



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:12 PM UTC

PDB ID : 2RKZ / pdb_00002rkz
Title : Crystal structure of the second and third fibronectin f1 modules in complex with a fragment of staphylococcus aureus fnbpa-1
Authors : Bingham, R.J.
Deposited on : 2007-10-18
Resolution : 2.00 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

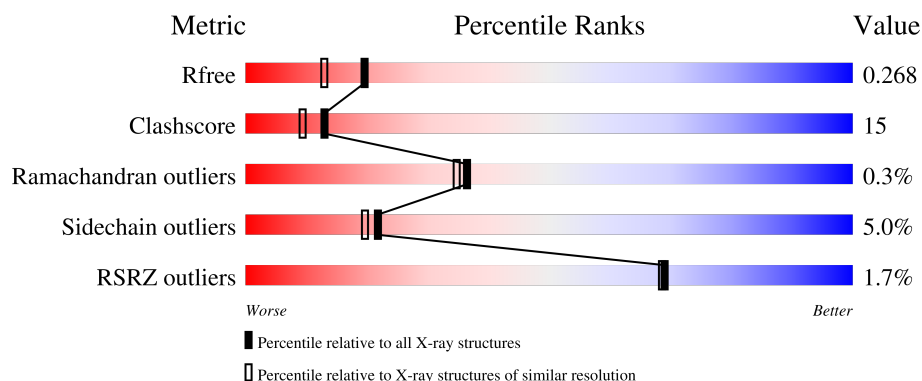
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	90	 83% 16% .
1	B	90	 79% 18% ..
1	C	90	 86% 13% .
1	D	90	 2% 71% 21% . .
1	E	90	 3% 69% 16% 6% 10%

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Mol	Chain	Length	Quality of chain
1	F	90	3% 78% 18% • •
2	M	23	78% • 17%
2	N	23	4% 52% 22% 9% 17%
2	O	23	78% 9% 13%
2	P	23	4% 78% 17% •
2	Q	23	4% 57% 22% 9% 13%
2	R	23	74% 9% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5928 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 Fibronectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	89	Total	C	N	O	S	0	1	0
			702	431	126	135	10			
1	B	89	Total	C	N	O	S	0	2	0
			707	435	126	135	11			
1	C	90	Total	C	N	O	S	0	0	0
			699	428	127	134	10			
1	D	86	Total	C	N	O	S	0	1	0
			683	421	123	129	10			
1	E	81	Total	C	N	O	S	0	0	0
			635	388	116	122	9			
1	F	89	Total	C	N	O	S	0	1	0
			702	430	126	136	10			

- Molecule 2 is a protein called peptide from Fibronectin-binding protein A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	19	Total	C	N	O	0	0	0
			143	87	20	36			
2	N	19	Total	C	N	O	0	1	0
			160	101	22	37			
2	O	20	Total	C	N	O	0	0	0
			164	101	23	40			
2	P	22	Total	C	N	O	0	0	1
			167	102	25	40			
2	Q	20	Total	C	N	O	0	0	0
			164	101	23	40			
2	R	19	Total	C	N	O	0	0	0
			156	97	22	37			

There are 12 discrepancies between the modelled and reference sequences:

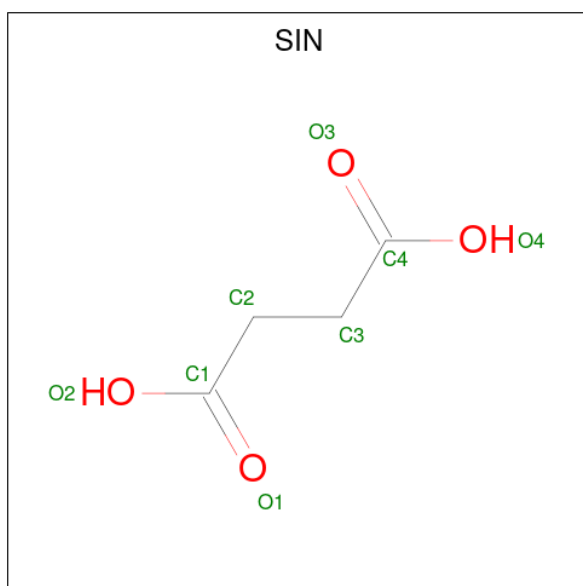
Chain	Residue	Modelled	Actual	Comment	Reference
M	528	ACE	-	acetylation	UNP P14738

