



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:04 PM GMT

PDB ID : 1WDA
Title : Crystal structure of human peptidylarginine deiminase type4 (PAD4) in complex with benzoyl-L-arginine amide
Authors : Arita, K.; Hashimoto, H.; Shimizu, T.; Nakashima, K.; Yamada, M.; Sato, M.
Deposited on : 2004-05-12
Resolution : 2.30 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

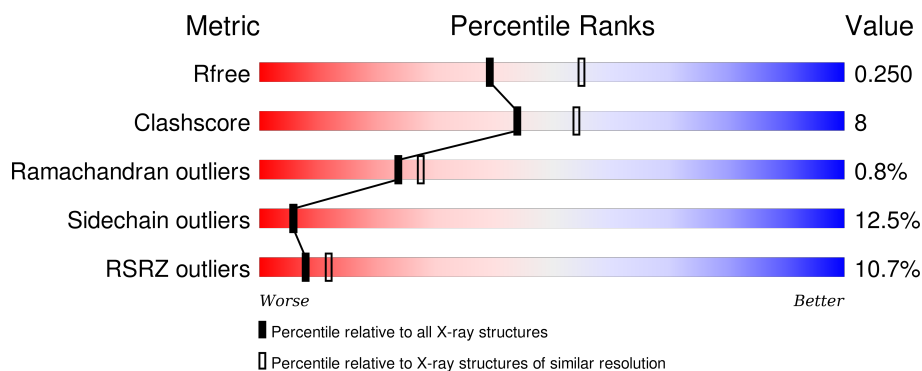
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	670	

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
3	SO4	A	906	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5145 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 Protein-arginine deiminase type IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	628	4946	3158	829	925	34	26	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP Q9UM07
A	-5	PRO	-	EXPRESSION TAG	UNP Q9UM07
A	-4	LEU	-	EXPRESSION TAG	UNP Q9UM07
A	-3	GLY	-	EXPRESSION TAG	UNP Q9UM07
A	-2	SER	-	EXPRESSION TAG	UNP Q9UM07
A	-1	PRO	-	EXPRESSION TAG	UNP Q9UM07
A	0	GLN	-	EXPRESSION TAG	UNP Q9UM07
A	645	ALA	CYS	ENGINEERED	UNP Q9UM07

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

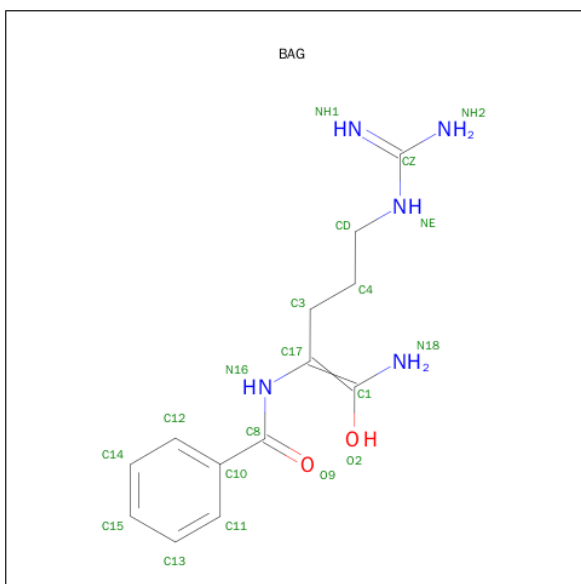
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Ca	0	0
			5	5		

- 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	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is N-[(E)-2-AMINO-1-(3-{[AMINO(IMINO)METHYL]AMINO}PROPYL)-2-HYDROXYVINYL]BENZAMIDE (three-letter code: BAG) (formula: C₁₃H₁₉N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			20	13	5	2		

