



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2018 – 11:33 AM EST

PDB ID : 5OYJ
Title : Crystal structure of VEGFR-2 domains 4-5 in complex with DARPin D4b
Authors : Piscitelli, C.L.; Thieltges, K.M.; Markovic-Mueller, S.; Binz, H.K.; Ballmer-Hofer, K.
Deposited on : 2017-09-10
Resolution : 2.38 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-20030736
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-20030736

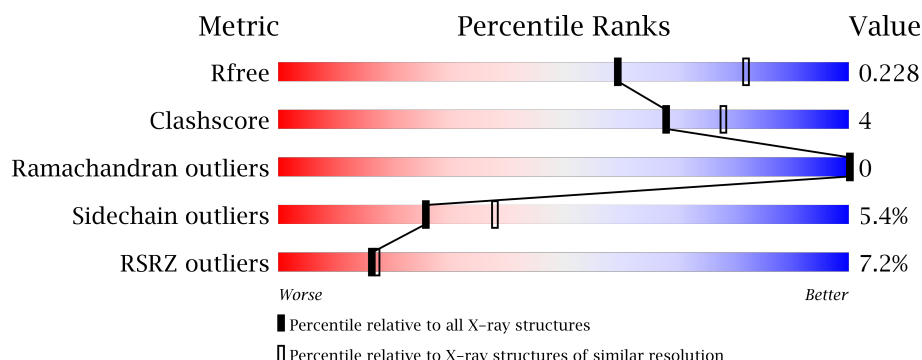
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	4388 (2.40-2.36)
Clashscore	112137	4984 (2.40-2.36)
Ramachandran outliers	110173	4907 (2.40-2.36)
Sidechain outliers	110143	4909 (2.40-2.36)
RSRZ outliers	101464	4423 (2.40-2.36)

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	169	<div> <div>4%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
1	B	169	<div> <div>11%</div> <div>82%</div> <div>9%</div> <div>7%</div> </div>
2	C	234	<div> <div>3%</div> <div>82%</div> <div>12%</div> <div>5%</div> </div>
2	D	234	<div> <div>10%</div> <div>80%</div> <div>12%</div> <div>7%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	TRE	B	201	-	-	-	X
5	TRE	C	612	-	-	-	X
5	TRE	D	607	-	-	-	X
6	NAG	C	601	-	-	-	X
6	NAG	C	607	-	-	-	X
7	CAC	C	610	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6506 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 DARPin D4b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	3	0
			1255	790	218	246	1			
1	B	157	Total	C	N	O	S	0	0	0
			1195	753	205	236	1			

- Molecule 2 is a protein called Vascular endothelial growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	223	Total	C	N	O	S	0	2	0
			1779	1137	304	332	6			
2	D	218	Total	C	N	O	S	0	0	0
			1728	1105	297	320	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	322	ALA	-	expression tag	UNP P35968
C	323	PRO	-	expression tag	UNP P35968
C	324	LEU	-	expression tag	UNP P35968
C	325	ALA	-	expression tag	UNP P35968
C	550	HIS	-	expression tag	UNP P35968
C	551	HIS	-	expression tag	UNP P35968
C	552	HIS	-	expression tag	UNP P35968
C	553	HIS	-	expression tag	UNP P35968
C	554	HIS	-	expression tag	UNP P35968
C	555	HIS	-	expression tag	UNP P35968
D	322	ALA	-	expression tag	UNP P35968
D	323	PRO	-	expression tag	UNP P35968
D	324	LEU	-	expression tag	UNP P35968
D	325	ALA	-	expression tag	UNP P35968
D	550	HIS	-	expression tag	UNP P35968
D	551	HIS	-	expression tag	UNP P35968

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Chain	Residue	Modelled	Actual	Comment	Reference
D	552	HIS	-	expression tag	UNP P35968
D	553	HIS	-	expression tag	UNP P35968
D	554	HIS	-	expression tag	UNP P35968
D	555	HIS	-	expression tag	UNP P35968

