



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:24 PM UTC

PDB ID : 8SPE / pdb_00008spe
Title : Crystal structure of Bax core domain BH3-groove dimer - tetrameric fraction P31
Authors : Miller, M.S.; Cowan, A.D.; Colman, P.M.; Czabotar, P.E.
Deposited on : 2023-05-03
Resolution : 2.30 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

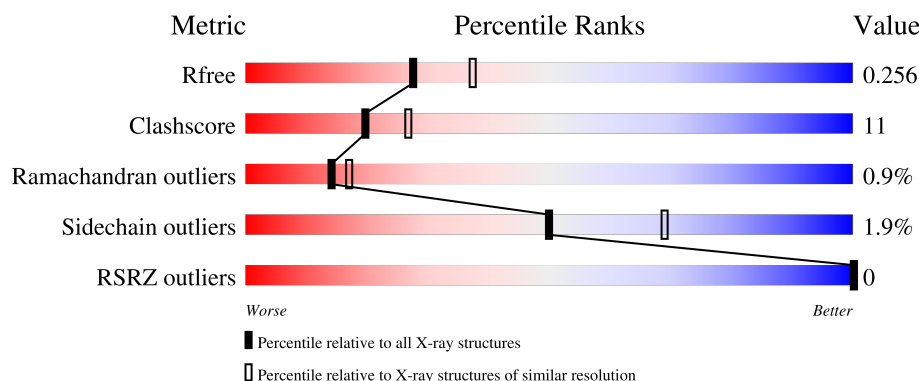
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	81	
1	B	81	
1	C	81	
1	D	81	
1	E	81	

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Mol	Chain	Length	Quality of chain
1	F	81	
1	G	81	
1	H	81	
1	I	81	
1	J	81	
1	K	81	
1	L	81	
1	M	81	
1	N	81	
1	O	81	
1	P	81	
1	Q	81	
1	R	81	
1	S	81	
1	T	81	
1	U	81	
1	V	81	
1	W	81	
1	X	81	
1	Y	81	
1	Z	81	
1	a	81	
1	b	81	
1	c	81	
1	d	81	

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Mol	Chain	Length	Quality of chain
1	e	81	
1	f	81	
1	g	81	
1	h	81	
1	i	81	
1	j	81	

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	PEG	F	201	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18988 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Apoptosis regulator BAX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	69	Total	C	N	O	S	0	0	0
			549	351	94	101	3			
1	B	71	Total	C	N	O	S	0	0	0
			562	358	96	105	3			
1	C	74	Total	C	N	O	S	0	0	0
			560	357	96	105	2			
1	D	71	Total	C	N	O	S	0	0	0
			558	356	96	103	3			
1	Q	71	Total	C	N	O	S	0	0	0
			554	353	95	103	3			
1	R	70	Total	C	N	O	S	0	0	0
			547	350	94	100	3			
1	S	70	Total	C	N	O	S	0	0	0
			547	350	94	100	3			
1	T	68	Total	C	N	O	S	0	0	0
			537	343	92	99	3			
1	G	59	Total	C	N	O	S	0	0	0
			458	296	79	82	1			
1	H	61	Total	C	N	O	S	0	0	0
			478	309	82	85	2			
1	U	69	Total	C	N	O	S	0	0	0
			524	337	89	96	2			
1	V	64	Total	C	N	O	S	0	0	0
			502	322	86	91	3			
1	E	72	Total	C	N	O	S	0	0	0
			560	357	96	104	3			
1	F	72	Total	C	N	O	S	0	0	0
			563	358	96	106	3			
1	I	68	Total	C	N	O	S	0	0	0
			511	326	87	96	2			
1	J	71	Total	C	N	O	S	0	0	0
			561	358	96	104	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	69	Total	C	N	O	S	0	0	0
			529	338	91	97	3			
1	L	62	Total	C	N	O	S	0	0	0
			463	306	72	82	3			
1	M	73	Total	C	N	O	S	0	0	0
			557	357	94	103	3			
1	N	70	Total	C	N	O	S	0	0	0
			550	352	92	103	3			
1	O	63	Total	C	N	O	S	0	0	0
			475	306	79	88	2			
1	P	66	Total	C	N	O	S	0	0	0
			472	308	78	84	2			
1	W	65	Total	C	N	O	S	0	0	0
			515	330	86	96	3			
1	X	65	Total	C	N	O	S	0	0	0
			508	326	87	92	3			
1	Y	70	Total	C	N	O	S	0	1	0
			545	349	93	100	3			
1	Z	69	Total	C	N	O	S	0	0	0
			543	347	93	100	3			
1	a	70	Total	C	N	O	S	0	0	0
			557	355	95	104	3			
1	b	72	Total	C	N	O	S	0	0	0
			562	359	96	104	3			
1	c	67	Total	C	N	O	S	0	0	0
			533	343	92	95	3			
1	d	71	Total	C	N	O	S	0	0	0
			555	354	95	103	3			
1	e	69	Total	C	N	O	S	0	0	0
			544	348	93	100	3			
1	f	68	Total	C	N	O	S	0	0	0
			524	337	89	96	2			
1	g	62	Total	C	N	O	S	0	0	0
			449	292	72	82	3			
1	h	65	Total	C	N	O	S	0	0	0
			465	299	75	89	2			
1	i	68	Total	C	N	O	S	0	0	0
			507	329	81	94	3			
1	j	68	Total	C	N	O	S	0	0	0
			486	314	79	90	3			

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLY	-	expression tag	UNP Q07812
A	49	PRO	-	expression tag	UNP Q07812
A	50	LEU	-	expression tag	UNP Q07812
A	51	GLY	-	expression tag	UNP Q07812
A	52	SER	-	expression tag	UNP Q07812
A	62	SER	CYS	conflict	UNP Q07812
A	126	SER	CYS	conflict	UNP Q07812
B	48	GLY	-	expression tag	UNP Q07812
B	49	PRO	-	expression tag	UNP Q07812
B	50	LEU	-	expression tag	UNP Q07812
B	51	GLY	-	expression tag	UNP Q07812
B	52	SER	-	expression tag	UNP Q07812
B	62	SER	CYS	conflict	UNP Q07812
B	126	SER	CYS	conflict	UNP Q07812
C	48	GLY	-	expression tag	UNP Q07812
C	49	PRO	-	expression tag	UNP Q07812
C	50	LEU	-	expression tag	UNP Q07812
C	51	GLY	-	expression tag	UNP Q07812
C	52	SER	-	expression tag	UNP Q07812
C	62	SER	CYS	conflict	UNP Q07812
C	126	SER	CYS	conflict	UNP Q07812
D	48	GLY	-	expression tag	UNP Q07812
D	49	PRO	-	expression tag	UNP Q07812
D	50	LEU	-	expression tag	UNP Q07812
D	51	GLY	-	expression tag	UNP Q07812
D	52	SER	-	expression tag	UNP Q07812
D	62	SER	CYS	conflict	UNP Q07812
D	126	SER	CYS	conflict	UNP Q07812
Q	48	GLY	-	expression tag	UNP Q07812
Q	49	PRO	-	expression tag	UNP Q07812
Q	50	LEU	-	expression tag	UNP Q07812
Q	51	GLY	-	expression tag	UNP Q07812
Q	52	SER	-	expression tag	UNP Q07812
Q	62	SER	CYS	conflict	UNP Q07812
Q	126	SER	CYS	conflict	UNP Q07812
R	48	GLY	-	expression tag	UNP Q07812
R	49	PRO	-	expression tag	UNP Q07812
R	50	LEU	-	expression tag	UNP Q07812
R	51	GLY	-	expression tag	UNP Q07812
R	52	SER	-	expression tag	UNP Q07812
R	62	SER	CYS	conflict	UNP Q07812
R	126	SER	CYS	conflict	UNP Q07812
S	48	GLY	-	expression tag	UNP Q07812

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Chain	Residue	Modelled	Actual	Comment	Reference
S	49	PRO	-	expression tag	UNP Q07812
S	50	LEU	-	expression tag	UNP Q07812
S	51	GLY	-	expression tag	UNP Q07812
S	52	SER	-	expression tag	UNP Q07812
S	62	SER	CYS	conflict	UNP Q07812
S	126	SER	CYS	conflict	UNP Q07812
T	48	GLY	-	expression tag	UNP Q07812
T	49	PRO	-	expression tag	UNP Q07812
T	50	LEU	-	expression tag	UNP Q07812
T	51	GLY	-	expression tag	UNP Q07812
T	52	SER	-	expression tag	UNP Q07812
T	62	SER	CYS	conflict	UNP Q07812
T	126	SER	CYS	conflict	UNP Q07812
G	48	GLY	-	expression tag	UNP Q07812
G	49	PRO	-	expression tag	UNP Q07812
G	50	LEU	-	expression tag	UNP Q07812
G	51	GLY	-	expression tag	UNP Q07812
G	52	SER	-	expression tag	UNP Q07812
G	62	SER	CYS	conflict	UNP Q07812
G	126	SER	CYS	conflict	UNP Q07812
H	48	GLY	-	expression tag	UNP Q07812
H	49	PRO	-	expression tag	UNP Q07812
H	50	LEU	-	expression tag	UNP Q07812
H	51	GLY	-	expression tag	UNP Q07812
H	52	SER	-	expression tag	UNP Q07812
H	62	SER	CYS	conflict	UNP Q07812
H	126	SER	CYS	conflict	UNP Q07812
U	48	GLY	-	expression tag	UNP Q07812
U	49	PRO	-	expression tag	UNP Q07812
U	50	LEU	-	expression tag	UNP Q07812
U	51	GLY	-	expression tag	UNP Q07812
U	52	SER	-	expression tag	UNP Q07812
U	62	SER	CYS	conflict	UNP Q07812
U	126	SER	CYS	conflict	UNP Q07812
V	48	GLY	-	expression tag	UNP Q07812
V	49	PRO	-	expression tag	UNP Q07812
V	50	LEU	-	expression tag	UNP Q07812
V	51	GLY	-	expression tag	UNP Q07812
V	52	SER	-	expression tag	UNP Q07812
V	62	SER	CYS	conflict	UNP Q07812
V	126	SER	CYS	conflict	UNP Q07812
E	48	GLY	-	expression tag	UNP Q07812

