



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2017 – 10:04 AM EST

PDB ID : 4DKT
Title : Crystal structure of human peptidylarginine deiminase 4 in complex with N-acetyl-L-threonyl-L-alpha-aspartyl-N5-[(1E)-2-fluoroethanimidoyl]-L-ornithinamide
Authors : Jones, J.E.; Slack, J.L.; Fang, P.; Zhang, X.; Subramanian, V.; Causey, C.P.; Coonrod, S.A.; Guo, M.; Thompson, P.R.
Deposited on : unknown
Resolution : 2.98 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

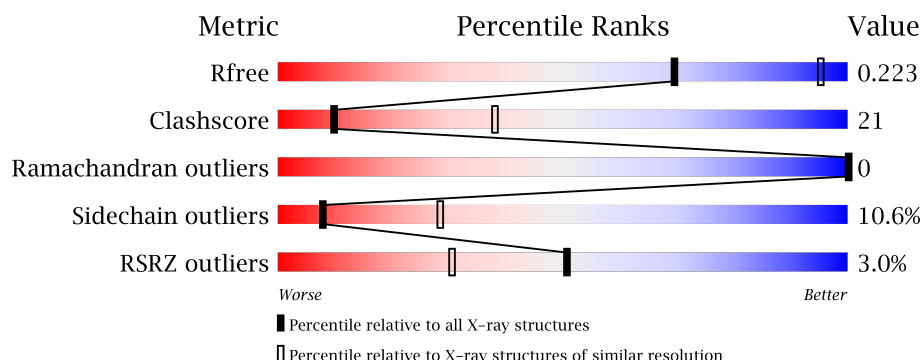
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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}	100719	2168 (3.00-2.96)
Clashscore	112137	2535 (3.00-2.96)
Ramachandran outliers	110173	2451 (3.00-2.96)
Sidechain outliers	110143	2454 (3.00-2.96)
RSRZ outliers	101464	2192 (3.00-2.96)

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	668	<div> <div>3%</div> <div>57%</div> <div>32%</div> <div>5%</div> <div>5%</div> </div>
2	B	5	<div> <div>20%</div> <div>40%</div> <div>20%</div> <div>40%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5076 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-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	636	Total	C	N	O	S	0	0	0
			4996	3185	840	935	36			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q9UM07
A	-3	PRO	-	EXPRESSION TAG	UNP Q9UM07
A	-2	LEU	-	EXPRESSION TAG	UNP Q9UM07
A	-1	GLY	-	EXPRESSION TAG	UNP Q9UM07
A	0	SER	-	EXPRESSION TAG	UNP Q9UM07
A	55	SER	GLY	CONFLICT	UNP Q9UM07
A	82	ALA	VAL	CONFLICT	UNP Q9UM07
A	112	ALA	GLY	CONFLICT	UNP Q9UM07

- Molecule 2 is a protein called Thr-Asp-F-amidine.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	1
			20	11	5	4			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