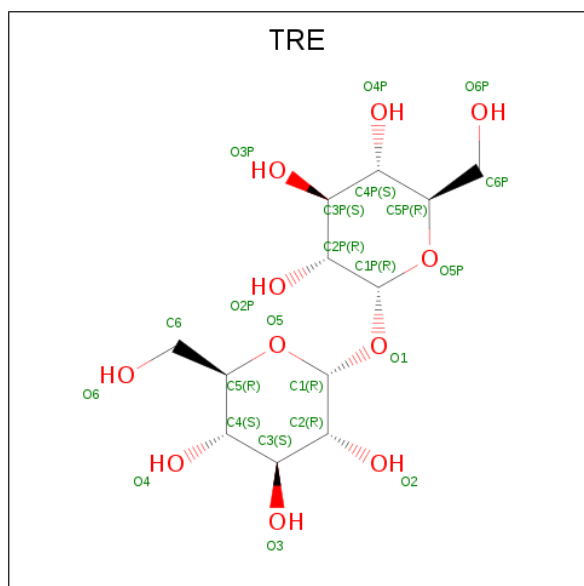
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Ca 3 3	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

- Molecule 5 is TREHALOSE (three-letter code: TRE) (formula: C₁₂H₂₂O₁₁).



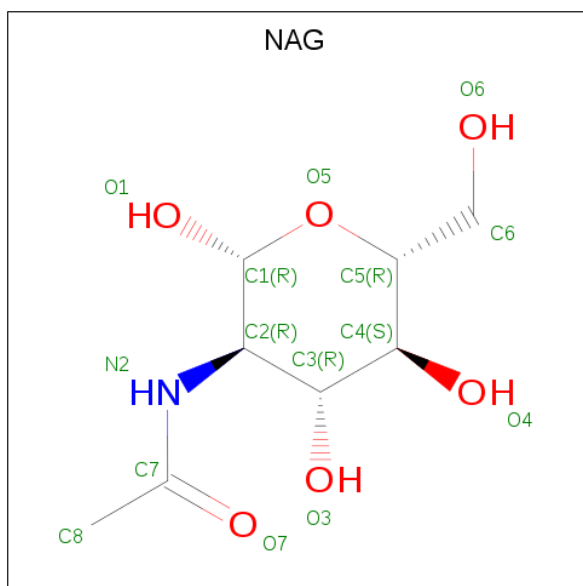
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 23 12 11	0	0
5	C	1	Total C O 23 12 11	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



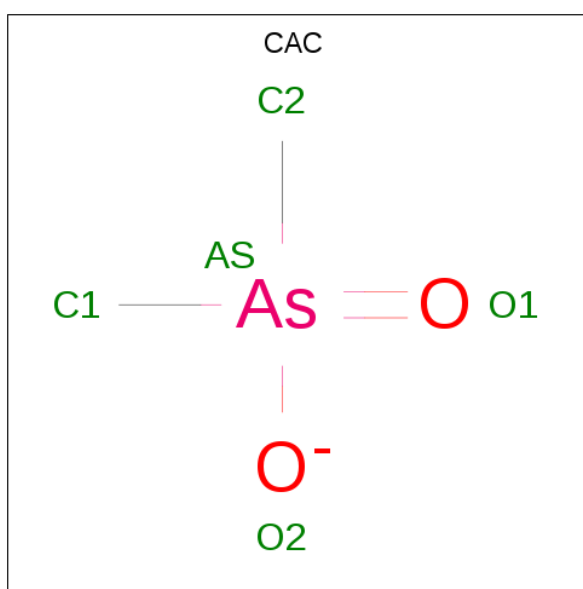
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

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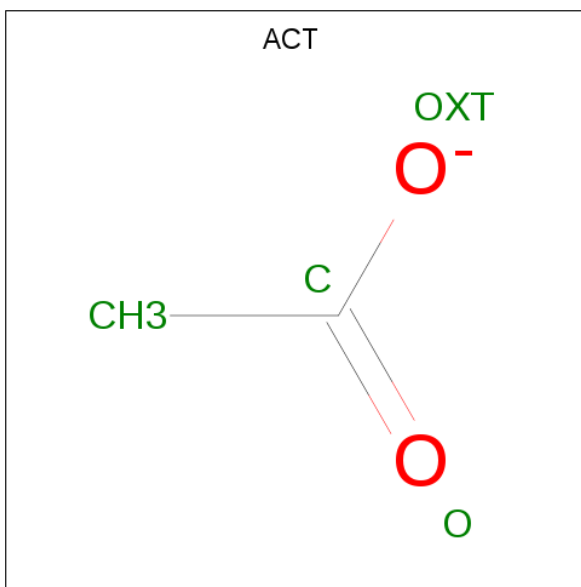
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	75	Total	O	0	0
			75	75		
9	B	43	Total	O	0	0
			43	43		
9	C	102	Total	O	0	0
			102	102		
9	D	50	Total	O	0	0
			50	50		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.49 Å 164.56 Å 70.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.75 – 2.38 53.65 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.75-2.38) 99.0 (53.65-2.38)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.37 Å)	Xtriage
Refinement program	PHENIX (dev_2722: ???)	Depositor
R, R_{free}	0.178 , 0.229 0.177 , 0.228	Depositor DCC
R_{free} test set	2581 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6506	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NA, CA, TRE, ACT, CAC

