



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 10:41 AM UTC

PDB ID : 8QTF / pdb_00008qtf
Title : Crystal structure of a C-terminally truncated version of Arabidopsis thaliana 14-3-3 omega in complex with a phosphopeptide from the transcription factor BZR1.
Authors : Hothorn, M.; Obergfell, E.
Deposited on : 2023-10-12
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

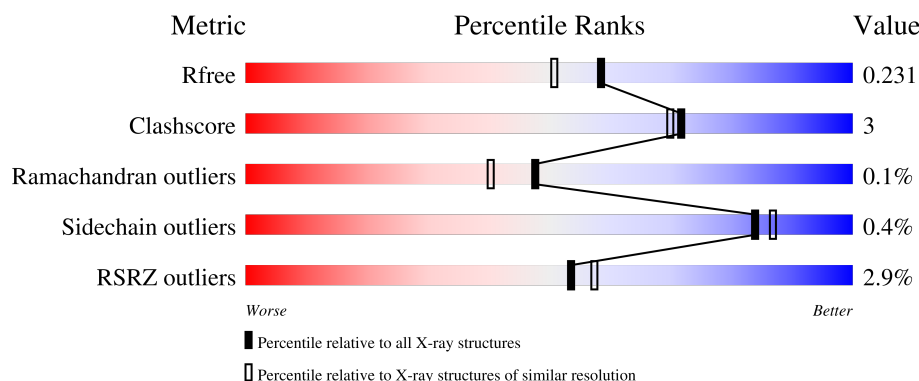
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

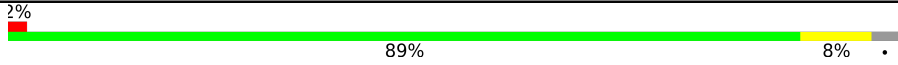
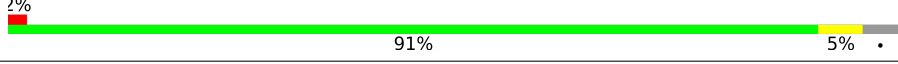
The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	242	
1	B	242	
1	C	242	
1	D	242	
1	E	242	

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Mol	Chain	Length	Quality of chain
1	F	242	
1	G	242	
1	H	242	
1	I	242	
1	J	242	
2	K	7	
2	L	7	
2	M	7	
2	N	7	
2	O	7	
2	P	7	
2	Q	7	
2	R	7	
2	S	7	
2	T	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	J	1202	-	-	X	-
7	CL	F	1201	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 39058 atoms, of which 18884 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 14-3-3-like protein GF14 omega.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	234	Total	C	H	N	O	S	0	2	0
			3696	1171	1826	322	370	7			
1	B	238	Total	C	H	N	O	S	0	2	0
			3760	1188	1863	325	376	8			
1	C	234	Total	C	H	N	O	S	0	1	0
			3709	1172	1839	321	370	7			
1	D	233	Total	C	H	N	O	S	0	0	0
			3669	1161	1820	316	365	7			
1	E	233	Total	C	H	N	O	S	0	1	0
			3689	1167	1831	319	365	7			
1	F	236	Total	C	H	N	O	S	0	0	0
			3687	1167	1826	319	367	8			
1	G	237	Total	C	H	N	O	S	0	1	0
			3712	1177	1834	319	374	8			
1	H	233	Total	C	H	N	O	S	0	1	0
			3686	1167	1825	317	370	7			
1	I	235	Total	C	H	N	O	S	0	0	0
			3672	1164	1816	317	368	7			
1	J	233	Total	C	H	N	O	S	0	2	0
			3707	1173	1835	321	371	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q01525
A	0	ALA	-	expression tag	UNP Q01525
B	-1	GLY	-	expression tag	UNP Q01525
B	0	ALA	-	expression tag	UNP Q01525
C	-1	GLY	-	expression tag	UNP Q01525
C	0	ALA	-	expression tag	UNP Q01525
D	-1	GLY	-	expression tag	UNP Q01525
D	0	ALA	-	expression tag	UNP Q01525
E	-1	GLY	-	expression tag	UNP Q01525