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Chain	Residue	Modelled	Actual	Comment	Reference
E	49	PRO	-	expression tag	UNP Q07812
E	50	LEU	-	expression tag	UNP Q07812
E	51	GLY	-	expression tag	UNP Q07812
E	52	SER	-	expression tag	UNP Q07812
E	62	SER	CYS	conflict	UNP Q07812
E	126	SER	CYS	conflict	UNP Q07812
F	48	GLY	-	expression tag	UNP Q07812
F	49	PRO	-	expression tag	UNP Q07812
F	50	LEU	-	expression tag	UNP Q07812
F	51	GLY	-	expression tag	UNP Q07812
F	52	SER	-	expression tag	UNP Q07812
F	62	SER	CYS	conflict	UNP Q07812
F	126	SER	CYS	conflict	UNP Q07812
I	48	GLY	-	expression tag	UNP Q07812
I	49	PRO	-	expression tag	UNP Q07812
I	50	LEU	-	expression tag	UNP Q07812
I	51	GLY	-	expression tag	UNP Q07812
I	52	SER	-	expression tag	UNP Q07812
I	62	SER	CYS	conflict	UNP Q07812
I	126	SER	CYS	conflict	UNP Q07812
J	48	GLY	-	expression tag	UNP Q07812
J	49	PRO	-	expression tag	UNP Q07812
J	50	LEU	-	expression tag	UNP Q07812
J	51	GLY	-	expression tag	UNP Q07812
J	52	SER	-	expression tag	UNP Q07812
J	62	SER	CYS	conflict	UNP Q07812
J	126	SER	CYS	conflict	UNP Q07812
K	48	GLY	-	expression tag	UNP Q07812
K	49	PRO	-	expression tag	UNP Q07812
K	50	LEU	-	expression tag	UNP Q07812
K	51	GLY	-	expression tag	UNP Q07812
K	52	SER	-	expression tag	UNP Q07812
K	62	SER	CYS	conflict	UNP Q07812
K	126	SER	CYS	conflict	UNP Q07812
L	48	GLY	-	expression tag	UNP Q07812
L	49	PRO	-	expression tag	UNP Q07812
L	50	LEU	-	expression tag	UNP Q07812
L	51	GLY	-	expression tag	UNP Q07812
L	52	SER	-	expression tag	UNP Q07812
L	62	SER	CYS	conflict	UNP Q07812
L	126	SER	CYS	conflict	UNP Q07812
M	48	GLY	-	expression tag	UNP Q07812

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Chain	Residue	Modelled	Actual	Comment	Reference
M	49	PRO	-	expression tag	UNP Q07812
M	50	LEU	-	expression tag	UNP Q07812
M	51	GLY	-	expression tag	UNP Q07812
M	52	SER	-	expression tag	UNP Q07812
M	62	SER	CYS	conflict	UNP Q07812
M	126	SER	CYS	conflict	UNP Q07812
N	48	GLY	-	expression tag	UNP Q07812
N	49	PRO	-	expression tag	UNP Q07812
N	50	LEU	-	expression tag	UNP Q07812
N	51	GLY	-	expression tag	UNP Q07812
N	52	SER	-	expression tag	UNP Q07812
N	62	SER	CYS	conflict	UNP Q07812
N	126	SER	CYS	conflict	UNP Q07812
O	48	GLY	-	expression tag	UNP Q07812
O	49	PRO	-	expression tag	UNP Q07812
O	50	LEU	-	expression tag	UNP Q07812
O	51	GLY	-	expression tag	UNP Q07812
O	52	SER	-	expression tag	UNP Q07812
O	62	SER	CYS	conflict	UNP Q07812
O	126	SER	CYS	conflict	UNP Q07812
P	48	GLY	-	expression tag	UNP Q07812
P	49	PRO	-	expression tag	UNP Q07812
P	50	LEU	-	expression tag	UNP Q07812
P	51	GLY	-	expression tag	UNP Q07812
P	52	SER	-	expression tag	UNP Q07812
P	62	SER	CYS	conflict	UNP Q07812
P	126	SER	CYS	conflict	UNP Q07812
W	48	GLY	-	expression tag	UNP Q07812
W	49	PRO	-	expression tag	UNP Q07812
W	50	LEU	-	expression tag	UNP Q07812
W	51	GLY	-	expression tag	UNP Q07812
W	52	SER	-	expression tag	UNP Q07812
W	62	SER	CYS	conflict	UNP Q07812
W	126	SER	CYS	conflict	UNP Q07812
X	48	GLY	-	expression tag	UNP Q07812
X	49	PRO	-	expression tag	UNP Q07812
X	50	LEU	-	expression tag	UNP Q07812
X	51	GLY	-	expression tag	UNP Q07812
X	52	SER	-	expression tag	UNP Q07812
X	62	SER	CYS	conflict	UNP Q07812
X	126	SER	CYS	conflict	UNP Q07812
Y	48	GLY	-	expression tag	UNP Q07812

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	49	PRO	-	expression tag	UNP Q07812
Y	50	LEU	-	expression tag	UNP Q07812
Y	51	GLY	-	expression tag	UNP Q07812
Y	52	SER	-	expression tag	UNP Q07812
Y	62	SER	CYS	conflict	UNP Q07812
Y	126	SER	CYS	conflict	UNP Q07812
Z	48	GLY	-	expression tag	UNP Q07812
Z	49	PRO	-	expression tag	UNP Q07812
Z	50	LEU	-	expression tag	UNP Q07812
Z	51	GLY	-	expression tag	UNP Q07812
Z	52	SER	-	expression tag	UNP Q07812
Z	62	SER	CYS	conflict	UNP Q07812
Z	126	SER	CYS	conflict	UNP Q07812
a	48	GLY	-	expression tag	UNP Q07812
a	49	PRO	-	expression tag	UNP Q07812
a	50	LEU	-	expression tag	UNP Q07812
a	51	GLY	-	expression tag	UNP Q07812
a	52	SER	-	expression tag	UNP Q07812
a	62	SER	CYS	conflict	UNP Q07812
a	126	SER	CYS	conflict	UNP Q07812
b	48	GLY	-	expression tag	UNP Q07812
b	49	PRO	-	expression tag	UNP Q07812
b	50	LEU	-	expression tag	UNP Q07812
b	51	GLY	-	expression tag	UNP Q07812
b	52	SER	-	expression tag	UNP Q07812
b	62	SER	CYS	conflict	UNP Q07812
b	126	SER	CYS	conflict	UNP Q07812
c	48	GLY	-	expression tag	UNP Q07812
c	49	PRO	-	expression tag	UNP Q07812
c	50	LEU	-	expression tag	UNP Q07812
c	51	GLY	-	expression tag	UNP Q07812
c	52	SER	-	expression tag	UNP Q07812
c	62	SER	CYS	conflict	UNP Q07812
c	126	SER	CYS	conflict	UNP Q07812
d	48	GLY	-	expression tag	UNP Q07812
d	49	PRO	-	expression tag	UNP Q07812
d	50	LEU	-	expression tag	UNP Q07812
d	51	GLY	-	expression tag	UNP Q07812
d	52	SER	-	expression tag	UNP Q07812
d	62	SER	CYS	conflict	UNP Q07812
d	126	SER	CYS	conflict	UNP Q07812
e	48	GLY	-	expression tag	UNP Q07812

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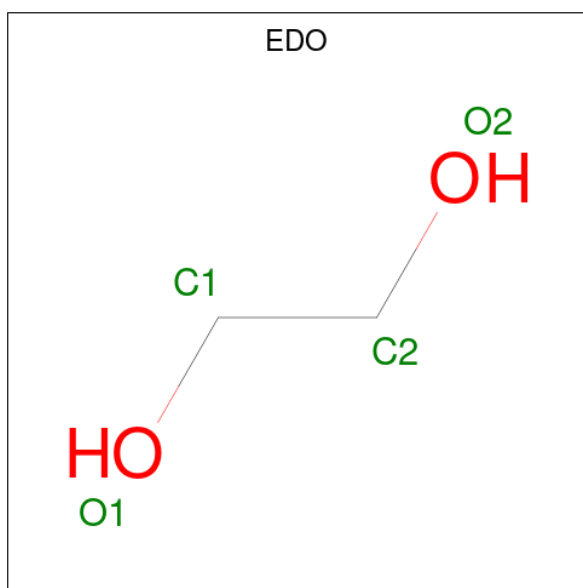
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Chain	Residue	Modelled	Actual	Comment	Reference
e	49	PRO	-	expression tag	UNP Q07812
e	50	LEU	-	expression tag	UNP Q07812
e	51	GLY	-	expression tag	UNP Q07812
e	52	SER	-	expression tag	UNP Q07812
e	62	SER	CYS	conflict	UNP Q07812
e	126	SER	CYS	conflict	UNP Q07812
f	48	GLY	-	expression tag	UNP Q07812
f	49	PRO	-	expression tag	UNP Q07812
f	50	LEU	-	expression tag	UNP Q07812
f	51	GLY	-	expression tag	UNP Q07812
f	52	SER	-	expression tag	UNP Q07812
f	62	SER	CYS	conflict	UNP Q07812
f	126	SER	CYS	conflict	UNP Q07812
g	48	GLY	-	expression tag	UNP Q07812
g	49	PRO	-	expression tag	UNP Q07812
g	50	LEU	-	expression tag	UNP Q07812
g	51	GLY	-	expression tag	UNP Q07812
g	52	SER	-	expression tag	UNP Q07812
g	62	SER	CYS	conflict	UNP Q07812
g	126	SER	CYS	conflict	UNP Q07812
h	48	GLY	-	expression tag	UNP Q07812
h	49	PRO	-	expression tag	UNP Q07812
h	50	LEU	-	expression tag	UNP Q07812
h	51	GLY	-	expression tag	UNP Q07812
h	52	SER	-	expression tag	UNP Q07812
h	62	SER	CYS	conflict	UNP Q07812
h	126	SER	CYS	conflict	UNP Q07812
i	48	GLY	-	expression tag	UNP Q07812
i	49	PRO	-	expression tag	UNP Q07812
i	50	LEU	-	expression tag	UNP Q07812
i	51	GLY	-	expression tag	UNP Q07812
i	52	SER	-	expression tag	UNP Q07812
i	62	SER	CYS	conflict	UNP Q07812
i	126	SER	CYS	conflict	UNP Q07812
j	48	GLY	-	expression tag	UNP Q07812
j	49	PRO	-	expression tag	UNP Q07812
j	50	LEU	-	expression tag	UNP Q07812
j	51	GLY	-	expression tag	UNP Q07812
j	52	SER	-	expression tag	UNP Q07812
j	62	SER	CYS	conflict	UNP Q07812
j	126	SER	CYS	conflict	UNP Q07812

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Zn 1	0	0
2	C	2	Total 2	Zn 2	0	0
2	D	1	Total 1	Zn 1	0	0
2	I	1	Total 1	Zn 1	0	0
2	J	1	Total 1	Zn 1	0	0
2	M	1	Total 1	Zn 1	0	0
2	c	1	Total 1	Zn 1	0	0
2	h	1	Total 1	Zn 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



