

Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 12:21 pm GMT

PDB ID	:	8QTF
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 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 <=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	А	242	88%	8%	·
1	В	242	88%	10%	••
1	С	242	87%	10%	·
1	D	242	4% 87%	9%	·
1	Е	242	.% 92%	5%	•



Mol	Chain	Length	Quality of chain	
1	F	242	6% 91%	7% •
1	G	242	2% 88%	10% •
1	Н	242	4% 87%	10% •
1	Ι	242	5% 92%	5% •
1	J	242	5% 89%	7% •
2	K	7	86%	14%
2	L	7	14%	14% 14%
2	М	7	29% 71%	14% 14%
2	Ν	7	86%	14%
2	О	7	29% 57% 14%	29%
2	Р	7	86%	14%
2	Q	7	86%	14%
2	R	7	71%	29%
2	S	7	29%	29%
2	Т	7	29%	14%

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	-	-	Х	-
7	CL	F	1201	-	-	Х	-



8QTF

2 Entry composition (i)

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.

Mol	Chain	Residues			Atoms	5			ZeroOcc	AltConf	Trace
1	Δ	234	Total	С	Η	Ν	0	S	0	9	0
	Л	234	3696	1171	1826	322	370	7	0	2	0
1	B	238	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	9	0
1	D	230	3760	1188	1863	325	376	8	0		0
1	C	234	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	1	0
L	U	204	3709	1172	1839	321	370	7	0	1	0
1	П	933	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	0	0
1	D	200	3669	1161	1820	316	365	7	0	0	0
1	E	233	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	1	0
		200	3689	1167	1831	319	365	7	0	1	0
1	F	236	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	0	0
1	1	250	3687	1167	1826	319	367	8	0	0	0
1	G	237	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	1	0
	u	201	3712	1177	1834	319	374	8	0	1	0
1	н	933	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	1	0
1	11	200	3686	1167	1825	317	370	7	0	I	0
1	т	235	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	0	0
	L	200	3672	1164	1816	317	368	7	0	0	0
1	Т	233	Total	\mathbf{C}	Н	N	0	S	0	2	0
	5	200	3707	1173	1835	321	371	7	0	2	0

• Molecule 1 is a protein called 14-3-3-like protein GF14 omega.

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	GLY	-	expression tag	UNP Q01525
А	0	ALA	-	expression tag	UNP Q01525
В	-1	GLY	-	expression tag	UNP Q01525
В	0	ALA	-	expression tag	UNP Q01525
С	-1	GLY	-	expression tag	UNP Q01525
С	0	ALA	-	expression tag	UNP Q01525
D	-1	GLY	-	expression tag	UNP Q01525
D	0	ALA	-	expression tag	UNP Q01525
Е	-1	GLY	-	expression tag	UNP Q01525



Chain	Residue	Modelled	Actual	Comment	Reference
Е	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
Н	-1	GLY	-	expression tag	UNP Q01525
Н	0	ALA	-	expression tag	UNP Q01525
Ι	-1	GLY	-	expression tag	UNP Q01525
Ι	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		A	Aton	ns			ZeroOcc	AltConf	Trace
9	K	7	Total	С	Η	Ν	0	Р	0	0	0
	К	1	107	30	51	11	14	1	0	0	0
2	T	7	Total	С	Η	Ν	Ο	Р	0	0	0
2		1	107	30	51	11	14	1	0	0	0
2	М	7	Total	С	Η	Ν	Ο	Р	0	0	0
2	111	1	107	30	51	11	14	1	0	0	0
2	N	7	Total	С	Η	Ν	Ο	Р	0	0	0
2	11	1	107	30	51	11	14	1		0	0
2	0	7	Total	\mathbf{C}	Η	Ν	Ο	Р	0	0	0
	0	1	107	30	51	11	14	1	0	0	0
2	Р	7	Total	С	Η	Ν	Ο	Р	0	0	0
	1	1	107	30	51	11	14	1	0	0	0
2	0	7	Total	\mathbf{C}	Η	Ν	Ο	Р	0	0	0
	્ય	•	107	30	51	11	14	1	0	0	0
2	B	7	Total	\mathbf{C}	Η	Ν	Ο	Р	0	0	0
	10	•	107	30	51	11	14	1	0	0	0
2	S	7	Total	С	Η	Ν	Ο	Р	0	0	0
	5	1	107	30	51	11	14	1	U	0	U
2	Т	7	Total	C	H	N	Ō	Р	0	0	0
2	1	1	107	30	51	11	14	1	0		0

• Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 5 & 1 & 2 & 2 \end{array}$	0	0
3	А	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 5 & 1 & 2 & 2 \end{array}$	0	0
3	С	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 5 & 1 & 2 & 2 \end{array}$	0	0
3	Е	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 5 & 1 & 2 & 2 \end{array}$	0	0
3	G	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 5 & 1 & 2 & 2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 5 & 1 & 2 & 2 \end{array}$	0	0
3	Ι	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 5 & 1 & 2 & 2 \end{array}$	0	0
3	J	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 5 & 1 & 2 & 2 \end{array}$	0	0
3	Q	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 5 & 1 & 2 & 2 \end{array}$	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf	
4	Λ	1	Total	С	Н	0	0	0	
4	Л	1	10	2	6	2	0	0	
4	Ц	1	Total	С	Η	Ο	0	0	
4	11	1	10	2	6	2	0	0	
4	т	1	Total	С	Η	Ο	0	0	
4	J	1	10	2	6	2	0	0	
4	K	1	Total	С	Н	0	0	0	
4	17	I	10	2	6	2	0	0	

• Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	3	Total Na 3 3	0	0
5	С	1	Total Na 1 1	0	0
5	Е	2	Total Na 2 2	0	0
5	G	1	Total Na 1 1	0	0
5	Н	2	Total Na 2 2	0	0
5	Ι	1	Total Na 1 1	0	0

• Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	С	Η	0	0	0
	-	-	22	6	14	2	Ŭ	Ŭ

• Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Ator	ns	ZeroOcc	AltConf
7	F	1	Total 1	Cl 1	0	0

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





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
8	G	1	Total 7	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	Н 3	0 2	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	91	Total O 91 91	0	0
9	В	124	Total O 124 124	0	0
9	С	96	Total O 96 96	0	0
9	D	56	Total O 56 56	0	0
9	Е	110	Total O 110 110	0	0
9	F	58	$\begin{array}{cc} \text{Total} & \text{O} \\ 58 & 58 \end{array}$	0	0
9	G	92	Total O 92 92	0	0
9	Н	93	Total O 93 93	0	0
9	Ι	48	Total O 48 48	0	0
9	J	54	$\begin{array}{cc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0
9	K	12	Total O 12 12	0	0
9	L	5	Total O 5 5	0	0
9	М	6	Total O 6 6	0	0
9	Ν	5	Total O 5 5	0	0
9	О	6	Total O 6 6	0	0
9	Р	2	Total O 2 2	0	0
9	Q	8	Total O 8 8	0	0
9	R	6	Total O 6 6	0	0
9	S	2	Total O 2 2	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	Т	2	Total O 2 2	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: 14-3-3-like protein GF14 omega







• Molecule 2: Protein BRASSINAZOLE-RESISTANT 1



Chain S:	29%	29%
R1169 • 11170 • S1173 A1174 P1175		
• Molecul	e 2: Protein BRASSINAZOLE-RESISTANT 1 29%	
Chain T:	86%	14%
R1169 11170 S1173 A1174 A1174 P1175		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	71.64Å 71.92Å 151.66Å	Depositor
a, b, c, α , β , γ	100.25° 94.84° 89.23°	Depositor
Bosolution(A)	59.91 - 1.90	Depositor
Resolution (A)	74.36 - 1.90	EDS
% Data completeness	97.1 (59.91 - 1.90)	Depositor
(in resolution range)	97.5(74.36-1.90)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.07 (at 1.90 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
P. P.	0.195 , 0.230	Depositor
II, II, <i>free</i>	0.193 , 0.230	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 $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.39 , 44.9	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=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.

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.



¹Intensities estimated from amplitudes.

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: SEP, FMT, ACT, EDO, NA, MPD, CL

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).

Mal	Chain	Bond	lengths	Bond	angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.37	0/1905	0.52	0/2568
1	В	0.37	0/1929	0.53	0/2599
1	С	0.36	0/1899	0.53	0/2559
1	D	0.33	0/1878	0.48	0/2532
1	Е	0.36	0/1890	0.53	0/2547
1	F	0.33	0/1890	0.50	0/2548
1	G	0.34	0/1910	0.51	0/2576
1	Н	0.37	0/1890	0.51	0/2548
1	Ι	0.33	0/1885	0.50	0/2543
1	J	0.33	0/1901	0.50	0/2562
2	Κ	0.34	0/45	0.65	0/57
2	L	0.30	0/45	0.65	0/57
2	М	0.29	0/45	0.59	0/57
2	Ν	0.34	0/45	0.55	0/57
2	0	0.29	0/45	0.63	0/57
2	Р	0.31	0/45	0.65	0/57
2	Q	0.36	0/45	0.54	0/57
2	R	0.27	0/45	0.54	0/57
2	S	0.28	0/45	0.54	0/57
2	Т	0.26	0/45	0.53	0/57
All	All	0.35	0/19427	0.51	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 (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	А	1870	1826	1833	11	1
1	В	1897	1863	1869	11	0
1	С	1870	1839	1840	17	0
1	D	1849	1820	1819	16	1
1	Е	1858	1831	1834	6	1
1	F	1861	1826	1828	13	1
1	G	1878	1834	1840	14	1
1	Н	1861	1825	1826	19	1
1	Ι	1856	1816	1815	14	1
1	J	1872	1835	1838	12	1
2	K	56	51	49	0	0
2	L	56	51	49	2	0
2	М	56	51	49	1	0
2	Ν	56	51	49	0	0
2	0	56	51	49	3	0
2	Р	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	Т	56	51	49	0	0
3	А	6	4	2	0	0
3	С	3	2	1	0	0
3	Ε	3	2	1	0	0
3	G	3	2	1	0	0
3	Н	3	2	1	0	0
3	Ι	3	2	1	0	0
3	J	3	2	1	0	0
3	Q	3	2	1	0	0
4	А	4	6	6	0	0
4	Н	4	6	6	1	0
4	J	4	6	6	4	0
4	K	4	6	6	0	0
5	В	3	0	0	0	0
5	С	1	0	0	0	0
5	E	2	0	0	0	0
5	G	1	0	0	0	0
5	Н	2	0	0	0	0