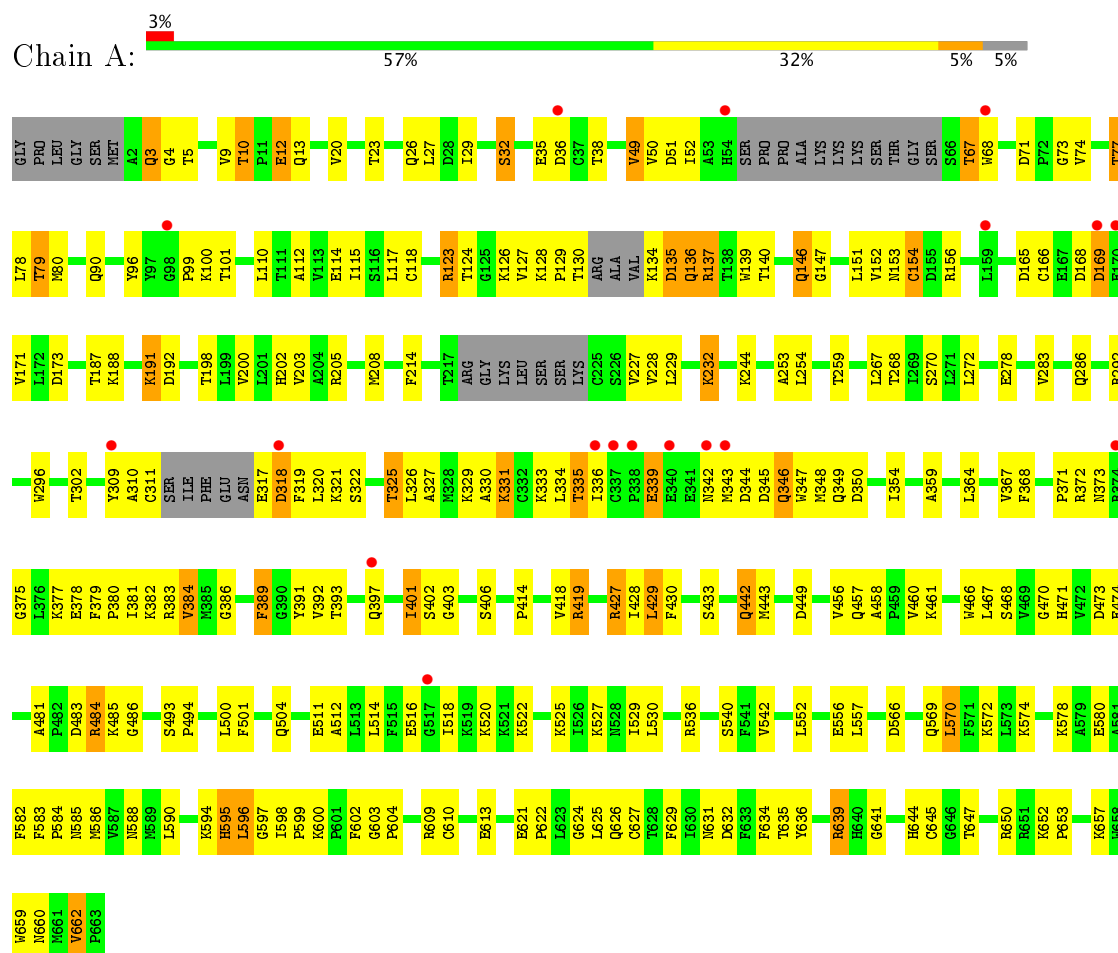
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total 36	O 36	0	0
6	B	1	Total 1	O 1	0	0

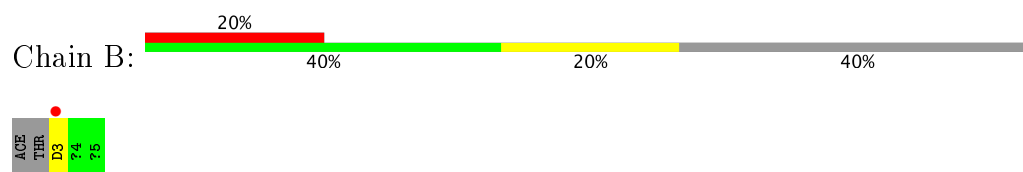
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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-4



• Molecule 2: Thr-Asp-F-amidine



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.65Å 61.08Å 115.38Å 90.00° 124.54° 90.00°	Depositor
Resolution (Å)	41.44 – 2.98 41.44 – 2.96	Depositor EDS
% Data completeness (in resolution range)	95.9 (41.44-2.98) 92.1 (41.44-2.96)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.191 , 0.230 0.186 , 0.223	Depositor DCC
R_{free} test set	837 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.7	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	5076	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: CA, NH2, EDO, FIO, 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	0.32	0/5116	0.54	0/6944
2	B	0.48	0/7	0.67	0/8
All	All	0.32	0/5123	0.54	0/6952

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

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	4996	0	4946	213	0
2	B	20	0	11	2	0
3	A	5	0	0	0	0
4	A	10	0	0	1	0
5	A	8	0	12	1	0
6	A	36	0	0	2	0
6	B	1	0	0	0	0
All	All	5076	0	4969	213	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 21.