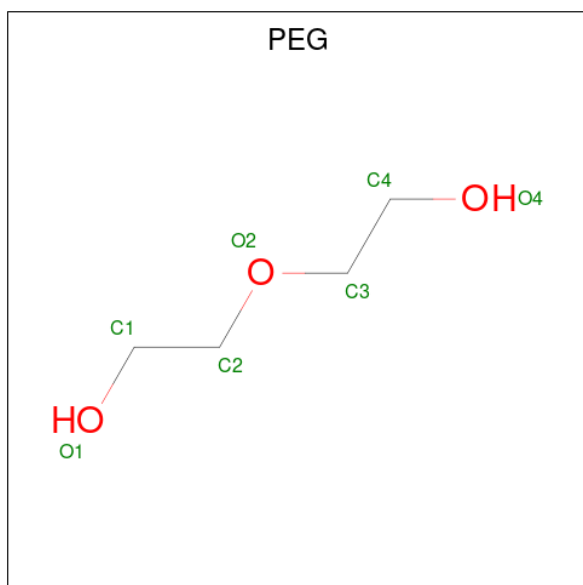
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	J	1	Total	C	O	0	0
			4	2	2		
3	N	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	B	5	Total	O	0	0
			5	5		
5	C	4	Total	O	0	0
			4	4		
5	D	1	Total	O	0	0
			1	1		
5	R	1	Total	O	0	0
			1	1		
5	T	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	2	Total O 2 2	0	0
5	V	1	Total O 1 1	0	0
5	E	1	Total O 1 1	0	0
5	F	5	Total O 5 5	0	0
5	I	1	Total O 1 1	0	0
5	J	2	Total O 2 2	0	0
5	L	1	Total O 1 1	0	0
5	M	3	Total O 3 3	0	0
5	N	3	Total O 3 3	0	0
5	X	1	Total O 1 1	0	0
5	a	1	Total O 1 1	0	0
5	d	1	Total O 1 1	0	0
5	e	1	Total O 1 1	0	0
5	i	1	Total O 1 1	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: Apoptosis regulator BAX

Chain A: 



- Molecule 1: Apoptosis regulator BAX

Chain B: 



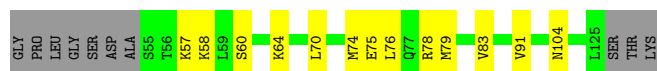
- Molecule 1: Apoptosis regulator BAX

Chain C: 



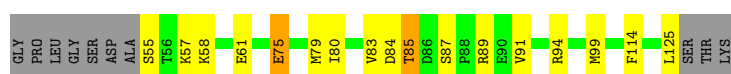
- Molecule 1: Apoptosis regulator BAX

Chain D: 



- Molecule 1: Apoptosis regulator BAX

Chain Q: 



- Molecule 1: Apoptosis regulator BAX

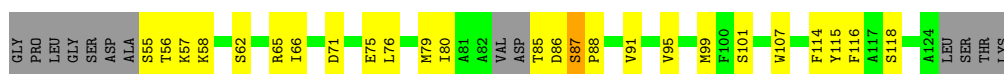
Chain R: 



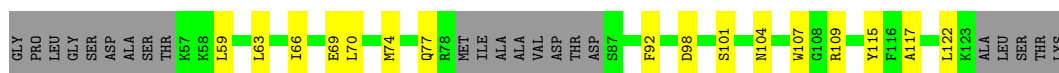
- Molecule 1: Apoptosis regulator BAX



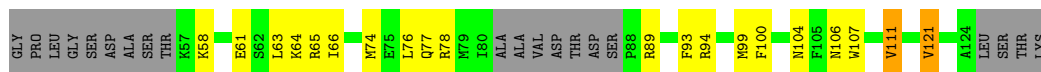
- Molecule 1: Apoptosis regulator BAX



- Molecule 1: Apoptosis regulator BAX



- Molecule 1: Apoptosis regulator BAX



- Molecule 1: Apoptosis regulator BAX

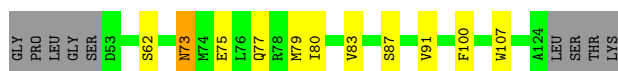


- Molecule 1: Apoptosis regulator BAX



- Molecule 1: Apoptosis regulator BAX





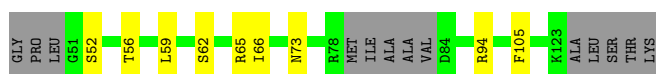
- Molecule 1: Apoptosis regulator BAX

Chain F: 74% 15% 11%



- Molecule 1: Apoptosis regulator BAX

Chain I: 73% 11% 16%



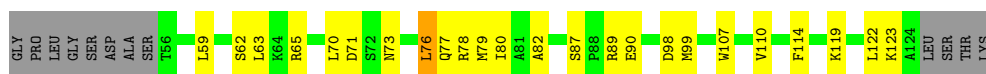
- Molecule 1: Apoptosis regulator BAX

Chain J: 64% 22% 12%



- Molecule 1: Apoptosis regulator BAX

Chain K: 56% 28% 15%



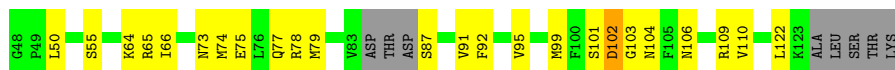
- Molecule 1: Apoptosis regulator BAX

Chain L: 47% 28% 23%



- Molecule 1: Apoptosis regulator BAX

Chain M: 60% 28% 10%



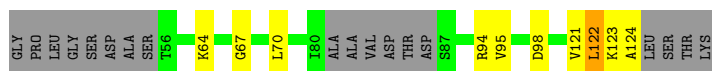
- Molecule 1: Apoptosis regulator BAX

Chain N:  64% 22% 14%



- Molecule 1: Apoptosis regulator BAX

Chain O:  65% 11% 22%



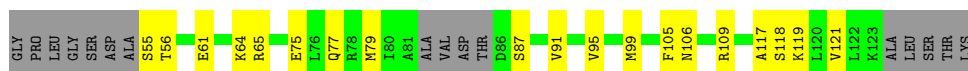
- Molecule 1: Apoptosis regulator BAX

Chain P:  65% 16% 19%



- Molecule 1: Apoptosis regulator BAX

Chain W:  57% 23% 20%



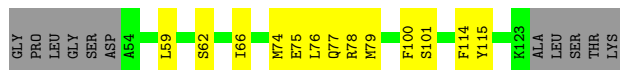
- Molecule 1: Apoptosis regulator BAX

Chain X:  57% 23% 20%



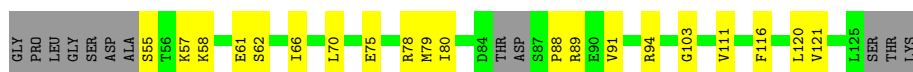
- Molecule 1: Apoptosis regulator BAX

Chain Y:  70% 16% 14%



- Molecule 1: Apoptosis regulator BAX

Chain Z:  60% 25% 15%



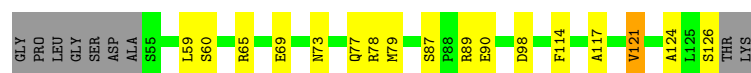
- Molecule 1: Apoptosis regulator BAX

Chain a: 



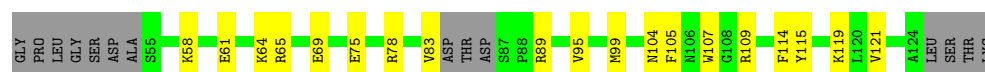
- Molecule 1: Apoptosis regulator BAX

Chain b: 



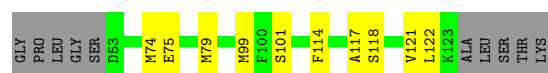
- Molecule 1: Apoptosis regulator BAX

Chain c: 



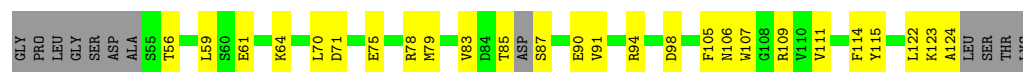
- Molecule 1: Apoptosis regulator BAX

Chain d: 



- Molecule 1: Apoptosis regulator BAX

Chain e: 



- Molecule 1: Apoptosis regulator BAX

Chain f: 

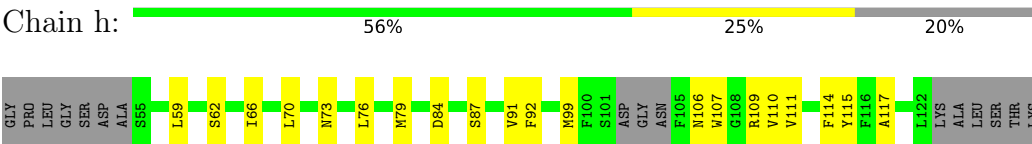


- Molecule 1: Apoptosis regulator BAX

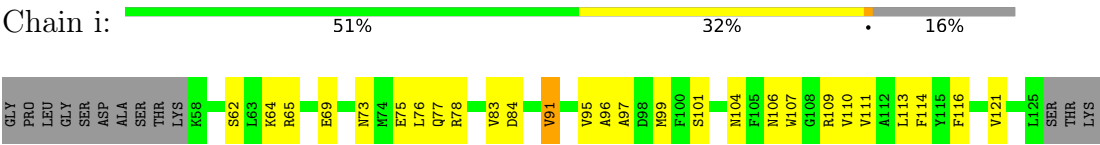
Chain g: 



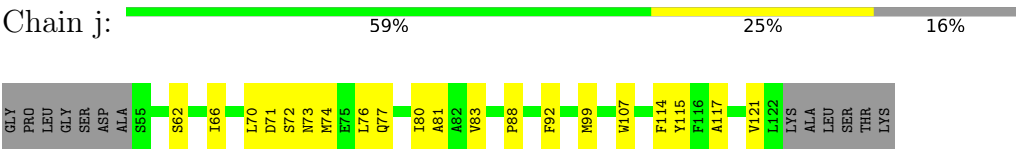
- Molecule 1: Apoptosis regulator BAX



● Molecule 1: Apoptosis regulator BAX



● Molecule 1: Apoptosis regulator BAX



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	141.35Å 141.35Å 110.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.43 – 2.30 35.43 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.43-2.30) 92.4 (35.43-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.09 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.229 , 0.256 0.229 , 0.256	Depositor DCC
R_{free} test set	1996 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l 0.053 for h,-h-k,-l 0.098 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18988	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.69% 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: EDO, PEG, ZN