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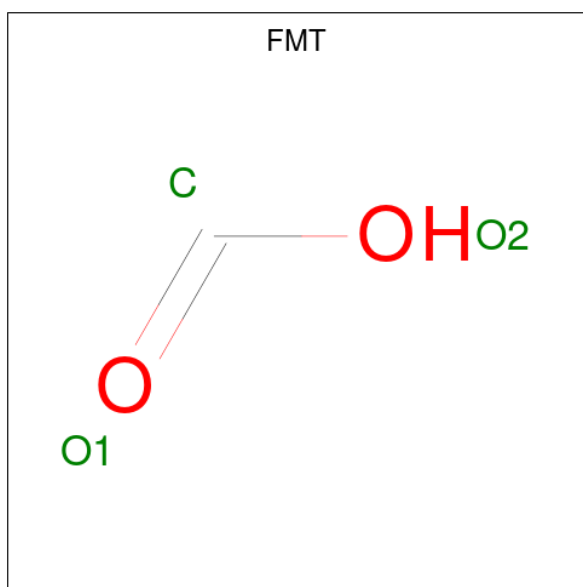
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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ALA	-	expression tag	UNP Q01525
F	-1	GLY	-	expression tag	UNP Q01525
F	0	ALA	-	expression tag	UNP Q01525
G	-1	GLY	-	expression tag	UNP Q01525
G	0	ALA	-	expression tag	UNP Q01525
H	-1	GLY	-	expression tag	UNP Q01525
H	0	ALA	-	expression tag	UNP Q01525
I	-1	GLY	-	expression tag	UNP Q01525
I	0	ALA	-	expression tag	UNP Q01525
J	-1	GLY	-	expression tag	UNP Q01525
J	0	ALA	-	expression tag	UNP Q01525

- Molecule 2 is a protein called Protein BRASSINAZOLE-RESISTANT 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	K	7	Total 107	C 30	H 51	N 11	O 14	P 1	0	0	0
2	L	7	Total 107	C 30	H 51	N 11	O 14	P 1	0	0	0
2	M	7	Total 107	C 30	H 51	N 11	O 14	P 1	0	0	0
2	N	7	Total 107	C 30	H 51	N 11	O 14	P 1	0	0	0
2	O	7	Total 107	C 30	H 51	N 11	O 14	P 1	0	0	0
2	P	7	Total 107	C 30	H 51	N 11	O 14	P 1	0	0	0
2	Q	7	Total 107	C 30	H 51	N 11	O 14	P 1	0	0	0
2	R	7	Total 107	C 30	H 51	N 11	O 14	P 1	0	0	0
2	S	7	Total 107	C 30	H 51	N 11	O 14	P 1	0	0	0
2	T	7	Total 107	C 30	H 51	N 11	O 14	P 1	0	0	0

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			5	1	2	2		
3	A	1	Total	C	H	O	0	0
			5	1	2	2		
3	C	1	Total	C	H	O	0	0
			5	1	2	2		
3	E	1	Total	C	H	O	0	0
			5	1	2	2		
3	G	1	Total	C	H	O	0	0
			5	1	2	2		
3	H	1	Total	C	H	O	0	0
			5	1	2	2		
3	I	1	Total	C	H	O	0	0
			5	1	2	2		
3	J	1	Total	C	H	O	0	0
			5	1	2	2		
3	Q	1	Total	C	H	O	0	0
			5	1	2	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

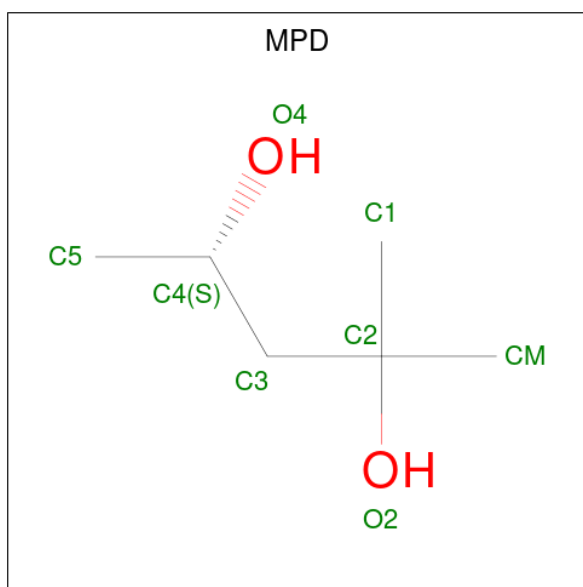


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	H	1	Total	C	H	O	0	0
			10	2	6	2		
4	J	1	Total	C	H	O	0	0
			10	2	6	2		
4	K	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Na	0	0
			3	3		
5	C	1	Total	Na	0	0
			1	1		
5	E	2	Total	Na	0	0
			2	2		
5	G	1	Total	Na	0	0
			1	1		
5	H	2	Total	Na	0	0
			2	2		
5	I	1	Total	Na	0	0
			1	1		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).