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	0.45	0/1279	0.60	0/1732
1	B	0.38	0/1215	0.57	0/1646
2	C	0.54	0/1833	0.68	0/2498
2	D	0.44	0/1775	0.61	0/2417
All	All	0.47	0/6102	0.62	0/8293

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	1255	0	1204	9	0
1	B	1195	0	1163	12	0
2	C	1779	0	1747	13	0
2	D	1728	0	1701	19	0
3	A	3	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
5	B	23	0	22	0	0
5	C	23	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	23	0	22	0	0
6	C	112	0	100	1	0
6	D	84	0	75	3	0
7	C	5	0	0	1	8
8	C	4	0	3	0	0
9	A	75	0	0	1	0
9	B	43	0	0	1	1
9	C	102	0	0	0	1
9	D	50	0	0	1	0
All	All	6506	0	6059	54	9

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 4.

All (54) 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:C:496:LYS:HD3	2:C:520:GLN:HG3	1.56	0.85
1:B:45:GLN:CD	1:B:45:GLN:H	1.93	0.71
2:C:330:VAL:HG12	2:C:407:GLU:HG2	1.71	0.71
2:D:423:ILE:HD12	2:D:447:VAL:HG22	1.75	0.67
2:C:358:PRO:HG2	2:C:403:PRO:HG2	1.77	0.67
2:D:541:ARG:HH21	2:D:541:ARG:HB2	1.61	0.65
1:A:61[B]:GLU:CD	1:A:61[B]:GLU:H	2.02	0.63
2:D:382:VAL:O	9:D:701:HOH:O	2.17	0.60
1:B:84:LEU:HD13	1:B:116:PRO:HG2	1.85	0.59
2:C:496:LYS:HG2	6:C:608:NAG:H82	1.87	0.56
2:D:329:PHE:CZ	2:D:356:GLY:HA2	2.41	0.56
2:D:367:ASN:O	2:D:369:ILE:HD12	2.07	0.55
1:A:56:TRP:CD1	1:A:86:LEU:HB3	2.42	0.54
2:C:362:ILE:HD12	2:C:381:HIS:HA	1.88	0.54
2:D:487:SER:OG	2:D:489:GLU:OE1	2.26	0.54
1:A:27:ASP:OD1	1:A:61[B]:GLU:HG2	2.07	0.54
2:D:391:ARG:HH12	6:D:602:NAG:H83	1.73	0.54
6:D:603:NAG:H62	6:D:604:NAG:HN2	1.73	0.53
1:A:126:LEU:HD12	1:A:161:LEU:HD13	1.91	0.53
2:D:329:PHE:CE1	2:D:356:GLY:HA2	2.44	0.52
1:B:93:LEU:HD11	1:B:131:VAL:HG21	1.92	0.51
2:D:497:ILE:HD13	2:D:517:LEU:HD21	1.93	0.51
2:D:497:ILE:HG21	2:D:517:LEU:HD11	1.94	0.48
1:A:31:ARG:NH2	9:A:503:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:GLY:O	1:B:68:LYS:HE3	2.13	0.48
2:C:430:SER:HB2	2:C:431:PRO:HD3	1.96	0.47
2:D:391:ARG:NH1	6:D:602:NAG:H83	2.30	0.47
1:B:26:GLN:O	1:B:30:VAL:HG13	2.15	0.47
2:C:448:TYR:OH	2:C:450:ILE:HD11	2.15	0.47
2:D:541:ARG:NH2	2:D:541:ARG:HB2	2.28	0.46
1:B:84:LEU:HD13	1:B:116:PRO:CG	2.44	0.46
2:C:464:GLU:OE1	7:C:610:CAC:AS	2.93	0.46
1:A:43:HIS:HA	1:A:48:PHE:O	2.17	0.45
2:C:421:PRO:HA	2:C:449:ALA:HB2	1.98	0.45
1:B:56:TRP:CD1	1:B:86:LEU:HB3	2.53	0.44
2:D:324:LEU:HA	2:D:324:LEU:HD12	1.69	0.44
1:B:84:LEU:CD1	1:B:116:PRO:HG2	2.46	0.44
1:B:42:ALA:O	1:B:50:PRO:HD3	2.18	0.44
2:C:483:GLU:HG3	2:C:484:GLU:HG3	2.00	0.44
2:D:428:LEU:HD11	2:D:543:ILE:CD1	2.48	0.44
2:D:506:LEU:HD21	2:D:509:GLY:HA2	2.01	0.43
2:C:426:LYS:HD3	2:C:426:LYS:HA	1.84	0.43
2:D:374:ASN:N	2:D:374:ASN:OD1	2.52	0.43
1:A:61[B]:GLU:CD	1:A:61[B]:GLU:N	2.70	0.43
1:B:94:GLU:O	1:B:98:VAL:HG23	2.19	0.42
2:C:436:GLN:O	2:C:439:THR:HG23	2.19	0.42
2:D:362:ILE:HD13	2:D:381:HIS:CD2	2.55	0.42
1:B:30:VAL:O	1:B:34:MET:HG2	2.20	0.41
2:D:421:PRO:HA	2:D:449:ALA:HB2	2.03	0.41
1:A:126:LEU:HD11	1:A:161:LEU:HB2	2.03	0.40
1:A:27:ASP:OD1	1:A:62:ILE:HG13	2.22	0.40
1:B:168:LEU:HD22	9:B:343:HOH:O	2.21	0.40
2:C:407:GLU:HG3	2:C:408:LYS:N	2.36	0.40
2:D:428:LEU:HD13	2:D:428:LEU:HA	1.80	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:610:CAC:C1	7:C:610:CAC:C2[2_465]	0.04	2.16
7:C:610:CAC:O1	7:C:610:CAC:O2[2_465]	0.12	2.08
7:C:610:CAC:AS	7:C:610:CAC:O2[2_465]	1.74	0.46
7:C:610:CAC:AS	7:C:610:CAC:O1[2_465]	1.74	0.46
7:C:610:CAC:C2	7:C:610:CAC:C2[2_465]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:610:CAC:AS	7:C:610:CAC:C1[2_465]	1.96	0.24
7:C:610:CAC:AS	7:C:610:CAC:C2[2_465]	1.96	0.24
7:C:610:CAC:C1	7:C:610:CAC:C1[2_465]	1.98	0.22
9:B:313:HOH:O	9:C:768:HOH:O[4_454]	2.01	0.19

