



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:45 am GMT

PDB ID : 4XTN
Title : Crystal structure of the light-driven sodium pump KR2 in the pentameric red form, pH 4.9
Authors : Gushchin, I.; Shevchenko, V.; Polovinkin, V.; Gordeliy, V.
Deposited on : 2015-01-23
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

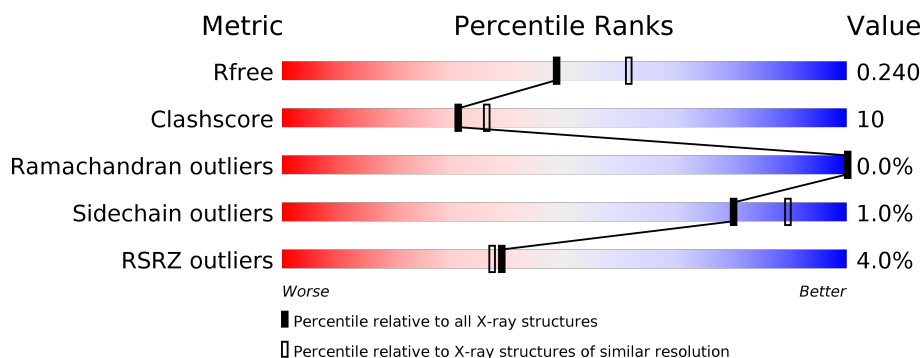
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	288	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>5%</div> </div> </div>
1	B	288	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>6%</div> </div> </div>
1	C	288	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>6%</div> </div> </div>
1	D	288	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>6%</div> </div> </div>
1	E	288	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>6%</div> </div> </div>
1	F	288	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	288	
1	H	288	
1	I	288	
1	J	288	

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
2	NA	A	301	-	-	-	X
3	LFA	A	302	-	-	-	X
3	LFA	A	304	-	-	-	X
3	LFA	A	305	-	-	-	X
3	LFA	A	306	-	-	-	X
3	LFA	A	307	-	-	-	X
3	LFA	A	309	-	-	-	X
3	LFA	A	311	-	-	-	X
3	LFA	B	302	-	-	-	X
3	LFA	B	303	-	-	-	X
3	LFA	B	304	-	-	-	X
3	LFA	B	307	-	-	-	X
3	LFA	B	308	-	-	-	X
3	LFA	B	309	-	-	-	X
3	LFA	B	310	-	-	-	X
3	LFA	C	302	-	-	-	X
3	LFA	C	306	-	-	-	X
3	LFA	C	307	-	-	-	X
3	LFA	C	309	-	-	-	X
3	LFA	C	310	-	-	-	X
3	LFA	C	312	-	-	-	X
3	LFA	D	302	-	-	-	X
3	LFA	D	303	-	-	-	X
3	LFA	D	306	-	-	-	X
3	LFA	D	309	-	-	-	X
3	LFA	D	312	-	-	-	X
3	LFA	E	302	-	-	-	X
3	LFA	E	303	-	-	-	X
3	LFA	E	305	-	-	-	X
3	LFA	E	311	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LFA	E	312	-	-	-	X
3	LFA	F	302	-	-	-	X
3	LFA	F	303	-	-	-	X
3	LFA	F	307	-	-	-	X
3	LFA	F	308	-	-	-	X
3	LFA	F	310	-	-	-	X
3	LFA	F	312	-	-	-	X
3	LFA	F	313	-	-	-	X
3	LFA	G	302	-	-	-	X
3	LFA	G	303	-	-	-	X
3	LFA	G	304	-	-	-	X
3	LFA	G	307	-	-	-	X
3	LFA	G	309	-	-	-	X
3	LFA	G	310	-	-	-	X
3	LFA	G	315	-	-	-	X
3	LFA	H	302	-	-	-	X
3	LFA	H	304	-	-	-	X
3	LFA	H	305	-	-	-	X
3	LFA	H	307	-	-	-	X
3	LFA	H	309	-	-	-	X
3	LFA	H	311	-	-	-	X
3	LFA	I	302	-	-	-	X
3	LFA	I	303	-	-	-	X
3	LFA	I	304	-	-	-	X
3	LFA	I	308	-	-	-	X
3	LFA	I	309	-	-	-	X
3	LFA	I	310	-	-	-	X
3	LFA	J	302	-	-	-	X
3	LFA	J	304	-	-	-	X
3	LFA	J	305	-	-	-	X
3	LFA	J	307	-	-	-	X
3	LFA	J	308	-	-	-	X
4	MPG	D	315	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23361 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 Sodium pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2174	1458	329	378	9			
1	B	270	Total	C	N	O	S	0	1	0
			2158	1449	324	376	9			
1	C	271	Total	C	N	O	S	0	2	0
			2170	1457	326	378	9			
1	D	271	Total	C	N	O	S	0	0	0
			2161	1449	326	377	9			
1	E	272	Total	C	N	O	S	0	0	0
			2166	1451	326	380	9			
1	F	271	Total	C	N	O	S	0	1	0
			2166	1454	326	377	9			
1	G	271	Total	C	N	O	S	0	3	0
			2178	1462	328	379	9			
1	H	273	Total	C	N	O	S	0	1	0
			2186	1464	331	382	9			
1	I	271	Total	C	N	O	S	0	0	0
			2152	1444	322	377	9			
1	J	272	Total	C	N	O	S	0	2	0
			2175	1458	328	380	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	LEU	-	expression tag	UNP N0DKS8
A	282	GLU	-	expression tag	UNP N0DKS8
A	283	HIS	-	expression tag	UNP N0DKS8
A	284	HIS	-	expression tag	UNP N0DKS8
A	285	HIS	-	expression tag	UNP N0DKS8
A	286	HIS	-	expression tag	UNP N0DKS8
A	287	HIS	-	expression tag	UNP N0DKS8
A	288	HIS	-	expression tag	UNP N0DKS8
B	281	LEU	-	expression tag	UNP N0DKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	282	GLU	-	expression tag	UNP N0DKS8
B	283	HIS	-	expression tag	UNP N0DKS8
B	284	HIS	-	expression tag	UNP N0DKS8
B	285	HIS	-	expression tag	UNP N0DKS8
B	286	HIS	-	expression tag	UNP N0DKS8
B	287	HIS	-	expression tag	UNP N0DKS8
B	288	HIS	-	expression tag	UNP N0DKS8
C	281	LEU	-	expression tag	UNP N0DKS8
C	282	GLU	-	expression tag	UNP N0DKS8
C	283	HIS	-	expression tag	UNP N0DKS8
C	284	HIS	-	expression tag	UNP N0DKS8
C	285	HIS	-	expression tag	UNP N0DKS8
C	286	HIS	-	expression tag	UNP N0DKS8
C	287	HIS	-	expression tag	UNP N0DKS8
C	288	HIS	-	expression tag	UNP N0DKS8
D	281	LEU	-	expression tag	UNP N0DKS8
D	282	GLU	-	expression tag	UNP N0DKS8
D	283	HIS	-	expression tag	UNP N0DKS8
D	284	HIS	-	expression tag	UNP N0DKS8
D	285	HIS	-	expression tag	UNP N0DKS8
D	286	HIS	-	expression tag	UNP N0DKS8
D	287	HIS	-	expression tag	UNP N0DKS8
D	288	HIS	-	expression tag	UNP N0DKS8
E	281	LEU	-	expression tag	UNP N0DKS8
E	282	GLU	-	expression tag	UNP N0DKS8
E	283	HIS	-	expression tag	UNP N0DKS8
E	284	HIS	-	expression tag	UNP N0DKS8
E	285	HIS	-	expression tag	UNP N0DKS8
E	286	HIS	-	expression tag	UNP N0DKS8
E	287	HIS	-	expression tag	UNP N0DKS8
E	288	HIS	-	expression tag	UNP N0DKS8
F	281	LEU	-	expression tag	UNP N0DKS8
F	282	GLU	-	expression tag	UNP N0DKS8
F	283	HIS	-	expression tag	UNP N0DKS8
F	284	HIS	-	expression tag	UNP N0DKS8
F	285	HIS	-	expression tag	UNP N0DKS8
F	286	HIS	-	expression tag	UNP N0DKS8
F	287	HIS	-	expression tag	UNP N0DKS8
F	288	HIS	-	expression tag	UNP N0DKS8
G	281	LEU	-	expression tag	UNP N0DKS8
G	282	GLU	-	expression tag	UNP N0DKS8
G	283	HIS	-	expression tag	UNP N0DKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	284	HIS	-	expression tag	UNP N0DKS8
G	285	HIS	-	expression tag	UNP N0DKS8
G	286	HIS	-	expression tag	UNP N0DKS8
G	287	HIS	-	expression tag	UNP N0DKS8
G	288	HIS	-	expression tag	UNP N0DKS8
H	281	LEU	-	expression tag	UNP N0DKS8
H	282	GLU	-	expression tag	UNP N0DKS8
H	283	HIS	-	expression tag	UNP N0DKS8
H	284	HIS	-	expression tag	UNP N0DKS8
H	285	HIS	-	expression tag	UNP N0DKS8
H	286	HIS	-	expression tag	UNP N0DKS8
H	287	HIS	-	expression tag	UNP N0DKS8
H	288	HIS	-	expression tag	UNP N0DKS8
I	281	LEU	-	expression tag	UNP N0DKS8
I	282	GLU	-	expression tag	UNP N0DKS8
I	283	HIS	-	expression tag	UNP N0DKS8
I	284	HIS	-	expression tag	UNP N0DKS8
I	285	HIS	-	expression tag	UNP N0DKS8
I	286	HIS	-	expression tag	UNP N0DKS8
I	287	HIS	-	expression tag	UNP N0DKS8
I	288	HIS	-	expression tag	UNP N0DKS8
J	281	LEU	-	expression tag	UNP N0DKS8
J	282	GLU	-	expression tag	UNP N0DKS8
J	283	HIS	-	expression tag	UNP N0DKS8
J	284	HIS	-	expression tag	UNP N0DKS8
J	285	HIS	-	expression tag	UNP N0DKS8
J	286	HIS	-	expression tag	UNP N0DKS8
J	287	HIS	-	expression tag	UNP N0DKS8
J	288	HIS	-	expression tag	UNP N0DKS8