All (213) 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:136:GLN:OE1	1:A:137:ARG:N	1.98	0.96
1:A:484:ARG:HG2	1:A:484:ARG:HH11	1.32	0.95
1:A:154:CYS:HB2	1:A:391:TYR:H	1.33	0.91
1:A:588:ASN:OD1	1:A:644:HIS:HB3	1.73	0.88
1:A:311:CYS:HB2	1:A:342:ASN:HD21	1.37	0.87
1:A:367:VAL:HG23	1:A:389:PHE:HE2	1.39	0.85
1:A:501:PHE:HD2	1:A:529:ILE:HD11	1.44	0.81
1:A:188:LYS:HD3	1:A:244:LYS:HG3	1.63	0.80
1:A:136:GLN:C	1:A:137:ARG:HG3	2.02	0.80
1:A:639:ARG:HD2	2:B:3:ASP:HB2	1.63	0.79
1:A:35:GLU:O	1:A:36:ASP:OD1	2.00	0.78
1:A:321:LYS:O	1:A:325:THR:HG23	1.85	0.76
1:A:501:PHE:CD2	1:A:529:ILE:HD11	2.20	0.75
1:A:191:LYS:O	1:A:191:LYS:HD2	1.86	0.75
1:A:348:MET:HE1	1:A:379:PHE:HE2	1.51	0.75
1:A:346:GLN:NE2	2:B:3:ASP:OD2	2.20	0.74
1:A:123:ARG:HH22	1:A:146:GLN:C	1.90	0.74
1:A:493:SER:HB2	1:A:566:ASP:HB3	1.68	0.74
1:A:168:ASP:OD1	1:A:169:ASP:N	2.21	0.73
1:A:484:ARG:CG	1:A:484:ARG:HH11	2.02	0.73
1:A:350:ASP:HB3	1:A:406:SER:HB2	1.70	0.73
1:A:232:LYS:HB3	1:A:232:LYS:NZ	2.06	0.71
1:A:639:ARG:HH21	1:A:639:ARG:CG	2.03	0.70
1:A:586:MET:HA	1:A:599:PRO:HG2	1.75	0.68
1:A:329:LYS:HE2	1:A:626:GLN:HE22	1.58	0.68
1:A:318:ASP:OD1	1:A:318:ASP:N	2.27	0.68
1:A:600:LYS:HD3	1:A:602:PHE:HE1	1.58	0.68
1:A:123:ARG:NH2	1:A:146:GLN:C	2.48	0.67
1:A:348:MET:HE1	1:A:379:PHE:CE2	2.30	0.67
1:A:632:ASP:HB2	1:A:636:TYR:HD1	1.59	0.66
1:A:327:ALA:CB	1:A:334:LEU:HD11	2.26	0.66
1:A:572:LYS:HE2	1:A:574:LYS:HD2	1.77	0.65
1:A:639:ARG:HH21	1:A:639:ARG:HG2	1.59	0.65
1:A:371:PRO:HB2	1:A:401:ILE:HD11	1.78	0.65
1:A:124:THR:OG1	1:A:126:LYS:HG2	1.97	0.65
1:A:367:VAL:HG23	1:A:389:PHE:CE2	2.27	0.65
1:A:456:VAL:HG13	1:A:457:GLN:HG3	1.78	0.65
1:A:71:ASP:O	1:A:74:VAL:HG12	1.98	0.64
1:A:326:LEU:HD23	1:A:590:LEU:HD23	1.81	0.63
1:A:530:LEU:O	1:A:536:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLN:O	1:A:137:ARG:HG3	1.99	0.62
1:A:632:ASP:HB2	1:A:636:TYR:HB2	1.81	0.62