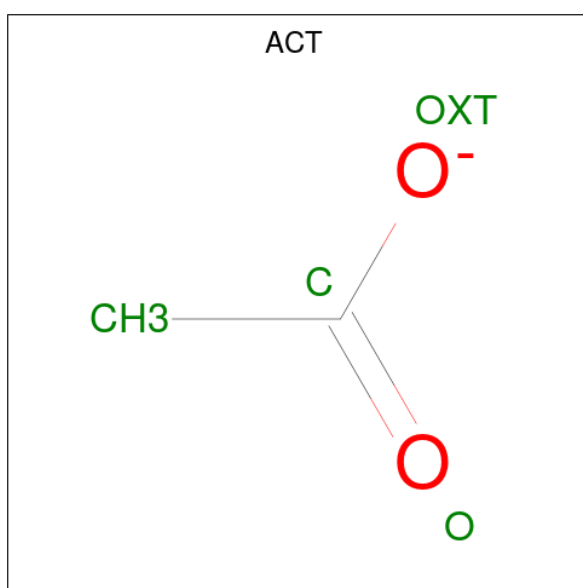


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	1	Total	Cl	0	0
			1	1		

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	91	Total	O			0	0
			91	91				
9	B	124	Total	O			0	0
			124	124				
9	C	96	Total	O			0	0
			96	96				
9	D	56	Total	O			0	0
			56	56				
9	E	110	Total	O			0	0
			110	110				
9	F	58	Total	O			0	0
			58	58				
9	G	92	Total	O			0	0
			92	92				
9	H	93	Total	O			0	0
			93	93				
9	I	48	Total	O			0	0
			48	48				
9	J	54	Total	O			0	0
			54	54				
9	K	12	Total	O			0	0
			12	12				
9	L	5	Total	O			0	0
			5	5				
9	M	6	Total	O			0	0
			6	6				
9	N	5	Total	O			0	0
			5	5				
9	O	6	Total	O			0	0
			6	6				
9	P	2	Total	O			0	0
			2	2				
9	Q	8	Total	O			0	0
			8	8				
9	R	6	Total	O			0	0
			6	6				
9	S	2	Total	O			0	0
			2	2				

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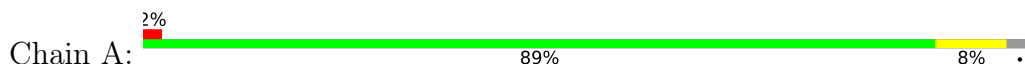
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	T	2	Total	O	0	0
			2	2		

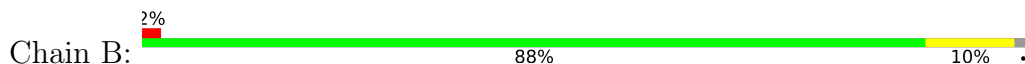
3 Residue-property plots [i](#)

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.

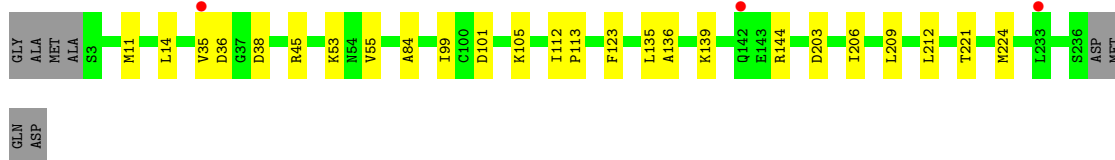
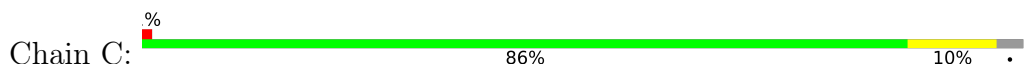
- Molecule 1: 14-3-3-like protein GF14 omega



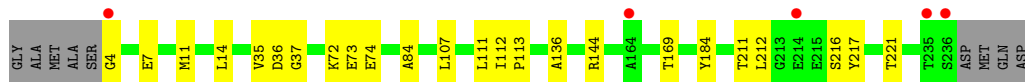
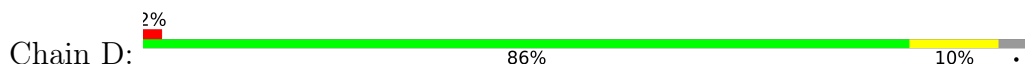
- Molecule 1: 14-3-3-like protein GF14 omega



