.42
1:A:360:ASN:HD22	1:A:360:ASN:HA	1.64	0.42
1:A:489:ASN:ND2	7:A:2082:HOH:O	2.53	0.42
1:A:519:ILE:N	1:A:520:PRO:CD	2.81	0.42
1:A:657:GLN:HB2	1:A:659:GLU:CD	2.39	0.42
1:B:110:TYR:CD1	1:B:396:GLN:HB2	2.55	0.42
1:B:346:GLU:HG2	1:B:586:ILE:HG12	2.02	0.42
1:B:739:VAL:HG23	1:B:748:VAL:HG21	2.01	0.42
1:A:494:ASN:HA	1:A:495:PRO:HD3	1.89	0.41
1:A:350:ARG:HD2	1:A:598:TYR:CE1	2.55	0.41
1:B:490:PHE:CE2	1:B:496:ILE:HG12	2.56	0.41
1:B:738:LYS:HA	1:B:746:VAL:O	2.20	0.41
1:A:424:ASN:HD22	1:A:674:GLY:HA2	1.86	0.41
1:B:382:GLU:OE2	1:B:388:TYR:OH	2.30	0.41
1:B:711:ILE:HA	1:B:711:ILE:HD12	1.98	0.41
1:A:352:TYR:CE2	1:A:376[B]:ARG:HG3	2.56	0.41
1:A:584:HIS:CG	1:A:600:TYR:CE2	3.09	0.41
1:A:610:LYS:O	1:A:614:THR:HG23	2.21	0.41
1:B:554:LEU:N	1:B:555:PRO:HD2	2.35	0.40
1:A:781:ASN:O	1:A:784:SER:HB3	2.22	0.40
1:A:105:ILE:HG21	7:A:2029:HOH:O	2.22	0.40
1:B:515:TYR:HB2	1:B:517:TRP:CD1	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2024:HOH:O	7:B:2219:HOH:O[3_645]	1.94	0.26

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	468/494 (95%)	436 (93%)	29 (6%)	3 (1%)	25	18
1	B	470/494 (95%)	442 (94%)	27 (6%)	1 (0%)	47	46
All	All	938/988 (95%)	878 (94%)	56 (6%)	4 (0%)	34	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	742	GLU
1	A	744	LYS
1	A	386	GLY
1	B	784	SER

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	388/408 (95%)	360 (93%)	28 (7%)	14	9
1	B	390/408 (96%)	373 (96%)	17 (4%)	28	25
All	All	778/816 (95%)	733 (94%)	45 (6%)	21	15

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	ASP
1	A	360	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	367	LYS
1	A	376[A]	ARG
1	A	376[B]	ARG
1	A	383	ILE
1	A	397	LYS
1	A	419	ARG
1	A	516	SER
1	A	519	ILE
1	A	569	ASN
1	A	595[A]	ARG
1	A	595[B]	ARG
1	A	597	VAL
1	A	657	GLN
1	A	681	ASN
1	A	714	ASN
1	A	727	GLU
1	A	738	LYS
1	A	740	SER
1	A	748	VAL
1	A	751	SER
1	A	760	LYS
1	A	767	SER
1	A	769	ARG
1	A	787	VAL
1	A	789	SER
1	A	790	LEU
1	B	123	LEU
1	B	337	ASP
1	B	364	LYS
1	B	367	LYS
1	B	455	LYS
1	B	477	MET
1	B	526	ARG
1	B	569	ASN
1	B	630	THR
1	B	738	LYS
1	B	744	LYS
1	B	749	THR
1	B	760	LYS
1	B	769	ARG
1	B	785	SER
1	B	789	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	790	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	ASN
1	A	385	ASN
1	A	403	GLN
1	A	442	ASN
1	A	448	ASN
1	A	489	ASN
1	A	645	ASN
1	A	657	GLN
1	A	692	ASN
1	A	714	ASN
1	B	385	ASN
1	B	442	ASN
1	B	448	ASN
1	B	645	ASN
1	B	692	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 33 ligands modelled in this entry, 28 are monoatomic - leaving 5 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
3	SO4	A	1100	-	4,4,4	0.41	0	6,6,6	0.15	0
6	EDO	A	1400	-	3,3,3	0.43	0	2,2,2	0.52	0
2	Z06	A	1000	1,5	14,16,17	4.16	4 (28%)	19,22,25	1.58	5 (26%)
3	SO4	B	1100	-	4,4,4	0.39	0	6,6,6	0.25	0
2	Z06	B	1000	1	14,16,17	4.42	4 (28%)	19,22,25	1.32	3 (15%)