1:A:600:LYS:HD3	1:A:602:PHE:CE1	2.35	0.62
1:A:136:GLN:HB3	1:A:137:ARG:HG2	1.81	0.62
1:A:632:ASP:HB2	1:A:636:TYR:CD1	2.35	0.61
1:A:427:ARG:NH1	1:A:458:ALA:HB3	2.15	0.61
1:A:514:LEU:HD13	1:A:604:PRO:HD3	1.82	0.61
1:A:379:PHE:HB3	1:A:380:PRO:HD3	1.81	0.61
1:A:154:CYS:HB2	1:A:391:TYR:N	2.13	0.61
1:A:493:SER:CB	1:A:566:ASP:HB3	2.30	0.61
1:A:494:PRO:HA	1:A:569:GLN:O	1.99	0.61
1:A:27:LEU:HD13	1:A:78:LEU:HD13	1.82	0.61
1:A:51:ASP:O	1:A:77:THR:HG23	2.02	0.60
1:A:333:LYS:HG2	1:A:334:LEU:N	2.15	0.60
1:A:529:ILE:HG13	1:A:530:LEU:N	2.16	0.60
1:A:333:LYS:C	1:A:334:LEU:HD12	2.21	0.60
1:A:169:ASP:O	1:A:227:VAL:HG21	2.02	0.60
1:A:327:ALA:HB1	1:A:334:LEU:HD11	1.83	0.60
1:A:156:ARG:HA	1:A:165:ASP:OD1	2.02	0.59
1:A:166:CYS:HB2	1:A:254:LEU:HD22	1.85	0.59
1:A:80:MET:SD	1:A:112:ALA:HB2	2.43	0.59
1:A:598:ILE:O	1:A:629:PHE:HA	2.01	0.59
1:A:136:GLN:C	1:A:137:ARG:CG	2.71	0.59
1:A:662:VAL:O	1:A:662:VAL:HG22	2.01	0.59
1:A:427:ARG:HG3	1:A:458:ALA:O	2.04	0.58
1:A:520:LYS:O	1:A:520:LYS:HG3	2.03	0.57
1:A:49:VAL:HG13	1:A:79:THR:HG23	1.86	0.57
1:A:156:ARG:O	1:A:156:ARG:HG3	2.04	0.57
1:A:29:ILE:HG23	1:A:96:TYR:HE1	1.70	0.56
1:A:329:LYS:HB3	1:A:595:HIS:CD2	2.41	0.56
1:A:319:PHE:HB3	1:A:320:LEU:HD12	1.88	0.56
1:A:639:ARG:CG	1:A:639:ARG:NH2	2.67	0.56
1:A:590:LEU:HD13	1:A:647:THR:HG21	1.88	0.56
1:A:272:LEU:HD23	1:A:283:VAL:HG22	1.87	0.56
1:A:309:TYR:HD1	1:A:348:MET:HE1	1.70	0.56
1:A:378:GLU:OE2	1:A:382:LYS:NZ	2.39	0.56
1:A:512:ALA:HB1	1:A:604:PRO:HB3	1.88	0.56
1:A:320:LEU:H	1:A:320:LEU:HD12	1.70	0.56
1:A:349:GLN:HB3	1:A:645:CYS:O	2.06	0.56
1:A:259:THR:CG2	1:A:449:ASP:HB3	2.36	0.56
1:A:594:LYS:HE2	1:A:624:GLY:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ASP:HB2	6:A:831:HOH:O	2.05	0.55
1:A:467:LEU:HD13	1:A:474:GLU:HB2	1.89	0.55
1:A:518:ILE:HG23	1:A:634:PHE:HZ	1.71	0.54
1:A:127:VAL:O	1:A:128:LYS:HD2	2.06	0.54
1:A:10:THR:HG22	1:A:12:GLU:HG3	1.89	0.54
