



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:23 AM UTC

PDB ID : 8QT5 / pdb_00008qt5
Title : Crystal structure of Arabidopsis thaliana 14-3-3 isoform lambda in complex with a phosphopeptide from the transcription factor BZR1.
Authors : Hothorn, M.; Obergfell, E.
Deposited on : 2023-10-12
Resolution : 2.69 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

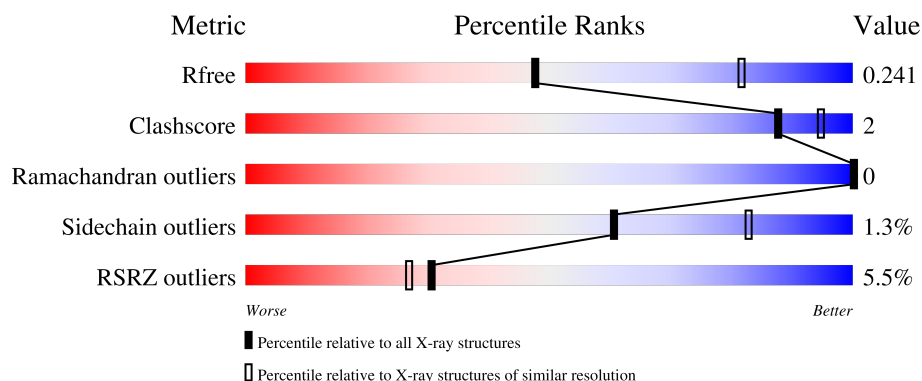
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	255	2% 92% 5% .
1	B	255	3% 91% 5% .
1	C	255	% 91% 5% .
1	D	255	2% 93% . .
1	E	255	% 90% 7% .

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Mol	Chain	Length	Quality of chain
1	F	255	7% 86% 10%
1	G	255	22% 86% 9% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27061 atoms, of which 13407 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.

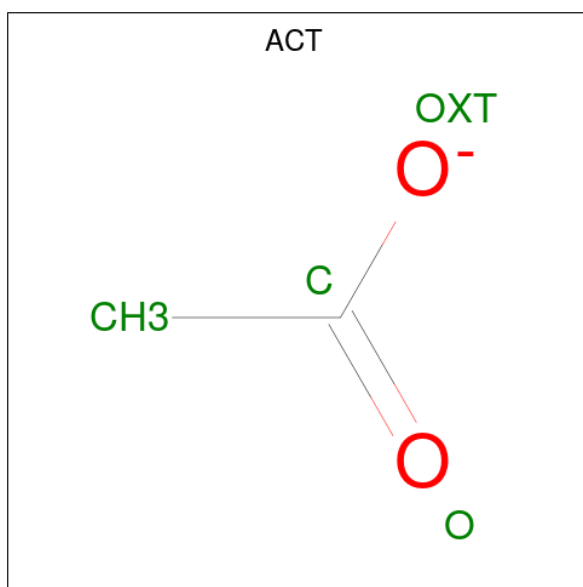
- Molecule 1 is a protein called 14-3-3-like protein G-BOX factor 14 lambda,Protein BRASSI NAZOLE-RESISTANT 1.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	248	Total	C	H	N	O	P	S	0	1	0
			3900	1230	1933	326	397	1	13			
1	B	247	Total	C	H	N	O	P	S	0	0	0
			3877	1222	1922	326	394	1	12			
1	C	246	Total	C	H	N	O	P	S	0	0	0
			3862	1217	1916	325	391	1	12			
1	D	247	Total	C	H	N	O	P	S	0	0	0
			3870	1221	1917	324	395	1	12			
1	E	247	Total	C	H	N	O	P	S	0	1	0
			3885	1226	1927	324	395	1	12			
1	F	245	Total	C	H	N	O	P	S	0	0	0
			3839	1211	1904	321	390	1	12			
1	G	242	Total	C	H	N	O	P	S	0	0	0
			3792	1197	1882	317	384	1	11			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1174	ALA	CYS	engineered mutation	UNP Q8S307
B	1174	ALA	CYS	engineered mutation	UNP Q8S307
C	1174	ALA	CYS	engineered mutation	UNP Q8S307
D	1174	ALA	CYS	engineered mutation	UNP Q8S307
E	1174	ALA	CYS	engineered mutation	UNP Q8S307
F	1174	ALA	CYS	engineered mutation	UNP Q8S307
G	1174	ALA	CYS	engineered mutation	UNP Q8S307