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
6	EDO	A	1400	-	-	1/1/1/1	-
2	Z06	A	1000	1,5	-	2/8/12/14	0/1/1/1
2	Z06	B	1000	1	-	2/8/12/14	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	Z06	B14-O15	11.55	1.56	1.36
2	B	1000	Z06	B14-O16	10.94	1.55	1.36
2	A	1000	Z06	B14-O16	10.75	1.54	1.36
2	A	1000	Z06	B14-O15	10.55	1.54	1.36
2	B	1000	Z06	C2-C11	3.28	1.50	1.47
2	A	1000	Z06	C2-C11	2.29	1.49	1.47
2	A	1000	Z06	C6-N7	-2.23	1.37	1.41
2	B	1000	Z06	C6-N7	-2.22	1.37	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	Z06	C3-C2-C11	-3.46	115.80	120.36
2	A	1000	Z06	O15-B14-C4	-2.53	112.39	119.95
2	B	1000	Z06	O15-B14-C4	-2.52	112.43	119.95
2	B	1000	Z06	C2-C3-C4	-2.27	119.52	121.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	Z06	C2-C3-C4	-2.18	119.59	121.33
2	A	1000	Z06	B14-C4-C3	-2.18	118.38	121.05
2	B	1000	Z06	C3-C2-C11	-2.06	117.65	120.36
2	A	1000	Z06	C1-C2-C3	2.02	121.29	118.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1000	Z06	O15-B14-C4-C5
2	B	1000	Z06	O15-B14-C4-C3
2	A	1000	Z06	O15-B14-C4-C5
2	A	1000	Z06	O15-B14-C4-C3
6	A	1400	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	Z06	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(Å ²)	Q<0.9
1	A	469/494 (94%)	0.07	21 (4%)	33 42	30, 46, 83, 129	0
1	B	474/494 (95%)	0.06	30 (6%)	20 27	28, 44, 89, 133	0
All	All	943/988 (95%)	0.06	51 (5%)	25 34	28, 45, 85, 133	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	364	LYS	5.4
1	B	789	SER	4.8
1	B	738	LYS	4.5
1	A	744	LYS	4.5
1	B	743	GLY	4.4
1	B	790	LEU	4.1
1	A	738	LYS	4.1
1	B	744	LYS	4.1
1	B	739	VAL	3.9
1	B	365	GLU	3.9
1	B	787	VAL	3.8
1	B	363	ALA	3.6
1	B	741	VAL	3.5
1	B	746	VAL	3.5
1	A	746	VAL	3.4
1	B	786	ILE	3.4
1	B	742	GLU	3.3
1	A	790	LEU	3.2
1	B	362	SER	3.2
1	A	783	TRP	3.1
1	A	739	VAL	3.1
1	B	444	GLN	3.1
1	B	366	LEU	3.0
1	B	367	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	592	ALA	2.9
1	B	788	GLY	2.9
1	A	748	VAL	2.9
1	A	742	GLU	2.8
1	B	748	VAL	2.8
1	B	368	ASN	2.8
1	B	360	ASN	2.7
1	A	364	LYS	2.7
1	B	745	GLU	2.6
1	B	357	GLN	2.6
1	A	115	VAL	2.6
1	A	741	VAL	2.5
1	A	743	GLY	2.5
1	A	760	LYS	2.5
1	A	787	VAL	2.4
1	A	745	GLU	2.3
1	B	105	ILE	2.3
1	A	119	ILE	2.3
1	A	786	ILE	2.2
1	A	749	THR	2.2
1	A	105	ILE	2.2
1	B	784	SER	2.2
1	B	445	GLU	2.1
1	B	361	VAL	2.1
1	B	594	GLY	2.1
1	A	789	SER	2.0
1	B	780	GLN	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. 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	B-factors(Å ²)	Q<0.9
4	CL	A	1206	1/1	0.45	0.35	126,126,126,126	0
4	CL	A	1207	1/1	0.53	0.24	87,87,87,87	0
4	CL	A	1208	1/1	0.65	0.31	90,90,90,90	0
4	CL	B	1203	1/1	0.76	0.23	84,84,84,84	0
4	CL	B	1207	1/1	0.79	0.20	74,74,74,74	0
4	CL	A	1209	1/1	0.83	0.22	85,85,85,85	0
4	CL	B	1209	1/1	0.85	0.18	73,73,73,73	0
4	CL	A	1205	1/1	0.88	0.17	80,80,80,80	0
5	NA	B	1301	1/1	0.90	0.09	58,58,58,58	0
4	CL	B	1206	1/1	0.90	0.16	83,83,83,83	0
4	CL	B	1224	1/1	0.92	0.15	74,74,74,74	0
2	Z06	B	1000	16/17	0.92	0.12	41,55,81,83	0
4	CL	B	1208	1/1	0.93	0.10	68,68,68,68	0
4	CL	A	1212	1/1	0.94	0.14	68,68,68,68	0
4	CL	A	1203	1/1	0.94	0.11	71,71,71,71	0
2	Z06	A	1000	16/17	0.94	0.13	51,70,90,94	0
4	CL	B	1216	1/1	0.94	0.08	63,63,63,63	0
4	CL	B	1204	1/1	0.95	0.11	53,53,53,53	0
6	EDO	A	1400	4/4	0.96	0.10	39,55,59,62	0
4	CL	A	1202	1/1	0.96	0.24	71,71,71,71	0
4	CL	A	1211	1/1	0.96	0.08	61,61,61,61	0
5	NA	A	1300	1/1	0.97	0.24	39,39,39,39	0
4	CL	B	1214	1/1	0.97	0.11	62,62,62,62	0
4	CL	A	1204	1/1	0.97	0.09	46,46,46,46	0
4	CL	A	1201	1/1	0.97	0.05	57,57,57,57	0
4	CL	A	1791	1/1	0.98	0.18	45,45,45,45	0
4	CL	B	1200	1/1	0.98	0.07	46,46,46,46	0
4	CL	A	1200	1/1	0.99	0.08	49,49,49,49	0
4	CL	B	1201	1/1	0.99	0.07	50,50,50,50	0
3	SO4	A	1100	5/5	0.99	0.10	47,62,72,76	0
4	CL	B	1211	1/1	0.99	0.10	59,59,59,59	0
3	SO4	B	1100	5/5	0.99	0.09	44,46,53,66	0
5	NA	B	1300	1/1	1.00	0.22	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.