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

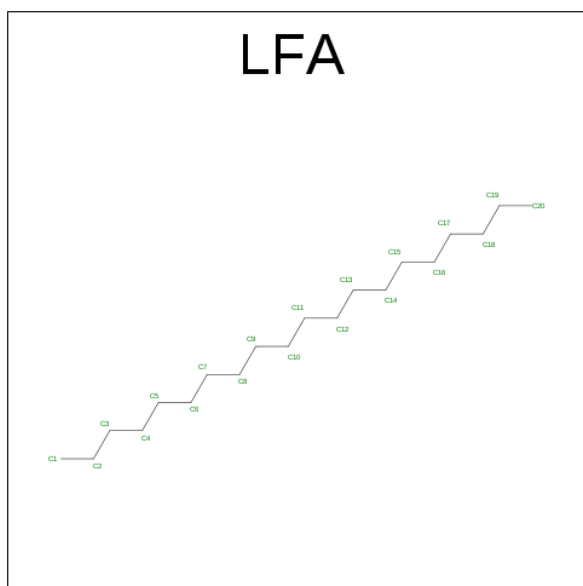
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Na 1 1	0	0
2	J	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	I	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	F	1	Total	Na	0	0
			1	1		

- Molecule 3 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			14	14		
3	A	1	Total	C	0	0
			6	6		
3	A	1	Total	C	0	0
			10	10		
3	A	1	Total	C	0	0
			10	10		
3	A	1	Total	C	0	0
			14	14		
3	A	1	Total	C	0	0
			18	18		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C 5 5	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C 14 14	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 16 16	0	0
3	B	1	Total C 18 18	0	0
3	B	1	Total C 13 13	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 8 8	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 10 10	0	0
3	C	1	Total C 6 6	0	0
3	C	1	Total C 10 10	0	0
3	C	1	Total C 16 16	0	0
3	C	1	Total C 18 18	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C 10 10	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 13 13	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 4 4	0	0
3	D	1	Total C 7 7	0	0
3	D	1	Total C 14 14	0	0
3	D	1	Total C 6 6	0	0
3	D	1	Total C 10 10	0	0
3	D	1	Total C 16 16	0	0
3	D	1	Total C 18 18	0	0
3	D	1	Total C 10 10	0	0
3	D	1	Total C 8 8	0	0
3	D	1	Total C 8 8	0	0
3	D	1	Total C 7 7	0	0
3	D	1	Total C 6 6	0	0
3	D	1	Total C 6 6	0	0
3	D	1	Total C 7 7	0	0
3	D	1	Total C 5 5	0	0
3	D	1	Total C 5 5	0	0
3	D	1	Total C 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C 14 14	0	0
3	E	1	Total C 18 18	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 6 6	0	0
3	E	1	Total C 12 12	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 14 14	0	0
3	E	1	Total C 6 6	0	0
3	E	1	Total C 10 10	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 8 8	0	0
3	F	1	Total C 7 7	0	0
3	F	1	Total C 14 14	0	0
3	F	1	Total C 10 10	0	0
3	F	1	Total C 6 6	0	0
3	F	1	Total C 10 10	0	0
3	F	1	Total C 6 6	0	0
3	F	1	Total C 8 8	0	0
3	F	1	Total C 10 10	0	0
3	F	1	Total C 18 18	0	0
3	F	1	Total C 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C 8 8	0	0
3	F	1	Total C 14 14	0	0
3	F	1	Total C 8 8	0	0
3	G	1	Total C 16 16	0	0
3	G	1	Total C 7 7	0	0
3	G	1	Total C 14 14	0	0
3	G	1	Total C 6 6	0	0
3	G	1	Total C 10 10	0	0
3	G	1	Total C 16 16	0	0
3	G	1	Total C 18 18	0	0
3	G	1	Total C 8 8	0	0
3	G	1	Total C 10 10	0	0
3	G	1	Total C 8 8	0	0
3	G	1	Total C 8 8	0	0
3	G	1	Total C 6 6	0	0
3	G	1	Total C 6 6	0	0
3	H	1	Total C 13 13	0	0
3	H	1	Total C 6 6	0	0
3	H	1	Total C 10 10	0	0
3	H	1	Total C 16 16	0	0
3	H	1	Total C 18 18	0	0

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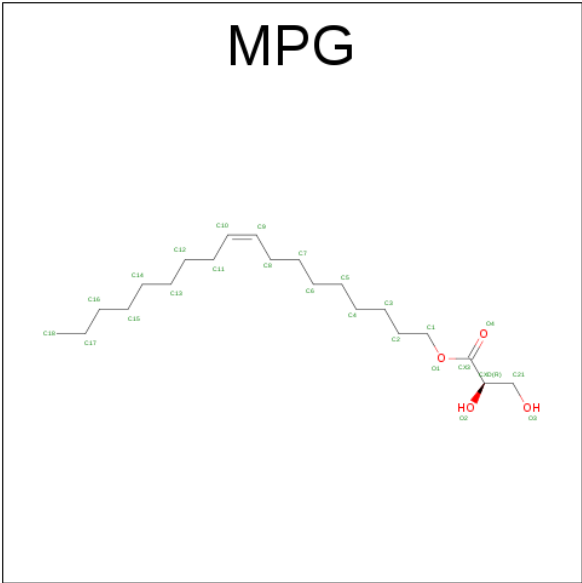
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C 14 14	0	0
3	H	1	Total C 8 8	0	0
3	H	1	Total C 5 5	0	0
3	H	1	Total C 8 8	0	0
3	H	1	Total C 7 7	0	0
3	H	1	Total C 6 6	0	0
3	I	1	Total C 7 7	0	0
3	I	1	Total C 7 7	0	0
3	I	1	Total C 14 14	0	0
3	I	1	Total C 6 6	0	0
3	I	1	Total C 10 10	0	0
3	I	1	Total C 6 6	0	0
3	I	1	Total C 16 16	0	0
3	I	1	Total C 18 18	0	0
3	I	1	Total C 14 14	0	0
3	I	1	Total C 8 8	0	0
3	I	1	Total C 7 7	0	0
3	I	1	Total C 4 4	0	0
3	J	1	Total C 16 16	0	0
3	J	1	Total C 18 18	0	0
3	J	1	Total C 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total C 14 14	0	0
3	J	1	Total C 8 8	0	0
3	J	1	Total C 7 7	0	0
3	J	1	Total C 14 14	0	0
3	J	1	Total C 10 10	0	0
3	J	1	Total C 10 10	0	0
3	J	1	Total C 4 4	0	0

- Molecule 4 is 1-MONOOLEOYL-RAC-GLYCEROL (three-letter code: MPG) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 14 11 3	0	0
4	B	1	Total C O 14 11 3	0	0
4	C	1	Total C O 13 10 3	0	0
4	D	1	Total C O 14 11 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			14	11	3		
4	F	1	Total	C	O	0	0
			14	11	3		
4	G	1	Total	C	O	0	0
			14	11	3		
4	H	1	Total	C	O	0	0
			14	11	3		
4	I	1	Total	C	O	0	0
			14	11	3		
4	J	1	Total	C	O	0	0
			14	11	3		

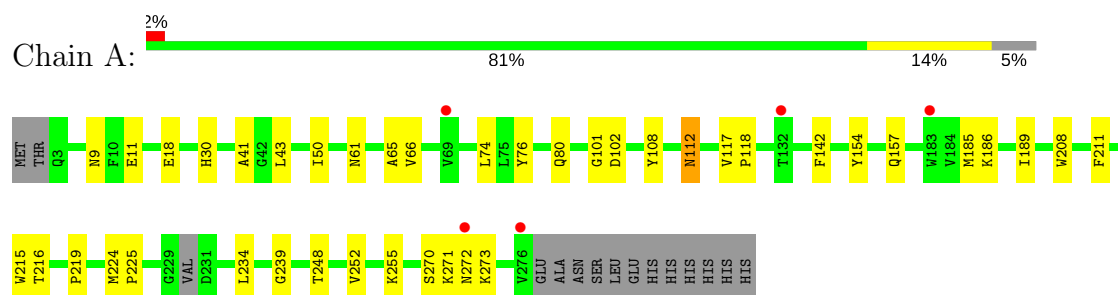
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	30	Total	O	0	0
			30	30		
5	C	31	Total	O	0	0
			31	31		
5	D	34	Total	O	0	0
			34	34		
5	E	30	Total	O	0	0
			30	30		
5	F	30	Total	O	0	0
			30	30		
5	G	35	Total	O	0	0
			35	35		
5	H	45	Total	O	0	0
			45	45		
5	I	40	Total	O	0	0
			40	40		
5	J	37	Total	O	0	0
			37	37		

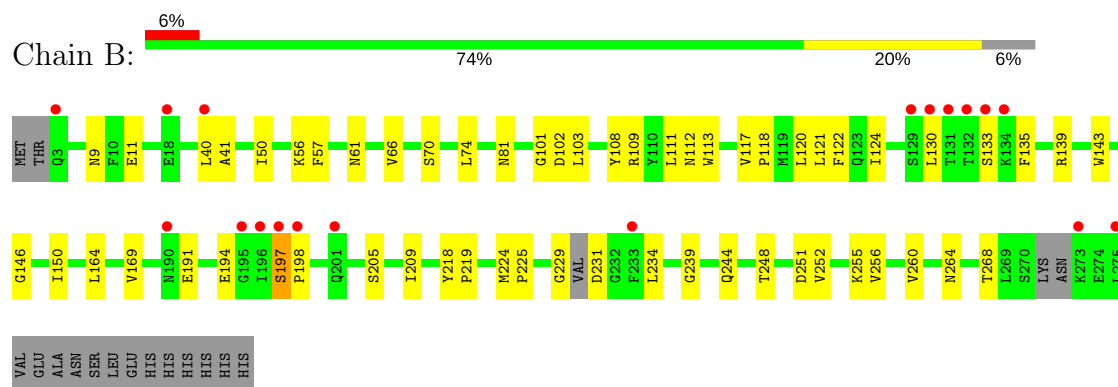
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