1:A:311:CYS:HB2	1:A:342:ASN:ND2	2.15	0.54
1:A:130:THR:O	1:A:134:LYS:HD3	2.08	0.54
1:A:333:LYS:HZ2	1:A:335:THR:HG22	1.72	0.54
1:A:259:THR:HG23	1:A:449:ASP:HB3	1.88	0.54
1:A:203:VAL:HG23	1:A:229:LEU:HD13	1.89	0.54
1:A:467:LEU:HB2	1:A:470:GLY:HA2	1.90	0.54
1:A:310:ALA:O	1:A:336:ILE:HA	2.07	0.54
1:A:354:ILE:CD1	1:A:367:VAL:HG22	2.39	0.53
1:A:135:ASP:OD2	1:A:135:ASP:N	2.35	0.53
1:A:367:VAL:HG21	1:A:384:VAL:HG21	1.91	0.53
1:A:354:ILE:HG21	1:A:650:ARG:HG3	1.91	0.53
1:A:518:ILE:HD11	1:A:602:PHE:CD2	2.44	0.53
1:A:347:TRP:CH2	1:A:641:GLY:HA3	2.43	0.52
1:A:393:THR:OG1	1:A:397:GLN:NE2	2.42	0.52
1:A:518:ILE:HG23	1:A:634:PHE:CZ	2.44	0.52
1:A:381:ILE:HG13	1:A:381:ILE:O	2.10	0.51
1:A:595:HIS:HA	1:A:626:GLN:HG2	1.92	0.51
1:A:123:ARG:NH1	1:A:140:THR:O	2.34	0.51
1:A:320:LEU:HD12	1:A:320:LEU:N	2.26	0.51
1:A:379:PHE:CE1	1:A:383:ARG:HB2	2.46	0.51
1:A:403:GLY:N	4:A:706:SO4:O4	2.43	0.51
1:A:169:ASP:C	1:A:169:ASP:OD1	2.49	0.51
1:A:333:LYS:O	1:A:334:LEU:HD12	2.12	0.50
1:A:329:LYS:HB3	1:A:595:HIS:HD2	1.75	0.50
1:A:38:THR:HG23	1:A:99:PRO:HD3	1.94	0.50
1:A:118:CYS:SG	1:A:129:PRO:HA	2.51	0.50
1:A:433:SER:O	5:A:709:EDO:H11	2.12	0.50
1:A:339:GLU:OE1	1:A:339:GLU:C	2.50	0.49
1:A:203:VAL:HG22	1:A:267:LEU:CD2	2.42	0.49
1:A:468:SER:HA	1:A:578:LYS:HB3	1.94	0.49
1:A:4:GLY:HA2	1:A:23:THR:HG23	1.95	0.49
1:A:317:GLU:O	1:A:321:LYS:HG2	2.13	0.49
1:A:401:ILE:HG23	1:A:402:SER:N	2.28	0.49
1:A:156:ARG:NH2	1:A:381:ILE:O	2.46	0.49
1:A:191:LYS:C	1:A:191:LYS:HD2	2.33	0.49
1:A:427:ARG:HH11	1:A:458:ALA:HB3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:PRO:O	1:A:384:VAL:HG22	2.13	0.49
1:A:296:TRP:CZ2	1:A:368:PHE:HB2	2.48	0.48
1:A:570:LEU:HB3	1:A:582:PHE:HB3	1.95	0.48
1:A:309:TYR:HE1	1:A:379:PHE:CZ	2.31	0.48
1:A:10:THR:HG21	1:A:12:GLU:OE2	2.13	0.48
1:A:114:GLU:O	1:A:187:THR:HA	2.14	0.48
1:A:320:LEU:H	1:A:320:LEU:CD1	2.26	0.48
1:A:188:LYS:HD3	1:A:244:LYS:CG	2.41	0.48