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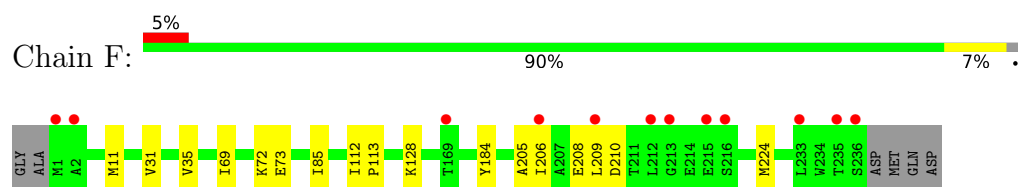
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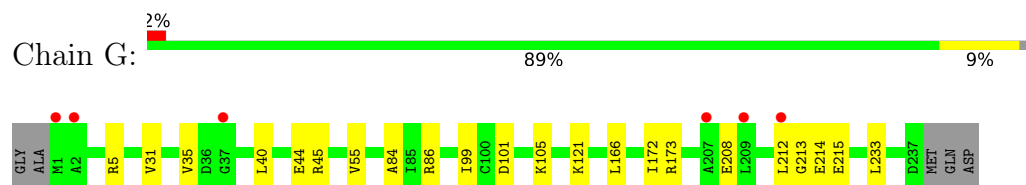
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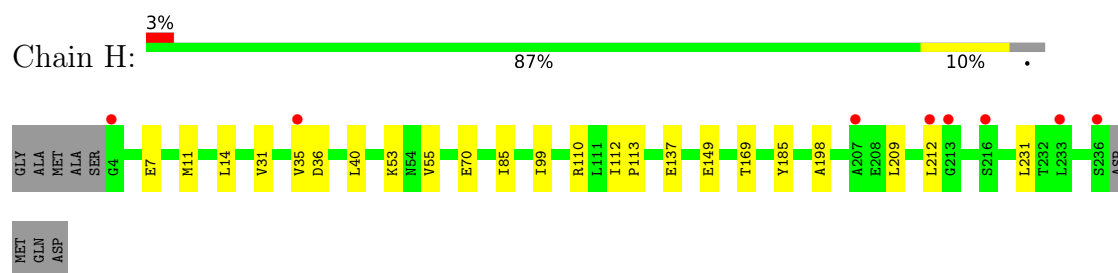
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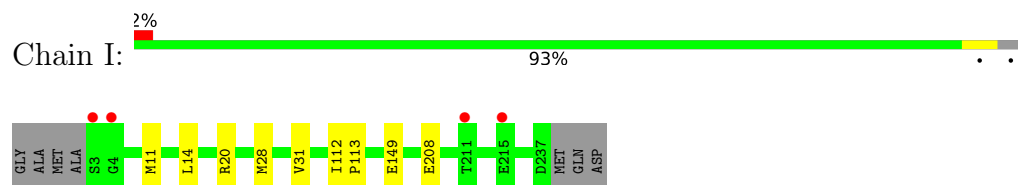
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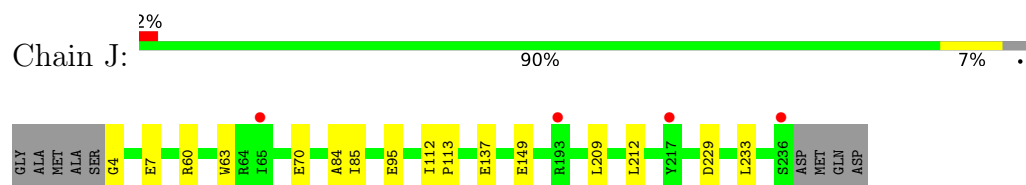
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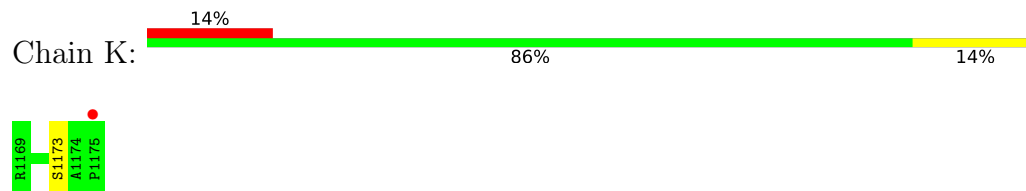
- Molecule 1: 14-3-3-like protein GF14 omega



- Molecule 1: 14-3-3-like protein GF14 omega



- Molecule 2: Protein BRASSINAZOLE-RESISTANT 1

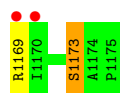
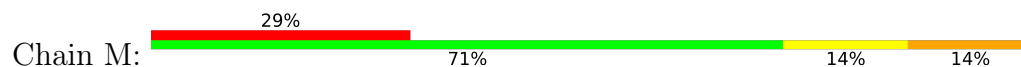


- Molecule 2: Protein BRASSINAZOLE-RESISTANT 1

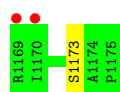
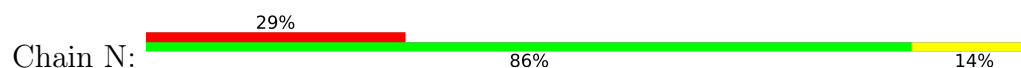




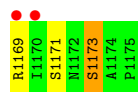
- Molecule 2: Protein BRASSINAZOLE-RESISTANT 1