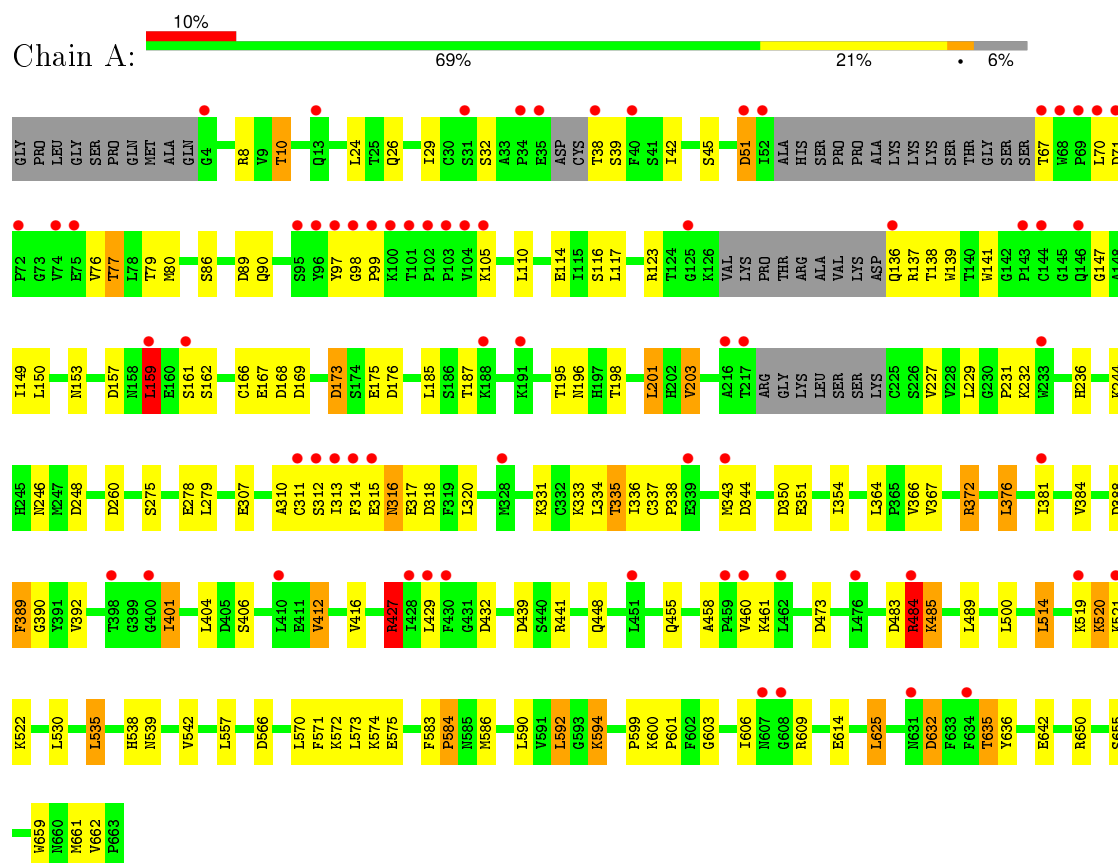
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	159	Total	O	0	0
			159	159		

3 Residue-property plots [i](#)

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

• Molecule 1: Protein-arginine deiminase type IV



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.13Å 60.05Å 115.41Å 90.00° 124.23° 90.00°	Depositor
Resolution (Å)	42.52 – 2.30 42.51 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (42.52-2.30) 97.9 (42.51-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.79 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.210 , 0.252 0.212 , 0.250	Depositor DCC
R_{free} test set	3661 reflections (11.21%)	DCC
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 36307 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5145	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: BAG, CA, 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	0.71	3/5065 (0.1%)	0.90	26/6873 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	519	LYS	CB-CG	-18.01	1.03	1.52
1	A	520	LYS	CB-CG	-8.38	1.29	1.52
1	A	521	LYS	CB-CG	5.90	1.68	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	VAL	CB-CA-C	-7.93	96.33	111.40
1	A	632	ASP	CB-CG-OD2	7.46	125.01	118.30
1	A	427	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	344	ASP	CB-CG-OD2	6.92	124.52	118.30
1	A	432	ASP	CB-CG-OD2	6.84	124.45	118.30
1	A	455	GLN	CB-CA-C	-6.59	97.22	110.40
1	A	51	ASP	CB-CG-OD2	6.55	124.20	118.30
1	A	137	ARG	CA-CB-CG	6.46	127.62	113.40
1	A	388	ASP	CB-CG-OD2	6.45	124.11	118.30
1	A	439	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	248	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	473	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	483	ASP	CB-CG-OD2	6.16	123.85	118.30
1	A	168	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	566	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	372	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	89	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	159	LEU	CA-CB-CG	5.44	127.80	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	260	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	203	VAL	CB-CA-C	-5.26	101.41	111.40
1	A	173	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	176	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	392	VAL	CB-CA-C	-5.14	101.64	111.40
1	A	318	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	455	GLN	CA-CB-CG	5.11	124.64	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4946	0	4906	79	0
2	A	5	0	0	0	0
3	A	15	0	0	0	0
4	A	20	0	18	0	0
5	A	159	0	0	6	0
All	All	5145	0	4924	79	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 8.