1:A:10:THR:CG2	1:A:12:GLU:HG3	2.42	0.48
1:A:67:THR:O	1:A:68:TRP:CD1	2.67	0.48
1:A:130:THR:C	1:A:134:LYS:HD3	2.34	0.47
1:A:200:VAL:HG13	1:A:270:SER:HB2	1.96	0.47
1:A:367:VAL:CG2	1:A:389:PHE:HE2	2.20	0.47
1:A:80:MET:CE	1:A:90:GLN:HG3	2.44	0.47
1:A:152:VAL:HA	1:A:253:ALA:O	2.15	0.47
1:A:484:ARG:CG	1:A:484:ARG:NH1	2.68	0.47
1:A:214:PHE:CE2	1:A:227:VAL:HG22	2.49	0.47
1:A:418:VAL:O	1:A:419:ARG:HG2	2.14	0.47
1:A:114:GLU:HB3	1:A:188:LYS:HB3	1.96	0.47
1:A:343:MET:O	1:A:344:ASP:CG	2.52	0.47
1:A:232:LYS:HB3	1:A:232:LYS:HZ3	1.79	0.47
1:A:596:LEU:HD21	1:A:625:LEU:HD13	1.97	0.47
1:A:657:LYS:HB3	1:A:659:TRP:CE2	2.49	0.47
1:A:228:VAL:HG23	1:A:229:LEU:H	1.80	0.47
1:A:428:ILE:HG12	1:A:457:GLN:HB2	1.95	0.47
1:A:574:LYS:HD3	1:A:580:GLU:OE1	2.15	0.47
1:A:192:ASP:OD2	1:A:192:ASP:N	2.44	0.47
1:A:20:VAL:O	1:A:23:THR:HB	2.14	0.47
1:A:354:ILE:HD12	1:A:367:VAL:HG22	1.96	0.46
1:A:67:THR:OG1	1:A:68:TRP:N	2.46	0.46
1:A:512:ALA:O	1:A:525:LYS:HA	2.15	0.46
1:A:514:LEU:HD12	1:A:603:GLY:HA2	1.97	0.46
1:A:442:GLN:NE2	1:A:443:MET:O	2.49	0.46
1:A:511:GLU:OE2	1:A:527:LYS:HE2	2.16	0.46
1:A:27:LEU:HD11	1:A:78:LEU:HD22	1.98	0.45
1:A:418:VAL:HG21	1:A:556:GLU:O	2.16	0.45
1:A:272:LEU:CD2	1:A:283:VAL:HG22	2.47	0.45
1:A:345:ASP:CB	1:A:375:GLY:HA3	2.46	0.45
1:A:10:THR:HG23	1:A:32:SER:CB	2.46	0.45
1:A:309:TYR:CD1	1:A:348:MET:HE1	2.50	0.45
1:A:345:ASP:HB2	1:A:375:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:O	1:A:32:SER:OG	2.25	0.45
1:A:3:GLN:NE2	1:A:286:GLN:O	2.50	0.45
1:A:590:LEU:HB3	1:A:597:GLY:HA3	1.98	0.45
1:A:202:HIS:CE1	1:A:268:THR:HB	2.51	0.45
1:A:333:LYS:HG2	1:A:334:LEU:H	1.80	0.45
1:A:610:CYS:SG	1:A:613:GLU:HG3	2.56	0.45
1:A:151:LEU:HD21	1:A:359:ALA:HB2	1.99	0.44
1:A:71:ASP:CG	1:A:73:GLY:H	2.20	0.44
1:A:406:SER:OG	1:A:471:HIS:CE1	2.70	0.44
1:A:585:ASN:O	1:A:599:PRO:HG3	2.17	0.44
1:A:427:ARG:O	1:A:429:LEU:HD13	2.16	0.44
1:A:205:ARG:O	1:A:208:MET:HG2	2.17	0.44
