



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:01 AM UTC

PDB ID : 1WD9 / pdb_00001wd9
Title : Calcium bound form of human peptidylarginine deiminase type4 (PAD4)
Authors : Arita, K.; Hashimoto, H.; Shimizu, T.; Nakashima, K.; Yamada, M.; Sato, M.
Deposited on : 2004-05-12
Resolution : 2.60 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

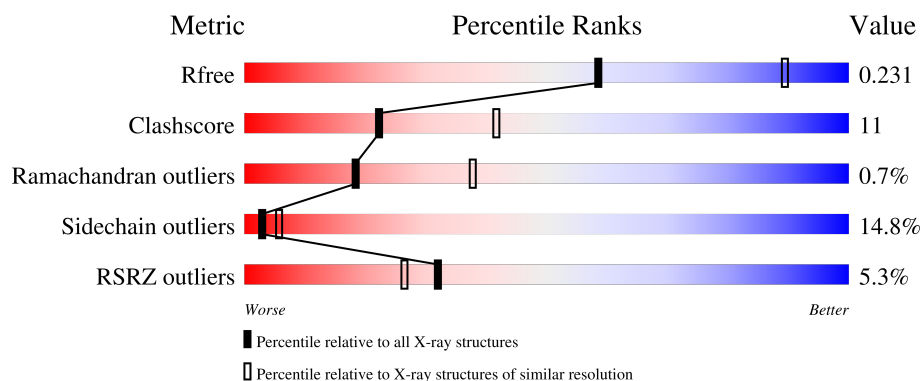
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. 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	5% 63% 22% • • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4829 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
1	A	603	Total	C	N	O	S	0	0	0
			4745	3035	797	880	33			

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 mutation	UNP Q9UM07

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is SULFATE ION (CCD ID: 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		

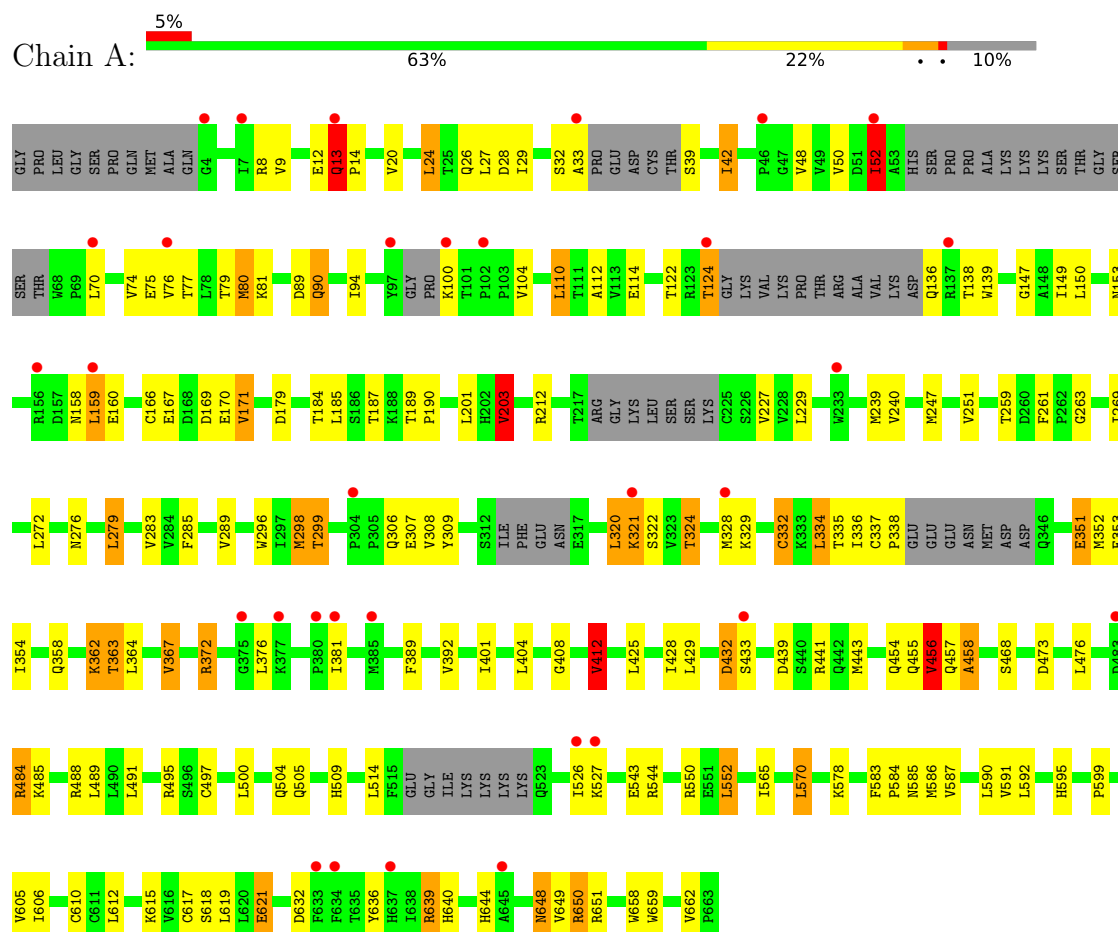
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		