All (79) 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:662:VAL:O	1:A:662:VAL:HG23	1.83	0.78
1:A:312:SER:HB2	1:A:316:ASN:HD21	1.54	0.73
1:A:311:CYS:O	1:A:311:CYS:SG	2.47	0.72
1:A:601:PRO:O	5:A:964:HOH:O	2.08	0.71
1:A:367:VAL:HG21	1:A:384:VAL:HG11	1.71	0.70
1:A:441:ARG:HH11	1:A:441:ARG:HG3	1.57	0.70
1:A:312:SER:OG	1:A:320:LEU:HG	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:VAL:HG21	1:A:384:VAL:CG1	2.27	0.64
1:A:484:ARG:O	1:A:485:LYS:HB2	1.99	0.62
1:A:351:GLU:OE2	1:A:372:ARG:HG3	2.00	0.62
1:A:123:ARG:HD3	1:A:659:TRP:CD1	2.36	0.60
1:A:310:ALA:O	1:A:336:ILE:HA	2.01	0.60
1:A:485:LYS:HB2	5:A:952:HOH:O	2.02	0.60
1:A:484:ARG:HG3	1:A:484:ARG:O	2.01	0.59
1:A:311:CYS:HB2	1:A:337:CYS:HB3	1.84	0.59
1:A:354:ILE:CD1	1:A:367:VAL:HG22	2.32	0.59
1:A:354:ILE:HD12	1:A:367:VAL:HG22	1.83	0.58
1:A:662:VAL:O	1:A:662:VAL:CG2	2.52	0.57
1:A:313:ILE:HB	1:A:338:PRO:HA	1.87	0.56
1:A:484:ARG:O	5:A:952:HOH:O	2.18	0.56
1:A:153:ASN:HB3	1:A:166:CYS:HB3	1.86	0.56
1:A:334:LEU:HD11	1:A:336:ILE:HD11	1.86	0.55
1:A:316:ASN:OD1	1:A:317:GLU:N	2.39	0.55
1:A:461:LYS:NZ	5:A:1052:HOH:O	2.40	0.54
1:A:67:THR:N	1:A:97:TYR:HH	2.05	0.53
1:A:586:MET:HA	1:A:599:PRO:HG2	1.90	0.53
1:A:26:GLN:OE1	1:A:77:THR:HB	2.07	0.53
1:A:195:THR:HG22	1:A:196:ASN:ND2	2.22	0.53
1:A:45:SER:OG	1:A:90:GLN:NE2	2.41	0.53
1:A:350:ASP:HB3	1:A:406:SER:HB2	1.92	0.52
1:A:307:GLU:OE2	1:A:335:THR:CG2	2.58	0.51
1:A:278:GLU:O	1:A:279:LEU:HD23	2.11	0.51
1:A:484:ARG:O	1:A:485:LYS:CB	2.59	0.51
1:A:600:LYS:NZ	5:A:995:HOH:O	2.43	0.51
1:A:351:GLU:HG3	1:A:376:LEU:HB3	1.93	0.50
1:A:10:THR:HG23	1:A:32:SER:HB3	1.94	0.50
1:A:594:LYS:N	1:A:594:LYS:HD2	2.27	0.50
1:A:203:VAL:HG23	1:A:229:LEU:HD13	1.94	0.50
1:A:203:VAL:CG2	1:A:229:LEU:HD13	2.41	0.50
1:A:367:VAL:HG23	1:A:389:PHE:CE2	2.48	0.49
1:A:307:GLU:OE2	1:A:335:THR:HG21	2.12	0.49
1:A:535:LEU:HD22	1:A:539:ASN:ND2	2.28	0.48
1:A:366:VAL:HG22	1:A:390:GLY:HA3	1.95	0.48
1:A:201:LEU:HD13	1:A:229:LEU:HD11	1.95	0.48
1:A:10:THR:HG23	1:A:32:SER:CB	2.44	0.48
1:A:514:LEU:HD23	1:A:603:GLY:HA2	1.96	0.47
1:A:311:CYS:CB	1:A:337:CYS:HB3	2.44	0.47
1:A:635:THR:HG23	1:A:636:TYR:HD1	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ARG:HG2	1:A:460:VAL:HG23	1.97	0.46
1:A:313:ILE:CB	1:A:338:PRO:HA	2.46	0.46
1:A:312:SER:O	1:A:320:LEU:HD11	2.16	0.45
1:A:67:THR:N	1:A:97:TYR:OH	2.50	0.45
1:A:307:GLU:OE1	1:A:650:ARG:NH1	2.51	0.44
1:A:594:LYS:HA	1:A:625:LEU:HD12	2.00	0.44
1:A:632:ASP:OD1	1:A:642:GLU:OE2	2.36	0.44
1:A:139:TRP:CD1	1:A:147:GLY:HA3	2.52	0.44
1:A:354:ILE:HG21	1:A:650:ARG:HG3	2.01	0.43
1:A:542:VAL:HG11	1:A:571:PHE:CD1	2.54	0.43
1:A:29:ILE:CD1	1:A:76:VAL:HG21	2.49	0.43
1:A:312:SER:O	1:A:316:ASN:ND2	2.51	0.43
1:A:114:GLU:O	1:A:187:THR:HA	2.18	0.42
1:A:401:ILE:HD12	1:A:401:ILE:HA	1.84	0.42
1:A:29:ILE:HD11	1:A:42:ILE:HD11	2.01	0.42
1:A:316:ASN:C	1:A:316:ASN:OD1	2.57	0.42
1:A:80:MET:CE	1:A:90:GLN:HG3	2.49	0.42
1:A:312:SER:HB2	1:A:320:LEU:CD1	2.50	0.41
1:A:123:ARG:HG2	1:A:149:ILE:HD13	2.01	0.41
1:A:448:GLN:HE22	1:A:461:LYS:HE2	1.84	0.41
1:A:538:HIS:CD2	1:A:573:LEU:H	2.38	0.41
1:A:484:ARG:CG	1:A:484:ARG:O	2.68	0.41
1:A:98:GLY:HA3	1:A:99:PRO:HD2	1.90	0.41
1:A:312:SER:HB2	1:A:320:LEU:HD11	2.01	0.41
1:A:201:LEU:HD13	1:A:229:LEU:CD1	2.51	0.41
1:A:141:TRP:HB3	1:A:661:MET:O	2.20	0.41
1:A:236:HIS:HE1	5:A:1047:HOH:O	2.03	0.41
1:A:231:PRO:O	1:A:232:LYS:HG2	2.21	0.41
1:A:590:LEU:HG	1:A:592:LEU:HD13	2.02	0.41
1:A:583:PHE:HB2	1:A:584:PRO:HD2	2.03	0.40
1:A:441:ARG:NH1	1:A:441:ARG:HG3	2.31	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	618/670 (92%)	584 (94%)	29 (5%)	5 (1%)	24	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	485	LYS
1	A	484	ARG
1	A	159	LEU
1	A	315	GLU
1	A	458	ALA