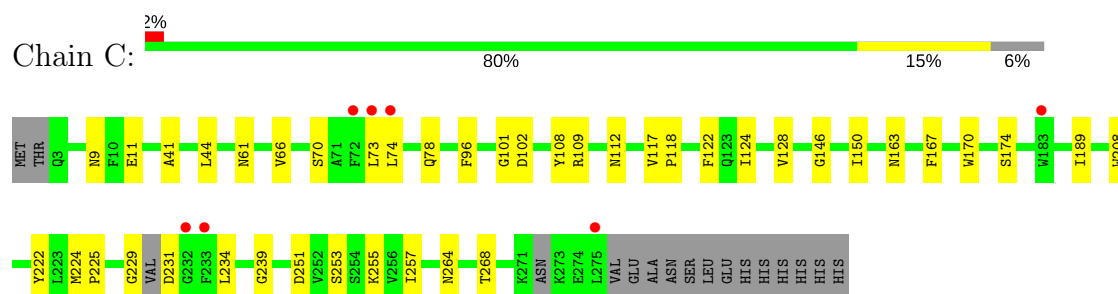
• Molecule 1: Sodium pumping rhodopsin



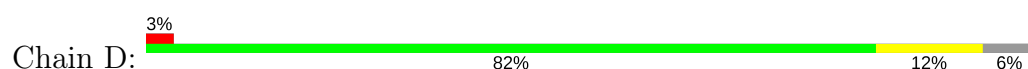
• Molecule 1: Sodium pumping rhodopsin



• Molecule 1: Sodium pumping rhodopsin



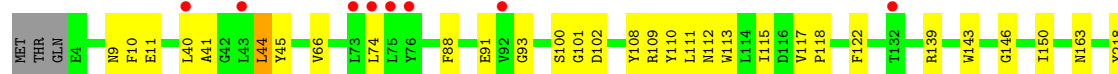
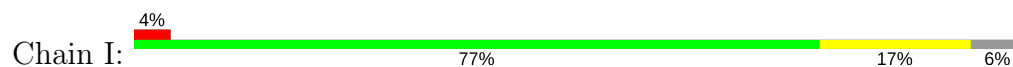
• Molecule 1: Sodium pumping rhodopsin



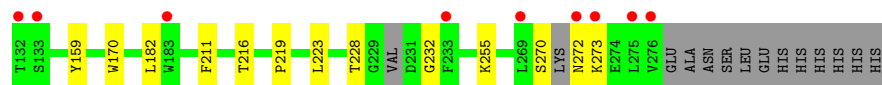
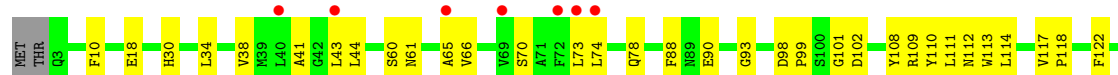
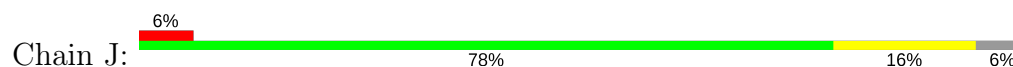




• Molecule 1: Sodium pumping rhodopsin



• Molecule 1: Sodium pumping rhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.69Å 107.00Å 240.80Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	48.90 – 2.20 48.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.90-2.20) 96.2 (48.89-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.195 , 0.236 0.203 , 0.240	Depositor DCC
R_{free} test set	9797 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23361	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: MPG, LFA, LYR, NA

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	0.29	0/2201	0.43	0/2990
1	B	0.28	0/2187	0.42	0/2972
1	C	0.29	0/2202	0.43	0/2992
1	D	0.30	0/2187	0.42	0/2970
1	E	0.29	0/2191	0.44	0/2976
1	F	0.29	0/2195	0.42	0/2982
1	G	0.29	0/2213	0.43	0/3007
1	H	0.30	0/2215	0.43	0/3008
1	I	0.30	0/2178	0.43	0/2963
1	J	0.29	0/2207	0.44	0/3000
All	All	0.29	0/21976	0.43	0/29860

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2174	0	2164	32	0
1	B	2158	0	2144	53	0
1	C	2170	0	2156	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2161	0	2145	34	0
1	E	2166	0	2140	67	0
1	F	2166	0	2155	60	0
1	G	2178	0	2174	58	0
1	H	2186	0	2177	51	0
1	I	2152	0	2117	52	0
1	J	2175	0	2156	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	108	0	199	3	0
3	B	108	0	200	3	0
3	C	110	0	206	6	0
3	D	138	0	260	10	0
3	E	112	0	204	9	0
3	F	129	0	245	7	0
3	G	133	0	250	5	0
3	H	111	0	208	2	0
3	I	117	0	219	7	0
3	J	109	0	205	5	0
4	A	14	0	19	0	0
4	B	14	0	19	0	0
4	C	13	0	17	1	0
4	D	14	0	19	1	0
4	E	14	0	19	3	0
4	F	14	0	19	1	0
4	G	14	0	19	2	0
4	H	14	0	19	0	0
4	I	14	0	19	0	0
4	J	14	0	19	2	0
5	A	39	0	0	3	0
5	B	30	0	0	2	0
5	C	31	0	0	1	0
5	D	34	0	0	0	0
5	E	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	30	0	0	3	0
5	G	35	0	0	3	0
5	H	45	0	0	6	0
5	I	40	0	0	3	0
5	J	37	0	0	6	0
All	All	23361	0	23912	482	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 10.