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	F	1	Total	C	H	O	0	0
			7	2	3	2		

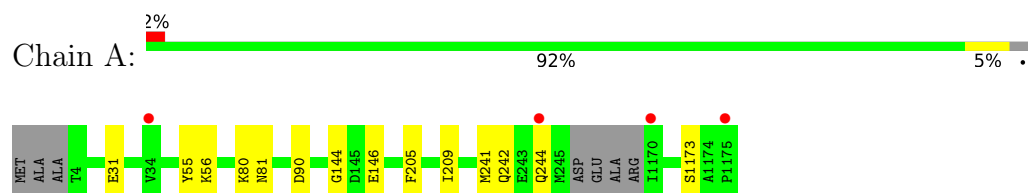
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	6	Total	O	0	0
			6	6		
3	C	2	Total	O	0	0
			2	2		
3	D	1	Total	O	0	0
			1	1		
3	E	6	Total	O	0	0
			6	6		

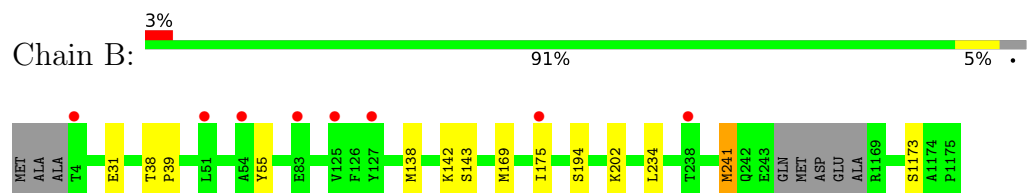
3 Residue-property plots [i](#)

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.

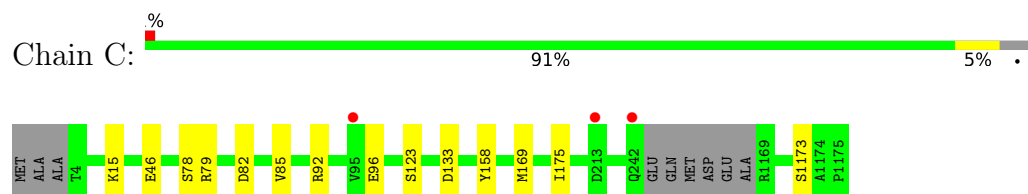
- Molecule 1: 14-3-3-like protein G-BOX factor 14 lambda,Protein BRASSINAZOLE-RESISTANT 1



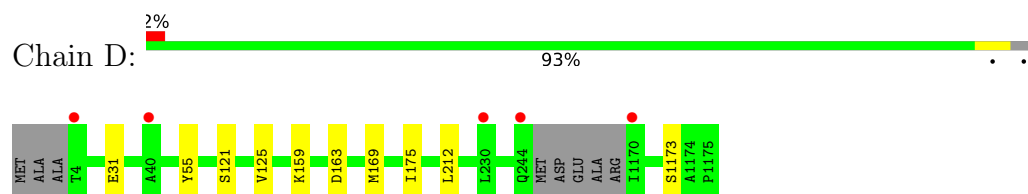
- Molecule 1: 14-3-3-like protein G-BOX factor 14 lambda,Protein BRASSINAZOLE-RESISTANT 1



- Molecule 1: 14-3-3-like protein G-BOX factor 14 lambda,Protein BRASSINAZOLE-RESISTANT 1



- Molecule 1: 14-3-3-like protein G-BOX factor 14 lambda,Protein BRASSINAZOLE-RESISTANT 1

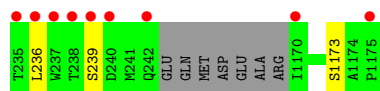
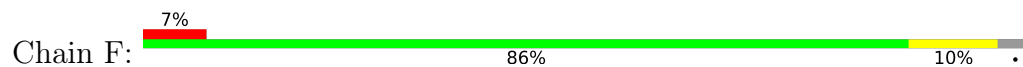


- Molecule 1: 14-3-3-like protein G-BOX factor 14 lambda,Protein BRASSINAZOLE-RESISTANT 1