8	O'	ΓF
$_{\circ}$	ve.	

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Ι	1	0	0	0	0
6	Е	8	14	14	0	0
7	F	1	0	0	3	0
8	G	4	3	3	0	0
9	А	91	0	0	0	0
9	В	124	0	0	1	0
9	С	96	0	0	0	0
9	D	56	0	0	0	0
9	Ε	110	0	0	1	0
9	F	58	0	0	2	0
9	G	92	0	0	1	0
9	Н	93	0	0	1	0
9	Ι	48	0	0	0	0
9	J	54	0	0	0	0
9	Κ	12	0	0	0	0
9	L	5	0	0	0	0
9	М	6	0	0	0	0
9	Ν	5	0	0	0	0
9	0	6	0	0	0	0
9	Р	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	Т	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.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:4:GLY:N	1:D:7:GLU:OE1	2.17	0.77
1:F:209:LEU:N	7:F:1201:CL:CL	2.58	0.74
1:D:72:LYS:NZ	1:D:73:GLU:OE2	2.22	0.71
1:B:39:GLU:OE2	9:B:1301:HOH:O	2.13	0.67
1:G:35:VAL:HG21	1:G:40:LEU:HD23	1.77	0.65
1:I:11:MET:HA	1:I:11:MET:HE2	1.79	0.63
1:A:233:LEU:HB3	1:D:72:LYS:HD3	1.82	0.60
1:B:101:ASP:O	1:B:105:LYS:HG2	2.01	0.60
1:J:137:GLU:OE1	4:J:1202:EDO:H12	2.01	0.60



UQ II

		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	$\frac{1}{1}$
1.C.84.ALA.HB1	1.H.11.MET.CE	2 32	0.59
1.C.35.VAL:HG13	1.C·38·ASP·HB2	1.84	0.55
1.1.60.ABG.HA	4. I.1202. EDO. H21	1.81	0.57
1.H.110.ARG.NE	9·H·1304·HOH·O	2.38	0.56
1.H.137.GLU.O	4·H·1202·EDO·O2	2.30	0.56
1:C:136:ALA:O	1.C.144.ABG.NH1	2.39	0.55
1:J:4:GLY:N	1.J.7.GLU.OE1	2.39	0.55
2.L.1169.ABC.NH2	2·L·1173·SEP·O1P	2.10	0.56
1·I·11·MET·CE	1:J:84:ALA:HB1	2.10	0.54
1.F.208.GLU.N	7·F·1201·CL·CL	2.31	0.53
1.1.200.0E0.IX	1.1.11201.01.01 1.1.113.PRO.HD3	1.91	0.53
1.H.112.IEE.IIE	1.H.14.LEU.HD12	1.91	0.53
1.C.84.ALA.HB1	1.D.11.MET.CE	2.39	0.52
1.D.36.ASP.OD1	1.D.37.GLV·N	2.03	0.52
1:A:236:SEB:O	1.D.37.ASP.HB2	2.10	0.52
1.1.250.5E1(.0	1.1.257.1151.1152 1.1.95.GLU.OE1	2.10	0.52
1.1.20.MET.HE2	1.J.31.VAL.:HG21	1.93	0.51
1:E:32:SEB:OG	1.E.106.LEU.HD11	2.11	0.51
1.1.02.0EIt.0G	1.1.100.1101.11011 1.1.14.LEU.HD12	1.94	0.30
1.H.11.MET.HE2	1.H.11.MET.HA	1.91	0.10
1.H.35.VAL.HG21	1.H.40.LEU.HD23	1.95	0.49
1:J:209:LEU:HD12	1:J:212:LEU:HD12	1.94	0.49
1.B.74.GLU:OE2	1.B.86.ARG.NH2	2.47	0.48
1:H:55:VAL:HG12	1:H:99:ILE:HD13	1.96	0.48
1:I:11:MET:HE1	1:J:84:ALA:HB1	1.95	0.48
1:A:39:GLU:OE2	1:A:116:ALA:N	2.42	0.48
2:0:1169:ARG:HG2	2:0:1171:SER:H	1.79	0.47
1:H:31:VAL:O	1:H:35:VAL:HG23	2.14	0.47
1:C:206:ILE:HD12	1:C:209:LEU:HD12	1.96	0.47
1:H:70:GLU:HB2	1:H:85:ILE:HG21	1.95	0.47
1:C:11:MET:CE	1:D:84:ALA:HB1	2.44	0.47
1:D:169:THR:HB	1:D:212:LEU:HD11	1.97	0.47
1:F:72:LYS:HE3	1:F:73:GLU:OE2	2.15	0.47
1:B:169:THR:O	1:B:220:SER:OG	2.24	0.47
1:D:11:MET:HA	1:D:11:MET:HE2	1.97	0.47
1:I:9:VAL:HA	1:I:28:MET:HE1	1.97	0.47
1:B:112:ILE:HB	1:B:113:PRO:HD3	1.98	0.46
1:C:135:LEU:O	1:C:139:LYS:HG2	2.16	0.46
1:D:35:VAL:HG12	1:D:35:VAL:O	2.16	0.46
1:H:35:VAL:O	1:H:36:ASP:HB3	2.16	0.46
1:I:28:MET:CE	1:I:31:VAL:HG21	2.46	0.46