1:A:483:ASP:N	1:A:483:ASP:OD2	2.50	0.44
1:A:169:ASP:O	1:A:227:VAL:CG2	2.66	0.44
1:A:329:LYS:CB	1:A:595:HIS:HD2	2.31	0.44
1:A:657:LYS:HB2	1:A:660:ASN:ND2	2.33	0.43
1:A:203:VAL:CG2	1:A:229:LEU:HD13	2.49	0.43
1:A:327:ALA:HB3	1:A:334:LEU:HD11	1.98	0.43
1:A:329:LYS:CE	1:A:626:GLN:HE22	2.28	0.43
1:A:631:ASN:C	1:A:631:ASN:OD1	2.57	0.43
1:A:333:LYS:NZ	1:A:335:THR:HG22	2.34	0.43
1:A:330:ALA:C	1:A:331:LYS:CG	2.87	0.43
1:A:481:ALA:O	1:A:486:GLY:HA2	2.19	0.43
1:A:430:PHE:CZ	1:A:461:LYS:HG2	2.54	0.42
1:A:171:VAL:HG23	1:A:214:PHE:CE2	2.53	0.42
1:A:652:LYS:HA	1:A:653:PRO:HD3	1.93	0.42
1:A:485:LYS:HB2	6:A:808:HOH:O	2.18	0.42
1:A:38:THR:CG2	1:A:99:PRO:HD3	2.48	0.42
1:A:552:LEU:HD12	1:A:552:LEU:HA	1.72	0.42
1:A:596:LEU:HD22	1:A:625:LEU:HB3	2.00	0.42
1:A:598:ILE:HD12	1:A:627:CYS:HB3	2.01	0.42
1:A:401:ILE:CG2	1:A:402:SER:N	2.82	0.42
1:A:466:TRP:CZ3	1:A:542:VAL:HG13	2.55	0.41
1:A:621:GLU:N	1:A:622:PRO:CD	2.84	0.41
1:A:339:GLU:O	1:A:342:ASN:N	2.53	0.41
1:A:372:ARG:HG3	1:A:373:ASN:N	2.35	0.41
1:A:514:LEU:CD1	1:A:603:GLY:HA2	2.50	0.41
1:A:302:THR:HG21	1:A:414:PRO:HB3	2.03	0.41
1:A:123:ARG:HD3	1:A:147:GLY:O	2.20	0.41
1:A:347:TRP:CZ3	1:A:641:GLY:HA3	2.56	0.41
1:A:136:GLN:HB3	1:A:137:ARG:CG	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:PHE:HB2	1:A:584:PRO:HD2	2.01	0.41
1:A:368:PHE:CD1	1:A:392:VAL:HG13	2.56	0.41
1:A:428:ILE:O	1:A:460:VAL:N	2.46	0.41
1:A:156:ARG:HG2	1:A:386:GLY:HA2	2.03	0.41
1:A:100:LYS:HE2	1:A:100:LYS:HB3	1.89	0.40
1:A:636:TYR:O	1:A:639:ARG:N	2.46	0.40
1:A:115:ILE:HD13	1:A:187:THR:HG22	2.02	0.40
1:A:139:TRP:CD1	1:A:147:GLY:HA3	2.57	0.40
1:A:10:THR:HG23	1:A:32:SER: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	626/668 (94%)	609 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	563/591 (95%)	503 (89%)	60 (11%)	8	28
2	B	1/2 (50%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	564/593 (95%)	504 (89%)	60 (11%)	8	28

