



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:59 AM GMT

PDB ID : 2Z2L
Title : Penicillin-Binding Protein 2X (PBP2X) from Streptococcus pneumoniae
Authors : Yamada, M.; Watanabe, T.; Takeuchi, Y.
Deposited on : 2007-05-23
Resolution : 2.85 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
<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

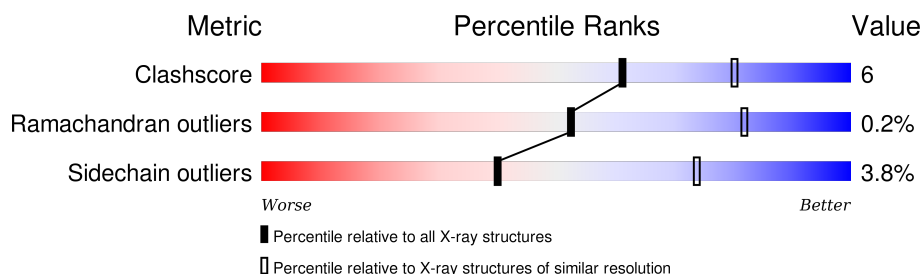
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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))
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	168	
1	D	168	
2	B	385	
2	E	385	
3	C	125	
3	F	125	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9852 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 2X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1224	766	204	250	4			
1	D	134	Total	C	N	O	S	0	0	0
			1021	634	172	212	3			

- Molecule 2 is a protein called Penicillin-binding protein 2X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	367	Total	C	N	O	S	0	0	0
			2814	1769	465	563	17			
2	E	367	Total	C	N	O	S	0	0	0
			2814	1769	465	563	17			

- Molecule 3 is a protein called Penicillin-binding protein 2X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	125	Total	C	N	O	S	0	0	0
			962	601	162	197	2			
3	F	125	Total	C	N	O	S	0	0	0
			962	601	162	197	2			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is water.

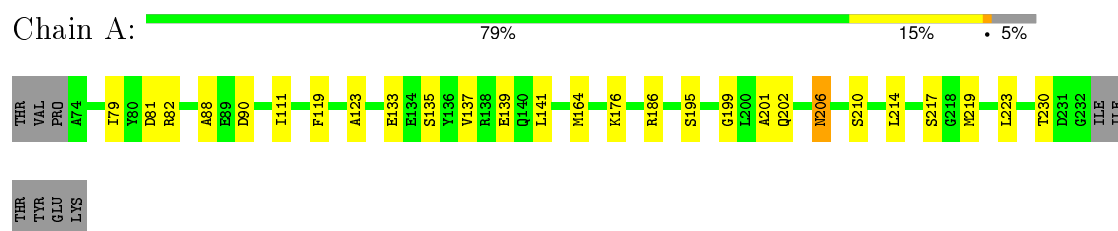
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	13	Total	O	0	0
			13	13		
5	C	3	Total	O	0	0
			3	3		
5	D	6	Total	O	0	0
			6	6		
5	E	19	Total	O	0	0
			19	19		
5	F	5	Total	O	0	0
			5	5		

3 Residue-property plots

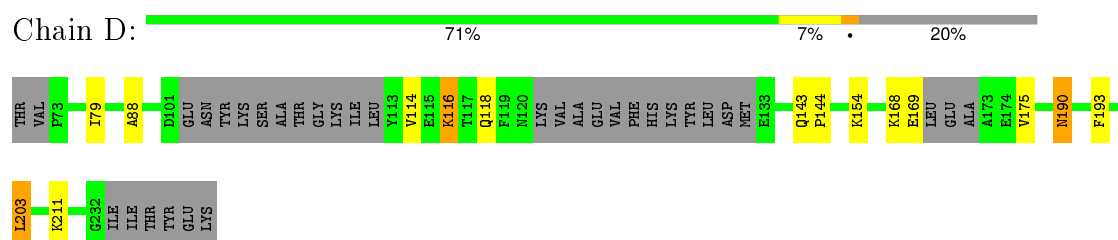
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