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Chain	Residue	Modelled	Actual	Comment	Reference
M	550	NH2	-	amidation	UNP P14738
N	528	ACE	-	acetylation	UNP P14738
N	550	NH2	-	amidation	UNP P14738
O	528	ACE	-	acetylation	UNP P14738
O	550	NH2	-	amidation	UNP P14738
P	528	ACE	-	acetylation	UNP P14738
P	550	NH2	-	amidation	UNP P14738
Q	528	ACE	-	acetylation	UNP P14738
Q	550	NH2	-	amidation	UNP P14738
R	528	ACE	-	acetylation	UNP P14738
R	550	NH2	-	amidation	UNP P14738

- Molecule 3 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	134	Total 134	O 134	0	0
4	C	106	Total 106	O 106	0	0
4	D	100	Total 100	O 100	0	0
4	E	77	Total 77	O 77	0	0
4	F	90	Total 90	O 90	0	0
4	M	26	Total 26	O 26	0	0
4	N	44	Total 44	O 44	0	0
4	O	41	Total 41	O 41	0	0
4	P	32	Total 32	O 32	0	0
4	Q	23	Total 23	O 23	0	0
4	R	30	Total 30	O 30	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Fibronectin

Chain A: 



- Molecule 1: Fibronectin

Chain B: 



- Molecule 1: Fibronectin

Chain C: 



- Molecule 1: Fibronectin

Chain D: 



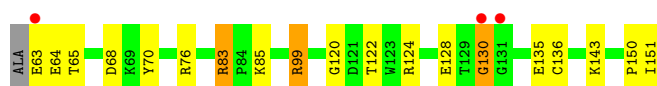
- Molecule 1: Fibronectin

Chain E: 

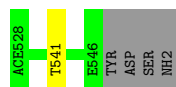
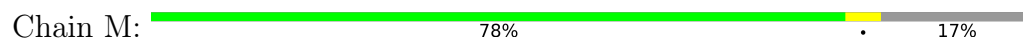


- Molecule 1: Fibronectin

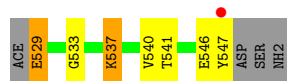
Chain F: 



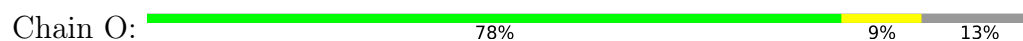
- Molecule 2: peptide from Fibronectin-binding protein A



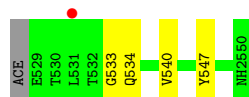
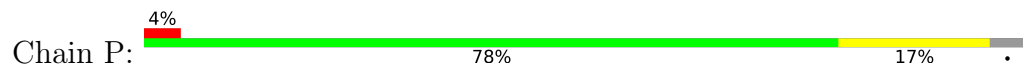
- Molecule 2: peptide from Fibronectin-binding protein A



- Molecule 2: peptide from Fibronectin-binding protein A



- Molecule 2: peptide from Fibronectin-binding protein A



- Molecule 2: peptide from Fibronectin-binding protein A



- Molecule 2: peptide from Fibronectin-binding protein A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.59Å 109.72Å 71.47Å 90.00° 96.94° 90.00°	Depositor
Resolution (Å)	25.58 – 2.00 25.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.58-2.00) 99.9 (25.58-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.4.0013	Depositor
R, R_{free}	0.197 , 0.261 (Not available) , 0.268	Depositor DCC
R_{free} test set	3086 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5928	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% 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: ACE, NH2, SIN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.87	0/721	0.92	1/970 (0.1%)
1	B	0.97	0/729	0.95	0/980
1	C	0.90	0/715	0.96	0/962
1	D	0.89	0/701	0.93	0/942
1	E	0.73	0/648	0.85	1/871 (0.1%)
1	F	0.78	0/721	0.88	1/970 (0.1%)
2	M	0.77	0/141	0.87	0/193
2	N	0.89	0/164	0.88	0/223
2	O	0.92	0/165	0.87	0/224
2	P	0.88	0/167	0.80	0/227
2	Q	0.89	0/165	0.88	0/224
2	R	0.81	0/157	0.82	0/213
All	All	0.86	0/5194	0.91	3/6999 (0.0%)