All (482) 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:C:74[B]:LEU:CD2	1:C:112[B]:ASN:CB	1.81	1.56
1:C:74[B]:LEU:CD2	1:C:112[B]:ASN:HB2	1.03	1.48
1:F:74[B]:LEU:CD2	1:F:112:ASN:HB2	1.41	1.48
1:C:74[B]:LEU:HD22	1:C:112[B]:ASN:CG	1.32	1.43
1:G:74[B]:LEU:CD1	1:G:112[B]:ASN:ND2	1.78	1.28
1:H:271:LYS:C	1:H:272:ASN:CA	2.10	1.20
1:C:74[B]:LEU:HD22	1:C:112[B]:ASN:CB	1.54	1.20
1:B:74[A]:LEU:HD11	1:B:108:TYR:O	1.43	1.17
1:G:74[B]:LEU:HD13	1:G:112[B]:ASN:ND2	1.39	1.17
1:G:74[B]:LEU:CD1	1:G:112[B]:ASN:HD21	1.48	1.15
1:F:74[B]:LEU:HD21	1:F:108:TYR:O	1.47	1.13
1:C:74[B]:LEU:HD21	1:C:112[B]:ASN:HB2	1.25	1.12
1:H:271:LYS:O	1:H:272:ASN:CA	1.98	1.12
1:B:74[A]:LEU:HD13	1:B:112:ASN:HB2	1.14	1.11
1:F:74[B]:LEU:HD23	1:F:112:ASN:CB	1.81	1.09
1:F:74[B]:LEU:HD11	1:F:108:TYR:HB3	1.29	1.08
1:F:74[B]:LEU:CD2	1:F:112:ASN:CB	2.32	1.08
1:F:74[B]:LEU:HD22	1:F:112:ASN:HB2	1.19	1.07
1:F:74[B]:LEU:HD23	1:F:112:ASN:HB2	1.16	1.06
1:B:74[A]:LEU:HD11	1:B:108:TYR:C	1.75	1.06
1:E:74:LEU:HD13	1:E:112:ASN:HB2	1.35	1.06
1:B:74[B]:LEU:HD23	1:B:112:ASN:HB2	1.37	1.05
1:G:74[B]:LEU:HD11	1:G:112[B]:ASN:ND2	1.69	1.03
3:C:306:LFA:C16	3:D:302:LFA:H11	1.89	1.01
1:B:219:PRO:HG3	1:B:255:LYR:H132	1.43	1.01
1:E:163:ASN:ND2	4:E:313:MPG:O3	1.93	0.99
1:B:74[A]:LEU:CD1	1:B:108:TYR:O	2.10	0.98
1:J:112[B]:ASN:ND2	5:J:429:HOH:O	1.97	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81[B]:ASN:ND2	5:G:415:HOH:O	1.97	0.96
1:C:44:LEU:HD12	1:D:69:VAL:HG21	1.48	0.96
1:H:271:LYS:C	1:H:272:ASN:CB	2.34	0.95
1:H:271:LYS:C	1:H:272:ASN:HB2	1.87	0.95
1:C:74[B]:LEU:CD2	1:C:112[B]:ASN:CG	2.22	0.93
1:C:74[B]:LEU:HD22	1:C:112[B]:ASN:ND2	1.85	0.91
3:C:306:LFA:C16	3:D:302:LFA:C1	2.49	0.90
1:H:18:GLU:OE2	5:H:432:HOH:O	1.90	0.89
1:C:74[B]:LEU:HD23	1:C:112[B]:ASN:HB2	0.89	0.89
1:B:74[A]:LEU:HD13	1:B:112:ASN:CB	2.01	0.88
1:E:163:ASN:HD22	4:E:313:MPG:H3	1.16	0.88
1:B:255:LYR:H9	1:B:255:LYR:H183	1.53	0.88
1:F:74[B]:LEU:CD2	1:F:108:TYR:O	2.23	0.87
1:C:74[B]:LEU:HD23	1:C:112[B]:ASN:CB	1.72	0.87
1:B:74[B]:LEU:CD2	1:B:112:ASN:HB2	2.05	0.86
1:B:197:SER:HB2	1:B:198:PRO:HD2	1.58	0.86
1:E:74:LEU:CD1	1:E:112:ASN:HB2	2.05	0.86
1:G:74[B]:LEU:HD11	1:G:112[B]:ASN:HD21	1.28	0.85
3:D:316:LFA:H12	3:D:317:LFA:H12	1.60	0.83
1:E:74:LEU:HD13	1:E:112:ASN:CB	2.09	0.83
1:B:74[A]:LEU:CD1	1:B:112:ASN:HB2	2.05	0.82
1:C:44:LEU:HD12	1:D:69:VAL:CG2	2.09	0.82
3:E:304:LFA:C3	3:E:305:LFA:C3	2.59	0.81
1:F:255:LYR:H183	1:F:255:LYR:H9	1.62	0.81
1:E:255:LYR:H183	1:E:255:LYR:H9	1.62	0.80
1:G:255:LYR:H9	1:G:255:LYR:H183	1.64	0.80
1:H:74:LEU:HD22	5:H:431:HOH:O	1.82	0.80
1:C:255:LYR:H183	1:C:255:LYR:H9	1.65	0.79
1:I:255:LYR:H183	1:I:255:LYR:H9	1.65	0.79
1:J:18:GLU:OE2	5:J:428:HOH:O	2.02	0.78
1:B:197:SER:HB2	1:B:198:PRO:CD	2.15	0.77
1:G:74[B]:LEU:HD11	1:G:112[B]:ASN:OD1	1.84	0.77
1:J:74[A]:LEU:HD13	1:J:112[A]:ASN:HB2	1.67	0.77
1:C:74[A]:LEU:HD21	1:C:109:ARG:HA	1.66	0.76
1:J:255:LYR:H183	1:J:255:LYR:H9	1.68	0.76
1:D:74:LEU:HD13	1:D:112:ASN:HB2	1.68	0.76
1:I:271:LYS:O	1:I:273:LYS:N	2.18	0.75
1:G:18:GLU:OE2	5:G:426:HOH:O	2.03	0.75
1:F:74[B]:LEU:HD21	1:F:108:TYR:C	2.06	0.75
1:J:270:SER:C	1:J:272:ASN:HB3	2.07	0.74
1:G:74[A]:LEU:HD11	1:G:108:TYR:C	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:302:LFA:H11	3:J:302:LFA:C16	2.18	0.74
1:A:255:LYR:H183	1:A:255:LYR:H9	1.70	0.74
3:D:302:LFA:C7	3:E:311:LFA:C8	2.65	0.73
1:G:273:LYS:O	5:G:433:HOH:O	2.07	0.73
1:A:101:GLY:O	1:A:102:ASP:HB2	1.90	0.72
1:F:74[B]:LEU:CD1	1:F:108:TYR:HB3	2.15	0.71
1:E:224:MET:HE3	1:E:234:LEU:HD22	1.72	0.71
1:I:224:MET:CE	1:I:234:LEU:HD13	2.21	0.71
1:J:18:GLU:OE1	5:J:427:HOH:O	2.08	0.70
1:D:255:LYR:H9	1:D:255:LYR:H183	1.72	0.70
5:H:433:HOH:O	1:I:108:TYR:CE2	2.43	0.70
1:D:101:GLY:O	1:D:102:ASP:HB2	1.90	0.70
1:E:74:LEU:CD1	1:E:112:ASN:CB	2.70	0.70
1:B:101:GLY:O	1:B:102:ASP:HB2	1.92	0.70
1:H:255:LYR:H183	1:H:255:LYR:H9	1.71	0.70
1:F:271:LYS:O	1:F:273:LYS:N	2.25	0.70
3:F:311:LFA:H61	3:F:312:LFA:C2	2.22	0.69
1:J:101:GLY:O	1:J:102:ASP:HB2	1.92	0.69
1:H:70:SER:OG	1:H:112[B]:ASN:OD1	2.09	0.69
1:E:89:ASN:HD21	1:G:89:ASN:HD21	1.41	0.69
1:G:74[A]:LEU:HD11	1:G:109:ARG:HA	1.74	0.69
1:H:101:GLY:O	1:H:102:ASP:HB2	1.91	0.69
1:G:74[A]:LEU:HD13	1:G:112[A]:ASN:HB2	1.74	0.69
1:B:70:SER:OG	1:B:112:ASN:ND2	2.26	0.69
1:B:255:LYR:C9	1:B:255:LYR:H183	2.23	0.69
1:F:113:TRP:CD1	1:F:255:LYR:HC2	2.28	0.69
1:H:74:LEU:CD2	5:H:431:HOH:O	2.37	0.68
1:D:41:ALA:HB1	1:E:66:VAL:HG13	1.76	0.68
1:B:74[B]:LEU:HD23	1:B:112:ASN:CB	2.21	0.68
1:C:74[B]:LEU:HD21	1:C:112[B]:ASN:CB	1.98	0.68
1:E:109:ARG:NH2	1:E:251:ASP:OD2	2.26	0.68
1:G:74[A]:LEU:HD13	1:G:112[A]:ASN:CB	2.24	0.68
1:I:101:GLY:O	5:I:416:HOH:O	2.10	0.68
1:J:74[A]:LEU:HD11	1:J:108:TYR:C	2.14	0.68
1:B:244:GLN:HG2	5:B:414:HOH:O	1.94	0.68
1:C:74[A]:LEU:HD13	1:C:112[A]:ASN:HB2	1.75	0.68
1:F:74[B]:LEU:HD11	1:F:108:TYR:CB	2.16	0.68
1:F:74[B]:LEU:HD22	1:F:112:ASN:CB	2.12	0.66
1:I:224:MET:HE1	1:I:234:LEU:HD13	1.77	0.66
1:G:74[A]:LEU:CD1	1:G:108:TYR:O	2.44	0.66
5:H:424:HOH:O	1:I:111:LEU:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:LEU:HD12	1:E:112:ASN:ND2	2.11	0.66
1:F:255:LYR:C9	1:F:255:LYR:H183	2.26	0.66
3:F:304:LFA:H61	3:J:304:LFA:H11	1.76	0.65
1:A:273:LYS:O	5:A:432:HOH:O	2.15	0.65
1:I:229:GLY:O	1:I:231:ASP:N	2.30	0.65
1:D:30:HIS:HB3	1:E:111:LEU:HD22	1.79	0.65
3:F:302:LFA:C1	3:J:302:LFA:C16	2.75	0.64
1:E:77:ALA:O	3:E:311:LFA:H21	1.98	0.64
1:B:50:ILE:HD13	1:B:61:ASN:HB3	1.79	0.64
1:G:9:ASN:HB3	1:G:11:GLU:OE1	1.97	0.64
1:D:89:ASN:HD21	1:H:89:ASN:HD21	1.45	0.64
1:F:264:ASN:O	1:F:268:THR:HG23	1.97	0.63
1:H:34:LEU:HD12	1:I:115:ILE:HD11	1.80	0.63
1:E:255:LYR:H183	1:E:255:LYR:C9	2.27	0.63
1:E:101:GLY:O	1:E:102:ASP:HB2	1.98	0.63
1:G:74[A]:LEU:HD11	1:G:109:ARG:N	2.13	0.63
1:I:267:ILE:HG21	1:I:275:LEU:HD23	1.81	0.62
1:E:224:MET:CE	1:E:234:LEU:HD13	2.29	0.62
1:G:44:LEU:HD11	1:H:43:LEU:HD11	1.82	0.62
1:I:163:ASN:HD21	3:I:306:LFA:H92	1.64	0.62
1:F:229:GLY:O	1:F:231:ASP:N	2.33	0.62
1:I:267:ILE:CG2	1:I:275:LEU:HD23	2.28	0.62
1:G:74[A]:LEU:HD11	1:G:109:ARG:CA	2.29	0.62
3:G:302:LFA:C16	3:G:303:LFA:H11	2.30	0.61
3:B:307:LFA:C16	3:C:302:LFA:H11	2.30	0.61
1:F:109:ARG:NH2	1:F:251:ASP:OD2	2.32	0.61
1:I:224:MET:HE3	1:I:234:LEU:HD22	1.82	0.61
1:J:255:LYR:H183	1:J:255:LYR:C9	2.30	0.61
1:I:255:LYR:H183	1:I:255:LYR:C9	2.30	0.61
1:A:65:ALA:HB1	1:E:44:LEU:CD1	2.31	0.61
1:B:229:GLY:O	1:B:231:ASP:N	2.33	0.61
1:C:255:LYR:H183	1:C:255:LYR:C9	2.31	0.61
3:C:306:LFA:C16	3:D:302:LFA:H12	2.31	0.60
1:B:74[B]:LEU:CD2	1:B:112:ASN:CB	2.78	0.60
1:G:101:GLY:O	1:G:102:ASP:HB2	2.02	0.60
1:E:113:TRP:CD1	1:E:255:LYR:HC2	2.36	0.60
1:A:41:ALA:HB1	1:B:66:VAL:HG13	1.82	0.60
1:B:219:PRO:HG3	1:B:255:LYR:C13	2.26	0.60
1:I:41:ALA:HB1	1:J:66:VAL:HG13	1.83	0.60
1:I:44:LEU:CD1	1:J:65:ALA:HB1	2.32	0.60
1:E:70:SER:OG	1:E:112:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:VAL:HB	1:F:118:PRO:HD3	1.84	0.60
1:F:247:TYR:OH	5:F:407:HOH:O	2.16	0.60
1:C:101:GLY:O	1:C:102:ASP:HB2	2.02	0.59
1:C:44:LEU:HD11	1:D:43:LEU:HD11	1.84	0.59
1:B:117:VAL:HB	1:B:118:PRO:HD3	1.83	0.59