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	0.12	0/558	0.28	0/748
1	B	0.07	0/571	0.21	0/766
1	C	0.08	0/569	0.23	0/764
1	D	0.14	0/567	0.33	0/761
1	E	0.11	0/569	0.31	0/765
1	F	0.13	0/572	0.25	0/769
1	G	0.11	0/466	0.28	0/626
1	H	0.11	0/486	0.29	0/650
1	I	0.08	0/519	0.24	0/698
1	J	0.11	0/570	0.28	0/765
1	K	0.20	0/538	0.41	0/726
1	L	0.19	0/470	0.42	0/631
1	M	0.13	0/566	0.32	0/760
1	N	0.10	0/559	0.28	0/751
1	O	0.15	0/483	0.28	0/651
1	P	0.11	0/480	0.29	0/650
1	Q	0.13	0/563	0.28	0/757
1	R	0.11	0/556	0.27	0/747
1	S	0.12	0/556	0.25	0/747
1	T	0.27	0/545	0.46	0/730
1	U	0.12	0/532	0.29	0/715
1	V	0.08	0/510	0.26	0/684
1	W	0.10	0/523	0.32	0/700
1	X	0.13	0/517	0.31	0/696
1	Y	0.13	0/557	0.40	0/750
1	Z	0.09	0/551	0.25	0/738
1	a	0.11	0/566	0.28	0/759
1	b	0.09	0/571	0.26	0/767
1	c	0.13	0/541	0.29	0/723
1	d	0.09	0/564	0.23	0/758
1	e	0.16	0/552	0.41	0/740
1	f	0.17	0/533	0.41	0/718

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	g	0.15	0/457	0.34	0/619
1	h	0.10	0/471	0.32	0/641
1	i	0.14	0/516	0.32	0/699
1	j	0.11	0/495	0.28	0/675
All	All	0.13	0/19219	0.31	0/25844

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	A	549	0	549	6	0
1	B	562	0	558	5	0
1	C	560	0	542	13	0
1	D	558	0	554	12	0
1	E	560	0	550	9	0
1	F	563	0	549	15	0
1	G	458	0	436	13	0
1	H	478	0	463	19	0
1	I	511	0	473	6	0
1	J	561	0	558	16	0
1	K	529	0	505	25	0
1	L	463	0	444	27	0
1	M	557	0	547	22	0
1	N	550	0	542	17	0
1	O	475	0	436	7	0
1	P	472	0	424	9	0
1	Q	554	0	543	17	0
1	R	547	0	541	13	0
1	S	547	0	535	19	0
1	T	537	0	528	22	0
1	U	524	0	500	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	502	0	483	10	0
1	W	515	0	503	15	0
1	X	508	0	491	15	0
1	Y	545	0	532	13	0
1	Z	543	0	535	15	0
1	a	557	0	556	17	0
1	b	562	0	554	14	0
1	c	533	0	537	19	0
1	d	555	0	545	11	0
1	e	544	0	537	24	0
1	f	524	0	506	22	0
1	g	449	0	401	19	0
1	h	465	0	419	17	0
1	i	507	0	479	21	0
1	j	486	0	430	17	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	M	1	0	0	0	0
2	c	1	0	0	0	0
2	h	1	0	0	0	0
3	C	4	0	6	3	0
3	D	4	0	6	1	0
3	F	4	0	6	1	0
3	I	4	0	6	1	0
3	J	4	0	6	1	0
3	N	4	0	6	3	0
4	F	7	0	10	4	0
5	A	2	0	0	0	0
5	B	5	0	0	0	0
5	C	4	0	0	1	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	5	0	0	0	0
5	H	2	0	0	1	0
5	I	1	0	0	0	0
5	J	2	0	0	0	0
5	L	1	0	0	0	0
5	M	3	0	0	0	0
5	N	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	1	0	0	0	0
5	T	1	0	0	0	0
5	V	1	0	0	0	0
5	X	1	0	0	0	0
5	a	1	0	0	0	0
5	d	1	0	0	1	0
5	e	1	0	0	0	0
5	i	1	0	0	0	0
All	All	18988	0	18331	428	0

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 11.