3 Residue-property plots

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: 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	146.39Å 60.09Å 115.34Å 90.00° 124.37° 90.00°	Depositor
Resolution (Å)	22.80 – 2.60 22.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.1 (22.80-2.60) 96.1 (22.80-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.05 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.224 , 0.269 0.229 , 0.231	Depositor DCC
R_{free} test set	2474 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	58.8	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4829	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CA

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	0.97	2/4857 (0.0%)	1.09	9/6590 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	MET	SD-CE	6.40	1.95	1.79
1	A	443	MET	SD-CE	-6.08	1.64	1.79

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	VAL	N-CA-C	13.09	122.99	110.42
1	A	412	VAL	CB-CA-C	-8.07	98.40	110.82
1	A	367	VAL	CB-CA-C	-7.79	100.28	111.34
1	A	456	VAL	CB-CA-C	6.53	120.33	111.97
1	A	13	GLN	N-CA-C	6.52	113.88	108.07
1	A	455	GLN	CA-C-N	6.26	128.46	120.56
1	A	455	GLN	C-N-CA	6.26	128.46	120.56
1	A	432	ASP	N-CA-C	6.20	116.19	108.19
1	A	203	VAL	CB-CA-C	-5.04	101.69	110.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	454	GLN	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	4745	0	4709	100	0
2	A	5	0	0	0	0
3	A	15	0	0	1	0
4	A	64	0	0	6	0
All	All	4829	0	4709	100	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 (100) 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:80:MET:HE2	1:A:112:ALA:HB2	1.45	0.96
1:A:354:ILE:HG21	1:A:650:ARG:HG2	1.52	0.92
1:A:136:GLN:N	4:A:970:HOH:O	2.13	0.80
1:A:39:SER:N	4:A:927:HOH:O	2.14	0.78
1:A:42:ILE:HG21	1:A:50:VAL:HG11	1.64	0.78
1:A:425:LEU:HD12	1:A:456:VAL:HG13	1.66	0.78
1:A:150:LEU:HD21	1:A:251:VAL:HG12	1.67	0.76
1:A:299:THR:CG2	1:A:299:THR:O	2.36	0.72
1:A:298:MET:HE3	1:A:353:GLU:CD	2.18	0.68
1:A:425:LEU:HD12	1:A:456:VAL:CG1	2.25	0.67
1:A:80:MET:HE1	1:A:110:LEU:HB3	1.78	0.66