1:F:74[B]:LEU:HD21	1:F:109:ARG:HA	1.85	0.59
3:A:311:LFA:C1	3:D:306:LFA:C16	2.81	0.58
1:C:170:TRP:HE1	4:C:313:MPG:HX31	1.67	0.58
1:H:9:ASN:HB3	1:H:11:GLU:OE1	2.03	0.58
1:I:74:LEU:HD12	1:I:112:ASN:HA	1.84	0.58
1:E:264:ASN:O	1:E:268:THR:HG23	2.04	0.58
1:F:44:LEU:HD21	1:G:65:ALA:HB1	1.86	0.58
1:J:74[A]:LEU:CD1	1:J:108:TYR:O	2.52	0.57
1:E:271:LYS:O	1:E:273:LYS:N	2.38	0.57
1:E:224:MET:HE1	1:E:234:LEU:HD13	1.87	0.57
1:H:74:LEU:HD21	1:H:109:ARG:HA	1.86	0.57
1:A:255:LYR:H183	1:A:255:LYR:C9	2.35	0.57
1:C:74[A]:LEU:CD2	1:C:109:ARG:HA	2.33	0.57
1:G:74[A]:LEU:CD1	1:G:109:ARG:HA	2.33	0.57
1:G:74[B]:LEU:HD13	1:G:112[B]:ASN:HD21	1.14	0.57
1:C:9:ASN:HB3	1:C:11:GLU:OE1	2.05	0.56
1:F:74[A]:LEU:HD13	1:F:112:ASN:HB2	1.86	0.56
1:H:255:LYR:H192	1:H:255:LYR:H9	1.88	0.56
1:H:255:LYR:H183	1:H:255:LYR:C9	2.34	0.56
1:A:185:MET:O	1:A:189:ILE:HG12	2.06	0.56
1:D:255:LYR:H9	1:D:255:LYR:H192	1.88	0.56
1:G:109:ARG:NH2	1:G:251:ASP:OD2	2.38	0.56
1:E:189:ILE:HD13	1:E:208:TRP:HB2	1.88	0.56
1:E:229:GLY:O	1:E:231:ASP:N	2.39	0.56
1:E:224:MET:HE1	1:E:234:LEU:CD1	2.35	0.56
1:A:50:ILE:HD13	1:A:61:ASN:HB3	1.87	0.56
1:F:41:ALA:HB1	1:G:66:VAL:HG13	1.88	0.56
1:G:255:LYR:C9	1:G:255:LYR:H183	2.32	0.55
1:G:117:VAL:HB	1:G:118:PRO:HD3	1.87	0.55
1:C:234:LEU:O	1:C:239:GLY:HA3	2.07	0.55
1:C:189:ILE:HD13	1:C:208:TRP:HB2	1.87	0.55
1:C:41:ALA:HB1	1:D:66:VAL:HG13	1.89	0.55
1:H:109:ARG:NH1	1:H:251:ASP:OD2	2.39	0.55
1:D:255:LYR:C9	1:D:255:LYR:H183	2.36	0.54
1:B:218:TYR:HB2	1:B:219:PRO:HD3	1.89	0.54
1:F:115:ILE:HD11	1:J:34:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:MET:HE1	1:I:234:LEU:CD1	2.38	0.54
1:F:74[A]:LEU:HD13	1:F:112:ASN:CB	2.37	0.54
1:A:255:LYR:H9	1:A:255:LYR:H192	1.87	0.54
1:F:62:ILE:O	1:F:66:VAL:HG23	2.07	0.54
1:F:66:VAL:HG13	1:J:41:ALA:HB1	1.90	0.54
1:A:9:ASN:HB3	1:A:11:GLU:OE1	2.08	0.54
1:B:133:SER:OG	1:B:191:GLU:OE2	2.26	0.53
1:C:255:LYR:H9	1:C:255:LYR:H192	1.90	0.53
1:H:272:ASN:C	1:H:273:LYS:HG3	2.29	0.53
1:J:70:SER:OG	1:J:112[B]:ASN:OD1	2.24	0.53
1:D:74:LEU:HD11	1:D:108:TYR:C	2.28	0.53
1:C:163:ASN:HD21	3:C:305:LFA:H92	1.73	0.53
1:B:234:LEU:O	1:B:239:GLY:HA3	2.09	0.53
1:F:234:LEU:O	1:F:239:GLY:HA3	2.08	0.53
1:J:255:LYR:H9	1:J:255:LYR:H192	1.91	0.53
3:F:311:LFA:H61	3:F:312:LFA:H22	1.90	0.53
1:G:111:LEU:O	1:G:114:LEU:HB2	2.09	0.53
1:D:159:TYR:CE1	4:D:315:MPG:H212	2.44	0.52
1:E:81:ASN:HA	3:E:311:LFA:H11	1.91	0.52
1:G:170:TRP:HE1	4:G:312:MPG:HX31	1.74	0.52
1:I:88:PHE:CZ	1:I:93:GLY:HA2	2.44	0.52
1:J:74[A]:LEU:HD11	1:J:108:TYR:O	2.08	0.52
1:C:70:SER:O	1:C:74[B]:LEU:HD13	2.09	0.52
1:F:109:ARG:O	1:F:112:ASN:HB3	2.09	0.52
1:F:76:TYR:O	1:F:80:GLN:HG2	2.09	0.52
1:A:66:VAL:HG13	1:E:41:ALA:HB1	1.92	0.52
3:G:302:LFA:C16	3:G:303:LFA:C1	2.87	0.52
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.91	0.52
1:A:234:LEU:O	1:A:239:GLY:HA3	2.10	0.52
1:A:65:ALA:HB1	1:E:44:LEU:HD11	1.90	0.52
1:D:117:VAL:HB	1:D:118:PRO:HD3	1.92	0.52
1:C:167:PHE:CE1	1:C:222:TYR:CE2	2.97	0.51
1:J:182:LEU:HD23	1:J:211:PHE:HE1	1.74	0.51
1:D:234:LEU:O	1:D:239:GLY:HA3	2.11	0.51
1:E:199:ALA:O	1:E:202:LYS:HE2	2.10	0.51
1:E:88:PHE:CZ	1:E:93:GLY:HA2	2.46	0.51
1:H:271:LYS:N	1:H:272:ASN:HB2	2.26	0.51
1:H:41:ALA:HB1	1:I:66:VAL:HG13	1.93	0.51
1:I:101:GLY:O	1:I:102:ASP:HB2	2.11	0.51
1:J:74[A]:LEU:HD11	1:J:109:ARG:HA	1.92	0.51
1:J:270:SER:O	1:J:272:ASN:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:311:LFA:H11	3:D:306:LFA:C16	2.41	0.50
3:F:311:LFA:H61	3:F:312:LFA:H21	1.93	0.50
1:G:44:LEU:HD22	1:G:48:LEU:CD1	2.40	0.50
1:I:224:MET:N	1:I:225:PRO:HD2	2.26	0.50
1:F:111:LEU:HD12	1:J:30:HIS:HB3	1.93	0.50
1:B:121:LEU:O	1:B:124:ILE:HG22	2.12	0.50
1:F:74[B]:LEU:HD21	1:F:109:ARG:CA	2.42	0.50
1:I:9:ASN:HB3	1:I:11:GLU:OE1	2.11	0.50
1:H:174:SER:HB3	1:H:255:LYR:H142	1.94	0.50
1:E:234:LEU:O	1:E:239:GLY:HA3	2.10	0.50
1:B:146:GLY:O	1:B:150:ILE:HG12	2.11	0.50
1:D:74:LEU:HD13	1:D:112:ASN:CB	2.39	0.50
1:H:101:GLY:O	1:H:102:ASP:CB	2.59	0.50
1:D:229:GLY:O	1:D:231:ASP:N	2.45	0.50
1:I:44:LEU:HD11	1:J:65:ALA:HB1	1.94	0.50
1:F:244:GLN:HG2	5:F:413:HOH:O	2.12	0.50
1:I:244:GLN:HG2	5:I:415:HOH:O	2.11	0.50
1:B:169:VAL:HG11	3:B:306:LFA:H32	1.94	0.50
3:D:316:LFA:H12	3:D:317:LFA:C1	2.39	0.49
3:H:305:LFA:C16	3:I:303:LFA:H11	2.42	0.49
1:I:110:TYR:O	1:I:113:TRP:HB2	2.12	0.49
1:J:216:THR:O	1:J:219:PRO:HG2	2.11	0.49
1:D:224:MET:N	1:D:225:PRO:HD2	2.27	0.49
1:E:163:ASN:ND2	4:E:313:MPG:H3	1.93	0.49
3:G:307:LFA:C16	3:I:302:LFA:H11	2.43	0.49
1:H:224:MET:HB3	1:H:225:PRO:CD	2.43	0.49
1:F:101:GLY:O	1:F:102:ASP:HB2	2.12	0.49
1:J:101:GLY:O	1:J:102:ASP:CB	2.60	0.49
1:B:40:LEU:HD23	1:C:73:LEU:HD11	1.94	0.49
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.94	0.49
1:G:118:PRO:O	1:G:122:PHE:HB2	2.12	0.49
1:H:117:VAL:HB	1:H:118:PRO:HD3	1.95	0.49
1:I:74:LEU:CD1	1:I:112:ASN:HA	2.42	0.49
1:C:109:ARG:NH1	1:C:251:ASP:OD2	2.46	0.49
3:C:302:LFA:C7	3:D:302:LFA:H42	2.42	0.49
1:B:197:SER:CB	1:B:198:PRO:CD	2.86	0.49
1:F:60:SER:OG	5:F:422:HOH:O	2.20	0.48
1:A:30:HIS:HB3	1:B:111:LEU:HD22	1.96	0.48
1:D:74:LEU:CD1	1:D:112:ASN:HB2	2.41	0.48
1:F:131:THR:OG1	1:F:132:THR:N	2.45	0.48
1:A:102:ASP:OD2	1:E:25:TYR:OH	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:LEU:HD11	1:D:109:ARG:HA	1.94	0.48
1:F:170:TRP:HE1	4:F:315:MPG:HX31	1.78	0.48
1:C:70:SER:OG	1:C:112[B]:ASN:ND2	2.45	0.48
1:F:38:VAL:CG2	1:G:115:ILE:HD11	2.44	0.48
1:G:51:LYS:HE2	3:G:302:LFA:H11	1.96	0.48
1:I:228:THR:O	1:I:232:GLY:HA3	2.13	0.48
1:J:88:PHE:CZ	1:J:93:GLY:HA2	2.49	0.48
1:C:74[A]:LEU:HD11	1:C:108:TYR:C	2.33	0.48
1:G:74[A]:LEU:HD23	1:G:75:LEU:HD23	1.96	0.48
1:H:33:THR:HG22	1:I:74:LEU:CD2	2.44	0.48
1:B:9:ASN:HB3	1:B:11:GLU:OE1	2.14	0.48
1:E:117:VAL:HB	1:E:118:PRO:HD3	1.96	0.47
1:A:101:GLY:O	1:A:102:ASP:CB	2.62	0.47
1:E:74:LEU:HD13	1:E:112:ASN:CA	2.43	0.47
1:H:34:LEU:CD1	1:I:115:ILE:HD11	2.44	0.47
1:E:81:ASN:HB2	3:E:311:LFA:C1	2.44	0.47
1:F:74[B]:LEU:CD2	1:F:109:ARG:HA	2.44	0.47
1:F:10:PHE:CE2	1:F:14:ILE:CD1	2.97	0.47
1:E:216:THR:O	1:E:219:PRO:HG2	2.14	0.47
1:G:44:LEU:HD22	1:G:48:LEU:HD11	1.96	0.47
1:I:109:ARG:NH1	1:I:251:ASP:OD2	2.46	0.47
1:E:224:MET:CE	1:E:234:LEU:HD22	2.42	0.47
1:E:81:ASN:CB	3:E:311:LFA:H11	2.45	0.47
1:G:70:SER:OG	1:G:112[A]:ASN:OD1	2.32	0.47
1:C:255:LYR:H192	1:C:255:LYR:C9	2.44	0.47
1:E:251:ASP:O	1:E:255:LYR:HB3	2.15	0.47
1:A:271:LYS:HA	1:A:272:ASN:HA	1.60	0.47
1:G:234:LEU:O	1:G:239:GLY:HA3	2.14	0.47
1:A:74:LEU:HD22	5:A:429:HOH:O	2.14	0.47
1:E:81:ASN:CA	3:E:311:LFA:H11	2.44	0.46
1:C:264:ASN:O	1:C:268:THR:HG23	2.15	0.46
1:D:113:TRP:CD1	1:D:255:LYR:HC2	2.49	0.46
1:H:74:LEU:HD21	1:H:109:ARG:HG3	1.96	0.46
1:J:78:GLN:OE1	1:J:78:GLN:HA	2.15	0.46
1:E:160:GLU:O	1:E:226:TYR:OH	2.25	0.46
1:E:255:LYR:H192	1:E:255:LYR:H9	1.98	0.46
1:G:44:LEU:CD1	1:H:65:ALA:HB1	2.45	0.46
1:J:74[A]:LEU:CD1	1:J:109:ARG:HA	2.46	0.46
1:J:61:ASN:ND2	5:J:431:HOH:O	2.47	0.46
1:D:91:GLU:HG2	1:H:96:PHE:CG	2.51	0.46
1:I:224:MET:HE3	1:I:234:LEU:HD13	1.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:45:TYR:CE1	3:I:309:LFA:H72	2.50	0.46
1:C:74[B]:LEU:CD2	1:C:112[B]:ASN:ND2	2.69	0.46
