Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 06:28 PM EST

PDB ID	:	4K91
Title	:	Crystal structure of Penicillin-Binding Protein 5 (PBP5) from Pseudomonas aeruginosa in apo state
Authors	:	Smith, J.; Toth, M.; Vakulenko, S.; Mobashery, S.; Chen, Y.
Deposited on	:	2013-04-19
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

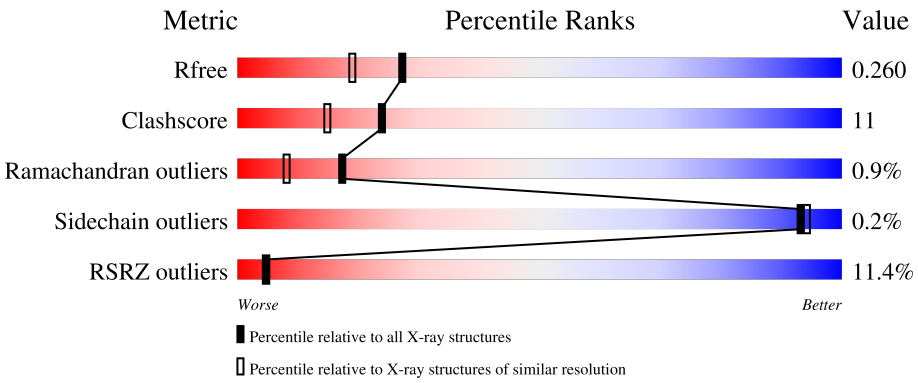
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (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 of 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 <=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	346	13% 79% 18% ··
1	B	346	10% 77% 21% ·

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
2	SIN	A	601	-	X	-	-
2	SIN	B	402	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5435 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.

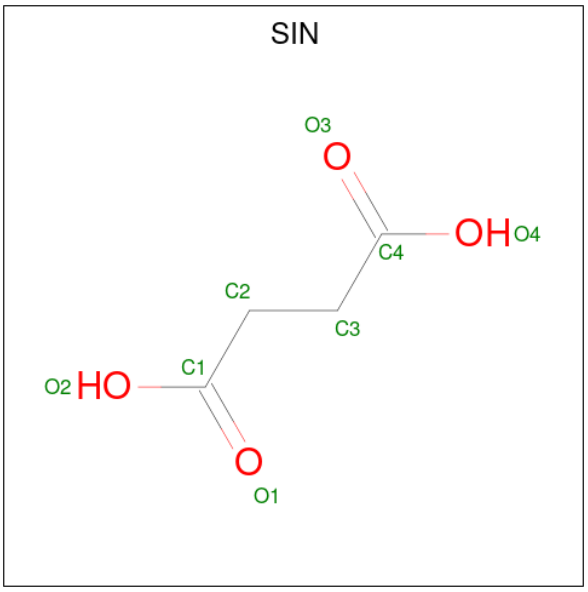
- Molecule 1 is a protein called D-ala-D-ala-carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	2639	1653	461	511	14	0	2	0
1	B	342	2617	1641	458	504	14	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q02SG6
B	1	MET	-	initiating methionine	UNP Q02SG6

- Molecule 2 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	8	4	4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	8	4	4	0	0
			Total	C	O		
2	B	1	8	4	4	0	0

- Molecule 3 is water.

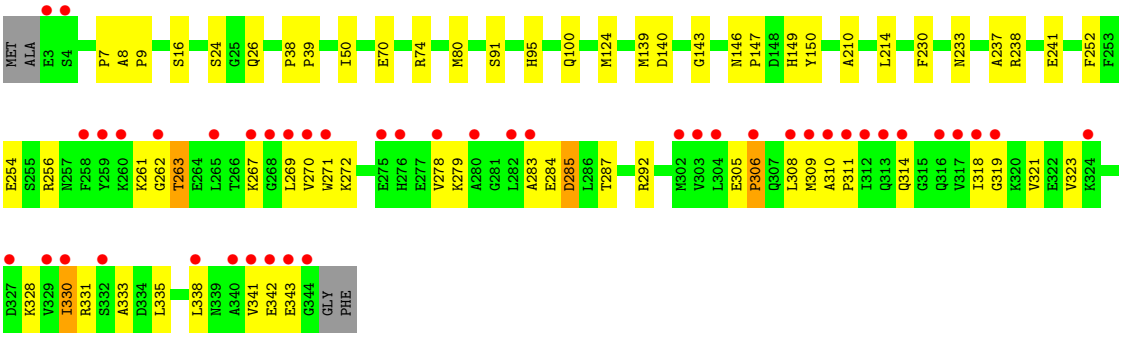
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	89	89	89	0	0
			Total	O		
3	B	66	66	66	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 (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.