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
2	N	0	1
2	Q	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	98	GLY	N-CA-C	-5.23	108.13	114.92
1	F	120	GLY	N-CA-C	-5.19	108.46	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
1	A	95	ILE	N-CA-C	-5.08	106.72	111.45

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	529	GLU	Peptide
2	Q	535	TYR	Peptide

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	702	0	654	8	0
1	B	707	0	663	20	0
1	C	699	0	646	11	0
1	D	683	0	639	37	0
1	E	635	0	589	27	0
1	F	702	0	652	24	0
2	M	143	0	127	1	0
2	N	160	0	152	13	0
2	O	164	0	147	3	0
2	P	167	0	148	6	0
2	Q	164	0	147	9	0
2	R	156	0	143	2	0
3	A	8	0	4	0	0
3	B	8	0	4	0	0
3	C	8	0	4	2	0
4	A	119	0	0	1	2
4	B	134	0	0	4	1
4	C	106	0	0	4	0
4	D	100	0	0	9	1
4	E	77	0	0	2	0
4	F	90	0	0	6	0
4	M	26	0	0	0	0
4	N	44	0	0	4	0
4	O	41	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	32	0	0	0	0
4	Q	23	0	0	2	0
4	R	30	0	0	0	0
All	All	5928	0	4719	147	2

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 15.

