



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2025 – 02:26 PM EDT

PDB ID : 5V65
Title : Crystal structure of macrocycles containing Abeta 17-23 (LV(PHI)FAED) and Abeta 30-36 (AII(SAR)L(ORN)V)
Authors : Kreutzer, A.G.; Salveson, P.J.; Nowick, J.S.
Deposited on : 2017-03-15
Resolution : 2.52 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

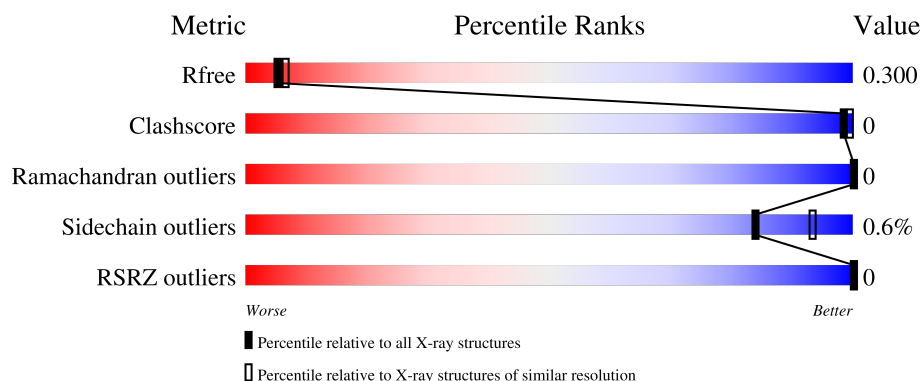
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 2.52 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}	164625	6935 (2.54-2.50)
Clashscore	180529	7778 (2.54-2.50)
Ramachandran outliers	177936	7674 (2.54-2.50)
Sidechain outliers	177891	7676 (2.54-2.50)
RSRZ outliers	164620	6935 (2.54-2.50)

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	16	 88% 12%
1	B	16	 81% 19%
1	C	16	 81% 19%
1	D	16	 81% 19%
1	E	16	 81% 19%

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Mol	Chain	Length	Quality of chain
1	F	16	 88%12%
1	G	16	 88%12%
1	H	16	 88%12%
1	I	16	 69%25%6%
1	J	16	 81%19%
1	K	16	 88%12%
1	L	16	 88%12%
1	M	16	 88%12%
1	N	16	 88%12%
1	O	16	 88%12%
1	P	16	 88%12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4218 atoms, of which 2148 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 ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-I LE-SAR-LEU-MET-VAL.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	16	Total	C	H	I	N	O	S	0	0	0
			259	85	134	1	18	20	1			
1	B	16	Total	C	H	I	N	O	S	0	0	0
			259	85	134	1	18	20	1			
1	C	16	Total	C	H	I	N	O	S	0	0	0
			259	85	134	1	18	20	1			
1	D	16	Total	C	H	I	N	O	S	0	0	0
			259	85	134	1	18	20	1			
1	E	16	Total	C	H	I	N	O	S	0	0	0
			259	85	134	1	18	20	1			
1	F	16	Total	C	H	I	N	O	S	0	0	0
			259	85	134	1	18	20	1			
1	G	16	Total	C	H	I	N	O	S	0	0	0
			259	85	134	1	18	20	1			
1	H	16	Total	C	H	I	N	O	S	0	0	0
			259	85	134	1	18	20	1			
1	I	16	Total	C	H	I	N	O	S	0	0	0
			260	85	135	1	18	20	1			
1	J	16	Total	C	H	I	N	O	S	0	0	0
			259	85	134	1	18	20	1			
1	K	16	Total	C	H	I	N	O	S	0	0	0
			260	85	135	1	18	20	1			
1	L	16	Total	C	H	I	N	O	S	0	0	0
			259	85	134	1	18	20	1			
1	M	16	Total	C	H	I	N	O	S	0	0	0
			259	85	134	1	18	20	1			
1	N	16	Total	C	H	I	N	O	S	0	0	0
			259	85	134	1	18	20	1			
1	O	16	Total	C	H	I	N	O	S	0	0	0
			260	85	135	1	18	20	1			
1	P	16	Total	C	H	I	N	O	S	0	0	0
			260	85	135	1	18	20	1			


- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total O 6 6	0	0
2	B	5	Total O 5 5	0	0
2	C	4	Total O 4 4	0	0
2	D	4	Total O 4 4	0	0
2	E	7	Total O 7 7	0	0
2	F	4	Total O 4 4	0	0
2	G	3	Total O 3 3	0	0
2	H	4	Total O 4 4	0	0
2	I	5	Total O 5 5	0	0
2	J	6	Total O 6 6	0	0
2	K	3	Total O 3 3	0	0
2	L	5	Total O 5 5	0	0
2	M	3	Total O 3 3	0	0
2	N	4	Total O 4 4	0	0
2	O	4	Total O 4 4	0	0
2	P	3	Total O 3 3	0	0

3 Residue-property plots


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: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL

Chain A:  88% 12%




- Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL

Chain B:  81% 19%




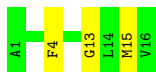
- Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL

Chain C:  81% 19%




- Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL

Chain D:  81% 19%



- Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL

Chain E:  81% 19%



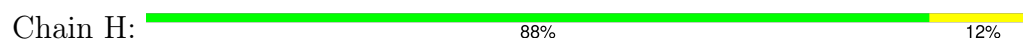
• Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL



• Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL



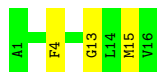
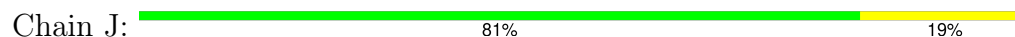
• Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL



• Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL




• Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL



• Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL



- Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL

Chain L:  88% 12%




- Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL

Chain M:  88% 12%




- Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL

Chain N:  88% 12%




- Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL

Chain O:  88% 12%



- Molecule 1: ORN-LEU-VAL-PHI-PHE-ALA-GLU-ASP-ORN-ALA-ILE-ILE-SAR-LEU-MET-VAL

Chain P:  88% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	67.72Å 67.72Å 169.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.86 – 2.52 33.86 – 2.52	Depositor EDS
% Data completeness (in resolution range)	94.8 (33.86-2.52) 95.5 (33.86-2.52)	Depositor EDS
R_{merge}	0.68	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.222 , 0.281 0.242 , 0.300	Depositor DCC
R_{free} test set	917 reflections (9.80%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.025 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.038 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.022 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$ 0.021 for $-h,2/3^*h+1/3^*k+1/3^*l,4/3^*h+8/3^*k-1/3^*l$ 0.025 for $1/3^*h+2/3^*k-1/3^*l,-k,-8/3^*h-4/3^*k-1/3^*l$ 0.038 for $-1/3^*h-2/3^*k+1/3^*l,-2/3^*h-1/3^*k-1/3^*l,4/3^*h-4/3^*k-1/3^*l$ 0.480 for $-h-k,k,-l$	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4218	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2844e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PHI, ORN, SAR

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	0.23	0/89	0.57	0/115
1	B	0.23	0/89	0.38	0/115
1	C	0.24	0/89	1.32	1/115 (0.9%)
1	D	0.23	0/89	1.15	1/115 (0.9%)
1	E	0.24	0/89	0.88	1/115 (0.9%)
1	F	0.24	0/89	0.38	0/115
1	G	0.22	0/89	0.45	0/115
1	H	0.24	0/89	0.42	0/115
1	I	0.32	0/89	1.49	2/115 (1.7%)
1	J	0.23	0/89	0.85	1/115 (0.9%)
1	K	0.24	0/89	0.45	0/115
1	L	0.24	0/89	0.56	0/115
1	M	0.24	0/89	0.49	0/115
1	N	0.23	0/89	0.50	0/115
1	O	0.23	0/89	0.45	0/115
1	P	0.24	0/89	0.51	0/115
All	All	0.24	0/1424	0.76	6/1840 (0.3%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	15	MET	C-N-CA	13.61	155.73	121.70
1	I	15	MET	C-N-CA	12.30	152.46	121.70
1	D	15	MET	C-N-CA	11.55	150.57	121.70
1	J	15	MET	C-N-CA	8.25	142.33	121.70
1	E	15	MET	C-N-CA	8.01	141.71	121.70
1	I	16	VAL	CG1-CB-CG2	6.81	121.80	110.90