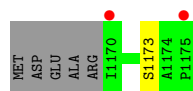
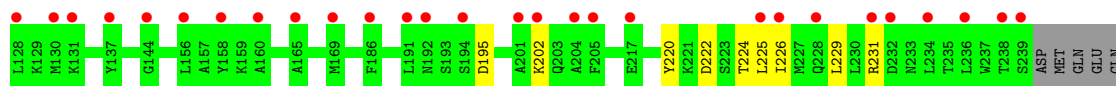
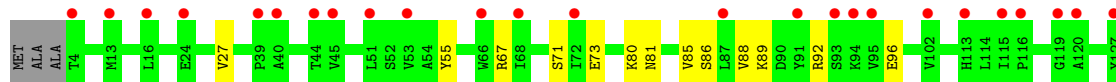
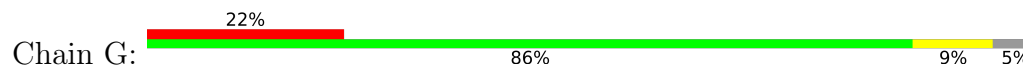




- Molecule 1: 14-3-3-like protein G-BOX factor 14 lambda,Protein BRASSINAZOLE-RESISTANT 1



- Molecule 1: 14-3-3-like protein G-BOX factor 14 lambda,Protein BRASSINAZOLE-RESISTANT 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	176.05Å 176.05Å 172.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	74.92 – 2.69 74.92 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.3 (74.92-2.69) 98.8 (74.92-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.241 , 0.262 (Not available) , 0.241	Depositor DCC
R_{free} test set	4235 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	86.3	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27061	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: SEP, ACT

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	0.11	0/1988	0.23	0/2676
1	B	0.10	0/1973	0.21	0/2656
1	C	0.10	0/1964	0.21	0/2644
1	D	0.10	0/1971	0.20	0/2654
1	E	0.11	0/1979	0.23	0/2665
1	F	0.12	0/1953	0.25	0/2630
1	G	0.10	0/1928	0.22	0/2597
All	All	0.11	0/13756	0.22	0/18522

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	1967	1933	1933	4	1
1	B	1955	1922	1921	8	0
1	C	1946	1916	1914	7	0
1	D	1953	1917	1916	5	0
1	E	1958	1927	1927	7	1
1	F	1935	1904	1901	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1910	1882	1880	13	0
2	A	4	3	3	0	0
2	F	4	3	3	0	0
3	A	7	0	0	1	0
3	B	6	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	6	0	0	0	0
All	All	13654	13407	13398	55	1

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 2.