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:F:209:LEU:HD12	1:F:210:ASP:N	2.30	0.46	
1:D:112:ILE:HB	1:D:113:PRO:HD3	1.98	0.45	
1:G:31:VAL:O	1:G:35:VAL:HG23	2.17	0.45	
1:F:11:MET:HE3	9:F:1326:HOH:O	2.17	0.45	
1:F:128:LYS:NZ	9:F:1303:HOH:O	2.49	0.45	
1:B:45[A]:ARG:HG3	1:B:46:ASN:N	2.31	0.45	
1:F:11:MET:HA	1:F:11:MET:HE2	1.98	0.45	
1:D:107:LEU:HD23	1:D:111:LEU:HD12	1.97	0.44	
1:A:69:ILE:HG22	1:A:85:ILE:HD13	1.99	0.44	
1:H:11:MET:CE	1:H:14:LEU:HD12	2.46	0.44	
1:H:7:GLU:OE1	1:H:7:GLU:N	2.46	0.44	
1:D:136:ALA:O	1:D:144:ARG:NH1	2.50	0.44	
1:D:211:THR:HG22	1:D:211:THR:O	2.18	0.44	
1:E:110:ARG:NH2	9:E:1310:HOH:O	2.49	0.44	
1:B:186:GLU:OE1	2:L:1169:ARG:NH1	2.50	0.44	
1:G:5:ARG:NH2	1:G:35:VAL:HG13	2.32	0.44	
1:I:28:MET:CE	1:I:28:MET:HA	2.48	0.44	
1:J:112:ILE:HB	1:J:113:PRO:HD3	1.99	0.44	
1:A:152:LEU:HG	1:E:207:ALA:HB1	1.99	0.44	
1:B:35:VAL:O	1:B:36:ASP:C	2.56	0.44	
1:G:5:ARG:HD3	1:G:44:GLU:OE2	2.18	0.44	
1:H:112:ILE:HB	1:H:113:PRO:HD3	2.00	0.44	
1:J:63:TRP:CE3	4:J:1202:EDO:H22	2.53	0.44	
1:D:212:LEU:HD22	1:D:216:SER:HB3	1.99	0.43	
1:I:11:MET:HA	1:I:11:MET:CE	2.48	0.43	
1:G:84:ALA:HB1	1:H:11:MET:HE1	1.98	0.43	
1:A:101:ASP:O	1:A:105:LYS:HG3	2.18	0.43	
1:F:72:LYS:HD3	1:G:233:LEU:HB3	2.00	0.43	
1:G:121:LYS:NZ	9:G:1304:HOH:O	2.51	0.43	
1:I:208:GLU:O	1:I:208:GLU:HG2	2.19	0.43	
1:E:186:GLU:OE2	2:0:1171:SER:HB2	2.18	0.43	
1:F:206:ILE:HA	1:F:209:LEU:HD23	1.99	0.43	
1:C:11:MET:CE	1:C:14:LEU:HD12	2.48	0.43	
1:C:45[B]:ARG:HD3	1:C:123:PHE:CE1	2.54	0.43	
1:C:101:ASP:OD2	1:C:105:LYS:HE2	2.19	0.43	
1:B:116:ALA:O	1:B:121:LYS:NZ	2.52	0.42	
1:A:123:PHE:CE1	1:A:127:MET:CE	3.02	0.42	
1:J:70:GLU:HB2	1:J:85:ILE:HG21	2.01	0.42	
1:D:11:MET:CE	1:D:14:LEU:HD12	2.50	0.42	
1:A:184:TYR:CE1	1:A:193[B]:ARG:HD2	2.55	0.42	

1:C:55:VAL:HG12

Continued on next page...