All (147) 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:E:124:ARG:CG	1:E:124:ARG:HH11	1.64	1.10
1:E:124:ARG:HH11	1:E:124:ARG:HG3	1.16	1.09
2:N:537:LYS:HG2	4:N:621:HOH:O	1.56	1.05
4:A:330:HOH:O	1:D:62:ALA:HB2	1.54	1.04
1:D:125:ARG:C	1:D:133:MET:CE	2.30	1.04
1:D:125:ARG:C	1:D:133:MET:HE1	1.83	1.02
1:F:99:ARG:HG2	1:F:99:ARG:HH11	0.85	1.00
1:F:99:ARG:HH11	1:F:99:ARG:CG	1.78	0.94
1:D:127:HIS:CD2	1:D:132:TYR:CE2	2.56	0.93
1:F:99:ARG:HG2	1:F:99:ARG:NH1	1.64	0.93
2:Q:531:LEU:H	2:Q:531:LEU:HD23	1.32	0.93
1:D:127:HIS:CD2	1:D:132:TYR:HE2	1.87	0.91
1:E:125:ARG:HB2	1:E:126:PRO:HD2	1.50	0.91
1:E:70:TYR:CZ	1:E:85:LYS:HD2	2.08	0.89
1:D:111:HIS:HB3	4:D:267:HOH:O	1.74	0.88
1:E:70:TYR:OH	1:E:85:LYS:HE3	1.74	0.88
2:N:547:TYR:HE2	4:N:633:HOH:O	1.58	0.87
1:E:124:ARG:HG3	1:E:124:ARG:NH1	1.85	0.86
1:F:63:GLU:HG3	1:F:63:GLU:O	1.77	0.83
1:D:125:ARG:C	1:D:133:MET:HE2	2.04	0.80
1:F:63:GLU:O	1:F:63:GLU:CG	2.30	0.80
1:D:126:PRO:HD3	4:D:225:HOH:O	1.81	0.79
1:E:88:MET:C	1:E:89:ILE:HD13	2.06	0.79
1:D:70:TYR:OH	1:D:85:LYS:HE3	1.82	0.78
1:D:126:PRO:CD	4:D:225:HOH:O	2.31	0.78
1:E:88:MET:O	1:E:89:ILE:HD13	1.84	0.78
1:D:126:PRO:N	1:D:133:MET:CE	2.46	0.78
1:D:125:ARG:O	1:D:133:MET:HE2	1.86	0.76
1:E:125:ARG:O	1:E:134:LEU:HB2	1.87	0.75
2:N:546:GLU:O	2:N:547:TYR:CD1	2.40	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ARG:HG2	1:D:151:ILE:HD11	1.70	0.74
1:E:125:ARG:CB	1:E:126:PRO:HD2	2.16	0.74
1:D:126:PRO:N	1:D:133:MET:HE1	2.05	0.72
1:D:125:ARG:CA	1:D:133:MET:HE1	2.20	0.71
2:Q:531:LEU:HD23	2:Q:531:LEU:N	2.04	0.71
1:E:70:TYR:CE2	1:E:85:LYS:HD2	2.25	0.71
1:F:76:ARG:NH2	4:F:203:HOH:O	2.24	0.69
1:C:108:ASN:OD1	4:C:301:HOH:O	2.09	0.69
2:Q:531:LEU:N	2:Q:531:LEU:CD2	2.56	0.69
1:F:150:PRO:HG2	2:R:529:GLU:HG3	1.76	0.68
1:E:85:LYS:O	1:E:86:ASP:HB2	1.94	0.67
1:E:124:ARG:HH11	1:E:124:ARG:HG2	1.58	0.67
1:B:99:ARG:NH1	1:B:99:ARG:HG2	2.09	0.67
2:Q:531:LEU:H	2:Q:531:LEU:CD2	2.07	0.66
2:Q:543:VAL:HG22	2:Q:544:GLU:N	2.09	0.66
1:D:127:HIS:HD2	1:D:132:TYR:CE2	2.12	0.65
2:N:546:GLU:O	2:N:547:TYR:HD1	1.81	0.64
1:F:68:ASP:OD2	1:F:83:ARG:HD3	1.99	0.63
2:N:546:GLU:C	2:N:547:TYR:CD1	2.78	0.62
1:D:62:ALA:HB1	4:D:268:HOH:O	2.00	0.61
1:D:126:PRO:CG	4:D:225:HOH:O	2.45	0.61
1:E:124:ARG:C	1:E:125:ARG:HG3	2.25	0.60
1:D:127:HIS:ND1	1:D:127:HIS:C	2.60	0.60
1:E:63:GLU:HG2	4:E:225:HOH:O	2.01	0.59
1:D:135:GLU:HG2	1:D:151:ILE:HG12	1.84	0.59
1:B:98:GLY:C	1:B:99:ARG:HG3	2.27	0.59
2:N:547:TYR:HA	4:N:630:HOH:O	2.01	0.59
1:F:70:TYR:CE2	1:F:85:LYS:HG3	2.39	0.58
2:Q:543:VAL:CG2	2:Q:544:GLU:N	2.67	0.58
1:F:99:ARG:CG	1:F:99:ARG:NH1	2.47	0.58
1:B:99:ARG:HG2	1:B:99:ARG:HH11	1.67	0.57
1:E:125:ARG:CB	1:E:126:PRO:CD	2.81	0.57
1:B:99:ARG:HH11	1:B:99:ARG:CG	2.16	0.57
1:E:124:ARG:CG	1:E:124:ARG:NH1	2.37	0.57
1:E:70:TYR:OH	1:E:85:LYS:CE	2.52	0.57
1:C:127:HIS:CE1	3:C:201:SIN:H21	2.40	0.56
1:F:124:ARG:HE	1:F:151:ILE:CD1	2.18	0.55
1:E:125:ARG:HB2	1:E:126:PRO:CD	2.28	0.55
2:N:540[A]:VAL:HG12	4:N:616:HOH:O	2.05	0.55
1:D:126:PRO:CA	1:D:133:MET:CE	2.85	0.55
1:D:70:TYR:CZ	1:D:85:LYS:HE3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LYS:NZ	4:D:205:HOH:O	2.40	0.54