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	558/592 (94%)	488 (88%)	70 (12%)	6	6

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	10	THR
1	A	24	LEU
1	A	38	THR
1	A	39	SER
1	A	51	ASP
1	A	70	LEU
1	A	71	ASP
1	A	77	THR
1	A	79	THR
1	A	86	SER
1	A	105	LYS
1	A	110	LEU
1	A	116	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	117	LEU
1	A	136	GLN
1	A	138	THR
1	A	150	LEU
1	A	159	LEU
1	A	161	SER
1	A	162	SER
1	A	167	GLU
1	A	169	ASP
1	A	173	ASP
1	A	175	GLU
1	A	185	LEU
1	A	198	THR
1	A	201	LEU
1	A	227	VAL
1	A	244	LYS
1	A	246	ASN
1	A	275	SER
1	A	314	PHE
1	A	316	ASN
1	A	331	LYS
1	A	333	LYS
1	A	335	THR
1	A	343	MET
1	A	364	LEU
1	A	376	LEU
1	A	381	ILE
1	A	389	PHE
1	A	401	ILE
1	A	404	LEU
1	A	412	VAL
1	A	416	VAL
1	A	427	ARG
1	A	429	LEU
1	A	484	ARG
1	A	489	LEU
1	A	500	LEU
1	A	514	LEU
1	A	520	LYS
1	A	522	LYS
1	A	530	LEU
1	A	535	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	557	LEU
1	A	570	LEU
1	A	572	LYS
1	A	574	LYS
1	A	575	GLU
1	A	584	PRO
1	A	592	LEU
1	A	594	LYS
1	A	606	ILE
1	A	609	ARG
1	A	614	GLU
1	A	625	LEU
1	A	635	THR
1	A	655	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	178	GLN
1	A	196	ASN
1	A	246	ASN
1	A	448	GLN
1	A	505	GLN
1	A	509	HIS
1	A	538	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 5 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$
4	BAG	A	801	-	14,20,20	4.95	9 (64%)	14,25,25	1.90	4 (28%)
3	SO4	A	905	-	4,4,4	0.17	0	6,6,6	0.35	0
3	SO4	A	906	-	4,4,4	0.30	0	6,6,6	0.37	0
3	SO4	A	907	-	4,4,4	0.17	0	6,6,6	0.14	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	BAG	A	801	-	-	0/12/19/19	0/1/1/1
3	SO4	A	905	-	-	0/0/0/0	0/0/0/0
3	SO4	A	906	-	-	0/0/0/0	0/0/0/0
3	SO4	A	907	-	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	BAG	C8-N16	-2.12	1.34	1.37
4	A	801	BAG	C3-C17	2.15	1.52	1.50
4	A	801	BAG	C14-C15	5.38	1.51	1.38
4	A	801	BAG	C15-C13	5.81	1.52	1.38
4	A	801	BAG	C14-C12	6.70	1.52	1.38
4	A	801	BAG	C13-C11	6.85	1.53	1.38
4	A	801	BAG	C17-N16	6.93	1.47	1.35
4	A	801	BAG	C12-C10	7.78	1.52	1.39
4	A	801	BAG	C11-C10	8.25	1.53	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	801	BAG	O9-C8-C10	-2.63	116.48	120.97
4	A	801	BAG	C4-C3-C17	-2.30	110.44	113.83
4	A	801	BAG	C11-C10-C8	-2.04	114.14	120.60
4	A	801	BAG	C10-C8-N16	5.08	123.58	116.21