1:D:255:LYR:C9	1:D:255:LYR:H192	2.45	0.46
1:E:118:PRO:O	1:E:122:PHE:HB2	2.16	0.46
1:F:99:PRO:HG3	1:J:90:GLU:CG	2.46	0.46
1:H:113:TRP:CD1	1:H:255:LYR:HC2	2.51	0.46
3:G:308:LFA:H151	3:H:302:LFA:H92	1.98	0.46
1:I:44:LEU:HD11	1:J:43:LEU:HD11	1.97	0.46
1:B:169:VAL:HG11	3:B:306:LFA:C3	2.46	0.46
1:G:114:LEU:O	1:G:118:PRO:HG2	2.15	0.46
1:I:224:MET:CE	1:I:234:LEU:HD22	2.46	0.45
1:J:111:LEU:O	1:J:114:LEU:HB2	2.16	0.45
1:A:255:LYR:C9	1:A:255:LYR:H192	2.46	0.45
1:C:146:GLY:O	1:C:150:ILE:HG12	2.17	0.45
1:C:61:ASN:ND2	5:C:425:HOH:O	2.49	0.45
1:E:89:ASN:ND2	1:G:89:ASN:HD21	2.11	0.45
5:H:433:HOH:O	1:I:108:TYR:HE2	1.93	0.45
1:E:163:ASN:HD21	3:E:310:LFA:H92	1.81	0.45
1:E:186:LYS:CD	1:E:190:ASN:HD21	2.29	0.45
1:G:74[A]:LEU:CD1	1:G:108:TYR:C	2.79	0.45
1:H:114:LEU:O	1:H:118:PRO:HG2	2.17	0.45
1:H:255:LYR:H192	1:H:255:LYR:C9	2.46	0.45
1:B:81:ASN:ND2	5:B:415:HOH:O	2.40	0.45
1:H:271:LYS:CA	1:H:272:ASN:HB2	2.47	0.45
1:I:118:PRO:O	1:I:122:PHE:HB2	2.17	0.45
1:F:38:VAL:HG23	1:G:115:ILE:HD11	1.99	0.45
1:G:74[A]:LEU:HD11	1:G:108:TYR:O	2.09	0.45
1:B:109:ARG:NH2	1:B:251:ASP:OD2	2.50	0.45
1:D:185:MET:O	1:D:189:ILE:HG12	2.17	0.45
1:D:33:THR:HG22	1:E:74:LEU:HD21	1.99	0.45
1:F:9:ASN:HB3	1:F:11:GLU:OE1	2.16	0.45
1:F:251:ASP:O	1:F:255:LYR:HB3	2.16	0.45
1:B:255:LYR:H81	1:B:255:LYR:H10	1.79	0.45
1:D:45:TYR:CE1	3:D:307:LFA:H72	2.51	0.45
1:H:118:PRO:O	1:H:122:PHE:HB2	2.17	0.45
1:A:74:LEU:HD11	1:A:108:TYR:C	2.38	0.44
1:G:218:TYR:N	1:G:219:PRO:HD2	2.33	0.44
1:B:56:LYS:HE3	1:B:57:PHE:CZ	2.52	0.44
1:C:124:ILE:O	1:C:128:VAL:HG22	2.17	0.44
1:F:88:PHE:CZ	1:F:93:GLY:HA2	2.52	0.44
1:G:34:LEU:O	1:G:38:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:159:TYR:CE1	4:J:312:MPG:H212	2.52	0.44
1:A:154:TYR:O	1:A:157:GLN:HG3	2.18	0.44
1:F:163:ASN:HD21	3:F:306:LFA:H92	1.82	0.44
1:G:41:ALA:HB1	1:H:66:VAL:HG13	1.99	0.44
1:J:113:TRP:CD1	1:J:255:LYR:HC2	2.52	0.44
1:H:3:GLN:HG2	1:H:4:GLU:N	2.31	0.44
3:A:307:LFA:H51	1:B:122:PHE:HE2	1.81	0.44
1:D:255:LYR:H81	1:D:255:LYR:H10	1.79	0.44
1:E:224:MET:HE3	1:E:234:LEU:HD13	2.00	0.44
1:H:255:LYR:H10	1:H:255:LYR:H81	1.72	0.44
1:J:255:LYR:H81	1:J:255:LYR:H10	1.81	0.44
1:C:224:MET:N	1:C:225:PRO:HD2	2.32	0.44
1:D:118:PRO:O	1:D:122:PHE:HB2	2.16	0.44
1:E:202:LYS:HE2	1:E:202:LYS:HB3	1.75	0.44
1:I:224:MET:HE2	1:I:242:ALA:CB	2.48	0.44
1:B:224:MET:N	1:B:225:PRO:HD2	2.33	0.44
1:I:117:VAL:HB	1:I:118:PRO:HD3	2.00	0.44
1:I:234:LEU:O	1:I:239:GLY:HA3	2.18	0.44
1:E:224:MET:HE2	1:E:242:ALA:CB	2.48	0.43
1:B:205:SER:O	1:B:209:ILE:HG12	2.18	0.43
1:G:159:TYR:CE1	4:G:312:MPG:H212	2.53	0.43
1:I:218:TYR:N	1:I:219:PRO:HD2	2.33	0.43
1:C:96:PHE:CG	1:I:91:GLU:HG2	2.53	0.43
1:D:74:LEU:HD11	1:D:108:TYR:O	2.18	0.43
1:F:255:LYR:H81	1:F:255:LYR:H10	1.80	0.43
1:J:223:LEU:HD21	3:J:311:LFA:H32	2.00	0.43
1:A:248:THR:O	1:A:252:VAL:HG23	2.19	0.43
1:F:255:LYR:H192	1:F:255:LYR:H9	2.00	0.43
1:H:224:MET:HB3	1:H:225:PRO:HD3	2.01	0.43
1:J:110:TYR:HA	1:J:113:TRP:CE3	2.53	0.43
1:D:218:TYR:N	1:D:219:PRO:HD2	2.34	0.43
1:A:43:LEU:HD11	1:E:44:LEU:HD11	2.01	0.43
1:B:248:THR:O	1:B:252:VAL:HG23	2.19	0.43
1:C:253:SER:HA	1:C:257:ILE:HD12	2.00	0.43
1:H:74:LEU:CD2	1:H:109:ARG:HA	2.48	0.43
1:E:89:ASN:HD21	1:G:89:ASN:ND2	2.13	0.43
1:G:216:THR:O	1:G:219:PRO:HG2	2.18	0.43
1:G:84:SER:O	1:G:101:GLY:HA3	2.19	0.43
1:H:78:GLN:HA	1:H:78:GLN:OE1	2.18	0.43
1:A:255:LYR:H10	1:A:255:LYR:H81	1.84	0.43
1:A:270:SER:O	5:A:432:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:TYR:O	1:A:80:GLN:HG2	2.19	0.43
1:F:180:HIS:O	1:F:184:VAL:HG23	2.19	0.43
1:J:117:VAL:HB	1:J:118:PRO:HD3	2.00	0.43
1:F:115:ILE:HD11	1:J:38:VAL:HG23	2.01	0.42
1:G:113:TRP:CD1	1:G:255:LYR:HC2	2.54	0.42
1:A:224:MET:N	1:A:225:PRO:HD2	2.34	0.42
1:E:74:LEU:HD12	1:E:112:ASN:CB	2.48	0.42
1:E:44:LEU:HD23	1:E:44:LEU:HA	1.88	0.42
1:B:139:ARG:HD2	1:B:143:TRP:CH2	2.53	0.42
1:D:33:THR:HG22	1:E:74:LEU:CD2	2.49	0.42
1:I:255:LYR:H9	1:I:255:LYR:H192	2.00	0.42
1:J:255:LYR:C9	1:J:255:LYR:H192	2.48	0.42
1:E:109:ARG:O	1:E:112:ASN:HB3	2.19	0.42
1:H:234:LEU:O	1:H:239:GLY:HA3	2.18	0.42
1:J:118:PRO:O	1:J:122:PHE:HB2	2.19	0.42
1:B:113:TRP:CD1	1:B:255:LYR:HC2	2.54	0.42
1:E:224:MET:CE	1:E:234:LEU:CD1	2.94	0.42
1:I:40:LEU:HD23	1:J:73:LEU:HD11	2.02	0.42
1:J:170:TRP:HE1	4:J:312:MPG:HX31	1.85	0.42
1:J:272:ASN:OD1	1:J:273:LYS:HG3	2.20	0.42
1:F:211:PHE:CE1	1:F:215:TRP:CE2	3.08	0.42
1:H:111:LEU:HA	1:H:111:LEU:HD12	1.85	0.42
1:B:120:LEU:HD11	1:B:255:LYR:HG3	2.02	0.42
1:C:174:SER:HB3	1:C:255:LYR:H142	2.01	0.42
1:E:255:LYR:H10	1:E:255:LYR:H81	1.74	0.42
1:G:142:PHE:CZ	1:G:184:VAL:HG12	2.55	0.42
1:E:91:GLU:HG2	1:G:96:PHE:CD2	2.55	0.42
1:J:74[A]:LEU:CD1	1:J:112[A]:ASN:HB2	2.45	0.42
1:E:174:SER:HB3	1:E:255:LYR:H142	2.02	0.41
1:E:74:LEU:HD12	1:E:112:ASN:CG	2.39	0.41
1:G:70:SER:O	1:G:74[B]:LEU:HD13	2.21	0.41
1:H:74:LEU:HD22	1:H:112[B]:ASN:HD22	1.84	0.41
1:H:251:ASP:O	1:H:255:LYR:HB3	2.20	0.41
1:J:74[A]:LEU:HD11	1:J:109:ARG:N	2.34	0.41
1:A:186:LYS:HD3	1:A:208:TRP:CZ2	2.55	0.41
1:F:71:ALA:O	1:F:75:LEU:HG	2.19	0.41
1:I:223:LEU:HD21	3:I:312:LFA:H61	2.01	0.41
3:I:308:LFA:C16	3:J:307:LFA:C1	2.98	0.41
1:J:60:SER:CB	5:J:425:HOH:O	2.67	0.41
1:B:255:LYR:H192	1:B:255:LYR:H9	2.03	0.41
1:B:256:VAL:O	1:B:260:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:268:THR:CG2	1:G:275:LEU:HD11	2.50	0.41
1:I:139:ARG:HD2	1:I:143:TRP:CH2	2.56	0.41
1:B:101:GLY:O	1:B:102:ASP:CB	2.64	0.41
1:C:229:GLY:O	1:C:231:ASP:N	2.53	0.41
1:E:167:PHE:CE1	1:E:222:TYR:CE2	3.09	0.41
1:F:114:LEU:HA	1:F:114:LEU:HD12	1.95	0.41
1:G:74[A]:LEU:HD13	1:G:112[A]:ASN:HB3	2.01	0.41
1:I:146:GLY:O	1:I:150:ILE:HG12	2.20	0.41
1:I:44:LEU:HD23	1:I:44:LEU:HA	1.89	0.41
1:C:118:PRO:O	1:C:122:PHE:HB2	2.20	0.41
1:J:60:SER:HB3	5:J:425:HOH:O	2.20	0.41
1:A:74:LEU:HD13	1:A:112:ASN:HB2	2.02	0.41
1:C:251:ASP:O	1:C:255:LYR:HB3	2.20	0.41
1:H:31:ILE:HD12	1:H:31:ILE:HA	1.94	0.41
1:H:3:GLN:HB3	1:H:3:GLN:HE21	1.69	0.41
1:H:25:TYR:OH	1:I:102:ASP:OD2	2.37	0.41
1:J:98:ASP:HA	1:J:99:PRO:HD2	1.89	0.41
1:B:41:ALA:HB1	1:C:66:VAL:HG13	2.01	0.41
1:F:118:PRO:O	1:F:122:PHE:HB2	2.20	0.41
1:C:78:GLN:HA	1:C:78:GLN:OE1	2.19	0.41
1:F:10:PHE:CE2	1:F:14:ILE:HD11	2.54	0.41
1:A:216:THR:O	1:A:219:PRO:HG2	2.20	0.41
1:C:255:LYR:H81	1:C:255:LYR:H10	1.71	0.41
1:D:9:ASN:HB3	1:D:11:GLU:OE1	2.21	0.41
1:F:175:SER:O	1:F:178:PHE:HB3	2.20	0.41
1:H:76:TYR:O	1:H:80:GLN:HG2	2.21	0.41
1:B:130:LEU:CD1	1:B:135:PHE:HA	2.51	0.41
1:E:40:LEU:HD12	1:E:40:LEU:HA	1.94	0.41
1:C:74[B]:LEU:HD21	1:C:112[B]:ASN:CA	2.49	0.41
1:I:45:TYR:CD1	3:I:309:LFA:H91	2.55	0.41
1:I:100:SER:O	5:I:440:HOH:O	2.22	0.40
1:I:255:LYR:H10	1:I:255:LYR:H81	1.77	0.40
1:J:228:THR:O	1:J:232:GLY:HA3	2.21	0.40
1:D:227:LEU:HD23	1:D:227:LEU:HA	1.85	0.40
1:B:264:ASN:O	1:B:268:THR:HG23	2.21	0.40
1:F:223:LEU:C	1:F:225:PRO:HD2	2.42	0.40
1:F:40:LEU:HD23	1:G:73:LEU:HD11	2.04	0.40
1:H:160:GLU:O	1:H:226:TYR:OH	2.28	0.40
1:E:189:ILE:CD1	1:E:208:TRP:HB2	2.49	0.40
1:H:33:THR:HA	1:H:36:TYR:CE2	2.57	0.40
1:A:211:PHE:CE1	1:A:215:TRP:CE2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ALA:HB1	3:E:311:LFA:H32	2.01	0.40