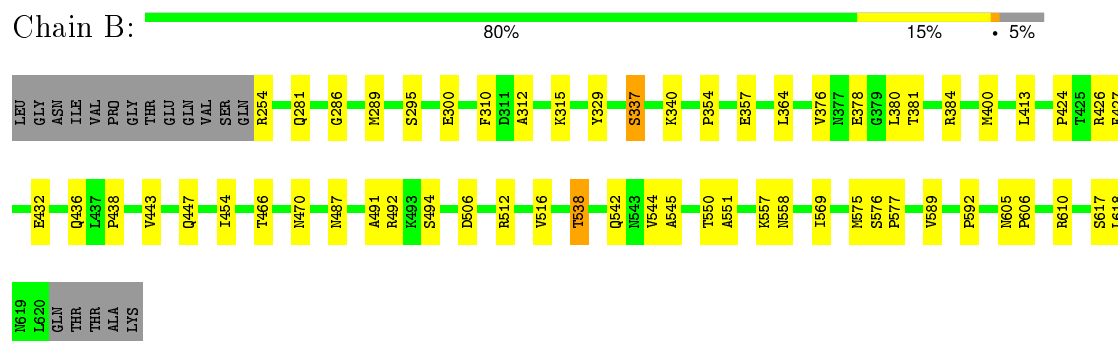
• Molecule 1: Penicillin-binding protein 2X



• Molecule 1: Penicillin-binding protein 2X

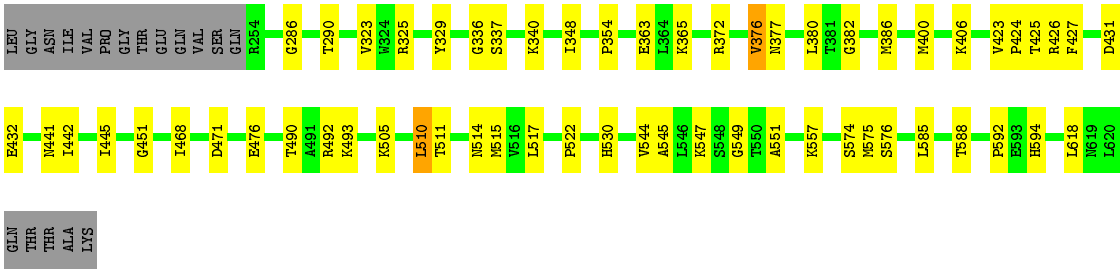


• Molecule 2: Penicillin-binding protein 2X

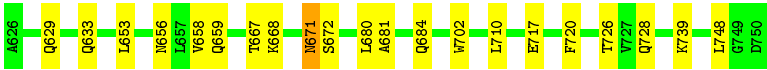
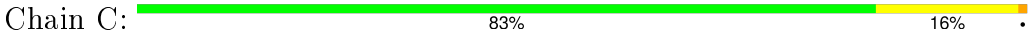


• Molecule 2: Penicillin-binding protein 2X

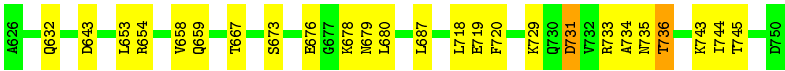
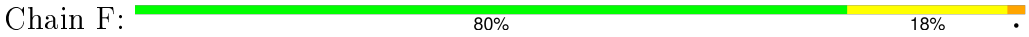




• Molecule 3: Penicillin-binding protein 2X



• Molecule 3: Penicillin-binding protein 2X



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.88Å 171.71Å 89.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.85	Depositor
% Data completeness (in resolution range)	99.7 (30.00-2.85)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.224 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9852	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

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: SO4

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	0.39	0/1244	0.53	0/1676
1	D	0.39	0/1035	0.53	0/1391
2	B	0.40	0/2868	0.55	0/3890
2	E	0.41	0/2868	0.56	0/3890
3	C	0.35	0/975	0.51	0/1320
3	F	0.38	0/975	0.55	0/1320
All	All	0.39	0/9965	0.54	0/13487

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 [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	1224	0	1191	15	0
1	D	1021	0	981	11	0
2	B	2814	0	2747	30	0
2	E	2814	0	2747	31	0
3	C	962	0	975	12	0
3	F	962	0	975	17	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	0	0	0
5	B	13	0	0	1	0
5	C	3	0	0	0	0
5	D	6	0	0	0	0
5	E	19	0	0	0	0
5	F	5	0	0	1	0
All	All	9852	0	9616	107	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 6.