All (55) 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:125:VAL:HG21	1:D:169:MET:SD	2.16	0.85
1:F:236:LEU:O	1:G:231:ARG:NH1	2.25	0.69
1:G:92:ARG:NH1	1:G:96:GLU:OE2	2.25	0.69
1:E:125:VAL:HG21	1:E:169:MET:SD	2.36	0.65
1:A:146:GLU:HB2	3:A:1302:HOH:O	1.99	0.62
1:D:121:SER:O	1:D:125:VAL:HG22	2.00	0.60
1:A:31:GLU:OE2	1:A:55:TYR:OH	2.23	0.56
1:C:92:ARG:NH1	1:C:96:GLU:OE2	2.40	0.55
1:E:31:GLU:OE2	1:E:55:TYR:OH	2.25	0.55
1:C:169:MET:HE1	1:C:175:ILE:HB	1.89	0.54
1:G:67:ARG:O	1:G:71:SER:N	2.34	0.54
1:D:31:GLU:OE2	1:D:55:TYR:OH	2.26	0.54
1:D:159:LYS:NZ	1:D:163:ASP:OD1	2.40	0.53
1:A:144:GLY:O	1:A:146:GLU:N	2.43	0.52
1:F:201:ALA:HB3	1:F:234:LEU:HD21	1.93	0.51
1:G:85:VAL:HA	1:G:88:VAL:HG12	1.94	0.50
1:F:139:ALA:O	1:F:147:ARG:NH1	2.44	0.49
1:F:38:THR:HB	1:F:39:PRO:HA	1.95	0.49
1:E:75:LYS:HE2	1:E:79:ARG:CZ	2.44	0.48
1:C:15:LYS:NZ	1:C:46:GLU:OE2	2.35	0.48
1:G:222:ASP:O	1:G:226:ILE:HD12	2.14	0.47
1:B:38:THR:HB	1:B:39:PRO:HA	1.97	0.47
1:E:139:ALA:O	1:E:147:ARG:NH1	2.46	0.47
1:F:218:GLU:OE1	1:F:218:GLU:N	2.42	0.47
1:G:89:LYS:CE	1:G:89:LYS:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LYS:CG	1:B:234:LEU:HD21	2.45	0.47
1:E:38:THR:HB	1:E:39:PRO:HA	1.97	0.46
1:B:169:MET:HE1	1:B:175:ILE:HB	1.97	0.46
1:C:82:ASP:HA	1:C:85:VAL:HG22	1.97	0.46
1:B:194:SER:OG	1:B:241:MET:SD	2.75	0.45
1:B:31:GLU:OE2	1:B:55:TYR:OH	2.34	0.45
1:D:169:MET:HE1	1:D:175:ILE:HB	1.97	0.45
1:G:225:LEU:O	1:G:229:LEU:HD23	2.16	0.45
1:F:225:LEU:O	1:F:229:LEU:HD23	2.16	0.45
1:G:89:LYS:HA	1:G:89:LYS:HE2	2.00	0.44
1:B:202:LYS:HG2	1:B:234:LEU:HD21	1.98	0.44
1:C:78:SER:O	1:C:79:ARG:HB3	2.18	0.44
1:F:44:THR:HG23	1:F:47:GLU:H	1.84	0.43
1:G:73:GLU:CD	1:G:89:LYS:HZ2	2.27	0.43
1:C:78:SER:O	1:C:79:ARG:CB	2.67	0.43
1:F:67:ARG:NE	1:G:195:ASP:OD2	2.46	0.43
1:F:14:ALA:CB	1:F:30:MET:HE2	2.49	0.42
1:F:165:ALA:HA	1:F:169:MET:HG2	2.02	0.42
1:F:222:ASP:O	1:F:226:ILE:HD12	2.19	0.42
1:A:205:PHE:CE2	1:A:209:ILE:HD11	2.55	0.42
1:E:133:ASP:OD1	1:E:158:TYR:OH	2.34	0.42
1:G:220:TYR:CZ	1:G:224:THR:HG21	2.55	0.42
1:C:133:ASP:OD1	1:C:158:TYR:OH	2.31	0.41
1:F:169:MET:O	1:F:176:ARG:NH1	2.54	0.41
1:F:236:LEU:HD11	1:G:202:LYS:HG3	2.03	0.41
1:B:138:MET:O	1:B:142:LYS:HG2	2.22	0.40
1:B:138:MET:HE3	1:B:142:LYS:CE	2.51	0.40
1:F:27:VAL:HG13	1:F:55:TYR:CE1	2.56	0.40
1:E:63:ARG:HH12	1:E:1173:SEP:P	2.44	0.40
1:G:27:VAL:HG13	1:G:55:TYR:CZ	2.56	0.40

All (1) 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:A:90:ASP:OD1	1:E:79:ARG:NH1[3_454]	2.11	0.09