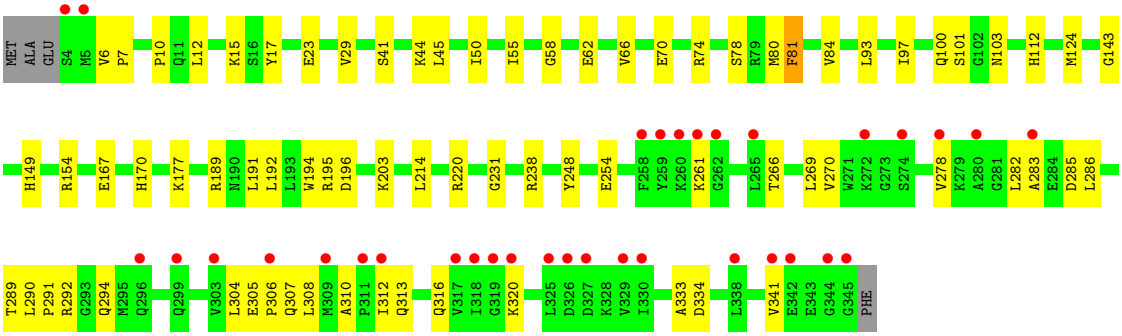
• Molecule 1: D-ala-D-ala-carboxypeptidase

Chain A:



• Molecule 1: D-ala-D-ala-carboxypeptidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	232.14Å 39.91Å 85.46Å 90.00° 111.03° 90.00°	Depositor
Resolution (Å)	39.89 – 2.05 39.88 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.89-2.05) 99.3 (39.88-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.05Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.212 , 0.263 0.212 , 0.260	Depositor DCC
R_{free} test set	2357 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5435	wwPDB-VP
Average B, all atoms (Å^2)	55.0	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 27.39 % 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 2.2186e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SIN

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	0/2684	0.61	0/3630
1	B	0.46	0/2662	0.64	0/3600
All	All	0.46	0/5346	0.63	0/7230