All (428) 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:h:107:TRP:HB2	1:i:121:VAL:HG11	1.46	0.96
1:O:94:ARG:HE	1:P:56:THR:HG21	1.30	0.95
1:I:65:ARG:HD2	3:I:202:EDO:H12	1.53	0.89
1:g:79:MET:HB2	1:h:59:LEU:HD13	1.59	0.84
1:Q:58:LYS:H	1:Q:58:LYS:HD2	1.42	0.83
1:f:58:LYS:H	1:f:58:LYS:HD2	1.42	0.83
1:M:55:SER:HB2	3:N:201:EDO:H11	1.61	0.83
1:Q:125:LEU:HG	1:H:78:ARG:CB	2.11	0.81
1:L:65:ARG:HG2	1:W:65:ARG:HD2	1.66	0.75
1:C:119:LYS:NZ	5:C:301:HOH:O	2.20	0.74
1:Z:88:PRO:HB3	1:Z:120:LEU:HD22	1.70	0.74
1:C:66:ILE:HG21	1:D:70:LEU:HG	1.68	0.73
1:K:89:ARG:HH21	1:N:103:GLY:HA2	1.51	0.73
1:N:79:MET:HB3	3:N:201:EDO:H21	1.71	0.72
1:K:70:LEU:O	1:K:77:GLN:NE2	2.23	0.71
1:J:102:ASP:OD1	1:J:103:GLY:N	2.22	0.71
1:U:106:ASN:ND2	1:V:71:ASP:OD2	2.26	0.69
1:Z:75:GLU:HG3	1:Z:79:MET:HE2	1.72	0.69
1:E:83:VAL:HB	1:E:91:VAL:HG11	1.75	0.68
1:g:121:VAL:HG11	1:j:107:TRP:HB2	1.75	0.68
1:C:107:TRP:H	3:D:202:EDO:H11	1.58	0.68
1:a:86:ASP:OD1	1:a:86:ASP:N	2.25	0.68
1:L:95:VAL:O	1:L:99:MET:HG3	1.92	0.68
1:A:87:SER:HB2	1:A:90:GLU:OE1	1.95	0.67
1:A:104:ASN:OD1	1:A:106:ASN:ND2	2.21	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:LEU:HA	1:D:79:MET:HE3	1.75	0.67
1:F:90:GLU:H	4:F:201:PEG:H21	1.59	0.67
1:Z:89:ARG:NE	1:a:100:PHE:O	2.27	0.67
1:i:83:VAL:HG23	1:i:84:ASP:H	1.60	0.66
1:K:63:LEU:HD23	1:L:76:LEU:HD11	1.78	0.66
1:i:73:ASN:HB3	1:i:76:LEU:HB3	1.77	0.65
1:X:75:GLU:O	1:X:79:MET:HG3	1.96	0.65
1:c:121:VAL:HG11	1:f:107:TRP:HB2	1.77	0.65
1:e:107:TRP:NE1	1:f:118:SER:OG	2.26	0.64
1:S:75:GLU:O	1:S:79:MET:HG3	1.98	0.64
1:T:58:LYS:H	1:T:58:LYS:HD3	1.63	0.64
1:i:106:ASN:ND2	1:j:71:ASP:OD2	2.31	0.64
1:U:109:ARG:CZ	1:V:64:LYS:HG3	2.28	0.64
1:J:89:ARG:NH1	1:J:90:GLU:OE2	2.31	0.63
1:Z:57:LYS:NZ	1:Z:61:GLU:OE2	2.26	0.63
1:D:58:LYS:NZ	1:T:85:THR:HG21	2.13	0.63
1:h:106:ASN:HB3	1:h:109:ARG:HG3	1.79	0.63
1:a:83:VAL:HG11	1:a:91:VAL:HG11	1.80	0.62
1:e:111:VAL:HG21	1:f:115:TYR:HD1	1.65	0.62
1:W:106:ASN:HB2	1:W:109:ARG:HG3	1.81	0.62
1:d:122:LEU:HB2	1:f:122:LEU:HD23	1.80	0.62
1:f:83:VAL:HB	1:f:91:VAL:HG21	1.81	0.62
1:g:66:ILE:HD13	1:h:70:LEU:HD13	1.81	0.62
1:Q:79:MET:HB2	1:R:59:LEU:HD13	1.82	0.61
1:T:87:SER:O	1:T:91:VAL:HG12	2.00	0.61
1:F:65:ARG:HD3	1:M:65:ARG:HG3	1.82	0.61
1:G:122:LEU:HB2	1:U:122:LEU:HD23	1.82	0.61
1:K:62:SER:OG	1:K:65:ARG:NH2	2.34	0.60
1:F:83:VAL:HG11	1:F:91:VAL:HG11	1.82	0.60
1:W:77:GLN:OE1	1:W:119:LYS:NZ	2.33	0.60
1:C:65:ARG:HA	3:C:203:EDO:H12	1.84	0.60
1:g:60:SER:HB3	1:h:99:MET:HA	1.82	0.60
1:I:94:ARG:HG2	1:J:56:THR:HG21	1.84	0.60
1:J:124:ALA:HA	1:M:78:ARG:HH21	1.67	0.60
1:D:58:LYS:HZ3	1:T:85:THR:HG21	1.66	0.59
1:Y:100:PHE:HB2	1:b:89:ARG:HD3	1.84	0.59
1:g:115:TYR:HD1	1:h:111:VAL:HG21	1.66	0.59
1:U:90:GLU:HA	1:U:93:PHE:HD2	1.67	0.59
1:a:75:GLU:O	1:a:79:MET:HG3	2.02	0.59
1:W:118:SER:OG	1:X:107:TRP:NE1	2.36	0.58
1:M:99:MET:HA	1:N:64:LYS:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:70:LEU:HD13	1:e:115:TYR:CZ	2.38	0.58
1:e:83:VAL:HG11	1:e:91:VAL:HG11	1.85	0.58
1:X:62:SER:O	1:X:66:ILE:HG13	2.03	0.58
1:K:70:LEU:HD21	1:L:66:ILE:HG21	1.86	0.58
1:e:75:GLU:O	1:e:79:MET:HG3	2.04	0.58
1:H:63:LEU:HA	1:H:66:ILE:HG22	1.86	0.58
1:M:91:VAL:O	1:M:95:VAL:HG23	2.04	0.58
1:d:75:GLU:HG2	1:d:79:MET:HE2	1.85	0.58
1:N:119:LYS:O	1:N:123:LYS:HG2	2.04	0.57
1:E:79:MET:SD	1:F:58:LYS:HD3	2.44	0.57
1:K:63:LEU:HD21	1:L:76:LEU:HD21	1.85	0.57
1:W:117:ALA:O	1:W:121:VAL:HG23	2.05	0.57
1:U:106:ASN:HB3	1:U:109:ARG:HG3	1.86	0.57
1:g:87:SER:HB3	1:g:90:GLU:HB3	1.85	0.57
1:W:75:GLU:O	1:W:79:MET:HG3	2.04	0.57
1:K:122:LEU:HD12	1:M:122:LEU:HD13	1.86	0.56
1:K:78:ARG:O	1:K:82:ALA:N	2.35	0.56
1:Y:75:GLU:O	1:Y:79:MET:HG3	2.06	0.56
1:R:83:VAL:HB	1:R:91:VAL:HG11	1.88	0.56
1:S:65:ARG:CZ	1:H:65:ARG:HG3	2.36	0.56
1:T:58:LYS:H	1:T:58:LYS:CD	2.19	0.56
1:K:79:MET:HE2	1:L:59:LEU:HB2	1.87	0.56
1:E:80:ILE:O	1:E:83:VAL:HG22	2.06	0.56
1:Y:74:MET:HA	1:Y:77:GLN:HG3	1.88	0.56
1:O:64:LYS:HD2	1:P:99:MET:HA	1.87	0.55
1:E:107:TRP:H	1:M:74:MET:HE1	1.72	0.55
1:D:83:VAL:HG11	1:D:91:VAL:HG11	1.87	0.55
1:e:83:VAL:CG1	1:e:91:VAL:HG21	2.36	0.55
1:i:65:ARG:O	1:i:69:GLU:HG3	2.06	0.55
1:K:99:MET:HA	1:L:64:LYS:HD2	1.88	0.55
1:j:66:ILE:O	1:j:70:LEU:HD12	2.07	0.55
1:B:106:ASN:HD21	1:B:109:ARG:HG3	1.72	0.55
1:K:62:SER:HB3	1:L:76:LEU:HD12	1.88	0.55
1:Z:75:GLU:OE2	1:Z:78:ARG:NE	2.38	0.55
1:M:102:ASP:HB2	1:M:109:ARG:HH12	1.72	0.55
1:f:56:THR:N	1:f:58:LYS:HZ2	2.05	0.54
1:D:104:ASN:HD21	1:R:73:ASN:HA	1.73	0.54
1:A:99:MET:HA	1:B:64:LYS:HD2	1.89	0.54
1:X:65:ARG:O	1:X:69:GLU:N	2.39	0.54
1:I:59:LEU:HD13	1:J:79:MET:HB3	1.90	0.54
1:a:73:ASN:HB3	1:a:76:LEU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:75:GLU:OE2	1:e:78:ARG:NH2	2.38	0.54
1:h:84:ASP:O	1:h:91:VAL:HG21	2.08	0.54
1:S:99:MET:O	1:S:109:ARG:NH1	2.41	0.54
1:c:89:ARG:HH12	1:f:103:GLY:H	1.55	0.53
1:C:61:GLU:OE1	1:C:65:ARG:NH2	2.32	0.53
1:Y:115:TYR:HD1	1:Z:111:VAL:HG21	1.72	0.53
1:i:107:TRP:O	1:i:111:VAL:HG23	2.09	0.53
1:G:104:ASN:HB3	1:G:109:ARG:NH1	2.22	0.53
1:i:104:ASN:HD21	1:i:109:ARG:NH2	2.06	0.53
1:T:66:ILE:HD12	1:T:66:ILE:H	1.74	0.53
1:D:75:GLU:HG3	1:D:79:MET:HE2	1.89	0.53
1:G:66:ILE:HD11	1:H:66:ILE:HG13	1.91	0.53
1:K:107:TRP:HB2	1:N:121:VAL:HG11	1.90	0.52
1:W:61:GLU:HA	1:W:64:LYS:HE2	1.91	0.52
1:R:87:SER:O	1:R:91:VAL:HG23	2.09	0.52
1:R:114:PHE:CE2	1:S:114:PHE:HB2	2.44	0.52
1:P:115:TYR:OH	1:P:119:LYS:NZ	2.39	0.52
1:S:75:GLU:HG2	1:S:78:ARG:HH21	1.74	0.52
1:a:57:LYS:HD2	1:b:98:ASP:HB3	1.92	0.52
1:G:107:TRP:HB2	1:V:121:VAL:HG11	1.90	0.52
1:g:106:ASN:O	1:g:110:VAL:HG23	2.09	0.52
1:T:75:GLU:O	1:T:79:MET:HG3	2.10	0.52
1:j:72:SER:O	1:j:74:MET:N	2.42	0.52
1:L:117:ALA:O	1:L:121:VAL:HG23	2.10	0.52
1:M:55:SER:O	3:N:201:EDO:O2	2.22	0.52
1:e:98:ASP:HB2	1:f:60:SER:OG	2.09	0.52
1:E:87:SER:O	1:E:91:VAL:HG23	2.10	0.51
1:Q:55:SER:N	1:Q:58:LYS:HZ2	2.09	0.51
1:S:107:TRP:NE1	1:T:118:SER:OG	2.42	0.51
1:Q:114:PHE:HB2	1:T:114:PHE:CE1	2.45	0.51
1:T:56:THR:H	1:T:57:LYS:HZ2	1.57	0.51
1:g:69:GLU:O	1:g:73:ASN:HB2	2.11	0.51
1:f:69:GLU:O	1:f:73:ASN:HB2	2.10	0.51
1:Q:83:VAL:O	1:Q:85:THR:N	2.44	0.51
1:F:88:PRO:HB2	1:I:105:PHE:CD2	2.45	0.51
1:J:122:LEU:O	1:J:124:ALA:N	2.43	0.51
1:L:73:ASN:HB3	1:L:76:LEU:HB2	1.92	0.51
1:L:74:MET:HE1	1:X:107:TRP:H	1.76	0.51
1:c:104:ASN:HB3	1:c:109:ARG:NH1	2.26	0.51
1:S:73:ASN:HA	1:G:104:ASN:OD1	2.11	0.51
1:i:99:MET:O	1:i:109:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:61:GLU:OE2	1:R:64:LYS:NZ	2.41	0.51
1:X:104:ASN:ND2	1:X:106:ASN:OD1	2.44	0.51
1:c:107:TRP:HB2	1:f:121:VAL:HG11	1.94	0.51
1:e:90:GLU:OE2	1:e:94:ARG:HD3	2.11	0.51
1:M:50:LEU:HD12	1:M:50:LEU:H	1.76	0.50
1:a:79:MET:HB2	1:b:59:LEU:HD13	1.93	0.50
1:e:56:THR:HG21	1:f:94:ARG:HH12	1.75	0.50
1:U:104:ASN:OD1	1:U:104:ASN:N	2.45	0.50
1:J:73:ASN:O	1:J:77:GLN:HG3	2.11	0.50
1:Q:80:ILE:O	1:Q:83:VAL:HG22	2.12	0.50
1:W:118:SER:OG	1:W:119:LYS:N	2.45	0.50
1:i:75:GLU:OE2	1:i:78:ARG:NH2	2.43	0.50
1:T:107:TRP:H	1:H:74:MET:HE3	1.76	0.50
1:G:63:LEU:HA	1:G:66:ILE:HG22	1.94	0.50
1:T:62:SER:O	1:T:65:ARG:N	2.42	0.50
1:T:75:GLU:HG3	1:T:76:LEU:H	1.76	0.50
1:L:100:PHE:CD1	1:L:105:PHE:HA	2.47	0.50
1:M:87:SER:O	1:M:91:VAL:HG23	2.12	0.50
1:j:62:SER:O	1:j:66:ILE:HG13	2.12	0.50
1:T:55:SER:N	1:T:57:LYS:HZ1	2.10	0.49
1:J:80:ILE:O	1:J:83:VAL:HG22	2.12	0.49
1:c:95:VAL:O	1:c:99:MET:HG3	2.12	0.49
1:U:95:VAL:O	1:U:99:MET:HG3	2.12	0.49
1:g:105:PHE:CD2	1:j:88:PRO:HB2	2.47	0.49
1:M:101:SER:C	1:M:103:GLY:H	2.21	0.49
1:h:87:SER:O	1:h:91:VAL:HG23	2.12	0.49
1:J:58:LYS:HA	1:J:61:GLU:HG3	1.93	0.49
1:i:96:ALA:HB2	1:i:113:LEU:HD21	1.95	0.49
1:L:88:PRO:HA	1:L:120:LEU:HD21	1.95	0.49
1:c:64:LYS:HD2	1:d:99:MET:HA	1.95	0.49
1:H:61:GLU:HA	1:H:64:LYS:HB2	1.95	0.49
1:Z:80:ILE:HG12	1:Z:116:PHE:CD1	2.48	0.49
1:g:114:PHE:HB2	1:j:114:PHE:CE2	2.48	0.49
1:h:92:PHE:CE1	1:h:117:ALA:HB2	2.48	0.49
1:L:61:GLU:O	1:L:65:ARG:HG3	2.12	0.49
1:i:97:ALA:O	1:i:101:SER:HB3	2.13	0.49
1:U:118:SER:O	1:U:122:LEU:HB2	2.13	0.48
1:F:122:LEU:HD22	1:J:122:LEU:HD22	1.95	0.48
1:P:61:GLU:OE2	1:P:64:LYS:NZ	2.47	0.48
1:d:117:ALA:O	1:d:121:VAL:HG22	2.14	0.48
1:e:83:VAL:HG12	1:e:83:VAL:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ASP:O	1:B:57:LYS:HE2	2.13	0.48
1:P:100:PHE:HE2	1:P:113:LEU:HD22	1.77	0.48
1:K:59:LEU:HD13	1:L:79:MET:HB3	1.96	0.48
1:Y:77:GLN:OE1	1:Y:78:ARG:N	2.46	0.48
1:H:58:LYS:H	1:H:58:LYS:HE2	1.78	0.48
1:I:52:SER:O	1:I:56:THR:HG23	2.13	0.48
1:N:70:LEU:O	1:N:77:GLN:NE2	2.47	0.48
1:Z:121:VAL:HG21	1:a:107:TRP:CE3	2.49	0.48
1:d:75:GLU:O	1:d:79:MET:HG3	2.13	0.48
1:j:77:GLN:O	1:j:81:ALA:N	2.47	0.48
1:S:79:MET:SD	1:T:58:LYS:HG2	2.54	0.48
1:H:99:MET:HE2	1:H:100:PHE:CE2	2.49	0.48
1:H:100:PHE:HD1	1:H:104:ASN:O	1.97	0.48
1:g:87:SER:CB	1:g:90:GLU:HB3	2.44	0.48
1:a:99:MET:HG3	1:b:60:SER:HB2	1.95	0.47
1:X:77:GLN:OE1	1:X:119:LYS:HE3	2.14	0.47
1:e:109:ARG:NE	1:f:68:ASP:OD1	2.47	0.47
1:D:74:MET:O	1:D:78:ARG:HG2	2.14	0.47
1:W:87:SER:O	1:W:91:VAL:HG23	2.15	0.47
1:Q:87:SER:O	1:Q:91:VAL:HG23	2.14	0.47
1:Y:74:MET:HA	1:Y:77:GLN:CG	2.44	0.47
1:a:119:LYS:O	1:a:123:LYS:HB2	2.14	0.47
1:b:87:SER:OG	1:b:90:GLU:OE1	2.32	0.47
1:E:75:GLU:O	1:E:79:MET:HG3	2.15	0.47