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 [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	628/670 (93%)	0.66	67 (10%) 8 12	33, 46, 71, 83	6 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	GLY	7.3
1	A	312	SER	7.1
1	A	103	PRO	6.1
1	A	104	VAL	6.0
1	A	99	PRO	5.8
1	A	74	VAL	5.7
1	A	217	THR	5.6
1	A	70	LEU	5.1
1	A	314	PHE	5.1
1	A	38	THR	4.8
1	A	68	TRP	4.7
1	A	96	TYR	4.5
1	A	67	THR	4.4
1	A	69	PRO	4.2
1	A	159	LEU	3.9
1	A	97	TYR	3.8
1	A	144	CYS	3.8
1	A	102	PRO	3.8
1	A	34	PRO	3.7
1	A	313	ILE	3.7
1	A	521	LYS	3.5
1	A	40	PHE	3.4
1	A	476	LEU	3.3
1	A	100	LYS	3.3
1	A	381	ILE	3.2
1	A	462	LEU	3.2
1	A	35	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	136	GLN	3.1
1	A	311	CYS	3.1
1	A	101	THR	3.1
1	A	161	SER	3.0
1	A	484	ARG	3.0
1	A	52	ILE	3.0
1	A	216	ALA	2.9
1	A	51	ASP	2.9
1	A	428	ILE	2.8
1	A	400	GLY	2.7
1	A	634	PHE	2.7
1	A	429	LEU	2.7
1	A	460	VAL	2.7
1	A	72	PRO	2.7
1	A	631	ASN	2.6
1	A	315	GLU	2.6
1	A	191	LYS	2.5
1	A	398	THR	2.4
1	A	146	GLN	2.4
1	A	343	MET	2.4
1	A	233	TRP	2.4
1	A	71	ASP	2.4
1	A	608	GLY	2.3
1	A	519	LYS	2.3
1	A	4	GLY	2.3
1	A	105	LYS	2.3
1	A	31	SER	2.2
1	A	95	SER	2.2
1	A	75	GLU	2.2
1	A	125	GLY	2.2
1	A	459	PRO	2.2
1	A	430	PHE	2.2
1	A	13	GLN	2.2
1	A	328	MET	2.1
1	A	607	ASN	2.1
1	A	143	PRO	2.1
1	A	188	LYS	2.1
1	A	410	LEU	2.0
1	A	451	LEU	2.0
1	A	339	GLU	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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	A	906	5/5	0.93	0.22	4.53	69,70,72,72	0
4	BAG	A	801	20/20	0.89	0.21	1.82	40,44,57,57	0
3	SO4	A	905	5/5	0.96	0.09	-1.23	69,71,71,73	0
2	CA	A	900	1/1	1.00	0.11	-1.50	35,35,35,35	0
2	CA	A	903	1/1	0.96	0.06	-2.20	50,50,50,50	0
2	CA	A	904	1/1	0.93	0.07	-2.82	47,47,47,47	0
2	CA	A	902	1/1	0.95	0.04	-3.20	51,51,51,51	0
2	CA	A	901	1/1	0.99	0.05	-5.71	41,41,41,41	0
3	SO4	A	907	5/5	0.93	0.20	-	72,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.