1:A:362:LYS:NZ	1:A:364:LEU:HD22	2.11	0.66
1:A:320:LEU:HD11	1:A:336:ILE:CD1	2.28	0.64
1:A:320:LEU:HD11	1:A:336:ILE:HD13	1.80	0.64
1:A:412:VAL:HG13	1:A:428:ILE:HD13	1.81	0.63
1:A:585:ASN:ND2	1:A:587:VAL:HG12	2.13	0.63
1:A:362:LYS:HZ1	1:A:364:LEU:HD22	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLN:HB2	1:A:14:PRO:HD2	1.80	0.62
1:A:509:HIS:CD2	1:A:606:ILE:HD12	2.34	0.62
1:A:8:ARG:HG2	1:A:28:ASP:HB3	1.82	0.61
1:A:33:ALA:C	4:A:928:HOH:O	2.43	0.61
1:A:24:LEU:HD21	1:A:77:THR:HG21	1.81	0.61
1:A:153:ASN:HB3	1:A:166:CYS:HB3	1.83	0.61
1:A:296:TRP:CH2	1:A:298:MET:HG3	2.36	0.60
1:A:441:ARG:HH11	1:A:441:ARG:HG3	1.67	0.59
1:A:299:THR:O	1:A:299:THR:HG23	2.04	0.58
1:A:48:VAL:HG23	1:A:90:GLN:HG3	1.86	0.57
1:A:20:VAL:HG21	1:A:285:PHE:CG	2.40	0.56
1:A:240:VAL:HG22	1:A:247:MET:HE3	1.87	0.56
1:A:362:LYS:HZ3	1:A:362:LYS:HB3	1.71	0.56
1:A:272:LEU:CD2	1:A:283:VAL:HG22	2.37	0.55
1:A:648:ASN:HD22	1:A:649:VAL:H	1.54	0.55
1:A:497:CYS:HB3	1:A:570:LEU:HD13	1.87	0.55
1:A:488:ARG:HG2	1:A:565:ILE:HG13	1.90	0.54
1:A:585:ASN:HD21	1:A:587:VAL:HG12	1.72	0.53
1:A:276:ASN:HB2	1:A:279:LEU:HD12	1.91	0.53
1:A:619:LEU:HA	4:A:935:HOH:O	2.09	0.52
1:A:149:ILE:HD13	1:A:659:TRP:CE3	2.46	0.51
1:A:495:ARG:NH1	3:A:906:SO4:O2	2.43	0.51
1:A:505:GLN:HE21	1:A:527:LYS:HA	1.75	0.51
1:A:495:ARG:HB2	1:A:543:GLU:OE2	2.10	0.51
1:A:9:VAL:HG21	1:A:94:ILE:HD13	1.93	0.50
1:A:358:GLN:HB2	1:A:363:THR:HB	1.93	0.50
1:A:362:LYS:CE	1:A:364:LEU:HD22	2.42	0.50
1:A:639:ARG:O	1:A:640:HIS:HB2	2.12	0.50
1:A:632:ASP:C	1:A:632:ASP:OD1	2.54	0.50
1:A:307:GLU:OE2	1:A:650:ARG:NH1	2.44	0.49
1:A:171:VAL:CG2	1:A:171:VAL:O	2.61	0.49
1:A:171:VAL:O	1:A:171:VAL:HG23	2.13	0.49
1:A:610:CYS:SG	1:A:612:LEU:HB2	2.53	0.49
1:A:362:LYS:NZ	1:A:362:LYS:HB3	2.25	0.49
1:A:473:ASP:OD2	1:A:644:HIS:CE1	2.66	0.48
1:A:189:THR:HB	1:A:190:PRO:HD2	1.96	0.47
1:A:114:GLU:O	1:A:187:THR:HA	2.14	0.47
1:A:329:LYS:HB3	1:A:595:HIS:CE1	2.50	0.47
1:A:617:CYS:O	1:A:621:GLU:HB2	2.13	0.47
1:A:80:MET:HE2	1:A:112:ALA:CB	2.32	0.47