1:B:81:TYR:OH	1:B:102:ILE:HD13	2.09	0.53
1:E:70:TYR:CZ	1:E:85:LYS:CD	2.87	0.53
1:C:62:ALA:N	4:C:309:HOH:O	2.42	0.53
1:C:80:THR:HB	4:C:331:HOH:O	2.09	0.53
2:O:547:TYR:CZ	2:P:540:VAL:HG22	2.44	0.53
1:F:63:GLU:HG2	4:F:261:HOH:O	2.08	0.52
1:B:99:ARG:NH1	1:B:99:ARG:CG	2.73	0.52
1:B:63:GLU:O	1:B:63:GLU:HG2	2.09	0.52
1:B:63:GLU:O	1:B:63:GLU:CG	2.56	0.52
1:B:151:ILE:HG22	4:B:388:HOH:O	2.09	0.52
1:F:70:TYR:CD1	1:F:83:ARG:HD2	2.45	0.51
1:C:85:LYS:O	1:C:86:ASP:HB2	2.10	0.51
1:F:130:GLY:CA	4:F:232:HOH:O	2.58	0.51
1:F:122[A]:THR:HG21	1:F:135:GLU:OE2	2.12	0.50
1:B:118:LYS:HD2	4:B:400:HOH:O	2.11	0.50
1:F:124:ARG:NE	1:F:151:ILE:HD12	2.27	0.50
2:Q:529:GLU:N	4:Q:602:HOH:O	2.45	0.49
2:Q:537:LYS:HE2	4:Q:617:HOH:O	2.12	0.49
1:E:86:ASP:C	1:E:87:SER:OG	2.55	0.49
1:C:97:ALA:HB3	1:C:101:ARG:HD3	1.94	0.49
2:O:540:VAL:HG22	2:P:547:TYR:CZ	2.48	0.49
1:C:70:TYR:OH	1:C:85:LYS:HE3	2.13	0.48
1:C:69:LYS:HE3	1:C:70:TYR:CZ	2.49	0.48
1:F:143:LYS:NZ	4:F:205:HOH:O	2.31	0.48
1:F:124:ARG:HE	1:F:151:ILE:HD12	1.79	0.48
1:A:135:GLU:HB2	1:A:151:ILE:HD13	1.95	0.48
1:F:64:GLU:OE1	4:F:201:HOH:O	2.20	0.48
2:N:546:GLU:C	2:N:547:TYR:CG	2.91	0.48
1:D:146:TRP:CZ2	2:P:533:GLY:HA3	2.49	0.47
1:D:133:MET:CE	4:D:225:HOH:O	2.64	0.46
2:N:547:TYR:O	2:N:547:TYR:CD2	2.68	0.46
1:C:80:THR:HG23	4:C:384:HOH:O	2.15	0.46
1:D:146:TRP:CE2	2:P:533:GLY:HA3	2.51	0.45
1:F:124:ARG:NE	1:F:151:ILE:CD1	2.79	0.45
1:B:64:GLU:HB3	1:B:77:VAL:HG23	1.99	0.45
1:D:126:PRO:CA	1:D:133:MET:HE3	2.47	0.45
1:E:124:ARG:O	1:E:125:ARG:HG3	2.15	0.45
1:E:134:LEU:HA	1:E:149:LYS:O	2.16	0.45
1:B:137[A]:VAL:HG12	1:B:147:THR:OG1	2.17	0.45
1:E:86:ASP:O	1:E:87:SER:OG	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:CD1	1:A:140:GLY:HA3	2.46	0.44
1:E:143:LYS:NZ	4:E:201:HOH:O	2.31	0.44
1:E:92:CYS:HA	1:E:103:SER:O	2.17	0.44
1:D:67:PHE:HE2	4:D:290:HOH:O	2.00	0.44
1:B:86:ASP:O	1:B:87:SER:HB2	2.18	0.43
1:D:126:PRO:HG3	4:D:225:HOH:O	2.14	0.43
1:B:105:THR:HA	2:N:541:THR:O	2.18	0.43
1:B:136:CYS:HA	1:B:147:THR:O	2.18	0.43
1:A:89:ILE:HD13	1:D:63:GLU:CD	2.44	0.43
1:A:137[B]:VAL:HG12	1:A:147:THR:OG1	2.18	0.43
1:E:148:CYS:O	2:Q:531:LEU:HD23	2.18	0.43
1:A:136:CYS:HA	1:A:147:THR:O	2.19	0.42
1:C:127:HIS:CE1	3:C:201:SIN:C2	3.02	0.42
1:D:143:LYS:O	2:P:534:GLN:HB2	2.19	0.42
1:D:127:HIS:CG	1:D:132:TYR:CE2	3.05	0.42
1:D:117:TYR:HB3	1:D:121:ASP:HB2	2.01	0.42
1:D:122:THR:HA	1:D:136:CYS:O	2.19	0.42
1:C:118:LYS:O	1:C:121:ASP:HB2	2.20	0.42
1:A:119:ILE:HD11	1:A:140:GLY:HA3	2.02	0.42
1:D:151:ILE:O	1:D:151:ILE:CG2	2.65	0.42
1:A:105:THR:HA	2:M:541:THR:O	2.19	0.42
1:F:122[A]:THR:HG23	1:F:136:CYS:O	2.20	0.41
1:F:150:PRO:CG	2:R:529:GLU:HG3	2.49	0.41
1:B:64:GLU:HB3	1:B:77:VAL:CG2	2.50	0.41
1:B:146:TRP:CE2	2:N:533:GLY:HA3	2.55	0.41
1:B:113:GLY:HA3	4:B:396:HOH:O	2.20	0.41
1:B:126:PRO:HD2	4:B:308:HOH:O	2.20	0.41
1:A:82:GLU:HB3	1:A:89:ILE:HG23	2.02	0.40
2:O:547:TYR:CE1	2:P:540:VAL:CG2	3.04	0.40
1:B:146:TRP:CZ2	2:N:533:GLY:HA3	2.57	0.40
1:D:70:TYR:CZ	1:D:85:LYS:CE	3.04	0.40
2:N:547:TYR:O	2:N:547:TYR:HD2	2.04	0.40
1:F:130:GLY:HA2	4:F:232:HOH:O	2.21	0.40
1:D:125:ARG:HA	1:D:133:MET:HE1	1.99	0.40
1:F:64:GLU:HG2	1:F:65:THR:N	2.36	0.40