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	125	134	131	0	0
1	B	125	134	130	1	0
1	C	125	134	130	0	0
1	D	125	134	130	0	0
1	E	125	134	131	0	0
1	F	125	134	131	0	0
1	G	125	134	131	0	0
1	H	125	134	131	0	0
1	I	125	135	129	1	0
1	J	125	134	131	0	0
1	K	125	135	131	0	0
1	L	125	134	131	0	0
1	M	125	134	130	0	0
1	N	125	134	131	0	0
1	O	125	135	131	0	0
1	P	125	135	131	0	0
2	A	6	0	0	0	0
2	B	5	0	0	1	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	7	0	0	0	0
2	F	4	0	0	0	0
2	G	3	0	0	0	1
2	H	4	0	0	0	1
2	I	5	0	0	1	0
2	J	6	0	0	0	0
2	K	3	0	0	0	0
2	L	5	0	0	0	0
2	M	3	0	0	0	0
2	N	4	0	0	0	0
2	O	4	0	0	0	1
2	P	3	0	0	0	1
All	All	2070	2148	2090	2	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 0.

All (2) 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:B:8:ASP:OD2	2:B:101:HOH:O	2.16	0.58
1:I:8:ASP:OD2	2:I:101:HOH:O	2.21	0.41

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)
2:O:101:HOH:O	2:O:101:HOH:O[2_665]	1.98	0.22
2:G:101:HOH:O	2:G:101:HOH:O[2_665]	2.01	0.19
2:H:101:HOH:O	2:H:101:HOH:O[2_665]	2.12	0.08
2:P:101:HOH:O	2:P:101:HOH:O[3_565]	2.16	0.04

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	10/16 (62%)	10 (100%)	0	0	100	100
1	B	10/16 (62%)	10 (100%)	0	0	100	100
1	C	10/16 (62%)	10 (100%)	0	0	100	100
1	D	10/16 (62%)	10 (100%)	0	0	100	100
1	E	10/16 (62%)	10 (100%)	0	0	100	100
1	F	10/16 (62%)	10 (100%)	0	0	100	100
1	G	10/16 (62%)	10 (100%)	0	0	100	100
1	H	10/16 (62%)	10 (100%)	0	0	100	100
1	I	10/16 (62%)	10 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	10/16 (62%)	10 (100%)	0	0	100	100
1	K	10/16 (62%)	10 (100%)	0	0	100	100
1	L	10/16 (62%)	10 (100%)	0	0	100	100
1	M	10/16 (62%)	10 (100%)	0	0	100	100
1	N	10/16 (62%)	10 (100%)	0	0	100	100
1	O	10/16 (62%)	10 (100%)	0	0	100	100
1	P	10/16 (62%)	10 (100%)	0	0	100	100
All	All	160/256 (62%)	160 (100%)	0	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	10/10 (100%)	10 (100%)	0	100	100
1	B	10/10 (100%)	10 (100%)	0	100	100
1	C	10/10 (100%)	10 (100%)	0	100	100
1	D	10/10 (100%)	10 (100%)	0	100	100
1	E	10/10 (100%)	10 (100%)	0	100	100
1	F	10/10 (100%)	10 (100%)	0	100	100
1	G	10/10 (100%)	10 (100%)	0	100	100
1	H	10/10 (100%)	10 (100%)	0	100	100
1	I	10/10 (100%)	9 (90%)	1 (10%)	6	12
1	J	10/10 (100%)	10 (100%)	0	100	100
1	K	10/10 (100%)	10 (100%)	0	100	100
1	L	10/10 (100%)	10 (100%)	0	100	100
1	M	10/10 (100%)	10 (100%)	0	100	100
1	N	10/10 (100%)	10 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	10/10 (100%)	10 (100%)	0	100	100
1	P	10/10 (100%)	10 (100%)	0	100	100
All	All	160/160 (100%)	159 (99%)	1 (1%)	84	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	16	VAL