1:K:119:LYS:HD3	1:K:123:LYS:HE2	1.95	0.47
1:L:62:SER:O	1:L:66:ILE:HD12	2.14	0.47
1:Q:75:GLU:O	1:Q:79:MET:HG3	2.14	0.47
1:S:74:MET:O	1:S:78:ARG:N	2.46	0.47
1:X:74:MET:HE2	1:X:74:MET:HB2	1.81	0.47
1:e:106:ASN:OD1	1:e:109:ARG:HG3	2.15	0.47
1:G:98:ASP:HA	1:G:101:SER:OG	2.15	0.47
1:R:110:VAL:O	1:R:114:PHE:HD1	1.97	0.47
1:K:87:SER:HB2	1:K:90:GLU:OE1	2.15	0.47
1:a:100:PHE:HE2	1:a:113:LEU:HD22	1.80	0.47
1:j:92:PHE:CE1	1:j:117:ALA:HB2	2.50	0.47
1:O:98:ASP:OD1	1:O:98:ASP:N	2.40	0.47
1:e:61:GLU:HA	1:e:64:LYS:HD3	1.96	0.46
1:N:75:GLU:O	1:N:79:MET:HG3	2.16	0.46
1:G:69:GLU:HB3	1:H:66:ILE:HD12	1.97	0.46
1:L:100:PHE:HD1	1:L:105:PHE:HA	1.81	0.46
1:W:55:SER:OG	1:W:56:THR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:ILE:O	1:H:66:ILE:HD11	2.15	0.46
1:K:65:ARG:HH22	1:L:73:ASN:HD21	1.62	0.46
1:O:67:GLY:HA2	1:O:70:LEU:HD12	1.97	0.46
1:P:87:SER:O	1:P:91:VAL:HG23	2.14	0.46
1:b:117:ALA:O	1:b:121:VAL:HG13	2.15	0.46
1:D:83:VAL:CG1	1:D:91:VAL:HG11	2.46	0.46
1:W:64:LYS:HD3	1:X:99:MET:HA	1.98	0.46
1:S:116:PHE:CE2	1:S:120:LEU:HD11	2.50	0.46
1:H:107:TRP:O	1:H:111:VAL:HG13	2.15	0.46
1:L:115:TYR:CZ	1:L:119:LYS:HD2	2.50	0.46
1:M:102:ASP:C	1:M:104:ASN:H	2.23	0.46
1:i:64:LYS:HE2	1:j:99:MET:HA	1.97	0.46
1:I:73:ASN:HD21	1:J:62:SER:HB2	1.80	0.46
1:e:70:LEU:HD12	1:e:71:ASP:N	2.31	0.46
1:g:99:MET:HB3	1:g:99:MET:HE2	1.76	0.46
1:H:65:ARG:NH2	5:H:201:HOH:O	2.48	0.46
1:g:114:PHE:HB2	1:j:114:PHE:CD2	2.50	0.46
1:U:79:MET:HB3	1:V:59:LEU:HB2	1.97	0.45
1:V:61:GLU:O	1:V:64:LYS:HB3	2.16	0.45
1:V:80:ILE:C	1:V:82:ALA:H	2.24	0.45
1:K:77:GLN:OE1	1:K:77:GLN:HA	2.15	0.45
1:Z:62:SER:O	1:Z:66:ILE:HG13	2.16	0.45
1:G:70:LEU:HD22	1:G:115:TYR:CD1	2.51	0.45
1:C:58:LYS:HD3	1:D:79:MET:SD	2.56	0.45
1:C:66:ILE:HD13	1:D:70:LEU:HD23	1.97	0.45
1:U:83:VAL:HG21	1:U:120:LEU:HB2	1.97	0.45
1:F:87:SER:HB3	4:F:201:PEG:H11	1.98	0.45
1:K:76:LEU:HD12	1:K:80:ILE:HD11	1.97	0.45
1:N:73:ASN:HD22	1:N:73:ASN:C	2.23	0.45
1:i:73:ASN:O	1:i:77:GLN:HG2	2.16	0.45
1:S:65:ARG:HH11	1:S:65:ARG:HG2	1.80	0.45
1:F:74:MET:HE1	1:N:107:TRP:H	1.81	0.45
1:M:92:PHE:CD1	1:M:92:PHE:C	2.95	0.45
1:c:61:GLU:OE2	1:c:64:LYS:NZ	2.46	0.45
1:S:58:LYS:H	1:S:58:LYS:HG2	1.62	0.45
1:H:121:VAL:HG12	1:U:105:PHE:CD2	2.51	0.45
1:N:104:ASN:ND2	1:N:106:ASN:HD22	2.14	0.45
1:Y:62:SER:O	1:Y:66:ILE:HG13	2.17	0.45
1:C:69:GLU:HG3	3:C:203:EDO:H22	1.99	0.45
1:S:102:ASP:OD2	1:S:104:ASN:ND2	2.50	0.45
1:T:75:GLU:HG3	1:T:76:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:83:VAL:HG11	1:X:120:LEU:HD11	1.98	0.45
1:R:90:GLU:HG3	1:R:94:ARG:HD2	1.99	0.45
1:A:80:ILE:HG12	1:A:116:PHE:HD1	1.83	0.44
1:Q:57:LYS:O	1:Q:61:GLU:HG3	2.17	0.44
1:E:75:GLU:HG2	1:E:79:MET:HE2	1.99	0.44
1:J:106:ASN:HD21	1:J:109:ARG:HG3	1.82	0.44
1:R:75:GLU:OE1	1:R:78:ARG:NH1	2.50	0.44
1:W:95:VAL:O	1:W:99:MET:HG3	2.17	0.44
1:c:107:TRP:NE1	1:d:118:SER:OG	2.49	0.44
1:i:95:VAL:O	1:i:99:MET:HG3	2.18	0.44
1:Q:114:PHE:HE2	1:S:114:PHE:HZ	1.64	0.44
1:T:101:SER:O	1:Z:103:GLY:HA3	2.17	0.44
1:O:95:VAL:HG21	1:P:59:LEU:HD23	1.99	0.44
1:a:92:PHE:CE1	1:a:117:ALA:HB2	2.53	0.44
1:a:98:ASP:HB3	1:b:60:SER:OG	2.18	0.44
1:h:70:LEU:HG	1:h:115:TYR:CZ	2.53	0.44
1:i:64:LYS:CE	1:j:99:MET:HA	2.47	0.44
1:G:59:LEU:HD21	1:H:76:LEU:HA	1.98	0.44
1:H:74:MET:HA	1:H:77:GLN:HG2	1.99	0.44
1:U:120:LEU:HG	1:U:121:VAL:HG13	2.00	0.44
1:f:106:ASN:HB2	1:f:109:ARG:HG3	2.00	0.44
1:S:65:ARG:HG2	1:S:65:ARG:NH1	2.33	0.44
1:U:104:ASN:O	1:U:106:ASN:N	2.48	0.44
1:K:73:ASN:O	1:K:77:GLN:HG2	2.18	0.44
1:c:78:ARG:C	1:c:78:ARG:HD3	2.43	0.44
1:K:98:ASP:HB2	1:L:57:LYS:NZ	2.32	0.44
1:h:73:ASN:OD1	1:h:76:LEU:N	2.45	0.44
1:B:53:ASP:O	1:B:56:THR:HG22	2.18	0.43
1:f:62:SER:O	1:f:66:ILE:HD12	2.17	0.43
1:f:91:VAL:HG13	1:f:120:LEU:HD21	1.99	0.43
1:B:77:GLN:OE1	1:B:119:LYS:HE2	2.18	0.43
1:C:64:LYS:HE2	1:C:65:ARG:NH2	2.33	0.43
1:D:57:LYS:HE3	1:D:57:LYS:HB3	1.85	0.43
1:F:65:ARG:HH22	1:N:109:ARG:HH21	1.66	0.43
1:L:74:MET:HE3	1:X:106:ASN:HB2	1.99	0.43
1:g:68:ASP:OD1	1:h:109:ARG:NE	2.46	0.43
1:c:114:PHE:HB2	1:f:114:PHE:CE1	2.54	0.43
1:U:58:LYS:HB3	1:U:58:LYS:HE2	1.71	0.43
1:c:114:PHE:HZ	1:e:114:PHE:CE2	2.37	0.43
1:T:71:ASP:OD1	1:T:115:TYR:OH	2.35	0.43
1:F:89:ARG:H	4:F:201:PEG:H32	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:123:LYS:O	1:e:123:LYS:HG2	2.19	0.43
1:g:59:LEU:HD13	1:h:79:MET:HB2	1.99	0.43
1:i:91:VAL:HG22	1:i:116:PHE:HZ	1.84	0.43
1:Y:114:PHE:HB2	1:b:114:PHE:CE2	2.53	0.43
1:E:100:PHE:HB3	1:J:89:ARG:HG3	2.01	0.43
1:F:89:ARG:HB3	4:F:201:PEG:H21	2.00	0.43
1:Y:114:PHE:HB2	1:b:114:PHE:CD2	2.54	0.43
1:M:64:LYS:HD3	1:N:99:MET:HA	2.00	0.43
1:T:95:VAL:O	1:T:99:MET:HG2	2.19	0.43
1:d:114:PHE:CG	1:e:114:PHE:HD1	2.37	0.43
1:W:99:MET:HE2	1:W:99:MET:HB3	1.87	0.43
1:Z:91:VAL:HG22	1:Z:94:ARG:NH2	2.33	0.43
1:a:58:LYS:HG2	1:b:79:MET:SD	2.58	0.43
1:O:122:LEU:O	1:O:124:ALA:N	2.47	0.42
1:e:87:SER:O	1:e:91:VAL:HG23	2.19	0.42
1:j:76:LEU:O	1:j:80:ILE:HG13	2.19	0.42
1:C:73:ASN:O	1:C:77:GLN:HG3	2.19	0.42
1:O:121:VAL:HG11	1:X:107:TRP:HB2	2.01	0.42
1:Y:76:LEU:HA	1:Y:79:MET:HG3	2.02	0.42
1:Y:79:MET:HE2	1:Y:79:MET:HB3	1.83	0.42
1:j:117:ALA:O	1:j:121:VAL:HG22	2.19	0.42
1:A:102:ASP:OD1	1:A:102:ASP:N	2.51	0.42
1:G:74:MET:HA	1:G:77:GLN:HB2	2.01	0.42
1:F:74:MET:CE	1:N:107:TRP:H	2.32	0.42
1:M:109:ARG:NH2	1:N:68:ASP:OD2	2.52	0.42
1:Y:66:ILE:HG21	1:Z:70:LEU:HD21	2.00	0.42
1:a:58:LYS:NZ	1:b:78:ARG:HH12	2.17	0.42
1:C:119:LYS:O	1:C:123:LYS:HB2	2.18	0.42
1:V:68:ASP:O	1:V:72:SER:OG	2.23	0.42
1:e:83:VAL:HG11	1:e:91:VAL:HG21	2.01	0.42
1:e:122:LEU:C	1:e:124:ALA:H	2.26	0.42
1:A:83:VAL:O	1:A:85:THR:N	2.53	0.42
3:C:203:EDO:O1	1:R:65:ARG:HA	2.20	0.42
1:G:92:PHE:CE1	1:G:117:ALA:HB2	2.55	0.42
1:U:117:ALA:HA	1:U:120:LEU:HD21	2.00	0.42
1:K:59:LEU:CD1	1:L:76:LEU:HA	2.50	0.42
1:N:73:ASN:O	1:N:77:GLN:HG2	2.20	0.42
1:a:83:VAL:O	1:a:85:THR:N	2.53	0.42
1:c:105:PHE:CD2	1:f:88:PRO:HB2	2.55	0.42
1:i:111:VAL:HG21	1:j:115:TYR:HD1	1.84	0.42
1:Q:99:MET:HG3	1:R:60:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:ARG:HD2	1:F:65:ARG:HA	1.82	0.42
1:M:75:GLU:O	1:M:79:MET:HG3	2.20	0.42
1:b:65:ARG:O	1:b:69:GLU:HG3	2.19	0.42
1:c:104:ASN:C	1:c:104:ASN:HD22	2.26	0.42
1:H:89:ARG:HG2	1:H:93:PHE:HE1	1.85	0.42
1:P:121:VAL:HG12	1:W:105:PHE:CD2	2.55	0.42
1:Z:80:ILE:HG12	1:Z:116:PHE:HD1	1.84	0.42
1:c:58:LYS:HG2	1:d:79:MET:SD	2.59	0.42
1:d:101:SER:OG	5:d:201:HOH:O	2.22	0.42
1:Q:75:GLU:OE1	1:Q:79:MET:HE2	2.20	0.42
1:F:57:LYS:HA	1:F:57:LYS:HD2	1.86	0.42
1:M:104:ASN:ND2	1:M:106:ASN:HD21	2.18	0.42
1:Y:59:LEU:HB2	1:Z:79:MET:HB3	2.01	0.42
1:T:80:ILE:HG12	1:T:116:PHE:CD1	2.55	0.42
1:E:73:ASN:O	1:E:77:GLN:HG2	2.19	0.42
1:J:65:ARG:HG2	3:J:202:EDO:H21	2.01	0.42
1:b:124:ALA:O	1:b:126:SER:N	2.53	0.42
1:H:99:MET:HE2	1:H:99:MET:HB3	1.86	0.41
1:J:106:ASN:ND2	1:J:109:ARG:HG3	2.35	0.41
1:K:71:ASP:HA	1:K:77:GLN:NE2	2.35	0.41
1:K:71:ASP:OD2	1:L:108:GLY:N	2.40	0.41
1:M:106:ASN:O	1:M:110:VAL:HG23	2.21	0.41
1:P:120:LEU:HD23	1:P:120:LEU:HA	1.88	0.41
1:c:65:ARG:O	1:c:69:GLU:HG3	2.20	0.41
1:d:122:LEU:HB2	1:f:122:LEU:CD2	2.50	0.41
1:C:54:ALA:HB1	3:F:202:EDO:H11	2.01	0.41
1:L:76:LEU:HD23	1:L:80:ILE:HD11	2.03	0.41
1:a:121:VAL:HG12	1:a:122:LEU:HD23	2.02	0.41
1:U:120:LEU:H	1:U:120:LEU:HD23	1.86	0.41
1:L:80:ILE:HG12	1:L:116:PHE:CE1	2.55	0.41
1:Z:55:SER:HB3	1:Z:58:LYS:HG3	2.01	0.41
1:h:114:PHE:CE2	1:i:114:PHE:HB2	2.54	0.41
1:V:104:ASN:CG	1:V:106:ASN:HD22	2.29	0.41
1:W:79:MET:HB3	1:X:59:LEU:HB2	2.03	0.41
1:h:62:SER:O	1:h:66:ILE:HG12	2.19	0.41
1:H:94:ARG:HG2	1:H:94:ARG:HH11	1.85	0.41
1:K:59:LEU:HD23	1:L:95:VAL:HG21	2.03	0.41
1:c:115:TYR:O	1:c:119:LYS:HG2	2.21	0.41
1:e:59:LEU:HD11	1:f:80:ILE:HG13	2.02	0.41
1:g:68:ASP:OD1	1:h:109:ARG:NH2	2.54	0.41
1:C:58:LYS:HE3	1:F:102:ASP:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:89:ARG:HH21	1:T:101:SER:HA	1.86	0.41
1:V:87:SER:O	1:V:91:VAL:HG23	2.21	0.41
1:c:89:ARG:NH1	1:f:103:GLY:H	2.19	0.41
1:g:114:PHE:CZ	1:i:114:PHE:HE2	2.39	0.41
1:S:107:TRP:O	1:S:111:VAL:HG23	2.20	0.41
1:J:124:ALA:HA	1:M:78:ARG:NH2	2.34	0.41
1:L:73:ASN:OD1	1:L:76:LEU:HB2	2.21	0.41
1:c:119:LYS:HA	1:c:119:LYS:HD2	1.94	0.41
1:e:56:THR:HG21	1:f:94:ARG:NH1	2.36	0.41
1:g:71:ASP:OD1	1:g:115:TYR:OH	2.39	0.41
1:T:85:THR:HG23	1:T:88:PRO:HD3	2.03	0.41
1:X:75:GLU:H	1:X:75:GLU:CD	2.28	0.41
1:h:106:ASN:O	1:h:110:VAL:HG23	2.21	0.41
1:Q:114:PHE:CZ	1:S:114:PHE:HE2	2.39	0.40
1:e:83:VAL:C	1:e:85:THR:H	2.28	0.40
1:Q:58:LYS:H	1:Q:58:LYS:CD	2.23	0.40
1:S:92:PHE:CE1	1:S:117:ALA:HB2	2.56	0.40
1:U:90:GLU:HA	1:U:93:PHE:CD2	2.51	0.40
1:K:110:VAL:O	1:K:114:PHE:HD2	2.05	0.40
1:N:90:GLU:HG3	1:N:94:ARG:CZ	2.52	0.40
1:g:71:ASP:O	1:g:77:GLN:NE2	2.54	0.40
1:i:106:ASN:O	1:i:110:VAL:HG23	2.21	0.40
1:R:89:ARG:NH1	1:S:100:PHE:O	2.55	0.40
1:V:80:ILE:O	1:V:82:ALA:N	2.54	0.40
1:M:66:ILE:HG21	1:N:70:LEU:HD21	2.02	0.40
1:M:73:ASN:O	1:M:77:GLN:HG2	2.21	0.40
1:b:73:ASN:O	1:b:77:GLN:HG2	2.20	0.40
1:c:75:GLU:OE1	1:c:75:GLU:HA	2.21	0.40
1:Q:94:ARG:HD3	1:R:56:THR:HG21	2.04	0.40
1:X:83:VAL:CG1	1:X:91:VAL:HG11	2.52	0.40
1:d:74:MET:HB3	1:d:74:MET:HE3	1.80	0.40
1:i:75:GLU:OE2	1:i:78:ARG:NE	2.52	0.40
1:j:74:MET:HA	1:j:77:GLN:HB2	2.04	0.40
1:j:81:ALA:O	1:j:83:VAL:N	2.47	0.40