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	162/169 (96%)	157 (97%)	5 (3%)	0	100	100
1	B	155/169 (92%)	154 (99%)	1 (1%)	0	100	100
2	C	221/234 (94%)	216 (98%)	5 (2%)	0	100	100
2	D	214/234 (92%)	210 (98%)	4 (2%)	0	100	100
All	All	752/806 (93%)	737 (98%)	15 (2%)	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	128/132 (97%)	122 (95%)	6 (5%)	30	45
1	B	122/132 (92%)	117 (96%)	5 (4%)	35	52
2	C	198/206 (96%)	186 (94%)	12 (6%)	22	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	192/206 (93%)	180 (94%)	12 (6%)	21	30
All	All	640/676 (95%)	605 (94%)	35 (6%)	26	37

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	12	SER
1	A	13	ASP
1	A	61[A]	GLU
1	A	61[B]	GLU
1	A	167	LYS
1	B	45	GLN
1	B	61	GLU
1	B	68	LYS
1	B	84	LEU
1	B	111	GLU
2	C	324	LEU
2	C	375	HIS
2	C	407	GLU
2	C	428	LEU
2	C	432	VAL
2	C	455	HIS
2	C	468	ASN
2	C	469	GLU
2	C	496	LYS
2	C	510	LYS
2	C	538	ARG
2	C	551	HIS
2	D	324	LEU
2	D	374	ASN
2	D	389	SER
2	D	422	GLN
2	D	428	LEU
2	D	466	CYS
2	D	507	ILE
2	D	536	VAL
2	D	541	ARG
2	D	544	SER
2	D	551	HIS
2	D	553	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 24 ligands modelled in this entry, 5 are monoatomic - leaving 19 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	$\# Z > 2$
5	TRE	B	201	-	24,24,24	0.48	0	35,35,35	0.82	2 (5%)
6	NAG	C	601	2,6	14,14,15	0.40	0	15,19,21	0.48	0
6	NAG	C	602	6	14,14,15	0.51	0	15,19,21	0.52	0
6	NAG	C	603	2,4,6	14,14,15	0.29	0	15,19,21	0.65	0
6	NAG	C	604	6	14,14,15	0.32	0	15,19,21	0.45	0
6	NAG	C	605	2,6	14,14,15	0.34	0	15,19,21	0.66	0
6	NAG	C	606	6	14,14,15	0.49	0	15,19,21	0.42	0
6	NAG	C	607	2,6	14,14,15	0.47	0	15,19,21	0.53	0
6	NAG	C	608	6	14,14,15	0.36	0	15,19,21	0.53	0
7	CAC	C	610	-	0,4,4	0.00	-	0,6,6	0.00	-
8	ACT	C	611	-	1,3,3	7.90	1 (100%)	0,3,3	0.00	-
5	TRE	C	612	-	24,24,24	0.61	0	35,35,35	0.82	0
6	NAG	D	601	2,6	14,14,15	0.34	0	15,19,21	0.62	0
6	NAG	D	602	6	14,14,15	0.44	0	15,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	603	2,6	14,14,15	0.43	0	15,19,21	0.54	0
6	NAG	D	604	6	14,14,15	0.46	0	15,19,21	0.51	0
6	NAG	D	605	2,6	14,14,15	1.19	1 (7%)	15,19,21	2.07	1 (6%)
6	NAG	D	606	6	14,14,15	0.27	0	15,19,21	0.57	0
5	TRE	D	607	-	24,24,24	0.53	0	35,35,35	1.26	4 (11%)