0.42



2.01

1:C:99:ILE:HD13

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:112:ILE:HB	1:C:113:PRO:HD3	2.01	0.42	
1:G:45[B]:ARG:HH22	1:G:172:ILE:HD11	1.84	0.42	
1:G:84:ALA:HB1	1:H:11:MET:HE3	2.01	0.42	
1:A:202:PHE:CE2	1:A:228:ARG:HG3	2.55	0.42	
1:H:198:ALA:HB3	1:H:231:LEU:HD21	2.01	0.42	
1:C:11:MET:HE1	1:D:84:ALA:HB1	2.01	0.41	
1:F:112:ILE:HB	1:F:113:PRO:HD3	2.02	0.41	
1:G:213:GLY:O	1:G:215:GLU:N	2.53	0.41	
1:H:169:THR:HB	1:H:212:LEU:HD11	2.02	0.41	
1:E:107:LEU:HA	1:E:111:LEU:HB2	2.02	0.41	
1:H:209:LEU:CD1	1:H:212:LEU:HD12	2.51	0.41	
1:F:31:VAL:O	1:F:35:VAL:HG23	2.20	0.41	
1:J:60:ARG:CA	4:J:1202:EDO:H21	2.51	0.41	
1:C:36:ASP:OD1	1:C:36:ASP:N	2.54	0.41	
1:J:229:ASP:O	1:J:233:LEU:HD13	2.21	0.41	
1:F:69:ILE:HG22	1:F:85:ILE:HD13	2.03	0.41	
1:C:209:LEU:HD23	1:C:212:LEU:HD12	2.01	0.41	
1:G:101:ASP:OD2	1:G:105:LYS:HE2	2.20	0.41	
1:A:52:TYR:HB3	1:A:131:TYR:OH	2.21	0.41	
1:B:90:SER:O	1:B:94:THR:HG23	2.21	0.41	
1:B:180:PHE:HB3	1:B:197:LEU:HD21	2.02	0.41	
1:C:203:ASP:O	1:C:206:ILE:HG22	2.20	0.41	
2:O:1169:ARG:NH2	2:O:1173:SEP:O2P	2.53	0.41	
1:A:123:PHE:HE1	1:A:127:MET:CE	2.34	0.41	
1:G:166:LEU:O	1:G:173:ARG:NH1	2.52	0.41	
2:M:1169:ARG:NH2	2:M:1173:SEP:O2P	2.54	0.41	
1:G:55:VAL:HG12	1:G:99:ILE:HD13	2.03	0.40	
1:C:11:MET:HA	1:C:11:MET:HE2	2.03	0.40	
1:E:45[B]:ARG:HG3	1:E:123:PHE:CE1	2.56	0.40	
1:F:206:ILE:O	7:F:1201:CL:CL	2.77	0.40	
1:H:185:TYR:CE2	2:R:1170:ILE:HD11	2.56	0.40	
1:I:11:MET:CE	1:I:14:LEU:HD12	2.50	0.40	
1:I:45:ARG:HG3	1:I:46:ASN:N	2.36	0.40	
1:C:11:MET:HE2	1:C:14:LEU:HD12	2.03	0.40	

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



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	Perce	ntiles
1	А	234/242~(97%)	230 (98%)	4 (2%)	0	100	100
1	В	238/242~(98%)	231 (97%)	5 (2%)	2 (1%)	19	9
1	С	233/242~(96%)	230~(99%)	3 (1%)	0	100	100
1	D	231/242~(96%)	225~(97%)	6 (3%)	0	100	100
1	Ε	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%)	34	24
1	Н	232/242~(96%)	225 (97%)	7 (3%)	0	100	100
1	Ι	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	М	4/7~(57%)	3(75%)	1 (25%)	0	100	100
2	Ν	4/7~(57%)	4 (100%)	0	0	100	100
2	Ο	4/7~(57%)	4 (100%)	0	0	100	100
2	Р	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



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
2	Т	4/7~(57%)	4 (100%)	0	0	100	100
All	All	2376/2490~(95%)	2317 (98%)	56 (2%)	3~(0%)	51	42

All (3) Ramachandran outliers are listed below:

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

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	А	196/201~(98%)	195 (100%)	1 (0%)	88 89
1	В	199/201~(99%)	194 (98%)	5(2%)	47 41
1	\mathbf{C}	197/201~(98%)	195~(99%)	2(1%)	76 76
1	D	194/201~(96%)	193 (100%)	1 (0%)	88 89
1	Ε	195/201~(97%)	194 (100%)	1 (0%)	88 89
1	F	194/201~(96%)	193 (100%)	1 (0%)	88 89
1	G	197/201~(98%)	194 (98%)	3~(2%)	65 62
1	Н	196/201~(98%)	195 (100%)	1 (0%)	88 89
1	Ι	194/201~(96%)	192~(99%)	2(1%)	76 76
1	J	197/201~(98%)	196 (100%)	1 (0%)	88 89
2	К	5/5~(100%)	5 (100%)	0	100 100
2	L	5/5~(100%)	5 (100%)	0	100 100
2	М	5/5~(100%)	5 (100%)	0	100 100
2	N	5/5~(100%)	5 (100%)	0	100 100
2	Ο	5/5~(100%)	4 (80%)	1 (20%)	1 0
2	Р	5/5~(100%)	5 (100%)	0	100 100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
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	Т	5/5~(100%)	5 (100%)	0	100	100
All	All	2009/2060~(98%)	1989~(99%)	20 (1%)	76	76

Continued from previous page...

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	180	PHE
1	В	119	ASP
1	В	180	PHE
1	В	193	ARG
1	В	215	GLU
1	В	218	LYS
1	С	180	PHE
1	С	192	ASP
1	D	180	PHE
1	Е	180	PHE
1	F	180	PHE
1	G	180	PHE
1	G	208	GLU
1	G	212	LEU
1	Н	180	PHE
1	Ι	20	ARG
1	Ι	180	PHE
1	J	180	PHE
2	0	1169	ARG
2	S	1170	ILE

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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).