There are no symmetry-related clashes.

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	67/81 (83%)	65 (97%)	1 (2%)	1 (2%)	8	8
1	B	69/81 (85%)	67 (97%)	2 (3%)	0	100	100
1	C	70/81 (86%)	66 (94%)	2 (3%)	2 (3%)	3	2
1	D	69/81 (85%)	65 (94%)	4 (6%)	0	100	100
1	E	70/81 (86%)	68 (97%)	1 (1%)	1 (1%)	9	9
1	F	70/81 (86%)	66 (94%)	4 (6%)	0	100	100
1	G	55/81 (68%)	52 (94%)	3 (6%)	0	100	100
1	H	57/81 (70%)	56 (98%)	1 (2%)	0	100	100
1	I	64/81 (79%)	62 (97%)	2 (3%)	0	100	100
1	J	69/81 (85%)	68 (99%)	0	1 (1%)	9	9
1	K	67/81 (83%)	64 (96%)	3 (4%)	0	100	100
1	L	56/81 (69%)	54 (96%)	2 (4%)	0	100	100
1	M	69/81 (85%)	63 (91%)	5 (7%)	1 (1%)	9	9
1	N	68/81 (84%)	66 (97%)	2 (3%)	0	100	100
1	O	59/81 (73%)	58 (98%)	0	1 (2%)	7	7
1	P	62/81 (76%)	60 (97%)	2 (3%)	0	100	100
1	Q	69/81 (85%)	65 (94%)	3 (4%)	1 (1%)	9	9
1	R	68/81 (84%)	65 (96%)	2 (3%)	1 (2%)	8	8
1	S	68/81 (84%)	66 (97%)	2 (3%)	0	100	100
1	T	64/81 (79%)	60 (94%)	3 (5%)	1 (2%)	7	7
1	U	65/81 (80%)	59 (91%)	4 (6%)	2 (3%)	3	2
1	V	60/81 (74%)	57 (95%)	1 (2%)	2 (3%)	3	2
1	W	61/81 (75%)	59 (97%)	2 (3%)	0	100	100
1	X	63/81 (78%)	60 (95%)	2 (3%)	1 (2%)	7	7
1	Y	69/81 (85%)	63 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	65/81 (80%)	63 (97%)	2 (3%)	0	100	100
1	a	68/81 (84%)	62 (91%)	5 (7%)	1 (2%)	8	8
1	b	70/81 (86%)	68 (97%)	2 (3%)	0	100	100
1	c	63/81 (78%)	58 (92%)	5 (8%)	0	100	100
1	d	69/81 (85%)	66 (96%)	3 (4%)	0	100	100
1	e	65/81 (80%)	56 (86%)	8 (12%)	1 (2%)	8	8
1	f	66/81 (82%)	61 (92%)	5 (8%)	0	100	100
1	g	58/81 (72%)	52 (90%)	4 (7%)	2 (3%)	3	2
1	h	61/81 (75%)	60 (98%)	1 (2%)	0	100	100
1	i	66/81 (82%)	61 (92%)	5 (8%)	0	100	100
1	j	66/81 (82%)	61 (92%)	4 (6%)	1 (2%)	8	8
All	All	2345/2916 (80%)	2222 (95%)	103 (4%)	20 (1%)	14	17