1:A:351:GLU:HG2	1:A:372:ARG:NE	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:PHE:HB2	1:A:584:PRO:HD2	1.97	0.47
1:A:296:TRP:CZ3	1:A:298:MET:HG3	2.50	0.46
1:A:158:ASN:O	1:A:159:LEU:C	2.58	0.46
1:A:320:LEU:O	1:A:324:THR:OG1	2.27	0.46
1:A:29:ILE:HD12	1:A:76:VAL:HG21	1.96	0.46
1:A:308:VAL:HB	1:A:334:LEU:HD23	1.97	0.46
1:A:457:GLN:O	1:A:458:ALA:C	2.59	0.46
1:A:484:ARG:O	1:A:485:LYS:HB2	2.14	0.46
1:A:299:THR:O	1:A:299:THR:HG22	2.13	0.45
1:A:321:LYS:HA	1:A:324:THR:OG1	2.16	0.45
1:A:122:THR:O	1:A:124:THR:HG22	2.16	0.45
1:A:491:LEU:CD1	1:A:550:ARG:HG3	2.46	0.45
1:A:632:ASP:HB2	1:A:636:TYR:HB2	1.99	0.45
1:A:337:CYS:HA	1:A:338:PRO:HD3	1.87	0.44
1:A:615:LYS:O	1:A:619:LEU:HG	2.17	0.44
1:A:473:ASP:OD2	1:A:644:HIS:ND1	2.50	0.44
1:A:203:VAL:CG2	1:A:229:LEU:HD13	2.46	0.44
1:A:299:THR:HG21	4:A:924:HOH:O	2.18	0.44
1:A:358:GLN:HG2	1:A:658:TRP:HD1	1.83	0.44
1:A:484:ARG:O	4:A:955:HOH:O	2.21	0.44
1:A:358:GLN:CB	1:A:363:THR:HB	2.47	0.43
1:A:358:GLN:HG2	1:A:658:TRP:CD1	2.53	0.43
1:A:139:TRP:CD1	1:A:147:GLY:HA3	2.54	0.42
1:A:52:ILE:O	1:A:52:ILE:HG23	2.19	0.42
1:A:74:VAL:O	1:A:74:VAL:HG13	2.19	0.42
1:A:351:GLU:OE2	1:A:372:ARG:O	2.37	0.42
1:A:179:ASP:OD1	1:A:362:LYS:CE	2.67	0.42
1:A:24:LEU:CD2	1:A:77:THR:HG21	2.47	0.42
1:A:261:PHE:CZ	1:A:263:GLY:HA2	2.54	0.42
1:A:552:LEU:HD12	1:A:552:LEU:HA	1.90	0.41
1:A:488:ARG:HG2	1:A:565:ILE:CG1	2.50	0.41
1:A:505:GLN:NE2	1:A:527:LYS:HA	2.36	0.41
1:A:298:MET:HE2	1:A:412:VAL:HG22	2.01	0.41
1:A:408:GLY:O	1:A:473:ASP:HB2	2.21	0.41
1:A:13:GLN:HE21	1:A:13:GLN:HB3	1.71	0.41
1:A:212:ARG:HD3	1:A:227:VAL:CG1	2.50	0.41
1:A:441:ARG:HG3	1:A:441:ARG:NH1	2.34	0.41
1:A:591:VAL:O	1:A:651:ARG:NH2	2.52	0.41
1:A:586:MET:HA	1:A:599:PRO:HD2	2.03	0.41
1:A:306:GLN:C	1:A:332:CYS:HB3	2.46	0.40
1:A:308:VAL:HG12	1:A:309:TYR:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:SER:HA	1:A:578:LYS:HB3	2.03	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	585/670 (87%)	553 (94%)	28 (5%)	4 (1%)	18 38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	LEU
1	A	484	ARG
1	A	52	ILE
1	A	458	ALA