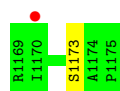
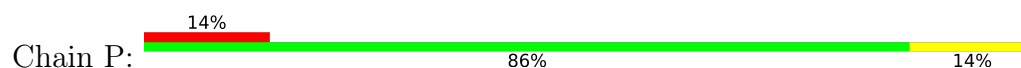
- Molecule 2: Protein BRASSINAZOLE-RESISTANT 1



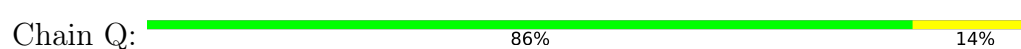
- Molecule 2: Protein BRASSINAZOLE-RESISTANT 1



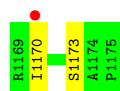
- Molecule 2: Protein BRASSINAZOLE-RESISTANT 1



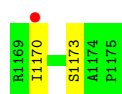
- Molecule 2: Protein BRASSINAZOLE-RESISTANT 1



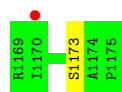
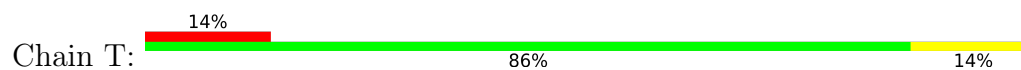
- Molecule 2: Protein BRASSINAZOLE-RESISTANT 1



- Molecule 2: Protein BRASSINAZOLE-RESISTANT 1



• Molecule 2: Protein BRASSINAZOLE-RESISTANT 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.64Å 71.92Å 151.66Å 100.25° 94.84° 89.23°	Depositor
Resolution (Å)	59.91 – 1.90 59.91 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (59.91-1.90) 97.4 (59.91-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.195 , 0.230 0.195 , 0.231	Depositor DCC
R_{free} test set	11382 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	39058	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.32% 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: CL, ACT, NA, FMT, MPD, EDO, SEP

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	0.28	0/1905	0.39	0/2568
1	B	0.27	0/1929	0.39	0/2599
1	C	0.28	0/1899	0.39	0/2559
1	D	0.24	0/1878	0.32	0/2532
1	E	0.29	0/1890	0.40	0/2547
1	F	0.25	0/1890	0.36	0/2548
1	G	0.27	0/1910	0.37	0/2576
1	H	0.27	0/1890	0.38	0/2548
1	I	0.25	0/1885	0.36	0/2543
1	J	0.24	0/1901	0.33	0/2562
2	K	0.29	0/45	0.51	0/57
2	L	0.25	0/45	0.40	0/57
2	M	0.25	0/45	0.34	0/57
2	N	0.31	0/45	0.29	0/57
2	O	0.24	0/45	0.40	0/57
2	P	0.24	0/45	0.39	0/57
2	Q	0.32	0/45	0.40	0/57
2	R	0.25	0/45	0.38	0/57
2	S	0.24	0/45	0.34	0/57
2	T	0.19	0/45	0.27	0/57
All	All	0.27	0/19427	0.37	0/26152

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	1870	1826	1833	11	1
1	B	1897	1863	1869	11	0
1	C	1870	1839	1840	19	0
1	D	1849	1820	1819	17	1
1	E	1858	1831	1834	7	1
1	F	1861	1826	1828	14	1
1	G	1878	1834	1840	13	1
1	H	1861	1825	1826	18	1
1	I	1856	1816	1815	10	1
1	J	1872	1835	1838	13	1
2	K	56	51	49	0	0
2	L	56	51	49	2	0
2	M	56	51	49	1	0
2	N	56	51	49	0	0
2	O	56	51	49	3	0
2	P	56	51	49	0	0
2	Q	56	51	49	0	0
2	R	56	51	49	1	0
2	S	56	51	49	0	0
2	T	56	51	49	0	0
3	A	6	4	2	0	0
3	C	3	2	1	0	0
3	E	3	2	1	0	0
3	G	3	2	1	0	0
3	H	3	2	1	0	0
3	I	3	2	1	0	0
3	J	3	2	1	0	0
3	Q	3	2	1	0	0
4	A	4	6	6	0	0
4	H	4	6	6	1	0
4	J	4	6	6	4	0
4	K	4	6	6	0	0
5	B	3	0	0	0	0
5	C	1	0	0	0	0
5	E	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	1	0	0	0	0
6	E	8	14	14	0	0
7	F	1	0	0	3	0
8	G	4	3	3	0	0
9	A	91	0	0	0	0
9	B	124	0	0	1	0
9	C	96	0	0	1	0
9	D	56	0	0	0	0
9	E	110	0	0	1	0
9	F	58	0	0	2	0
9	G	92	0	0	1	0
9	H	93	0	0	2	0
9	I	48	0	0	0	0
9	J	54	0	0	0	0
9	K	12	0	0	0	0
9	L	5	0	0	0	0
9	M	6	0	0	0	0
9	N	5	0	0	0	0
9	O	6	0	0	0	0
9	P	2	0	0	0	0
9	Q	8	0	0	0	0
9	R	6	0	0	0	0
9	S	2	0	0	0	0
9	T	2	0	0	0	0
All	All	20174	18884	18882	125	4

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 3.