All (2) 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)
4:A:377:HOH:O	4:B:351:HOH:O[1_556]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:348:HOH:O	4:D:239:HOH:O[2_545]	2.16	0.04

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	88/90 (98%)	84 (96%)	4 (4%)	0	100	100
1	B	89/90 (99%)	83 (93%)	6 (7%)	0	100	100
1	C	88/90 (98%)	84 (96%)	4 (4%)	0	100	100
1	D	83/90 (92%)	80 (96%)	3 (4%)	0	100	100
1	E	77/90 (86%)	72 (94%)	5 (6%)	0	100	100
1	F	88/90 (98%)	80 (91%)	6 (7%)	2 (2%)	5	2
2	M	17/23 (74%)	17 (100%)	0	0	100	100
2	N	18/23 (78%)	17 (94%)	1 (6%)	0	100	100
2	O	18/23 (78%)	16 (89%)	2 (11%)	0	100	100
2	P	20/23 (87%)	19 (95%)	1 (5%)	0	100	100
2	Q	18/23 (78%)	16 (89%)	2 (11%)	0	100	100
2	R	17/23 (74%)	17 (100%)	0	0	100	100
All	All	621/678 (92%)	585 (94%)	34 (6%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	128	GLU
1	F	130	GLY

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	75/74 (101%)	72 (96%)	3 (4%)	28	27
1	B	76/74 (103%)	74 (97%)	2 (3%)	40	44
1	C	73/74 (99%)	71 (97%)	2 (3%)	39	42
1	D	73/74 (99%)	68 (93%)	5 (7%)	14	11
1	E	68/74 (92%)	61 (90%)	7 (10%)	7	4
1	F	75/74 (101%)	73 (97%)	2 (3%)	39	42
2	M	16/20 (80%)	16 (100%)	0	100	100
2	N	19/20 (95%)	17 (90%)	2 (10%)	6	4
2	O	19/20 (95%)	19 (100%)	0	100	100
2	P	19/20 (95%)	19 (100%)	0	100	100
2	Q	19/20 (95%)	16 (84%)	3 (16%)	2	1
2	R	18/20 (90%)	17 (94%)	1 (6%)	19	16
All	All	550/564 (98%)	523 (95%)	27 (5%)	22	20

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	143	LYS
1	A	149	LYS
1	B	63	GLU
1	B	99	ARG
1	C	80	THR
1	C	149	LYS
1	D	69	LYS
1	D	108	ASN
1	D	127	HIS
1	D	133	MET
1	D	135	GLU
1	E	87	SER
1	E	89	ILE