All (107) 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)
2:B:340:LYS:HG2	2:B:400:MET:HG3	1.58	0.84
2:E:340:LYS:HG2	2:E:400:MET:HG3	1.70	0.74
2:E:290:THR:HG1	2:E:588:THR:HG1	1.35	0.74
2:E:337:SER:HB2	2:E:549:GLY:HA2	1.69	0.74
3:F:653:LEU:HB3	3:F:658:VAL:HB	1.71	0.72
1:A:135:SER:O	1:A:139:GLU:HG2	1.90	0.71
3:F:676:GLU:HB2	5:F:38:HOH:O	1.98	0.64
1:D:190:ASN:ND2	1:D:190:ASN:H	1.95	0.64
3:F:719:GLU:HB3	3:F:745:THR:HG23	1.79	0.63
1:D:190:ASN:HD22	1:D:190:ASN:H	1.47	0.62
2:B:424:PRO:HG2	2:B:426:ARG:HD3	1.81	0.62
2:E:363:GLU:HG2	2:E:372:ARG:HG2	1.80	0.61
2:E:426:ARG:O	3:F:654:ARG:HD2	2.01	0.60
3:C:671:ASN:HD22	3:C:672:SER:H	1.48	0.59
2:E:468:ILE:HG21	2:E:515:MET:HE2	1.84	0.59
2:B:329:TYR:HB2	2:B:432:GLU:HG3	1.85	0.58
2:E:380:LEU:C	2:E:382:GLY:H	2.07	0.57
3:C:653:LEU:HB3	3:C:658:VAL:HB	1.86	0.57
2:E:336:GLY:HA3	2:E:551:ALA:HB2	1.87	0.57
2:E:492:ARG:NH1	3:F:680:LEU:O	2.37	0.57
2:B:544:VAL:HG13	2:B:576:SER:HB3	1.88	0.55
2:E:348:ILE:HD13	2:E:510:LEU:HB3	1.88	0.55
3:F:673:SER:HB3	3:F:687:LEU:HB2	1.89	0.55
1:A:82:ARG:NH1	2:B:300:GLU:OE1	2.41	0.54
2:E:286:GLY:HA2	2:E:592:PRO:HA	1.91	0.53
3:F:658:VAL:HG12	3:F:659:GLN:N	2.23	0.53
3:C:702:TRP:O	3:C:726:THR:HA	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:557:LYS:HB3	2:B:558:ASN:OD1	2.09	0.53
2:E:522:PRO:O	2:E:530:HIS:HE1	1.92	0.52
3:F:733:ARG:O	3:F:736:THR:OG1	2.25	0.52
1:D:203:LEU:HD11	1:D:211:LYS:HD3	1.91	0.51
3:F:718:LEU:HD23	3:F:720:PHE:CZ	2.46	0.51
2:E:471:ASP:HB3	2:E:505:LYS:HG3	1.93	0.51
2:B:312:ALA:O	2:B:315:LYS:NZ	2.44	0.50
2:B:545:ALA:HB3	2:B:575:MET:HB2	1.94	0.49
2:E:514:ASN:HA	2:E:517:LEU:HD12	1.92	0.49
2:B:376:VAL:HG22	2:B:381:THR:HG23	1.94	0.49
2:B:378:GLU:HB3	2:B:380:LEU:HG	1.95	0.49
2:B:542:GLN:HG2	2:B:577:PRO:HB3	1.95	0.49
1:D:190:ASN:ND2	1:D:190:ASN:N	2.60	0.48
2:B:466:THR:O	2:B:470:ASN:HB3	2.13	0.48
1:A:79:ILE:HB	1:A:88:ALA:HB3	1.96	0.48
3:F:734:ALA:O	3:F:735:ASN:HB2	2.14	0.48
3:F:743:LYS:HG2	3:F:744:ILE:N	2.28	0.48
3:C:667:THR:HG23	3:C:668:LYS:HD3	1.96	0.48
2:B:286:GLY:HA2	2:B:592:PRO:HA	1.94	0.48
3:F:718:LEU:HD23	3:F:720:PHE:HZ	1.79	0.47
2:B:492:ARG:NH1	3:C:680:LEU:O	2.47	0.47
2:B:443:VAL:O	2:B:447:GLN:HG3	2.13	0.47
2:E:441:ASN:O	2:E:445:ILE:HG13	2.14	0.47
1:A:201:ALA:HA	1:A:214:LEU:O	2.15	0.47
2:E:329:TYR:HB2	2:E:432:GLU:HG3	1.97	0.47
1:A:206:ASN:HD21	1:A:210:SER:HB3	1.80	0.47
1:D:114:VAL:HG23	1:D:118:GLN:HB2	1.97	0.46
3:C:702:TRP:CH2	3:C:710:LEU:HD22	2.50	0.46
2:B:354:PRO:HB2	2:B:357:GLU:HB2	1.96	0.46
2:E:545:ALA:HB3	2:E:575:MET:HB2	1.98	0.46
1:A:111:ILE:O	1:A:176:LYS:HE3	2.16	0.46
1:A:219:MET:HG2	1:A:223:LEU:HD12	1.97	0.46
2:E:425:THR:O	2:E:476:GLU:OE2	2.34	0.46
1:A:119:PHE:CD1	1:A:141:LEU:HD13	2.51	0.45
2:E:363:GLU:HG2	2:E:372:ARG:CG	2.46	0.45
2:B:487:ASN:HD22	2:B:487:ASN:N	2.15	0.44