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

64 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	ORN	O	1	1	6,7,8	0.62	0	2,7,9	0.41	0
1	ORN	B	9	1	6,7,8	0.66	0	2,7,9	0.42	0
1	SAR	G	13	1	3,4,5	2.16	1 (33%)	1,3,5	1.21	0
1	PHI	O	4	1	11,12,13	1.14	1 (9%)	10,15,17	0.53	0
1	ORN	F	1	1	6,7,8	0.54	0	2,7,9	0.29	0
1	PHI	A	4	1	11,12,13	1.15	1 (9%)	10,15,17	0.48	0
1	SAR	B	13	1	3,4,5	2.17	1 (33%)	1,3,5	1.29	0
1	SAR	C	13	1	3,4,5	2.16	1 (33%)	1,3,5	1.32	0
1	PHI	I	4	1	11,12,13	1.13	1 (9%)	10,15,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	ORN	M	9	1	6,7,8	0.73	0	2,7,9	0.24	0
1	ORN	D	1	1	6,7,8	0.53	0	2,7,9	0.29	0
1	PHI	G	4	1	11,12,13	1.15	1 (9%)	10,15,17	0.48	0
1	SAR	L	13	1	3,4,5	2.16	1 (33%)	1,3,5	1.25	0
1	SAR	M	13	1	3,4,5	2.19	1 (33%)	1,3,5	1.38	0
1	ORN	G	1	1	6,7,8	0.59	0	2,7,9	0.16	0
1	ORN	A	1	1	6,7,8	0.57	0	2,7,9	0.37	0
1	SAR	P	13	1	3,4,5	2.17	1 (33%)	1,3,5	1.28	0
1	ORN	G	9	1	6,7,8	0.63	0	2,7,9	0.42	0
1	ORN	B	1	1	6,7,8	0.66	0	2,7,9	0.53	0
1	ORN	N	1	1	6,7,8	0.60	0	2,7,9	0.26	0
1	SAR	F	13	1	3,4,5	2.16	1 (33%)	1,3,5	1.31	0
1	SAR	H	13	1	3,4,5	2.16	1 (33%)	1,3,5	1.26	0
1	ORN	J	1	1	6,7,8	0.54	0	2,7,9	0.11	0
1	PHI	L	4	1	11,12,13	1.14	1 (9%)	10,15,17	0.61	0
1	SAR	D	13	1	3,4,5	2.17	1 (33%)	1,3,5	1.32	0
1	PHI	M	4	1	11,12,13	1.14	1 (9%)	10,15,17	0.53	0
1	PHI	N	4	1	11,12,13	1.17	1 (9%)	10,15,17	0.48	0
1	ORN	K	9	1	6,7,8	0.59	0	2,7,9	0.11	0
1	ORN	L	1	1	6,7,8	0.53	0	2,7,9	0.15	0
1	PHI	J	4	1	11,12,13	1.15	1 (9%)	10,15,17	0.49	0
1	ORN	O	9	1	6,7,8	0.66	0	2,7,9	0.18	0
1	ORN	K	1	1	6,7,8	0.64	0	2,7,9	0.14	0
1	ORN	C	9	1	6,7,8	0.65	0	2,7,9	0.43	0
1	ORN	H	9	1	6,7,8	0.63	0	2,7,9	0.16	0
1	PHI	H	4	1	11,12,13	1.15	1 (9%)	10,15,17	0.54	0
1	PHI	P	4	1	11,12,13	1.15	1 (9%)	10,15,17	0.51	0
1	ORN	A	9	1	6,7,8	0.58	0	2,7,9	0.25	0
1	SAR	I	13	1	3,4,5	2.17	1 (33%)	1,3,5	1.33	0
1	SAR	N	13	1	3,4,5	2.16	1 (33%)	1,3,5	1.28	0
1	ORN	P	1	1	6,7,8	0.63	0	2,7,9	0.46	0
1	ORN	I	9	1	6,7,8	0.68	0	2,7,9	0.37	0
1	SAR	K	13	1	3,4,5	2.15	1 (33%)	1,3,5	1.18	0