The worst 5 of 125 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:D:4:GLY:N	1:D:7:GLU:OE1	2.17	0.77
1:I:11:MET:HA	1:I:11:MET:HE2	1.67	0.75
1:F:209:LEU:N	7:F:1201:CL:CL	2.58	0.74
1:I:28:MET:HA	1:I:28:MET:HE2	1.71	0.72
1:D:72:LYS:NZ	1:D:73:GLU:OE2	2.22	0.71

All (4) 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)
1:F:184:TYR:OH	1:I:149:GLU:OE2[1_556]	1.98	0.22
1:A:165:GLU:OE1	1:G:86:ARG:HH12[1_565]	1.50	0.10
1:D:184:TYR:OH	1:J:149:GLU:OE2[1_665]	2.17	0.03
1:E:184:TYR:OH	1:H:149:GLU:OE2[1_665]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	234/242 (97%)	230 (98%)	4 (2%)	0	100	100
1	B	238/242 (98%)	231 (97%)	5 (2%)	2 (1%)	16	8
1	C	233/242 (96%)	230 (99%)	3 (1%)	0	100	100
1	D	231/242 (96%)	225 (97%)	6 (3%)	0	100	100
1	E	232/242 (96%)	227 (98%)	5 (2%)	0	100	100
1	F	234/242 (97%)	227 (97%)	7 (3%)	0	100	100
1	G	236/242 (98%)	232 (98%)	3 (1%)	1 (0%)	30	22
1	H	232/242 (96%)	225 (97%)	7 (3%)	0	100	100
1	I	233/242 (96%)	225 (97%)	8 (3%)	0	100	100
1	J	233/242 (96%)	226 (97%)	7 (3%)	0	100	100
2	K	4/7 (57%)	4 (100%)	0	0	100	100
2	L	4/7 (57%)	4 (100%)	0	0	100	100
2	M	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	N	4/7 (57%)	4 (100%)	0	0	100	100
2	O	4/7 (57%)	4 (100%)	0	0	100	100
2	P	4/7 (57%)	4 (100%)	0	0	100	100
2	Q	4/7 (57%)	4 (100%)	0	0	100	100
2	R	4/7 (57%)	4 (100%)	0	0	100	100
2	S	4/7 (57%)	4 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	4/7 (57%)	4 (100%)	0	0	100	100
All	All	2376/2490 (95%)	2317 (98%)	56 (2%)	3 (0%)	48	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	214	GLU
1	B	215	GLU
1	B	214	GLU

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	196/201 (98%)	196 (100%)	0	100	100
1	B	199/201 (99%)	197 (99%)	2 (1%)	68	70
1	C	197/201 (98%)	197 (100%)	0	100	100
1	D	194/201 (96%)	193 (100%)	1 (0%)	81	84
1	E	195/201 (97%)	194 (100%)	1 (0%)	81	84
1	F	194/201 (96%)	194 (100%)	0	100	100
1	G	197/201 (98%)	195 (99%)	2 (1%)	68	70
1	H	196/201 (98%)	196 (100%)	0	100	100
1	I	194/201 (96%)	194 (100%)	0	100	100
1	J	197/201 (98%)	197 (100%)	0	100	100
2	K	5/5 (100%)	5 (100%)	0	100	100
2	L	5/5 (100%)	5 (100%)	0	100	100
2	M	5/5 (100%)	5 (100%)	0	100	100
2	N	5/5 (100%)	5 (100%)	0	100	100
2	O	5/5 (100%)	5 (100%)	0	100	100
2	P	5/5 (100%)	5 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	5/5 (100%)	5 (100%)	0	100	100
2	R	5/5 (100%)	5 (100%)	0	100	100
2	S	5/5 (100%)	4 (80%)	1 (20%)	1	0
2	T	5/5 (100%)	5 (100%)	0	100	100
All	All	2009/2060 (98%)	2002 (100%)	7 (0%)	84	88