Mal	Tuno	Chain	Dog	Link	B	ond leng	$_{ m gths}$	B	Bond ang	gles
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	SEP	М	1173	2	8,9,10	1.50	1 (12%)	8,12,14	1.62	2 (25%)
2	SEP	Р	1173	2	8,9,10	1.40	1 (12%)	8,12,14	2.03	3 (37%)
2	SEP	0	1173	2	8,9,10	1.50	1 (12%)	8,12,14	2.05	2 (25%)
2	SEP	R	1173	2	8,9,10	1.67	1 (12%)	8,12,14	1.84	3 (37%)
2	SEP	Т	1173	2	8,9,10	1.47	1 (12%)	8,12,14	1.82	3 (37%)
2	SEP	S	1173	2	8,9,10	1.72	2 (25%)	8,12,14	1.76	2 (25%)
2	SEP	Ν	1173	2	8,9,10	1.57	1 (12%)	8,12,14	1.61	3 (37%)
2	SEP	Q	1173	2	8,9,10	1.57	2 (25%)	8,12,14	1.40	1 (12%)
2	SEP	L	1173	2	8,9,10	1.53	1 (12%)	8,12,14	2.00	3 (37%)
2	SEP	Κ	1173	2	8,9,10	1.60	1 (12%)	8,12,14	1.68	2 (25%)

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	М	1173	2	-	0/5/8/10	-
2	SEP	Р	1173	2	-	0/5/8/10	-
2	SEP	0	1173	2	-	0/5/8/10	-
2	SEP	R	1173	2	-	0/5/8/10	-
2	SEP	Т	1173	2	-	0/5/8/10	-
2	SEP	S	1173	2	-	0/5/8/10	-
2	SEP	N	1173	2	-	0/5/8/10	-
2	SEP	Q	1173	2	-	0/5/8/10	-
2	SEP	L	1173	2	-	0/5/8/10	-
2	SEP	K	1173	2	-	0/5/8/10	-

All (12) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
2	R	1173	SEP	P-01P	4.17	1.64	1.50
2	Κ	1173	SEP	P-O1P	3.72	1.62	1.50
2	S	1173	SEP	P-O1P	3.59	1.62	1.50
2	L	1173	SEP	P-01P	3.57	1.62	1.50
2	0	1173	SEP	P-O1P	3.46	1.61	1.50
2	Ν	1173	SEP	P-O1P	3.25	1.61	1.50
2	М	1173	SEP	P-O1P	3.25	1.61	1.50
2	Q	1173	SEP	P-O1P	3.15	1.60	1.50
2	Т	1173	SEP	P-O1P	3.12	1.60	1.50
2	Р	1173	SEP	P-O1P	2.83	1.59	1.50
2	S	1173	SEP	P-O3P	2.42	1.64	1.54
2	Q	1173	SEP	P-O3P	2.22	1.63	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Р	1173	SEP	OG-CB-CA	4.28	112.31	108.14
2	0	1173	SEP	OG-CB-CA	4.23	112.26	108.14
2	Κ	1173	SEP	OG-CB-CA	3.36	111.41	108.14
2	R	1173	SEP	O3P-P-OG	3.27	115.43	106.73
2	L	1173	SEP	P-OG-CB	-3.26	109.31	118.30
2	Т	1173	SEP	OG-CB-CA	3.24	111.30	108.14
2	S	1173	SEP	P-OG-CB	-3.10	109.74	118.30
2	М	1173	SEP	OG-CB-CA	2.99	111.06	108.14
2	L	1173	SEP	OG-CB-CA	2.86	110.93	108.14
2	Q	1173	SEP	P-OG-CB	-2.86	110.42	118.30
2	S	1173	SEP	OG-CB-CA	2.71	110.78	108.14
2	Р	1173	SEP	P-OG-CB	-2.54	111.29	118.30
2	Т	1173	SEP	O3P-P-OG	2.50	113.39	106.73
2	Ν	1173	SEP	OG-CB-CA	2.49	110.57	108.14
2	Κ	1173	SEP	P-OG-CB	-2.41	111.66	118.30
2	R	1173	SEP	P-OG-CB	-2.40	111.67	118.30
2	0	1173	SEP	O2P-P-OG	2.39	113.10	106.73
2	Ν	1173	SEP	P-OG-CB	-2.35	111.83	118.30
2	Р	1173	SEP	OG-P-O1P	2.25	112.79	106.47
2	L	1173	SEP	OG-P-O1P	2.24	112.74	106.47
2	Т	1173	SEP	O2P-P-OG	2.17	112.50	106.73
2	М	1173	SEP	P-OG-CB	-2.04	112.67	118.30
2	N	1173	SEP	OG-P-O1P	2.03	112.17	106.47
2	R	1173	SEP	O2P-P-OG	2.01	112.08	106.73