1	ORN	L	9	1	6,7,8	0.60	0	2,7,9	0.19	0
1	ORN	E	9	1	6,7,8	0.62	0	2,7,9	0.34	0
1	PHI	B	4	1	11,12,13	1.15	1 (9%)	10,15,17	0.50	0
1	PHI	E	4	1	11,12,13	1.17	1 (9%)	10,15,17	0.48	0
1	PHI	C	4	1	11,12,13	1.13	1 (9%)	10,15,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	ORN	I	1	1	6,7,8	0.66	0	2,7,9	0.33	0
1	ORN	N	9	1	6,7,8	0.60	0	2,7,9	0.19	0
1	ORN	C	1	1	6,7,8	0.62	0	2,7,9	0.29	0
1	ORN	H	1	1	6,7,8	0.65	0	2,7,9	0.55	0
1	SAR	O	13	1	3,4,5	2.17	1 (33%)	1,3,5	1.20	0
1	ORN	F	9	1	6,7,8	0.63	0	2,7,9	0.44	0
1	SAR	J	13	1	3,4,5	2.18	1 (33%)	1,3,5	1.35	0
1	PHI	F	4	1	11,12,13	1.15	1 (9%)	10,15,17	0.58	0
1	ORN	J	9	1	6,7,8	0.67	0	2,7,9	0.17	0
1	ORN	E	1	1	6,7,8	0.56	0	2,7,9	0.14	0
1	ORN	D	9	1	6,7,8	0.60	0	2,7,9	0.25	0
1	ORN	M	1	1	6,7,8	0.59	0	2,7,9	0.17	0
1	PHI	D	4	1	11,12,13	1.15	1 (9%)	10,15,17	0.48	0
1	ORN	P	9	1	6,7,8	0.61	0	2,7,9	0.24	0
1	SAR	E	13	1	3,4,5	2.16	1 (33%)	1,3,5	1.25	0
1	PHI	K	4	1	11,12,13	1.15	1 (9%)	10,15,17	0.56	0
1	SAR	A	13	1	3,4,5	2.18	1 (33%)	1,3,5	1.31	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
1	ORN	O	1	1	-	2/5/6/8	-
1	ORN	B	9	1	-	2/5/6/8	-
1	SAR	G	13	1	-	1/1/2/3	-
1	PHI	O	4	1	-	0/5/6/8	0/1/1/1
1	ORN	F	1	1	-	2/5/6/8	-
1	PHI	A	4	1	-	0/5/6/8	0/1/1/1
1	SAR	B	13	1	-	1/1/2/3	-
1	SAR	C	13	1	-	1/1/2/3	-
1	PHI	I	4	1	-	0/5/6/8	0/1/1/1
1	ORN	M	9	1	-	1/5/6/8	-
1	ORN	D	1	1	-	0/5/6/8	-
1	PHI	G	4	1	-	0/5/6/8	0/1/1/1
1	SAR	L	13	1	-	1/1/2/3	-
1	SAR	M	13	1	-	1/1/2/3	-
1	ORN	G	1	1	-	0/5/6/8	-
1	ORN	A	1	1	-	2/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SAR	P	13	1	-	1/1/2/3	-
1	ORN	G	9	1	-	2/5/6/8	-
1	ORN	B	1	1	-	2/5/6/8	-
1	ORN	N	1	1	-	1/5/6/8	-
1	SAR	F	13	1	-	1/1/2/3	-
1	SAR	H	13	1	-	1/1/2/3	-
1	ORN	J	1	1	-	1/5/6/8	-
1	PHI	L	4	1	-	0/5/6/8	0/1/1/1
1	SAR	D	13	1	-	1/1/2/3	-
1	PHI	M	4	1	-	0/5/6/8	0/1/1/1
1	PHI	N	4	1	-	0/5/6/8	0/1/1/1
1	ORN	K	9	1	-	1/5/6/8	-
1	ORN	L	1	1	-	0/5/6/8	-
1	PHI	J	4	1	-	0/5/6/8	0/1/1/1
1	ORN	O	9	1	-	0/5/6/8	-
1	ORN	K	1	1	-	0/5/6/8	-
1	ORN	C	9	1	-	2/5/6/8	-