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	244/255 (96%)	237 (97%)	7 (3%)	0	100	100
1	B	242/255 (95%)	239 (99%)	3 (1%)	0	100	100
1	C	241/255 (94%)	236 (98%)	5 (2%)	0	100	100
1	D	242/255 (95%)	239 (99%)	3 (1%)	0	100	100
1	E	243/255 (95%)	239 (98%)	4 (2%)	0	100	100
1	F	240/255 (94%)	235 (98%)	5 (2%)	0	100	100
1	G	237/255 (93%)	233 (98%)	4 (2%)	0	100	100
All	All	1689/1785 (95%)	1658 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	212/215 (99%)	206 (97%)	6 (3%)	38	68
1	B	210/215 (98%)	208 (99%)	2 (1%)	68	86
1	C	209/215 (97%)	208 (100%)	1 (0%)	81	92
1	D	210/215 (98%)	209 (100%)	1 (0%)	81	92
1	E	211/215 (98%)	207 (98%)	4 (2%)	50	77
1	F	208/215 (97%)	206 (99%)	2 (1%)	68	86
1	G	205/215 (95%)	202 (98%)	3 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1465/1505 (97%)	1446 (99%)	19 (1%)	61 83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	80	LYS
1	A	81	ASN
1	A	241	MET
1	A	242	GLN
1	A	244	GLN
1	B	143	SER
1	B	241	MET
1	C	123	SER
1	D	212	LEU
1	E	86	SER
1	E	122	GLU
1	E	211	GLU
1	E	215	LEU
1	F	196	LYS
1	F	239	SER
1	G	80	LYS
1	G	81	ASN
1	G	86	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	244	GLN
1	B	81	ASN
1	B	113	HIS
1	B	228	GLN
1	C	57	ASN
1	D	57	ASN
1	D	228	GLN
1	E	57	ASN
1	F	57	ASN
1	F	74	GLN
1	F	162	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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
1	SEP	E	1173	1	8,9,10	1.60	2 (25%)	7,12,14	1.85	1 (14%)
1	SEP	D	1173	1	8,9,10	1.67	1 (12%)	7,12,14	1.76	1 (14%)
1	SEP	F	1173	1	8,9,10	1.65	1 (12%)	7,12,14	1.60	1 (14%)
1	SEP	C	1173	1	8,9,10	1.61	1 (12%)	7,12,14	1.87	1 (14%)
1	SEP	A	1173	1	8,9,10	1.71	2 (25%)	7,12,14	1.64	1 (14%)
1	SEP	G	1173	1	8,9,10	1.62	1 (12%)	7,12,14	1.34	1 (14%)
1	SEP	B	1173	1	8,9,10	1.70	1 (12%)	7,12,14	1.42	1 (14%)

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
1	SEP	E	1173	1	-	0/6/8/10	-
1	SEP	D	1173	1	-	0/6/8/10	-
1	SEP	F	1173	1	-	0/6/8/10	-
1	SEP	C	1173	1	-	0/6/8/10	-
1	SEP	A	1173	1	-	0/6/8/10	-
1	SEP	G	1173	1	-	0/6/8/10	-
1	SEP	B	1173	1	-	0/6/8/10	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1173	SEP	P-O1P	3.84	1.62	1.50
1	A	1173	SEP	P-O1P	3.76	1.62	1.50
1	D	1173	SEP	P-O1P	3.67	1.61	1.50
1	F	1173	SEP	P-O1P	3.64	1.61	1.50
1	G	1173	SEP	P-O1P	3.55	1.61	1.50
1	C	1173	SEP	P-O1P	3.35	1.60	1.50
1	E	1173	SEP	P-O1P	3.30	1.60	1.50
1	E	1173	SEP	P-O2P	2.10	1.62	1.54
1	A	1173	SEP	P-O2P	2.02	1.62	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1173	SEP	OG-CB-CA	4.40	112.43	108.14
1	E	1173	SEP	OG-CB-CA	4.22	112.25	108.14
1	D	1173	SEP	OG-CB-CA	4.19	112.23	108.14
1	A	1173	SEP	OG-CB-CA	3.90	111.94	108.14
1	F	1173	SEP	OG-CB-CA	3.72	111.77	108.14
1	B	1173	SEP	OG-CB-CA	3.42	111.48	108.14
1	G	1173	SEP	OG-CB-CA	2.88	110.94	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	1173	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	ACT	A	1201	-	3,3,3	1.23	0	3,3,3	1.40	0
2	ACT	F	1201	-	3,3,3	1.23	0	3,3,3	1.45	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.