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	\mathbf{Res}	Type	Clashes	Symm-Clashes
2	М	1173	SEP	1	0
2	0	1173	SEP	1	0
2	L	1173	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	Bog	Link	B	ond leng	gths	Bond angles		
IVIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	EDO	Н	1202	-	3,3,3	0.47	0	$2,\!2,\!2$	0.26	0
3	FMT	А	1201	-	2,2,2	0.69	0	$1,\!1,\!1$	0.48	0
3	FMT	Е	1201	-	2,2,2	0.72	0	$1,\!1,\!1$	0.40	0
3	FMT	Q	1201	-	2,2,2	0.59	0	$1,\!1,\!1$	0.44	0
3	FMT	Ι	1201	-	2,2,2	0.69	0	$1,\!1,\!1$	0.47	0
4	EDO	K	1201	-	3,3,3	0.49	0	$2,\!2,\!2$	0.60	0
3	FMT	С	1201	-	2,2,2	0.75	0	$1,\!1,\!1$	0.49	0
4	EDO	J	1202	-	3,3,3	0.69	0	$2,\!2,\!2$	0.49	0
3	FMT	G	1201	-	2,2,2	0.72	0	$1,\!1,\!1$	0.51	0
3	FMT	Н	1201	-	2,2,2	0.71	0	$1,\!1,\!1$	0.44	0
6	MPD	E	1202	-	7,7,7	0.35	0	$9,\!10,\!10$	0.48	0
8	ACT	G	1202	-	3,3,3	1.01	0	$3,\!3,\!3$	1.62	1 (33%)
3	FMT	J	1201	-	2,2,2	0.69	0	$1,\!1,\!1$	0.46	0
3	FMT	A	1202	-	2,2,2	0.70	0	1,1,1	0.48	0
4	EDO	A	1203	-	3,3,3	0.54	0	2,2,2	0.32	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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	А	1203	-	-	0/1/1/1	-
4	EDO	Κ	1201	-	-	0/1/1/1	-
4	EDO	J	1202	-	-	1/1/1/1	-
4	EDO	Н	1202	-	-	0/1/1/1	-
6	MPD	Е	1202	-	-	2/5/5/5	-

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	G	1202	ACT	O-C-CH3	-2.02	114.48	122.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Е	1202	MPD	C2-C3-C4-O4
6	Е	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	Н	1202	EDO	1	0
4	J	1202	EDO	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	А	234/242~(96%)	0.32	4 (1%) 70 72	32, 47, 86, 136	0
1	В	238/242~(98%)	0.36	9 (3%) 40 43	31, 46, 93, 151	0
1	С	234/242~(96%)	0.14	2 (0%) 84 85	31, 46, 82, 103	0
1	D	233/242~(96%)	0.22	10 (4%) 35 38	36, 57, 112, 144	0
1	Ε	233/242~(96%)	0.26	3 (1%) 77 79	29, 43, 79, 106	0
1	F	236/242~(97%)	0.38	14 (5%) 22 25	33, 54, 110, 141	0
1	G	237/242~(97%)	0.37	5 (2%) 63 66	31, 48, 98, 135	0
1	Н	233/242~(96%)	0.32	10 (4%) 35 38	31, 49, 104, 162	0
1	Ι	235/242~(97%)	0.30	11 (4%) 31 34	43, 59, 101, 134	0
1	J	233/242~(96%)	0.25	13 (5%) 24 27	41, 58, 101, 137	0
2	Κ	6/7~(85%)	0.08	0 100 100	45, 46, 51, 58	0
2	L	6/7~(85%)	0.68	1 (16%) 1 1	41, 55, 75, 88	0
2	М	6/7~(85%)	1.33	2 (33%) 0 0	42, 56, 89, 103	0
2	Ν	6/7~(85%)	1.34	1 (16%) 1 1	58, 72, 108, 110	0
2	Ο	6/7~(85%)	1.65	2 (33%) 0 0	42, 59, 100, 116	0
2	Р	6/7~(85%)	0.53	0 100 100	57, 68, 95, 117	0
2	Q	6/7~(85%)	-0.11	0 100 100	43, 45, 48, 64	0
2	R	6/7~(85%)	0.60	1 (16%) 1 1	44, 59, 70, 82	0
2	S	6/7~(85%)	1.07	2 (33%) 0 0	51, 67, 85, 93	0
2	Т	6/7~(85%)	1.59	2 (33%) 0 0	55, 69, 85, 85	0
All	All	2406/2490~(96%)	0.31	92 (3%) 40 43	29, 51, 99, 162	0

All (92) RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
1	Н	212	LEU	13.2
1	В	211	THR	11.4
1	В	212	LEU	11.2
1	А	214	GLU	8.7
1	Н	211	THR	7.8
1	D	212	LEU	7.0
1	А	212	LEU	6.8
1	F	209	LEU	6.6
1	G	209	LEU	6.5
1	Н	213	GLY	6.4
1	Ι	213	GLY	6.4
1	А	215	GLU	6.4
1	G	212	LEU	5.9
1	В	214	GLU	5.8
1	F	1	MET	5.5
1	В	213	GLY	5.4
1	Н	36	ASP	5.2
1	F	213	GLY	5.2
2	М	1169	ARG	5.1
2	Ν	1170	ILE	4.8
2	0	1169	ARG	4.7
1	J	211	THR	4.5
1	D	213	GLY	4.5
1	J	215	GLU	4.4
1	F	216	SER	4.3
1	D	209	LEU	4.2
1	G	216	SER	4.0
1	Н	210	ASP	4.0
1	Ι	214	GLU	3.9
1	J	233	LEU	3.7
1	Н	35	VAL	3.7
2	L	1170	ILE	3.6
1	D	214	GLU	3.6
1	Е	214	GLU	3.6
1	D	211	THR	3.6
2	Т	1170	ILE	3.6
1	F	210	ASP	3.5
2	Ο	1170	ILE	3.5
1	В	209	LEU	3.5
2	R	1170	ILE	3.4
1	J	212	LEU	3.3
1	В	218	LYS	3.3
1	В	215	GLU	3.3