1	ORN	H	9	1	-	0/5/6/8	-
1	PHI	H	4	1	-	0/5/6/8	0/1/1/1
1	PHI	P	4	1	-	0/5/6/8	0/1/1/1
1	ORN	A	9	1	-	0/5/6/8	-
1	SAR	I	13	1	-	1/1/2/3	-
1	SAR	N	13	1	-	1/1/2/3	-
1	ORN	P	1	1	-	2/5/6/8	-
1	ORN	I	9	1	-	2/5/6/8	-
1	SAR	K	13	1	-	1/1/2/3	-
1	ORN	L	9	1	-	2/5/6/8	-
1	ORN	E	9	1	-	0/5/6/8	-
1	PHI	B	4	1	-	0/5/6/8	0/1/1/1
1	PHI	E	4	1	-	0/5/6/8	0/1/1/1
1	PHI	C	4	1	-	0/5/6/8	0/1/1/1
1	ORN	I	1	1	-	1/5/6/8	-
1	ORN	N	9	1	-	2/5/6/8	-
1	ORN	C	1	1	-	1/5/6/8	-
1	ORN	H	1	1	-	2/5/6/8	-
1	SAR	O	13	1	-	1/1/2/3	-
1	ORN	F	9	1	-	3/5/6/8	-
1	SAR	J	13	1	-	1/1/2/3	-
1	PHI	F	4	1	-	0/5/6/8	0/1/1/1
1	ORN	J	9	1	-	0/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ORN	E	1	1	-	0/5/6/8	-
1	ORN	D	9	1	-	1/5/6/8	-
1	ORN	M	1	1	-	0/5/6/8	-
1	PHI	D	4	1	-	0/5/6/8	0/1/1/1
1	ORN	P	9	1	-	1/5/6/8	-
1	SAR	E	13	1	-	1/1/2/3	-
1	PHI	K	4	1	-	0/5/6/8	0/1/1/1
1	SAR	A	13	1	-	1/1/2/3	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	13	SAR	CA-C	-3.78	1.35	1.49
1	J	13	SAR	CA-C	-3.77	1.35	1.49
1	A	13	SAR	CA-C	-3.76	1.36	1.49
1	O	13	SAR	CA-C	-3.75	1.36	1.49
1	D	13	SAR	CA-C	-3.75	1.36	1.49
1	B	13	SAR	CA-C	-3.75	1.36	1.49
1	I	13	SAR	CA-C	-3.75	1.36	1.49
1	P	13	SAR	CA-C	-3.74	1.36	1.49
1	E	13	SAR	CA-C	-3.74	1.36	1.49
1	N	13	SAR	CA-C	-3.73	1.36	1.49
1	F	13	SAR	CA-C	-3.73	1.36	1.49
1	C	13	SAR	CA-C	-3.73	1.36	1.49
1	L	13	SAR	CA-C	-3.72	1.36	1.49
1	G	13	SAR	CA-C	-3.72	1.36	1.49
1	K	13	SAR	CA-C	-3.72	1.36	1.49
1	H	13	SAR	CA-C	-3.72	1.36	1.49
1	E	4	PHI	CZ-I	-2.98	2.02	2.10
1	N	4	PHI	CZ-I	-2.96	2.02	2.10
1	D	4	PHI	CZ-I	-2.91	2.02	2.10
1	B	4	PHI	CZ-I	-2.88	2.02	2.10
1	M	4	PHI	CZ-I	-2.86	2.02	2.10
1	P	4	PHI	CZ-I	-2.85	2.02	2.10
1	G	4	PHI	CZ-I	-2.85	2.02	2.10
1	A	4	PHI	CZ-I	-2.83	2.02	2.10
1	O	4	PHI	CZ-I	-2.82	2.02	2.10
1	I	4	PHI	CZ-I	-2.82	2.02	2.10
1	J	4	PHI	CZ-I	-2.80	2.02	2.10
1	H	4	PHI	CZ-I	-2.77	2.03	2.10
1	C	4	PHI	CZ-I	-2.77	2.03	2.10
1	K	4	PHI	CZ-I	-2.77	2.03	2.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	4	PHI	CZ-I	-2.74	2.03	2.10
1	L	4	PHI	CZ-I	-2.69	2.03	2.10