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
5	TRE	B	201	-	-	0/8/48/48	0/2/2/2
6	NAG	C	601	2,6	-	0/6/23/26	0/1/1/1
6	NAG	C	602	6	-	0/6/23/26	0/1/1/1
6	NAG	C	603	2,4,6	-	0/6/23/26	0/1/1/1
6	NAG	C	604	6	-	0/6/23/26	0/1/1/1
6	NAG	C	605	2,6	-	0/6/23/26	0/1/1/1
6	NAG	C	606	6	-	0/6/23/26	0/1/1/1
6	NAG	C	607	2,6	-	0/6/23/26	0/1/1/1
6	NAG	C	608	6	-	0/6/23/26	0/1/1/1
7	CAC	C	610	-	-	0/0/0/0	0/0/0/0
8	ACT	C	611	-	-	0/0/0/0	0/0/0/0
5	TRE	C	612	-	-	0/8/48/48	0/2/2/2
6	NAG	D	601	2,6	-	0/6/23/26	0/1/1/1
6	NAG	D	602	6	-	0/6/23/26	0/1/1/1
6	NAG	D	603	2,6	-	0/6/23/26	0/1/1/1
6	NAG	D	604	6	-	0/6/23/26	0/1/1/1
6	NAG	D	605	2,6	-	0/6/23/26	0/1/1/1
6	NAG	D	606	6	-	0/6/23/26	0/1/1/1
5	TRE	D	607	-	-	0/8/48/48	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	605	NAG	O5-C1	4.34	1.50	1.43
8	C	611	ACT	CH3-C	7.90	1.58	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	607	TRE	C4-C3-C2	-2.68	106.12	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	201	TRE	C1P-O1-C1	-2.21	110.38	114.37
5	D	607	TRE	C1-C2-C3	-2.14	106.00	109.98
5	D	607	TRE	C3P-C4P-C5P	-2.01	106.67	110.22
5	B	201	TRE	O1-C1-C2	2.13	112.91	108.11
5	D	607	TRE	C1P-O1-C1	2.82	119.47	114.37
6	D	605	NAG	C1-O5-C5	7.78	122.88	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	608	NAG	1	0
7	C	610	CAC	1	8
6	D	602	NAG	2	0
6	D	603	NAG	1	0
6	D	604	NAG	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	161/169 (95%)	0.59	6 (3%) 42 45	33, 46, 72, 213	0
1	B	157/169 (92%)	0.56	18 (11%) 5 6	43, 67, 118, 138	0
2	C	223/234 (95%)	0.31	8 (3%) 43 46	32, 49, 118, 158	0
2	D	218/234 (93%)	0.64	23 (10%) 7 7	39, 64, 136, 172	0
All	All	759/806 (94%)	0.52	55 (7%) 16 17	32, 56, 124, 213	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	427	SER	9.6
2	D	428	LEU	7.0
2	C	324	LEU	6.4
1	A	10	HIS	6.1
2	D	426	LYS	6.0
2	D	482	CYS	5.7
1	A	9	HIS	5.3
1	B	32	ILE	5.3
1	B	33	LEU	5.1
1	B	35	ALA	5.0
2	C	322	ALA	4.8
2	D	429	ILE	4.8
2	D	481	PRO	4.6
2	D	483	GLU	4.5