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	2639	0	2624	59	0
1	B	2617	0	2611	57	0
2	A	8	0	4	0	0
2	B	16	0	8	5	0
3	A	89	0	0	0	0
3	B	66	0	0	3	0
All	All	5435	0	5247	117	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 (117) 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:261:LYS:HB3	1:A:284:GLU:HA	1.34	1.04
1:A:314:GLN:HG3	1:A:338:LEU:O	1.62	0.99
1:A:261:LYS:HB3	1:A:284:GLU:CA	1.95	0.96
1:A:330:ILE:HG13	1:A:331:ARG:H	1.28	0.95
1:A:261:LYS:CB	1:A:284:GLU:HA	1.99	0.92
1:B:41:SER:HB2	2:B:402:SIN:H21	1.59	0.85
1:A:261:LYS:HD3	1:A:284:GLU:HA	1.56	0.84
1:A:271:TRP:HB2	1:A:309:MET:HG3	1.61	0.81
1:B:41:SER:CB	2:B:402:SIN:H21	2.13	0.78
1:B:17:TYR:HE1	1:B:29:VAL:HG12	1.47	0.77
1:A:328:LYS:HA	1:A:328:LYS:HE2	1.67	0.77
1:A:269:LEU:O	1:A:269:LEU:HD12	1.85	0.76
1:A:310:ALA:HB1	1:A:311:PRO:HA	1.71	0.73
1:B:70:GLU:OE1	1:B:74:ARG:NH2	2.22	0.72
1:A:261:LYS:CD	1:A:284:GLU:HA	2.19	0.72
1:B:270:VAL:HG21	1:B:278:VAL:HG13	1.72	0.71
1:B:254:GLU:OE2	1:B:292:ARG:HA	1.91	0.70
1:A:38:PRO:HG2	1:A:210:ALA:HB2	1.72	0.69
1:A:323:VAL:HG12	1:A:331:ARG:O	1.94	0.67
2:B:402:SIN:H31	3:B:549:HOH:O	1.94	0.66
1:A:261:LYS:CG	1:A:284:GLU:HA	2.25	0.66
1:A:279:LYS:O	1:A:338:LEU:HG	1.95	0.66
1:A:261:LYS:HD3	1:A:284:GLU:CA	2.27	0.65
1:A:318:ILE:HG13	1:A:319:GLY:H	1.62	0.65
1:A:269:LEU:HD11	1:A:306:PRO:O	1.97	0.64
1:A:321:VAL:HB	1:A:335:LEU:HD11	1.80	0.62
1:B:289:THR:O	1:B:290:LEU:HD12	2.00	0.61
1:B:84:VAL:HG12	3:B:516:HOH:O	2.00	0.61
1:B:304:LEU:N	1:B:304:LEU:HD12	2.16	0.61
1:A:91:SER:O	1:A:95:HIS:HD2	1.84	0.60
1:A:330:ILE:HG13	1:A:331:ARG:N	2.09	0.59
1:B:167:GLU:HB2	1:B:170:HIS:ND1	2.18	0.58
1:B:191:LEU:O	1:B:195:ARG:HG3	2.04	0.57
1:A:328:LYS:HA	1:A:328:LYS:CE	2.34	0.57
1:A:261:LYS:HD3	1:A:283:ALA:O	2.05	0.56
1:B:313:GLN:O	1:B:316:GLN:HB3	2.05	0.56
1:B:17:TYR:HE1	1:B:29:VAL:CG1	2.17	0.56
1:A:271:TRP:O	1:A:272:LYS:HB2	2.05	0.56
1:B:44:LYS:NZ	1:B:103:ASN:OD1	2.39	0.56
1:B:289:THR:O	1:B:290:LEU:CD1	2.55	0.54
1:A:342:GLU:H	1:A:342:GLU:CD	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASN:ND2	1:A:147:PRO:HD2	2.23	0.54
1:A:139:MET:HG3	1:A:146:ASN:OD1	2.07	0.54
1:B:12:LEU:HD12	1:B:17:TYR:CD2	2.43	0.53
1:B:23:GLU:HG3	3:B:559:HOH:O	2.07	0.53
1:B:55:ILE:HD13	1:B:62:GLU:HG2	1.90	0.53
1:B:50:ILE:HD11	1:B:124:MET:HA	1.91	0.53
1:A:278:VAL:CG1	1:A:341:VAL:HG21	2.41	0.51
1:B:80:MET:HA	1:B:100:GLN:NE2	2.26	0.51
1:B:278:VAL:HG12	1:B:341:VAL:HG21	1.93	0.51
1:A:214:LEU:HB2	1:A:238:ARG:HD2	1.92	0.50
1:A:261:LYS:HB3	1:A:284:GLU:C	2.31	0.50
1:B:278:VAL:HG12	1:B:341:VAL:CG2	2.42	0.50
1:B:313:GLN:O	1:B:316:GLN:CB	2.60	0.49
1:B:269:LEU:O	1:B:308:LEU:HB3	2.13	0.49
1:A:50:ILE:HD11	1:A:124:MET:HA	1.95	0.49
1:B:261:LYS:HD2	1:B:283:ALA:O	2.12	0.49
1:B:214:LEU:HB2	1:B:238:ARG:HD2	1.94	0.48
1:A:271:TRP:O	1:A:272:LYS:CB	2.62	0.47
1:B:41:SER:OG	2:B:402:SIN:H21	2.15	0.47
1:B:80:MET:O	1:B:81:PHE:HB2	2.15	0.47
1:A:24:SER:OG	1:A:26:GLN:HG3	2.15	0.47
1:A:321:VAL:CG1	1:A:333:ALA:HB3	2.44	0.47
1:B:78:SER:OG	1:B:189:ARG:NH2	2.48	0.47
1:B:266:THR:HG21	1:B:304:LEU:HD11	1.96	0.47
1:A:80:MET:HA	1:A:100:GLN:HE22	1.80	0.46
1:B:291:PRO:HB2	1:B:294:GLN:HG3	1.96	0.46
1:B:196:ASP:OD1	1:B:220:ARG:NH1	2.49	0.46
1:A:70:GLU:O	1:A:74:ARG:HG3	2.16	0.46
1:A:343:GLU:O	1:A:343:GLU:HG2	2.15	0.46
1:A:323:VAL:CG1	1:A:331:ARG:HB3	2.46	0.46
1:B:10:PRO:HD3	1:B:248:TYR:CD1	2.50	0.46
1:B:80:MET:HA	1:B:100:GLN:HE22	1.81	0.46
1:A:284:GLU:O	1:A:285:ASP:C	2.55	0.45
1:B:320:LYS:HE2	1:B:334:ASP:OD1	2.16	0.45
1:A:16:SER:OG	1:A:230:PHE:HB2	2.17	0.45
1:B:41:SER:OG	2:B:402:SIN:C2	2.64	0.45
1:A:272:LYS:O	1:A:343:GLU:HA	2.17	0.45
1:A:7:PRO:HG2	1:A:252:PHE:CZ	2.51	0.45
1:A:262:GLY:O	1:A:263:THR:C	2.55	0.44
1:B:282:LEU:HD13	1:B:286:LEU:HD12	1.99	0.44
1:B:310:ALA:HA	1:B:312:ILE:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:VAL:HG22	1:A:308:LEU:HD11	1.99	0.44
1:B:70:GLU:OE1	1:B:74:ARG:CZ	2.65	0.44
1:A:254:GLU:OE2	1:A:292:ARG:HA	2.17	0.44
1:B:45:LEU:HD21	1:B:203:LYS:HB2	1.99	0.44
1:B:192:LEU:HD23	1:B:192:LEU:HA	1.84	0.43
1:B:261:LYS:HB3	1:B:285:ASP:N	2.33	0.43
1:B:286:LEU:HD13	1:B:333:ALA:HB2	1.99	0.43
1:A:267:LYS:N	1:A:267:LYS:HD2	2.33	0.43
1:B:286:LEU:HD13	1:B:333:ALA:CB	2.48	0.43
1:B:308:LEU:HG	1:B:312:ILE:HD11	2.00	0.43
1:B:143:GLY:HA2	1:B:149:HIS:NE2	2.33	0.43
1:A:237:ALA:O	1:A:241:GLU:HG2	2.19	0.43
1:B:154:ARG:HD3	1:B:154:ARG:C	2.40	0.42
1:A:8:ALA:HB1	1:A:9:PRO:HD2	2.00	0.42
1:A:261:LYS:HD3	1:A:284:GLU:HB3	2.01	0.42
1:B:177:LYS:HB3	1:B:194:TRP:CZ2	2.54	0.42
1:A:318:ILE:HG13	1:A:319:GLY:N	2.30	0.42
1:A:140:ASP:OD2	1:A:140:ASP:C	2.58	0.42
1:B:6:VAL:HA	1:B:7:PRO:HD3	1.86	0.42
1:A:261:LYS:HD3	1:A:284:GLU:CB	2.50	0.41
1:A:39:PRO:HD3	1:A:150:TYR:HA	2.00	0.41
1:A:328:LYS:HE2	1:A:328:LYS:CA	2.44	0.41
1:A:143:GLY:HA2	1:A:149:HIS:NE2	2.35	0.41
1:A:256:ARG:O	1:A:287:THR:HG23	2.20	0.41
1:B:44:LYS:CE	1:B:103:ASN:OD1	2.69	0.41
1:B:93:LEU:O	1:B:97:ILE:HG13	2.20	0.41
1:A:269:LEU:HD13	1:A:271:TRP:HE1	1.85	0.41
1:B:15:LYS:HG3	1:B:231:GLY:HA3	2.03	0.41
1:B:305:GLU:HA	1:B:306:PRO:HD3	1.87	0.41
1:A:80:MET:HA	1:A:100:GLN:NE2	2.36	0.40
1:A:305:GLU:HA	1:A:306:PRO:HD2	1.90	0.40
1:B:17:TYR:CD1	1:B:17:TYR:C	2.94	0.40
1:B:55:ILE:O	1:B:58:GLY:N	2.39	0.40
1:B:97:ILE:O	1:B:101:SER:HA	2.21	0.40
1:B:66:VAL:HG13	1:B:112:HIS:HB2	2.02	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	342/346 (99%)	321 (94%)	17 (5%)	4 (1%)	13 5
1	B	340/346 (98%)	327 (96%)	11 (3%)	2 (1%)	25 15
All	All	682/692 (99%)	648 (95%)	28 (4%)	6 (1%)	17 8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	ASP
1	B	81	PHE
1	A	263	THR
1	B	307	GLN
1	A	306	PRO
1	A	330	ILE