There are no bond angle outliers.

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	9	ORN	O-C-CA-CB
1	F	9	ORN	O-C-CA-CB
1	N	9	ORN	C-CA-CB-CG
1	A	13	SAR	C-CA-N-CN
1	B	13	SAR	C-CA-N-CN
1	C	13	SAR	C-CA-N-CN
1	D	13	SAR	C-CA-N-CN
1	E	13	SAR	C-CA-N-CN
1	F	13	SAR	C-CA-N-CN
1	G	13	SAR	C-CA-N-CN
1	H	13	SAR	C-CA-N-CN
1	I	13	SAR	C-CA-N-CN
1	J	13	SAR	C-CA-N-CN
1	K	13	SAR	C-CA-N-CN
1	L	13	SAR	C-CA-N-CN
1	M	13	SAR	C-CA-N-CN
1	N	13	SAR	C-CA-N-CN
1	O	13	SAR	C-CA-N-CN
1	P	13	SAR	C-CA-N-CN
1	C	1	ORN	CA-CB-CG-CD
1	I	1	ORN	CA-CB-CG-CD
1	F	1	ORN	NE-CD-CG-CB
1	K	9	ORN	NE-CD-CG-CB
1	A	1	ORN	CA-CB-CG-CD
1	H	1	ORN	CA-CB-CG-CD
1	N	1	ORN	CA-CB-CG-CD
1	P	1	ORN	CA-CB-CG-CD
1	B	1	ORN	CA-CB-CG-CD
1	O	1	ORN	CA-CB-CG-CD
1	B	1	ORN	NE-CD-CG-CB
1	O	1	ORN	NE-CD-CG-CB
1	L	9	ORN	NE-CD-CG-CB
1	C	9	ORN	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	N	9	ORN	CA-CB-CG-CD
1	P	9	ORN	CA-CB-CG-CD
1	B	9	ORN	CA-CB-CG-CD
1	F	9	ORN	CA-CB-CG-CD
1	I	9	ORN	CA-CB-CG-CD
1	L	9	ORN	CA-CB-CG-CD
1	F	1	ORN	CA-CB-CG-CD
1	G	9	ORN	CA-CB-CG-CD
1	H	1	ORN	NE-CD-CG-CB
1	P	1	ORN	NE-CD-CG-CB
1	C	9	ORN	NE-CD-CG-CB
1	F	9	ORN	NE-CD-CG-CB
1	G	9	ORN	NE-CD-CG-CB
1	I	9	ORN	NE-CD-CG-CB
1	B	9	ORN	NE-CD-CG-CB
1	M	9	ORN	CA-CB-CG-CD
1	A	1	ORN	NE-CD-CG-CB
1	J	1	ORN	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	12/16 (75%)	-1.22	0 100 100	36, 43, 52, 53	0
1	B	12/16 (75%)	-1.27	0 100 100	30, 33, 52, 55	0
1	C	12/16 (75%)	-1.10	0 100 100	36, 48, 58, 65	0
1	D	12/16 (75%)	-1.24	0 100 100	25, 34, 52, 54	0
1	E	12/16 (75%)	-1.24	0 100 100	28, 42, 50, 64	0
1	F	12/16 (75%)	-1.23	0 100 100	32, 43, 60, 60	0
1	G	12/16 (75%)	-1.14	0 100 100	36, 45, 55, 69	0
1	H	12/16 (75%)	-1.10	0 100 100	35, 47, 62, 63	0
1	I	12/16 (75%)	-1.22	0 100 100	31, 34, 58, 62	0
1	J	12/16 (75%)	-1.29	0 100 100	34, 40, 49, 49	0
1	K	12/16 (75%)	-1.21	0 100 100	33, 44, 59, 62	0
1	L	12/16 (75%)	-1.23	0 100 100	28, 40, 57, 67	0
1	M	12/16 (75%)	-1.19	0 100 100	29, 35, 45, 46	0
1	N	12/16 (75%)	-1.24	0 100 100	26, 41, 52, 62	0
1	O	12/16 (75%)	-1.05	0 100 100	35, 44, 57, 61	0
1	P	12/16 (75%)	-1.09	0 100 100	33, 44, 64, 66	0
All	All	192/256 (75%)	-1.19	0 100 100	25, 43, 62, 69	0

There are no RSRZ outliers to report.