2:E:511:THR:HG22	2:E:515:MET:CE	2.47	0.44
3:C:681:ALA:O	3:C:684:GLN:HB2	2.18	0.44
1:A:195:SER:HB3	2:B:310:PHE:CZ	2.53	0.43
1:A:199:GLY:HA3	1:A:217:SER:O	2.18	0.43
3:C:658:VAL:HG12	3:C:659:GLN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:HB3	2:B:310:PHE:CE2	2.52	0.43
2:B:605:ASN:HB2	2:B:606:PRO:HD3	2.00	0.43
2:B:512:ARG:O	2:B:516:VAL:HG23	2.18	0.43
2:E:574:SER:OG	2:E:585:LEU:HB3	2.19	0.43
3:C:728:GLN:HB3	3:C:728:GLN:HE21	1.66	0.43
1:D:190:ASN:HB2	1:D:193:PHE:HB2	2.00	0.43
2:E:544:VAL:HG13	2:E:576:SER:HB3	2.01	0.43
2:E:511:THR:HG22	2:E:515:MET:HE2	2.00	0.43
2:B:492:ARG:NH2	3:C:656:ASN:O	2.52	0.43
2:B:438:PRO:HD3	2:B:454:ILE:HD12	2.00	0.43
2:B:538:THR:HA	2:B:544:VAL:HG21	2.01	0.43
2:E:323:VAL:HG12	2:E:325:ARG:HB3	2.01	0.43
2:B:538:THR:HG22	5:B:9:HOH:O	2.18	0.42
1:D:118:GLN:HB3	1:D:175:VAL:HG13	2.01	0.42
2:E:376:VAL:O	2:E:377:ASN:HB2	2.20	0.42
1:D:79:ILE:HB	1:D:88:ALA:HB3	2.01	0.42
3:F:731:ASP:OD1	3:F:745:THR:N	2.52	0.42
2:B:491:ALA:O	3:C:633:GLN:HA	2.20	0.42
1:D:143:GLN:HA	1:D:144:PRO:HD3	1.92	0.42
3:F:729:LYS:HB2	3:F:729:LYS:HE3	1.89	0.42
2:E:490:THR:HG22	3:F:632:GLN:HB3	2.01	0.41
3:C:720:PHE:HB3	3:C:748:LEU:HD21	2.01	0.41
1:D:168:LYS:HG3	1:D:169:GLU:HG3	2.02	0.41
1:A:164:MET:HA	1:A:164:MET:HE3	2.03	0.41
1:A:90:ASP:OD1	1:A:186:ARG:NH2	2.53	0.41
2:E:468:ILE:HG21	2:E:515:MET:CE	2.51	0.41
3:F:678:LYS:HG2	3:F:679:ASN:N	2.36	0.41
2:E:423:VAL:HA	2:E:424:PRO:HD2	1.91	0.41
2:B:337:SER:O	2:B:340:LYS:HB2	2.21	0.41
2:E:354:PRO:HG3	2:E:406:LYS:HE3	2.03	0.41
2:B:289:MET:HG2	2:B:589:VAL:HG13	2.03	0.41
3:F:658:VAL:CG1	3:F:659:GLN:N	2.84	0.41
2:E:365:LYS:HE3	2:E:365:LYS:HB2	1.94	0.40
2:E:336:GLY:O	2:E:451:GLY:HA3	2.21	0.40
1:A:123:ALA:HA	1:A:137:VAL:HG11	2.02	0.40
2:B:551:ALA:HB3	2:B:569:ILE:HB	2.03	0.40
2:B:381:THR:HG21	2:B:384:ARG:HD2	2.03	0.40
1:A:164:MET:HA	1:A:164:MET:CE	2.51	0.40
1:D:116:LYS:H	1:D:116:LYS:HD2	1.86	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	157/168 (94%)	147 (94%)	10 (6%)	0	100	100
1	D	126/168 (75%)	122 (97%)	4 (3%)	0	100	100
2	B	365/385 (95%)	347 (95%)	18 (5%)	0	100	100
2	E	365/385 (95%)	343 (94%)	20 (6%)	2 (0%)	34	67
3	C	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
3	F	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
All	All	1259/1356 (93%)	1195 (95%)	62 (5%)	2 (0%)	52	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	557	LYS
2	E	376	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	132/141 (94%)	127 (96%)	5 (4%)	40	74
1	D	111/141 (79%)	107 (96%)	4 (4%)	42	75
2	B	307/322 (95%)	292 (95%)	15 (5%)	31	63
2	E	307/322 (95%)	298 (97%)	9 (3%)	50	81
3	C	108/108 (100%)	104 (96%)	4 (4%)	41	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	108/108 (100%)	104 (96%)	4 (4%)	41	74
All	All	1073/1142 (94%)	1032 (96%)	41 (4%)	40	74