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Mol	Chain	Res	Type
1	E	99	ARG
1	E	124	ARG
1	E	125	ARG
1	E	135	GLU
1	E	143	LYS
1	F	83	ARG
1	F	99	ARG
2	N	529	GLU
2	N	537	LYS
2	Q	529	GLU
2	Q	531	LEU
2	Q	548	ASP
2	R	531	LEU

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

Mol	Chain	Res	Type
1	A	73	ASN
1	B	73	ASN
1	C	73	ASN
1	C	108	ASN
1	D	108	ASN
1	D	127	HIS
1	F	73	ASN
2	O	534	GLN
2	P	538	ASN
2	R	538	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SIN	A	201	-	7,7,7	1.12	0	8,8,8	1.52	1 (12%)
3	SIN	B	201	-	7,7,7	1.04	0	8,8,8	1.58	1 (12%)
3	SIN	C	201	-	7,7,7	0.98	0	8,8,8	1.42	1 (12%)

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
3	SIN	A	201	-	-	5/5/5/5	-
3	SIN	B	201	-	-	2/5/5/5	-
3	SIN	C	201	-	-	5/5/5/5	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	SIN	C3-C2-C1	-3.40	104.63	113.67
3	A	201	SIN	C2-C3-C4	-2.64	106.66	113.67
3	C	201	SIN	O4-C4-C3	2.04	120.46	114.00

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	201	SIN	C1-C2-C3-C4
3	A	201	SIN	C1-C2-C3-C4
3	B	201	SIN	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	C	201	SIN	O1-C1-C2-C3
3	A	201	SIN	C2-C3-C4-O3
3	A	201	SIN	C2-C3-C4-O4
3	B	201	SIN	O2-C1-C2-C3
3	C	201	SIN	O2-C1-C2-C3
3	A	201	SIN	O2-C1-C2-C3
3	A	201	SIN	O1-C1-C2-C3
3	C	201	SIN	C2-C3-C4-O3
3	C	201	SIN	C2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	201	SIN	2	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	89/90 (98%)	-0.45	0 100 100	7, 16, 33, 50	1 (1%)
1	B	89/90 (98%)	-0.50	0 100 100	7, 15, 32, 50	2 (2%)
1	C	90/90 (100%)	-0.42	0 100 100	11, 18, 33, 37	0
1	D	86/90 (95%)	-0.14	2 (2%) 61 60	9, 19, 47, 71	1 (1%)
1	E	81/90 (90%)	0.14	3 (3%) 45 44	15, 27, 52, 70	0
1	F	89/90 (98%)	-0.06	3 (3%) 48 47	11, 24, 43, 62	1 (1%)
2	M	18/23 (78%)	-0.19	0 100 100	13, 20, 30, 39	0
2	N	19/23 (82%)	-0.17	1 (5%) 32 31	8, 17, 39, 52	1 (5%)
2	O	20/23 (86%)	-0.17	0 100 100	14, 20, 35, 54	0
2	P	21/23 (91%)	0.15	1 (4%) 35 34	15, 23, 43, 48	0
2	Q	20/23 (86%)	0.30	1 (5%) 34 33	17, 30, 52, 54	0
2	R	19/23 (82%)	-0.24	0 100 100	14, 22, 38, 41	0
All	All	641/678 (94%)	-0.21	11 (1%) 69 68	7, 20, 43, 71	6 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	150	PRO	3.4
2	N	547	TYR	3.4
1	D	132	TYR	3.4
1	E	126	PRO	3.3
1	F	130	GLY	2.5
1	E	124	ARG	2.3
2	Q	548	ASP	2.2
1	F	63	GLU	2.2
1	F	131	GLY	2.2
1	D	126	PRO	2.1
2	P	531	LEU	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($\text{\AA}^2$)	Q<0.9
3	SIN	C	201	8/8	0.83	0.15	33,52,71,77	0
3	SIN	B	201	8/8	0.90	0.11	18,27,53,54	0
3	SIN	A	201	8/8	0.94	0.09	16,24,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.