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(\AA^2)	Q<0.9
1	ORN	O	1	8/9	0.95	0.10	52,71,80,80	0
1	ORN	G	1	8/9	0.96	0.09	51,65,72,72	0
1	ORN	E	9	8/9	0.96	0.10	72,102,124,124	0
1	ORN	F	9	8/9	0.96	0.11	74,89,106,106	0
1	ORN	N	9	8/9	0.96	0.08	62,80,96,96	0
1	ORN	O	9	8/9	0.96	0.07	57,73,82,82	0
1	ORN	F	1	8/9	0.97	0.07	44,53,63,63	0
1	ORN	P	1	8/9	0.97	0.07	50,65,70,70	0
1	ORN	G	9	8/9	0.97	0.07	56,67,78,78	0
1	ORN	K	9	8/9	0.97	0.10	68,81,96,96	0
1	ORN	L	9	8/9	0.97	0.11	76,94,112,112	0
1	ORN	A	9	8/9	0.97	0.08	48,62,75,75	0
1	ORN	C	9	8/9	0.97	0.07	60,72,83,83	0
1	ORN	P	9	8/9	0.97	0.06	55,71,74,75	0
1	SAR	O	13	5/6	0.97	0.06	35,37,43,43	0
1	ORN	I	1	8/9	0.98	0.06	50,69,73,73	0
1	ORN	J	1	8/9	0.98	0.06	44,57,64,64	0
1	ORN	H	9	8/9	0.98	0.06	59,78,85,85	0
1	ORN	J	9	8/9	0.98	0.06	42,51,62,62	0
1	ORN	N	1	8/9	0.98	0.06	33,39,48,48	0
1	ORN	D	1	8/9	0.98	0.06	49,62,72,72	0
1	ORN	M	9	8/9	0.98	0.06	35,41,51,51	0
1	ORN	E	1	8/9	0.98	0.06	35,46,53,53	0
1	ORN	A	1	8/9	0.98	0.07	41,55,64,64	0
1	ORN	C	1	8/9	0.98	0.07	52,67,80,80	0
1	SAR	D	13	5/6	0.98	0.04	24,27,30,30	0
1	SAR	G	13	5/6	0.98	0.05	34,37,44,44	0
1	SAR	H	13	5/6	0.98	0.05	35,38,43,43	0
1	SAR	J	13	5/6	0.98	0.04	28,29,35,35	0
1	SAR	K	13	5/6	0.98	0.04	28,31,34,34	0
1	SAR	L	13	5/6	0.98	0.04	28,31,35,35	0
1	ORN	H	1	8/9	0.98	0.07	47,61,69,69	0
1	SAR	P	13	5/6	0.98	0.04	29,31,36,36	0
1	ORN	M	1	8/9	0.99	0.04	39,49,54,54	0
1	ORN	B	9	8/9	0.99	0.03	24,29,33,33	0
1	ORN	B	1	8/9	0.99	0.04	40,52,59,59	0
1	ORN	D	9	8/9	0.99	0.05	37,46,50,50	0
1	SAR	A	13	5/6	0.99	0.04	29,35,42,42	0
1	SAR	B	13	5/6	0.99	0.04	31,35,40,40	0
1	SAR	C	13	5/6	0.99	0.03	30,32,39,39	0
1	ORN	K	1	8/9	0.99	0.04	40,48,53,53	0
1	SAR	E	13	5/6	0.99	0.03	26,28,34,34	0
1	SAR	F	13	5/6	0.99	0.04	29,34,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	ORN	L	1	8/9	0.99	0.05	37,45,54,54	0
1	PHI	B	4	12/13	0.99	0.06	26,39,51,52	0
1	SAR	I	13	5/6	0.99	0.04	29,35,39,39	0
1	PHI	H	4	12/13	0.99	0.05	34,43,52,53	0
1	ORN	I	9	8/9	0.99	0.04	27,33,35,35	0
1	PHI	I	4	12/13	0.99	0.05	29,41,53,55	0
1	SAR	M	13	5/6	0.99	0.04	24,29,33,33	0
1	SAR	N	13	5/6	0.99	0.03	22,23,28,28	0
1	PHI	L	4	12/13	0.99	0.05	21,26,35,35	0
1	PHI	P	4	12/13	0.99	0.05	31,41,49,49	0
1	PHI	E	4	12/13	1.00	0.05	24,29,36,37	0
1	PHI	F	4	12/13	1.00	0.04	29,35,42,43	0
1	PHI	G	4	12/13	1.00	0.05	31,37,45,45	0
1	PHI	A	4	12/13	1.00	0.04	30,39,50,52	0
1	PHI	C	4	12/13	1.00	0.05	30,39,51,51	0
1	PHI	J	4	12/13	1.00	0.04	30,37,49,49	0
1	PHI	K	4	12/13	1.00	0.05	28,37,48,49	0
1	PHI	D	4	12/13	1.00	0.04	27,40,53,53	0
1	PHI	M	4	12/13	1.00	0.04	27,40,53,55	0
1	PHI	N	4	12/13	1.00	0.05	23,32,40,42	0
1	PHI	O	4	12/13	1.00	0.05	31,39,48,49	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.