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	235	THR
1	G	208	GLU
2	S	1170	ILE
1	G	212	LEU
1	D	74	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	54	ASN
1	I	71	GLN
1	J	142	GLN
1	J	71	GLN
1	H	81	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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
2	SEP	S	1173	2	8,9,10	1.78	2 (25%)	7,12,14	1.49	1 (14%)
2	SEP	K	1173	2	8,9,10	1.66	1 (12%)	7,12,14	1.55	1 (14%)
2	SEP	N	1173	2	8,9,10	1.63	1 (12%)	7,12,14	1.51	2 (28%)
2	SEP	M	1173	2	8,9,10	1.56	1 (12%)	7,12,14	1.57	1 (14%)
2	SEP	Q	1173	2	8,9,10	1.62	2 (25%)	7,12,14	1.05	0
2	SEP	R	1173	2	8,9,10	1.74	1 (12%)	7,12,14	1.78	2 (28%)
2	SEP	L	1173	2	8,9,10	1.59	1 (12%)	7,12,14	1.78	2 (28%)
2	SEP	T	1173	2	8,9,10	1.53	2 (25%)	7,12,14	1.86	3 (42%)
2	SEP	P	1173	2	8,9,10	1.46	1 (12%)	7,12,14	1.97	2 (28%)
2	SEP	O	1173	2	8,9,10	1.56	1 (12%)	7,12,14	2.08	2 (28%)

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	SEP	S	1173	2	-	0/6/8/10	-
2	SEP	K	1173	2	-	0/6/8/10	-
2	SEP	N	1173	2	-	0/6/8/10	-
2	SEP	M	1173	2	-	0/6/8/10	-
2	SEP	Q	1173	2	-	0/6/8/10	-
2	SEP	R	1173	2	-	0/6/8/10	-
2	SEP	L	1173	2	-	0/6/8/10	-
2	SEP	T	1173	2	-	0/6/8/10	-
2	SEP	P	1173	2	-	0/6/8/10	-
2	SEP	O	1173	2	-	0/6/8/10	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	1173	SEP	P-O1P	4.35	1.64	1.50
2	K	1173	SEP	P-O1P	3.88	1.62	1.50
2	S	1173	SEP	P-O1P	3.75	1.62	1.50
2	L	1173	SEP	P-O1P	3.73	1.62	1.50
2	O	1173	SEP	P-O1P	3.61	1.61	1.50

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1173	SEP	OG-CB-CA	4.29	112.32	108.14
2	O	1173	SEP	OG-CB-CA	4.23	112.26	108.14
2	R	1173	SEP	O3P-P-OG	3.36	115.43	106.67
2	K	1173	SEP	OG-CB-CA	3.36	111.41	108.14
2	T	1173	SEP	OG-CB-CA	3.23	111.29	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	1173	SEP	1	0
2	L	1173	SEP	1	0
2	O	1173	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 11 are monoatomic - leaving 15 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	FMT	I	1201	-	2,2,2	0.71	0	1,1,1	0.47	0
3	FMT	Q	1201	-	2,2,2	0.62	0	1,1,1	0.44	0
4	EDO	J	1202	-	3,3,3	0.64	0	2,2,2	0.52	0
3	FMT	A	1202	-	2,2,2	0.72	0	1,1,1	0.47	0
3	FMT	A	1201	-	2,2,2	0.72	0	1,1,1	0.48	0
3	FMT	J	1201	-	2,2,2	0.72	0	1,1,1	0.45	0
4	EDO	K	1201	-	3,3,3	0.46	0	2,2,2	0.63	0
3	FMT	H	1201	-	2,2,2	0.73	0	1,1,1	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	H	1202	-	3,3,3	0.44	0	2,2,2	0.31	0
8	ACT	G	1202	-	3,3,3	1.08	0	3,3,3	1.60	0
3	FMT	E	1201	-	2,2,2	0.74	0	1,1,1	0.39	0
6	MPD	E	1202	-	7,7,7	0.33	0	9,10,10	0.48	0
4	EDO	A	1203	-	3,3,3	0.51	0	2,2,2	0.37	0
3	FMT	G	1201	-	2,2,2	0.74	0	1,1,1	0.50	0
3	FMT	C	1201	-	2,2,2	0.77	0	1,1,1	0.49	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	EDO	J	1202	-	-	1/1/1/1	-
4	EDO	K	1201	-	-	0/1/1/1	-
4	EDO	H	1202	-	-	0/1/1/1	-
6	MPD	E	1202	-	-	2/5/5/5	-
4	EDO	A	1203	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	1202	MPD	C2-C3-C4-O4
6	E	1202	MPD	C2-C3-C4-C5
4	J	1202	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1202	EDO	4	0
4	H	1202	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