5.7 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	247/255 (96%)	0.15	4 (1%) 70 68	68, 93, 142, 175	1 (0%)
1	B	246/255 (96%)	0.25	8 (3%) 49 45	77, 102, 158, 240	0
1	C	245/255 (96%)	0.05	3 (1%) 76 75	82, 100, 162, 202	0
1	D	246/255 (96%)	0.20	5 (2%) 65 62	90, 115, 161, 194	0
1	E	246/255 (96%)	0.20	3 (1%) 76 75	65, 101, 148, 213	1 (0%)
1	F	244/255 (95%)	0.45	17 (6%) 22 19	75, 133, 185, 242	0
1	G	241/255 (94%)	1.33	55 (22%) 2 2	157, 234, 277, 326	0
All	All	1715/1785 (96%)	0.37	95 (5%) 30 27	65, 110, 242, 326	2 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1170	ILE	7.2
1	F	238	THR	5.0
1	F	1170	ILE	4.6
1	G	115	ILE	4.3
1	G	1170	ILE	4.2
1	G	202	LYS	4.2
1	G	128	LEU	3.8
1	G	68	ILE	3.8
1	G	232	ASP	3.5
1	F	187	TYR	3.5
1	B	4	THR	3.4
1	E	1170	ILE	3.3
1	G	1175	PRO	3.3
1	G	238	THR	3.2
1	G	102	VAL	3.2
1	G	225	LEU	3.2
1	G	40	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	236	LEU	3.0
1	G	94	LYS	3.0
1	G	160	ALA	3.0
1	B	125	VAL	3.0
1	G	205	PHE	3.0
1	G	156	LEU	3.0
1	G	116	PRO	3.0
1	G	4	THR	3.0
1	F	237	TRP	3.0
1	G	13	MET	2.9
1	G	91	TYR	2.9
1	G	119	GLY	2.9
1	G	87	LEU	2.9
1	C	242	GLN	2.9
1	A	34	VAL	2.9
1	G	72	ILE	2.9
1	D	40	ALA	2.8
1	G	127	TYR	2.8
1	F	197	ALA	2.8
1	F	239	SER	2.7
1	A	1175	PRO	2.7
1	A	244	GLN	2.7
1	F	79	ARG	2.7
1	G	120	ALA	2.7
1	F	205	PHE	2.7
1	F	242	GLN	2.6
1	G	158	TYR	2.6
1	G	239	SER	2.5
1	G	130	MET	2.5
1	F	191	LEU	2.5
1	B	127	TYR	2.5
1	E	244	GLN	2.5
1	G	204	ALA	2.5
1	B	54	ALA	2.5
1	G	236	LEU	2.4
1	G	113	HIS	2.4
1	G	131	LYS	2.4
1	G	44	THR	2.4
1	F	227	MET	2.4
1	G	191	LEU	2.4
1	G	194	SER	2.4
1	G	39	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	51	LEU	2.3
1	G	66	TRP	2.3
1	F	1175	PRO	2.3
1	G	95	VAL	2.3
1	G	165	ALA	2.3
1	A	1170	ILE	2.3
1	D	4	THR	2.3
1	F	128	LEU	2.3
1	C	213	ASP	2.3
1	B	51	LEU	2.3
1	G	234	LEU	2.3
1	E	226	ILE	2.2
1	G	24	GLU	2.2
1	G	53	VAL	2.2
1	B	238	THR	2.2
1	G	201	ALA	2.2
1	G	228	GLN	2.2
1	D	230	LEU	2.2
1	B	175	ILE	2.2
1	G	137	TYR	2.2
1	F	240	ASP	2.2
1	D	244	GLN	2.1
1	G	144	GLY	2.1
1	G	93	SER	2.1
1	F	235	THR	2.1
1	G	217	GLU	2.1
1	G	169	MET	2.1
1	G	16	LEU	2.1
1	C	95	VAL	2.1
1	F	183	PHE	2.1
1	G	192	ASN	2.0
1	G	226	ILE	2.0
1	B	83	GLU	2.0
1	G	186	PHE	2.0
1	G	231	ARG	2.0
1	G	45	VAL	2.0

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

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
1	SEP	G	1173	10/11	0.78	0.11	173,186,215,215	0
1	SEP	E	1173	10/11	0.85	0.13	75,82,99,104	0
1	SEP	D	1173	10/11	0.87	0.11	80,87,106,108	0
1	SEP	C	1173	10/11	0.88	0.10	75,78,97,98	0
1	SEP	F	1173	10/11	0.89	0.11	81,94,115,120	0
1	SEP	A	1173	10/11	0.90	0.12	62,76,93,99	0
1	SEP	B	1173	10/11	0.92	0.10	79,81,100,102	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
2	ACT	A	1201	4/4	0.81	0.26	89,91,108,108	0
2	ACT	F	1201	4/4	0.87	0.23	103,112,136,136	0

6.5 Other polymers [i](#)

There are no such residues in this entry.