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	535/592 (90%)	456 (85%)	79 (15%)	3 6

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	13	GLN
1	A	24	LEU
1	A	26	GLN
1	A	27	LEU
1	A	32	SER
1	A	42	ILE
1	A	52	ILE
1	A	70	LEU
1	A	75	GLU
1	A	79	THR
1	A	80	MET
1	A	81	LYS
1	A	89	ASP
1	A	90	GLN
1	A	100	LYS
1	A	104	VAL
1	A	110	LEU
1	A	124	THR
1	A	138	THR
1	A	160	GLU
1	A	167	GLU
1	A	169	ASP
1	A	170	GLU
1	A	171	VAL
1	A	184	THR
1	A	185	LEU
1	A	201	LEU
1	A	203	VAL
1	A	259	THR
1	A	269	ILE
1	A	279	LEU
1	A	289	VAL
1	A	298	MET
1	A	299	THR
1	A	320	LEU
1	A	321	LYS
1	A	322	SER
1	A	324	THR
1	A	328	MET
1	A	332	CYS
1	A	334	LEU
1	A	335	THR

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Mol	Chain	Res	Type
1	A	351	GLU
1	A	352	MET
1	A	362	LYS
1	A	363	THR
1	A	367	VAL
1	A	372	ARG
1	A	376	LEU
1	A	381	ILE
1	A	389	PHE
1	A	392	VAL
1	A	401	ILE
1	A	404	LEU
1	A	412	VAL
1	A	429	LEU
1	A	432	ASP
1	A	433	SER
1	A	439	ASP
1	A	456	VAL
1	A	476	LEU
1	A	489	LEU
1	A	500	LEU
1	A	504	GLN
1	A	514	LEU
1	A	526	ILE
1	A	544	ARG
1	A	552	LEU
1	A	570	LEU
1	A	590	LEU
1	A	592	LEU
1	A	605	VAL
1	A	618	SER
1	A	621	GLU
1	A	639	ARG
1	A	648	ASN
1	A	650	ARG
1	A	662	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	26	GLN

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Mol	Chain	Res	Type
1	A	136	GLN
1	A	146	GLN
1	A	197	HIS
1	A	202	HIS
1	A	236	HIS
1	A	276	ASN
1	A	286	GLN
1	A	306	GLN
1	A	445	GLN
1	A	448	GLN
1	A	502	GLN
1	A	505	GLN
1	A	506	ASN
1	A	509	HIS
1	A	523	GLN
1	A	524	GLN
1	A	585	ASN
1	A	631	ASN
1	A	648	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	905	-	4,4,4	0.45	0	6,6,6	0.51	0
3	SO4	A	906	-	4,4,4	0.31	0	6,6,6	0.45	0
3	SO4	A	907	-	4,4,4	0.32	0	6,6,6	0.33	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	906	SO4	1	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	603/670 (90%)	0.45	32 (5%) 32 26	41, 58, 79, 90	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	ARG	4.1
1	A	375	GLY	3.9
1	A	645	ALA	3.6
1	A	377	LYS	3.6
1	A	33	ALA	3.3
1	A	527	LYS	3.2
1	A	156	ARG	3.0
1	A	76	VAL	3.0
1	A	483	ASP	3.0
1	A	4	GLY	2.9
1	A	637	HIS	2.9
1	A	46	PRO	2.8
1	A	97	TYR	2.7
1	A	385	MET	2.5
1	A	13	GLN	2.5
1	A	100	LYS	2.4
1	A	124	THR	2.4
1	A	328	MET	2.4
1	A	526	ILE	2.3
1	A	159	LEU	2.3
1	A	233	TRP	2.3
1	A	381	ILE	2.2
1	A	634	PHE	2.2
1	A	304	PRO	2.2
1	A	7	ILE	2.2
1	A	380	PRO	2.2
1	A	321	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	633	PHE	2.1
1	A	70	LEU	2.1
1	A	52	ILE	2.1
1	A	433	SER	2.0
1	A	102	PRO	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 oligosaccharides 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
3	SO4	A	906	5/5	0.81	0.15	75,75,77,77	0
3	SO4	A	907	5/5	0.84	0.15	77,77,79,80	0
2	CA	A	904	1/1	0.88	0.11	71,71,71,71	0
3	SO4	A	905	5/5	0.90	0.17	76,76,79,80	0
2	CA	A	903	1/1	0.94	0.09	67,67,67,67	0
2	CA	A	902	1/1	0.96	0.05	75,75,75,75	0
2	CA	A	900	1/1	0.98	0.09	57,57,57,57	0
2	CA	A	901	1/1	0.99	0.08	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.