2	D	466	CYS	4.3
2	D	465	GLU	4.3
1	B	30	VAL	4.2
1	B	28	ASP	4.2
1	B	34	MET	4.1
1	B	31	ARG	4.0
2	C	430	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	169	ASN	3.8
1	B	36	ASN	3.7
2	D	507	ILE	3.7
2	D	508	GLU	3.6
2	D	425	GLU	3.6
1	A	11	GLY	3.5
2	C	478	ASN	3.2
2	D	322	ALA	3.1
1	A	168	LEU	3.0
2	D	464	GLU	3.0
2	D	506	LEU	3.0
2	D	553	HIS	3.0
2	C	480	TYR	2.9
1	B	14	LEU	2.8
1	B	27	ASP	2.8
2	C	431	PRO	2.7
1	B	37	GLY	2.7
1	B	169	ASN	2.7
2	C	552	HIS	2.7
2	D	541	ARG	2.6
1	B	13	ASP	2.6
2	D	485	TRP	2.5
1	B	168	LEU	2.5
1	B	29	GLU	2.4
1	A	76[A]	PHE	2.4
1	B	18	LEU	2.3
1	B	65	VAL	2.3
2	D	423	ILE	2.3
2	D	492	GLN	2.3
2	C	428	LEU	2.2
2	D	462	LEU	2.2
2	D	461	GLN	2.2
1	B	40	VAL	2.1
2	D	489	GLU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
5	TRE	C	612	23/23	0.77	0.28	5.49	78,122,132,138	0
5	TRE	D	607	23/23	0.51	0.40	3.84	103,133,150,158	0
6	NAG	C	607	14/15	0.87	0.23	3.13	73,94,111,120	0
6	NAG	C	601	14/15	0.84	0.27	2.85	91,109,125,142	0
5	TRE	B	201	23/23	0.73	0.25	2.23	87,121,129,132	0
3	CA	A	402	1/1	0.97	0.20	1.58	64,64,64,64	0
8	ACT	C	611	4/4	0.90	0.18	1.14	48,72,73,86	0
6	NAG	D	601	14/15	0.83	0.24	1.03	79,96,109,121	0
4	NA	A	404	1/1	0.92	0.14	-	63,63,63,63	0
6	NAG	C	606	14/15	0.88	0.23	-	66,101,113,115	0
6	NAG	D	602	14/15	0.86	0.40	-	126,130,135,135	0
6	NAG	D	603	14/15	0.86	0.31	-	89,116,127,143	0
3	CA	C	609	1/1	0.89	0.22	-	83,83,83,83	0
6	NAG	D	605	14/15	0.85	0.39	-	99,116,125,133	0
6	NAG	D	606	14/15	0.72	0.37	-	129,145,151,152	0
7	CAC	C	610	5/5	0.90	0.19	-	141,149,155,155	0
3	CA	A	403	1/1	0.93	0.08	-	106,106,106,106	0
6	NAG	C	603	14/15	0.94	0.12	-	56,70,88,100	0
3	CA	A	401	1/1	0.95	0.16	-	87,87,87,87	0
6	NAG	D	604	14/15	0.32	0.55	-	140,153,157,157	0
6	NAG	C	602	14/15	0.66	0.34	-	143,162,168,168	0
6	NAG	C	608	14/15	0.83	0.38	-	133,139,140,140	0
6	NAG	C	605	14/15	0.96	0.11	-	36,57,68,71	0
6	NAG	C	604	14/15	0.85	0.13	-	90,106,121,129	0

6.5 Other polymers ⓘ

There are no such residues in this entry.