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	5	THR
1	A	10	THR
1	A	12	GLU
1	A	13	GLN
1	A	26	GLN
1	A	32	SER
1	A	49	VAL
1	A	50	VAL
1	A	52	ILE
1	A	67	THR
1	A	77	THR
1	A	79	THR
1	A	101	THR
1	A	110	LEU
1	A	117	LEU
1	A	123	ARG
1	A	135	ASP
1	A	136	GLN
1	A	137	ARG
1	A	146	GLN
1	A	153	ASN
1	A	154	CYS
1	A	169	ASP
1	A	173	ASP
1	A	191	LYS
1	A	198	THR
1	A	232	LYS
1	A	278	GLU
1	A	292	ARG
1	A	318	ASP
1	A	322	SER
1	A	325	THR
1	A	331	LYS
1	A	335	THR
1	A	339	GLU
1	A	346	GLN

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Mol	Chain	Res	Type
1	A	364	LEU
1	A	377	LYS
1	A	384	VAL
1	A	389	PHE
1	A	401	ILE
1	A	419	ARG
1	A	427	ARG
1	A	429	LEU
1	A	442	GLN
1	A	484	ARG
1	A	500	LEU
1	A	504	GLN
1	A	516	GLU
1	A	522	LYS
1	A	540	SER
1	A	557	LEU
1	A	570	LEU
1	A	595	HIS
1	A	596	LEU
1	A	609	ARG
1	A	635	THR
1	A	639	ARG
1	A	662	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	626	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
2	FIO	B	4	1,2	9,10,12	0.44	0	5,11,14	1.08	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	FIO	B	4	1,2	-	0/6/9/13	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.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	SO4	A	706	-	4,4,4	0.22	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	707	-	4,4,4	0.19	0	6,6,6	0.09	0
5	EDO	A	708	-	3,3,3	0.50	0	2,2,2	0.31	0
5	EDO	A	709	-	3,3,3	0.54	0	2,2,2	0.33	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	A	706	-	-	0/0/0/0	0/0/0/0
4	SO4	A	707	-	-	0/0/0/0	0/0/0/0
5	EDO	A	708	-	-	0/1/1/1	0/0/0/0
5	EDO	A	709	-	-	0/1/1/1	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	706	SO4	1	0
5	A	709	EDO	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 [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	636/668 (95%)	-0.08	18 (2%) 53 33	15, 40, 80, 112	0
2	B	1/5 (20%)	2.44	1 (100%) 0 0	69, 69, 69, 69	0
All	All	637/673 (94%)	-0.08	19 (2%) 51 30	15, 40, 80, 112	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	GLY	4.5
1	A	159	LEU	3.6
1	A	170	GLU	3.3
1	A	342	ASN	3.3
1	A	169	ASP	2.9
1	A	36	ASP	2.9
1	A	337	CYS	2.6
1	A	340	GLU	2.5
2	B	3	ASP	2.4
1	A	343	MET	2.3
1	A	309	TYR	2.3
1	A	318	ASP	2.3
1	A	98	GLY	2.2
1	A	374	ARG	2.2
1	A	54	HIS	2.1
1	A	338	PRO	2.1
1	A	68	TRP	2.1
1	A	336	ILE	2.0
1	A	397	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	FIO	B	4	11/13	0.91	0.32	-	49,55,63,65	0

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
4	SO4	A	706	5/5	0.92	0.29	1.65	51,65,83,96	0
5	EDO	A	708	4/4	0.95	0.20	1.21	25,27,29,34	0
3	CA	A	705	1/1	0.73	0.29	0.51	70,70,70,70	0
5	EDO	A	709	4/4	0.93	0.18	-0.68	25,33,34,37	0
3	CA	A	701	1/1	0.88	0.14	-1.37	39,39,39,39	0
3	CA	A	704	1/1	0.94	0.12	-1.55	56,56,56,56	0
3	CA	A	702	1/1	0.60	0.11	-1.63	60,60,60,60	0
3	CA	A	703	1/1	0.85	0.06	-2.76	64,64,64,64	0
4	SO4	A	707	5/5	0.95	0.17	-	61,68,84,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.