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	234/242 (96%)	0.07	5 (2%) 63 67	29, 51, 94, 147	2 (0%)
1	B	238/242 (98%)	0.01	5 (2%) 63 67	24, 50, 102, 164	2 (0%)
1	C	234/242 (96%)	0.01	3 (1%) 75 78	21, 50, 91, 113	1 (0%)
1	D	233/242 (96%)	0.24	5 (2%) 63 67	41, 62, 120, 156	0
1	E	233/242 (96%)	0.07	5 (2%) 63 67	20, 48, 88, 115	1 (0%)
1	F	236/242 (97%)	0.25	12 (5%) 33 36	36, 59, 118, 157	0
1	G	237/242 (97%)	0.21	6 (2%) 58 62	30, 52, 105, 144	1 (0%)
1	H	233/242 (96%)	0.05	8 (3%) 48 51	23, 53, 113, 179	1 (0%)
1	I	235/242 (97%)	0.28	4 (1%) 69 72	47, 65, 109, 143	0
1	J	233/242 (96%)	0.31	4 (1%) 69 72	32, 64, 113, 148	2 (0%)
2	K	6/7 (85%)	0.25	1 (16%) 4 4	49, 51, 59, 63	0
2	L	6/7 (85%)	0.92	1 (16%) 4 4	44, 59, 82, 101	0
2	M	6/7 (85%)	1.45	2 (33%) 1 1	46, 61, 96, 117	0
2	N	6/7 (85%)	1.77	2 (33%) 1 1	63, 78, 118, 124	0
2	O	6/7 (85%)	2.22	2 (33%) 1 1	47, 63, 109, 132	0
2	P	6/7 (85%)	1.53	1 (16%) 4 4	62, 75, 101, 132	0
2	Q	6/7 (85%)	0.17	0 100 100	46, 49, 55, 69	0
2	R	6/7 (85%)	0.80	1 (16%) 4 4	48, 63, 75, 94	0
2	S	6/7 (85%)	0.78	1 (16%) 4 4	56, 74, 95, 100	0
2	T	6/7 (85%)	0.89	1 (16%) 4 4	59, 77, 94, 96	0
All	All	2406/2490 (96%)	0.17	69 (2%) 53 57	20, 57, 107, 179	10 (0%)

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	1170	ILE	5.4
1	G	37	GLY	5.2
2	P	1170	ILE	4.9
2	M	1170	ILE	4.2
1	E	236	SER	4.1

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. 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
2	SEP	P	1173	10/11	0.96	0.07	41,53,59,64	0
2	SEP	S	1173	10/11	0.96	0.06	40,50,59,60	0
2	SEP	T	1173	10/11	0.96	0.07	43,52,62,66	0
2	SEP	N	1173	10/11	0.97	0.08	48,51,59,63	0
2	SEP	M	1173	10/11	0.97	0.07	36,43,51,54	0
2	SEP	L	1173	10/11	0.98	0.05	33,38,46,46	0
2	SEP	K	1173	10/11	0.98	0.07	33,40,46,51	0
2	SEP	R	1173	10/11	0.99	0.05	29,39,47,49	0
2	SEP	O	1173	10/11	0.99	0.05	35,39,48,49	0
2	SEP	Q	1173	10/11	0.99	0.05	32,41,47,51	0

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
7	CL	F	1201	1/1	0.65	0.13	123,123,123,123	0
8	ACT	G	1202	4/4	0.72	0.17	58,59,82,82	0
3	FMT	H	1201	3/3	0.78	0.25	56,66,68,79	0
4	EDO	A	1203	4/4	0.78	0.15	58,69,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FMT	A	1201	3/3	0.80	0.20	61,61,73,75	0
6	MPD	E	1202	8/8	0.80	0.20	57,69,85,85	0
5	NA	E	1203	1/1	0.81	0.23	70,70,70,70	0
4	EDO	H	1202	4/4	0.82	0.15	49,59,71,71	0
5	NA	E	1204	1/1	0.83	0.11	80,80,80,80	0
3	FMT	C	1201	3/3	0.83	0.20	69,71,83,85	0
4	EDO	K	1201	4/4	0.84	0.13	52,63,73,73	0
3	FMT	G	1201	3/3	0.85	0.14	53,60,65,72	0
3	FMT	Q	1201	3/3	0.85	0.11	52,52,62,62	0
5	NA	H	1204	1/1	0.88	0.17	57,57,57,57	0
4	EDO	J	1202	4/4	0.88	0.24	44,54,65,68	0
3	FMT	A	1202	3/3	0.88	0.13	58,60,70,72	0
5	NA	H	1203	1/1	0.88	0.19	58,58,58,58	0
5	NA	C	1202	1/1	0.89	0.10	61,61,61,61	0
3	FMT	J	1201	3/3	0.89	0.12	61,65,81,97	0
3	FMT	I	1201	3/3	0.90	0.17	58,64,77,88	0
5	NA	I	1202	1/1	0.91	0.11	63,63,63,63	0
5	NA	G	1203	1/1	0.91	0.11	58,58,58,58	0
3	FMT	E	1201	3/3	0.94	0.08	48,54,58,66	0
5	NA	B	1201	1/1	0.94	0.19	56,56,56,56	0
5	NA	B	1202	1/1	0.95	0.12	57,57,57,57	0
5	NA	B	1203	1/1	0.95	0.17	60,60,60,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.