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	280/280 (100%)	279 (100%)	1 (0%)	91 91
1	B	277/280 (99%)	277 (100%)	0	100 100
All	All	557/560 (100%)	556 (100%)	1 (0%)	93 94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	100	GLN
1	A	206	HIS
1	A	233	ASN
1	A	257	ASN
1	B	11	GLN
1	B	35	GLN
1	B	100	GLN
1	B	129	GLN
1	B	299	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are 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	$\#\|Z\| > 2$
2	SIN	A	601	-	7,7,7	1.17	0	8,8,8	1.67	3 (37%)
2	SIN	B	402	-	7,7,7	1.18	0	8,8,8	1.41	0
2	SIN	B	401	-	7,7,7	1.11	0	8,8,8	1.50	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	SIN	A	601	-	-	5/5/5/5	-
2	SIN	B	402	-	-	3/5/5/5	-
2	SIN	B	401	-	-	0/5/5/5	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	SIN	O4-C4-O3	-2.61	116.79	123.30
2	A	601	SIN	C2-C3-C4	2.41	118.80	113.60
2	A	601	SIN	O4-C4-C3	2.15	120.95	114.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	402	SIN	C1-C2-C3-C4
2	A	601	SIN	C1-C2-C3-C4
2	B	402	SIN	O1-C1-C2-C3
2	A	601	SIN	O2-C1-C2-C3
2	B	402	SIN	O2-C1-C2-C3
2	A	601	SIN	O1-C1-C2-C3
2	A	601	SIN	C2-C3-C4-O4
2	A	601	SIN	C2-C3-C4-O3