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ASP
1	j	73	ASN
1	Q	84	ASP
1	R	123	LYS
1	V	73	ASN
1	J	123	LYS
1	X	73	ASN
1	g	73	ASN
1	C	123	LYS
1	a	73	ASN
1	U	89	ARG
1	V	81	ALA
1	E	73	ASN
1	e	105	PHE
1	C	86	ASP
1	U	73	ASN
1	M	102	ASP
1	O	123	LYS
1	g	75	GLU
1	T	87	SER

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	59/68 (87%)	57 (97%)	2 (3%)	32	49
1	B	60/68 (88%)	58 (97%)	2 (3%)	33	50
1	C	57/68 (84%)	55 (96%)	2 (4%)	32	48
1	D	59/68 (87%)	57 (97%)	2 (3%)	32	49
1	E	58/68 (85%)	57 (98%)	1 (2%)	53	72
1	F	59/68 (87%)	59 (100%)	0	100	100
1	G	46/68 (68%)	46 (100%)	0	100	100
1	H	48/68 (71%)	45 (94%)	3 (6%)	16	23
1	I	50/68 (74%)	48 (96%)	2 (4%)	28	42
1	J	59/68 (87%)	58 (98%)	1 (2%)	53	72
1	K	53/68 (78%)	52 (98%)	1 (2%)	50	69
1	L	45/68 (66%)	44 (98%)	1 (2%)	45	65
1	M	58/68 (85%)	58 (100%)	0	100	100
1	N	58/68 (85%)	58 (100%)	0	100	100
1	O	46/68 (68%)	45 (98%)	1 (2%)	45	65
1	P	41/68 (60%)	41 (100%)	0	100	100
1	Q	58/68 (85%)	56 (97%)	2 (3%)	32	49
1	R	57/68 (84%)	54 (95%)	3 (5%)	20	30
1	S	56/68 (82%)	56 (100%)	0	100	100
1	T	56/68 (82%)	55 (98%)	1 (2%)	51	70
1	U	51/68 (75%)	48 (94%)	3 (6%)	18	26
1	V	51/68 (75%)	50 (98%)	1 (2%)	48	67
1	W	55/68 (81%)	55 (100%)	0	100	100
1	X	52/68 (76%)	51 (98%)	1 (2%)	50	69
1	Y	56/68 (82%)	55 (98%)	1 (2%)	51	70
1	Z	57/68 (84%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	60/68 (88%)	58 (97%)	2 (3%)	33	50
1	b	59/68 (87%)	58 (98%)	1 (2%)	53	72
1	c	56/68 (82%)	55 (98%)	1 (2%)	51	70
1	d	58/68 (85%)	58 (100%)	0	100	100
1	e	57/68 (84%)	57 (100%)	0	100	100
1	f	53/68 (78%)	52 (98%)	1 (2%)	50	69
1	g	41/68 (60%)	41 (100%)	0	100	100
1	h	43/68 (63%)	43 (100%)	0	100	100
1	i	50/68 (74%)	48 (96%)	2 (4%)	28	42
1	j	44/68 (65%)	44 (100%)	0	100	100
All	All	1926/2448 (79%)	1889 (98%)	37 (2%)	50	69

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	SER
1	A	106	ASN
1	B	55	SER
1	B	65	ARG
1	C	60	SER
1	C	76	LEU
1	D	60	SER
1	D	64	LYS
1	Q	75	GLU
1	Q	85	THR
1	R	60	SER
1	R	70	LEU
1	R	122	LEU
1	T	86	ASP
1	H	106	ASN
1	H	111	VAL
1	H	121	VAL
1	U	60	SER
1	U	102	ASP
1	U	104	ASN
1	V	101	SER
1	E	62	SER
1	I	62	SER

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Mol	Chain	Res	Type
1	I	66	ILE
1	J	56	THR
1	K	76	LEU
1	L	76	LEU
1	O	122	LEU
1	X	87	SER
1	Y	101	SER
1	a	75	GLU
1	a	86	ASP
1	b	121	VAL
1	c	83	VAL
1	f	101	SER
1	i	62	SER
1	i	91	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	77	GLN
1	R	104	ASN
1	S	77	GLN
1	V	106	ASN
1	F	104	ASN
1	J	73	ASN
1	M	77	GLN
1	M	104	ASN
1	M	106	ASN
1	N	73	ASN
1	N	104	ASN
1	N	106	ASN
1	b	106	ASN
1	c	104	ASN
1	e	77	GLN
1	i	77	GLN
1	j	77	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	N	201	-	3,3,3	0.39	0	2,2,2	0.34	0
3	EDO	D	202	-	3,3,3	0.41	0	2,2,2	0.41	0
3	EDO	I	202	-	3,3,3	0.11	0	2,2,2	0.08	0
3	EDO	C	203	-	3,3,3	0.41	0	2,2,2	0.24	0
3	EDO	J	202	-	3,3,3	0.41	0	2,2,2	0.32	0
3	EDO	F	202	-	3,3,3	0.42	0	2,2,2	0.39	0
4	PEG	F	201	-	6,6,6	0.09	0	5,5,5	0.04	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
3	EDO	N	201	-	-	1/1/1/1	-
3	EDO	D	202	-	-	1/1/1/1	-
3	EDO	I	202	-	-	0/1/1/1	-
3	EDO	C	203	-	-	0/1/1/1	-
3	EDO	J	202	-	-	1/1/1/1	-
3	EDO	F	202	-	-	0/1/1/1	-
4	PEG	F	201	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	201	PEG	O2-C3-C4-O4
3	D	202	EDO	O1-C1-C2-O2
4	F	201	PEG	C4-C3-O2-C2
4	F	201	PEG	O1-C1-C2-O2
3	J	202	EDO	O1-C1-C2-O2
3	N	201	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	201	EDO	3	0
3	D	202	EDO	1	0
3	I	202	EDO	1	0
3	C	203	EDO	3	0
3	J	202	EDO	1	0
3	F	202	EDO	1	0
4	F	201	PEG	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, 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	69/81 (85%)	-1.25	0 100 100	33, 50, 79, 114	0
1	B	71/81 (87%)	-1.41	0 100 100	29, 41, 68, 78	0
1	C	74/81 (91%)	-1.28	0 100 100	28, 42, 79, 95	0
1	D	71/81 (87%)	-1.30	0 100 100	31, 48, 67, 76	0
1	E	72/81 (88%)	-1.24	0 100 100	28, 50, 83, 130	0
1	F	72/81 (88%)	-1.26	0 100 100	29, 40, 71, 116	0
1	G	59/81 (72%)	-0.97	0 100 100	44, 79, 115, 130	0
1	H	61/81 (75%)	-1.07	0 100 100	49, 79, 107, 119	0
1	I	68/81 (83%)	-1.32	0 100 100	30, 42, 71, 92	0
1	J	71/81 (87%)	-1.27	0 100 100	31, 50, 71, 82	0
1	K	69/81 (85%)	-1.03	0 100 100	41, 80, 144, 167	0
1	L	62/81 (76%)	-1.02	0 100 100	49, 79, 128, 133	0
1	M	73/81 (90%)	-1.15	0 100 100	35, 63, 114, 168	0
1	N	70/81 (86%)	-1.23	0 100 100	33, 51, 89, 105	0
1	O	63/81 (77%)	-1.08	0 100 100	40, 64, 104, 119	0
1	P	66/81 (81%)	-1.14	0 100 100	39, 69, 109, 121	0
1	Q	71/81 (87%)	-1.14	0 100 100	35, 58, 86, 162	0
1	R	70/81 (86%)	-1.24	0 100 100	36, 51, 81, 97	0
1	S	70/81 (86%)	-1.11	0 100 100	46, 63, 94, 124	0
1	T	68/81 (83%)	-1.12	0 100 100	40, 70, 102, 157	0
1	U	69/81 (85%)	-1.12	0 100 100	41, 73, 108, 124	0
1	V	64/81 (79%)	-1.06	0 100 100	40, 70, 103, 120	0
1	W	65/81 (80%)	-1.04	0 100 100	52, 74, 97, 120	0
1	X	65/81 (80%)	-1.04	0 100 100	45, 74, 103, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9	
1	Y	70/81 (86%)	-1.10	0	100100	41, 71, 116, 184	1 (1%)
1	Z	69/81 (85%)	-1.20	0	100100	43, 65, 84, 106	0
1	a	70/81 (86%)	-1.17	0	100100	33, 53, 85, 197	0
1	b	72/81 (88%)	-1.29	0	100100	37, 55, 89, 103	0
1	c	67/81 (82%)	-1.22	0	100100	37, 57, 73, 87	0
1	d	71/81 (87%)	-1.13	0	100100	34, 55, 86, 129	0
1	e	69/81 (85%)	-1.09	0	100100	46, 69, 109, 143	0
1	f	68/81 (83%)	-1.03	0	100100	48, 82, 141, 181	0
1	g	62/81 (76%)	-1.17	0	100100	58, 85, 116, 159	0
1	h	65/81 (80%)	-0.98	0	100100	62, 86, 135, 183	0
1	i	68/81 (83%)	-1.04	0	100100	64, 89, 146, 186	0
1	j	68/81 (83%)	-1.04	0	100100	55, 93, 125, 186	0
All	All	2452/2916 (84%)	-1.15	0	100100	28, 62, 113, 197	1 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	D	202	4/4	0.97	0.05	58,64,66,68	0
3	EDO	F	202	4/4	0.97	0.11	50,51,57,58	0
3	EDO	J	202	4/4	0.98	0.04	49,55,56,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	C	203	4/4	0.99	0.06	42,47,54,61	0
3	EDO	I	202	4/4	0.99	0.05	50,53,54,56	0
2	ZN	h	201	1/1	0.99	0.04	152,152,152,152	0
3	EDO	N	201	4/4	0.99	0.08	42,43,46,49	0
4	PEG	F	201	7/7	0.99	0.15	42,50,53,53	0
2	ZN	B	201	1/1	1.00	0.03	49,49,49,49	0
2	ZN	C	201	1/1	1.00	0.02	80,80,80,80	0
2	ZN	C	202	1/1	1.00	0.01	67,67,67,67	0
2	ZN	D	201	1/1	1.00	0.02	85,85,85,85	0
2	ZN	I	201	1/1	1.00	0.02	70,70,70,70	0
2	ZN	J	201	1/1	1.00	0.01	105,105,105,105	0
2	ZN	M	201	1/1	1.00	0.03	63,63,63,63	0
2	ZN	c	201	1/1	1.00	0.01	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.