There are no symmetry-related clashes.

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	Percentiles	
1	A	268/288 (93%)	261 (97%)	7 (3%)	0	100	100
1	B	264/288 (92%)	252 (96%)	11 (4%)	1 (0%)	38	41
1	C	266/288 (92%)	261 (98%)	5 (2%)	0	100	100
1	D	264/288 (92%)	258 (98%)	6 (2%)	0	100	100
1	E	265/288 (92%)	259 (98%)	6 (2%)	0	100	100
1	F	265/288 (92%)	259 (98%)	6 (2%)	0	100	100
1	G	267/288 (93%)	260 (97%)	7 (3%)	0	100	100
1	H	267/288 (93%)	262 (98%)	5 (2%)	0	100	100
1	I	264/288 (92%)	259 (98%)	5 (2%)	0	100	100
1	J	267/288 (93%)	262 (98%)	5 (2%)	0	100	100
All	All	2657/2880 (92%)	2593 (98%)	63 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	197	SER

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	A	226/247 (92%)	223 (99%)	3 (1%)	73	85
1	B	224/247 (91%)	221 (99%)	3 (1%)	73	85
1	C	225/247 (91%)	225 (100%)	0	100	100
1	D	224/247 (91%)	222 (99%)	2 (1%)	82	91
1	E	224/247 (91%)	223 (100%)	1 (0%)	93	97
1	F	225/247 (91%)	224 (100%)	1 (0%)	93	97
1	G	228/247 (92%)	224 (98%)	4 (2%)	64	77
1	H	228/247 (92%)	224 (98%)	4 (2%)	64	77
1	I	221/247 (90%)	219 (99%)	2 (1%)	82	91
1	J	226/247 (92%)	224 (99%)	2 (1%)	82	91
All	All	2251/2470 (91%)	2229 (99%)	22 (1%)	80	89