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	SIN	5	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	342/346 (98%)	0.45	44 (12%)	3	3	26, 45, 111, 118	0
1	B	342/346 (98%)	0.37	34 (9%)	7	8	25, 45, 96, 108	0
All	All	684/692 (98%)	0.41	78 (11%)	5	5	25, 45, 106, 118	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	345	GLY	10.7
1	A	317	VAL	6.6
1	A	278	VAL	6.1
1	B	278	VAL	6.0
1	A	265	LEU	5.8
1	A	311	PRO	5.6
1	A	344	GLY	5.1
1	A	341	VAL	4.9
1	B	341	VAL	4.5
1	A	4	SER	4.5
1	A	258	PHE	4.5
1	B	4	SER	4.4
1	A	271	TRP	4.4
1	B	338	LEU	4.4
1	A	327	ASP	4.2
1	A	309	MET	4.2
1	B	344	GLY	4.0
1	B	326	ASP	4.0
1	A	262	GLY	3.9
1	B	325	LEU	3.8
1	B	265	LEU	3.8
1	B	262	GLY	3.7
1	A	3	GLU	3.7
1	A	268	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	267	LYS	3.6
1	A	318	ILE	3.6
1	A	329	VAL	3.5
1	B	330	ILE	3.5
1	A	340	ALA	3.4
1	A	269	LEU	3.3
1	B	342	GLU	3.2
1	A	312	ILE	3.2
1	B	258	PHE	3.1
1	B	306	PRO	3.1
1	B	318	ILE	3.1
1	A	338	LEU	3.1
1	A	304	LEU	3.0
1	B	261	LYS	3.0
1	A	316	GLN	3.0
1	A	313	GLN	2.9
1	A	306	PRO	2.9
1	A	343	GLU	2.9
1	B	320	LYS	2.9
1	B	327	ASP	2.9
1	B	299	GLN	2.9
1	B	280	ALA	2.9
1	A	308	LEU	2.8
1	A	324	LYS	2.8
1	A	259	TYR	2.8
1	B	259	TYR	2.7
1	B	274	SER	2.7
1	B	312	ILE	2.7
1	B	303	VAL	2.7
1	A	275	GLU	2.7
1	A	330	ILE	2.6
1	B	311	PRO	2.6
1	B	5	MET	2.6
1	A	283	ALA	2.6
1	A	314	GLN	2.6
1	A	280	ALA	2.6
1	A	342	GLU	2.6
1	A	310	ALA	2.5
1	B	283	ALA	2.5
1	A	302	MET	2.5
1	B	317	VAL	2.5
1	A	332	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	309	MET	2.4
1	A	260	LYS	2.2
1	A	303	VAL	2.2
1	A	282	LEU	2.2
1	B	260	LYS	2.2
1	A	276	HIS	2.2
1	A	319	GLY	2.2
1	B	296	GLN	2.1
1	B	272	LYS	2.0
1	B	319	GLY	2.0
1	B	329	VAL	2.0
1	A	270	VAL	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 monosaccharides 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
2	SIN	B	402	8/8	0.78	0.20	46,59,61,64	0
2	SIN	B	401	8/8	0.97	0.10	37,40,43,43	0
2	SIN	A	601	8/8	0.97	0.11	43,45,47,48	0

6.5 Other polymers (i)

There are no such residues in this entry.