Mol	Chain	Res	Type	RSRZ
1	Ι	212	LEU	3.3
2	М	1170	ILE	3.3
1	Н	214	GLU	3.2
1	Ι	3	SER	3.2
1	J	228	ARG	3.1
1	А	207	ALA	3.1
1	J	210	ASP	3.0
1	Ι	210	ASP	3.0
1	D	231	LEU	2.9
1	F	212	LEU	2.8
1	G	215	GLU	2.8
1	F	217	TYR	2.8
1	F	233	LEU	2.8
2	Т	1169	ARG	2.8
1	F	211	THR	2.7
1	J	226	LEU	2.7
1	Ι	216	SER	2.7
1	С	35	VAL	2.7
1	G	214	GLU	2.6
1	С	3	SER	2.6
2	S	1170	ILE	2.6
1	Ι	211	THR	2.6
1	Н	209	LEU	2.5
1	D	217	TYR	2.5
1	J	217	TYR	2.5
1	J	216	SER	2.5
1	Ι	35	VAL	2.5
1	В	210	ASP	2.5
1	J	214	GLU	2.5
1	Ι	209	LEU	2.5
1	J	218	LYS	2.4
1	Ι	79	ASP	2.4
1	Н	207	ALA	2.4
1	D	236	SER	2.3
1	F	193	ARG	2.3
2	S	1169	ARG	2.3
1	D	215	GLU	2.3
1	Ι	215	GLU	2.3
1	D	164	ALA	2.2
1	F	200	GLN	2.2
1	В	236	SER	2.2
1	F	36	ASP	2.1



Continued	from	previous	page
-----------	------	----------	------

Mol	Chain	Res	Type	RSRZ
1	F	169	THR	2.1
1	J	65	ILE	2.1
1	Н	233	LEU	2.1
1	F	223	ILE	2.1
1	Е	233	LEU	2.1
1	J	213	GLY	2.1
1	E	235	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	$B-factors(Å^2)$	Q<0.9
2	SEP	М	1173	10/11	0.98	0.15	36,43,51,54	0
2	SEP	N	1173	10/11	0.98	0.15	48,51,59,63	0
2	SEP	S	1173	10/11	0.98	0.10	40,50,59,60	0
2	SEP	Т	1173	10/11	0.98	0.12	43,52,62,66	0
2	SEP	0	1173	10/11	0.99	0.15	35,39,48,49	0
2	SEP	Р	1173	10/11	0.99	0.13	41,53,59,64	0
2	SEP	Q	1173	10/11	0.99	0.15	32,41,47,51	0
2	SEP	R	1173	10/11	0.99	0.14	29,39,47,49	0
2	SEP	K	1173	10/11	0.99	0.16	33,40,46,51	0
2	SEP	L	1173	10/11	0.99	0.15	33,38,46,46	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	FMT	J	1201	3/3	0.83	0.10	$61,\!65,\!81,\!97$	0



8	Ω'	TF
O	ve.	T T

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q<0.9
5	NA	Н	1203	1/1	0.83	0.33	58, 58, 58, 58	0
6	MPD	Е	1202	8/8	0.83	0.21	57,69,85,85	0
8	ACT	G	1202	4/4	0.84	0.17	58,59,82,82	0
3	FMT	С	1201	3/3	0.86	0.11	69,71,83,85	0
4	EDO	Н	1202	4/4	0.87	0.27	49,59,71,71	0
7	CL	F	1201	1/1	0.87	0.35	123,123,123,123	0
5	NA	Н	1204	1/1	0.87	0.34	57,57,57,57	0
5	NA	Е	1204	1/1	0.88	0.27	80,80,80,80	0
5	NA	С	1202	1/1	0.88	0.14	61,61,61,61	0
5	NA	G	1203	1/1	0.89	0.08	58,58,58,58	0
5	NA	Е	1203	1/1	0.89	0.53	70,70,70,70	0
4	EDO	K	1201	4/4	0.90	0.20	52,63,73,73	0
3	FMT	Q	1201	3/3	0.90	0.11	52,52,62,62	0
4	EDO	J	1202	4/4	0.91	0.33	44,54,65,68	0
3	FMT	G	1201	3/3	0.91	0.14	53,60,65,72	0
5	NA	Ι	1202	1/1	0.91	0.06	$63,\!63,\!63,\!63$	0
4	EDO	А	1203	4/4	0.92	0.20	58,69,81,81	0
3	FMT	Н	1201	3/3	0.93	0.20	$56,\!66,\!68,\!79$	0
5	NA	В	1203	1/1	0.93	0.23	60,60,60,60	0
3	FMT	Ι	1201	3/3	0.94	0.13	$58,\!64,\!77,\!88$	0
3	FMT	A	1202	3/3	0.95	0.09	$5\overline{8,60,70,72}$	0
3	FMT	A	1201	3/3	0.95	0.10	61,61,73,75	0
5	NA	В	1202	1/1	0.96	0.12	57, 57, 57, 57	0
3	FMT	Е	1201	3/3	0.98	0.09	48,54,58,66	0
5	NA	В	1201	1/1	0.98	0.35	56, 56, 56, 56	0

6.5 Other polymers (i)

There are no such residues in this entry.