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ASP
1	A	133	GLU
1	A	202	GLN
1	A	206	ASN
1	A	230	THR
2	B	254	ARG
2	B	281	GLN
2	B	295	SER
2	B	337	SER
2	B	364	LEU
2	B	413	LEU
2	B	427	PHE
2	B	436	GLN
2	B	494	SER
2	B	506	ASP
2	B	538	THR
2	B	550	THR
2	B	610	ARG
2	B	617	SER
2	B	618	LEU
3	C	629	GLN
3	C	671	ASN
3	C	717	GLU
3	C	739	LYS
1	D	116	LYS
1	D	154	LYS
1	D	190	ASN
1	D	203	LEU
2	E	386	MET
2	E	427	PHE
2	E	431	ASP
2	E	442	ILE
2	E	493	LYS
2	E	510	LEU
2	E	547	LYS
2	E	594	HIS

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Mol	Chain	Res	Type
2	E	618	LEU
3	F	643	ASP
3	F	667	THR
3	F	731	ASP
3	F	736	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	206	ASN
2	B	405	GLN
2	B	458	GLN
2	B	470	ASN
2	B	487	ASN
2	B	542	GLN
3	C	671	ASN
3	C	728	GLN
1	D	118	GLN
1	D	185	ASN
1	D	190	ASN
1	D	202	GLN
2	E	350	ASN
2	E	377	ASN
2	E	530	HIS
2	E	580	ASN
3	F	671	ASN
3	F	715	ASN
3	F	728	GLN

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

1 ligand is modelled in this entry.

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	SO4	B	801	-	4,4,4	0.17	0	6,6,6	0.12	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	SO4	B	801	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.