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	112	ASN
1	A	142	PHE
1	B	103	LEU
1	B	164	LEU
1	B	194	GLU
1	D	91	GLU
1	D	92	VAL
1	E	44	LEU
1	F	132	THR
1	G	44	LEU
1	G	84	SER
1	G	114	LEU
1	G	141	GLN
1	H	3	GLN
1	H	10	PHE
1	H	55	LYS
1	H	111	LEU
1	I	10	PHE
1	I	44	LEU

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Mol	Chain	Res	Type
1	J	10	PHE
1	J	44	LEU

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

Mol	Chain	Res	Type
1	A	112	ASN
1	B	112	ASN
1	C	61	ASN
1	C	89	ASN
1	C	141	GLN
1	C	180	HIS
1	E	112	ASN
1	E	163	ASN
1	E	180	HIS
1	E	190	ASN
1	F	81	ASN
1	F	112	ASN
1	G	89	ASN
1	H	3	GLN
1	H	89	ASN
1	I	112	ASN
1	J	180	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LYR	A	255	1	29,29,30	1.55	4 (13%)	32,37,39	1.83	6 (18%)
1	LYR	B	255	1	29,29,30	1.47	3 (10%)	32,37,39	2.00	8 (25%)
1	LYR	C	255	1	29,29,30	1.54	4 (13%)	32,37,39	2.03	6 (18%)
1	LYR	D	255	1	29,29,30	1.52	3 (10%)	32,37,39	1.87	7 (21%)
1	LYR	E	255	1	29,29,30	1.54	4 (13%)	32,37,39	1.92	6 (18%)
1	LYR	F	255	1	29,29,30	1.56	5 (17%)	32,37,39	1.96	6 (18%)
1	LYR	G	255	1	29,29,30	1.54	5 (17%)	32,37,39	1.99	9 (28%)
1	LYR	H	255	1	29,29,30	1.52	4 (13%)	32,37,39	1.93	6 (18%)
1	LYR	I	255	1	29,29,30	1.45	4 (13%)	32,37,39	2.08	6 (18%)
1	LYR	J	255	1	29,29,30	1.48	5 (17%)	32,37,39	2.00	8 (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
1	LYR	A	255	1	-	0/21/40/42	0/1/1/1
1	LYR	B	255	1	-	0/21/40/42	0/1/1/1
1	LYR	C	255	1	-	0/21/40/42	0/1/1/1
1	LYR	D	255	1	-	0/21/40/42	0/1/1/1
1	LYR	E	255	1	-	0/21/40/42	0/1/1/1
1	LYR	F	255	1	-	0/21/40/42	0/1/1/1
1	LYR	G	255	1	-	0/21/40/42	0/1/1/1
1	LYR	H	255	1	-	0/21/40/42	0/1/1/1
1	LYR	I	255	1	-	0/21/40/42	0/1/1/1
1	LYR	J	255	1	-	0/21/40/42	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	255	LYR	C1-NZ	-5.21	1.31	1.47
1	C	255	LYR	C1-NZ	-4.99	1.32	1.47
1	F	255	LYR	C1-NZ	-4.93	1.32	1.47
1	E	255	LYR	C1-NZ	-4.91	1.32	1.47
1	G	255	LYR	C1-NZ	-4.90	1.32	1.47
1	D	255	LYR	C1-NZ	-4.80	1.32	1.47
1	B	255	LYR	C1-NZ	-4.78	1.32	1.47
1	J	255	LYR	C1-NZ	-4.75	1.33	1.47
1	H	255	LYR	C1-NZ	-4.72	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	LYR	C1-NZ	-4.68	1.33	1.47
1	G	255	LYR	C5-C3	-2.17	1.41	1.45
1	F	255	LYR	C5-C3	-2.11	1.41	1.45
1	I	255	LYR	C5-C3	-2.06	1.41	1.45
1	J	255	LYR	C5-C3	-2.05	1.41	1.45
1	J	255	LYR	CA-C	2.02	1.52	1.50
1	A	255	LYR	C6-C5	2.02	1.39	1.34
1	H	255	LYR	CA-C	2.16	1.53	1.50
1	I	255	LYR	C2-C3	2.16	1.40	1.33
1	G	255	LYR	C2-C3	2.22	1.40	1.33
1	J	255	LYR	C2-C3	2.25	1.40	1.33
1	F	255	LYR	CA-C	2.30	1.53	1.50
1	E	255	LYR	C2-C3	2.35	1.40	1.33
1	H	255	LYR	C2-C3	2.40	1.40	1.33
1	D	255	LYR	C2-C3	2.40	1.40	1.33
1	F	255	LYR	C2-C3	2.40	1.40	1.33
1	A	255	LYR	C2-C3	2.42	1.40	1.33
1	B	255	LYR	C2-C3	2.42	1.40	1.33
1	E	255	LYR	CA-C	2.49	1.53	1.50
1	C	255	LYR	C2-C3	2.50	1.41	1.33
1	I	255	LYR	C7-C80	2.56	1.39	1.35
1	C	255	LYR	C7-C80	2.63	1.39	1.35
1	G	255	LYR	CA-C	2.64	1.53	1.50
1	J	255	LYR	C7-C80	2.67	1.39	1.35
1	C	255	LYR	CA-C	2.69	1.53	1.50
1	H	255	LYR	C7-C80	2.72	1.39	1.35
1	G	255	LYR	C7-C80	2.72	1.39	1.35
1	E	255	LYR	C7-C80	2.78	1.39	1.35
1	B	255	LYR	C7-C80	2.84	1.39	1.35
1	D	255	LYR	C7-C80	2.96	1.39	1.35
1	F	255	LYR	C7-C80	2.99	1.39	1.35
1	A	255	LYR	C7-C80	3.15	1.40	1.35

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	255	LYR	C13-C12-C11	-5.15	118.74	124.51
1	B	255	LYR	C13-C12-C11	-5.02	118.89	124.51
1	J	255	LYR	C13-C12-C11	-4.92	119.00	124.51
1	C	255	LYR	C13-C12-C11	-4.82	119.11	124.51
1	I	255	LYR	C13-C12-C11	-4.78	119.15	124.51
1	E	255	LYR	C13-C12-C11	-4.73	119.22	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	LYR	C10-C9-C80	-4.71	119.13	126.21
1	A	255	LYR	C13-C12-C11	-4.68	119.26	124.51
1	H	255	LYR	C10-C9-C80	-4.64	119.24	126.21
1	F	255	LYR	C13-C12-C11	-4.61	119.35	124.51
1	B	255	LYR	C7-C6-C5	-4.33	109.94	123.23
1	E	255	LYR	C10-C9-C80	-4.28	119.79	126.21
1	I	255	LYR	C10-C9-C80	-4.20	119.91	126.21
1	F	255	LYR	C10-C9-C80	-4.16	119.97	126.21
1	F	255	LYR	C7-C6-C5	-4.15	110.51	123.23
1	H	255	LYR	C7-C6-C5	-4.12	110.59	123.23
1	H	255	LYR	C13-C12-C11	-4.12	119.89	124.51
1	E	255	LYR	C7-C6-C5	-4.08	110.71	123.23
1	I	255	LYR	C7-C6-C5	-4.03	110.87	123.23
1	B	255	LYR	C10-C9-C80	-4.01	120.19	126.21
1	C	255	LYR	C7-C6-C5	-3.99	110.98	123.23
1	G	255	LYR	C7-C6-C5	-3.99	111.00	123.23
1	J	255	LYR	C7-C6-C5	-3.85	111.43	123.23
1	A	255	LYR	C7-C6-C5	-3.77	111.66	123.23
1	D	255	LYR	C10-C9-C80	-3.65	120.73	126.21
1	D	255	LYR	C13-C12-C11	-3.64	120.44	124.51
1	J	255	LYR	C10-C9-C80	-3.62	120.78	126.21
1	D	255	LYR	C7-C6-C5	-3.61	112.16	123.23
1	G	255	LYR	C10-C9-C80	-3.42	121.08	126.21
1	H	255	LYR	C15-C14-C12	-3.36	108.01	113.78
1	C	255	LYR	C15-C14-C12	-3.34	108.04	113.78
1	F	255	LYR	C15-C14-C12	-3.24	108.21	113.78
1	J	255	LYR	C15-C14-C12	-3.15	108.36	113.78
1	I	255	LYR	C15-C14-C12	-3.09	108.47	113.78
1	I	255	LYR	C8-C80-C7	-3.00	118.72	122.92
1	D	255	LYR	C15-C14-C12	-2.98	108.65	113.78
1	J	255	LYR	C8-C80-C7	-2.88	118.89	122.92
1	D	255	LYR	C8-C80-C7	-2.87	118.91	122.92
1	A	255	LYR	C10-C9-C80	-2.86	121.91	126.21
1	A	255	LYR	C15-C14-C12	-2.84	108.90	113.78
1	B	255	LYR	C15-C14-C12	-2.83	108.92	113.78
1	G	255	LYR	C15-C14-C12	-2.79	108.98	113.78
1	E	255	LYR	C15-C14-C12	-2.73	109.08	113.78
1	C	255	LYR	C8-C80-C7	-2.61	119.27	122.92
1	F	255	LYR	C8-C80-C7	-2.59	119.29	122.92
1	G	255	LYR	C8-C80-C7	-2.49	119.44	122.92
1	B	255	LYR	C19-C17-C11	-2.44	106.35	110.31
1	B	255	LYR	CB-CA-C	-2.42	107.67	111.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	LYR	C8-C80-C7	-2.34	119.64	122.92
1	A	255	LYR	C8-C80-C7	-2.31	119.68	122.92
1	H	255	LYR	C8-C80-C7	-2.24	119.78	122.92
1	D	255	LYR	C6-C7-C80	-2.16	124.23	127.31
1	J	255	LYR	C6-C7-C80	-2.14	124.26	127.31
1	E	255	LYR	C8-C80-C7	-2.07	120.02	122.92
1	J	255	LYR	C18-C17-C11	-2.06	106.97	110.31
1	G	255	LYR	C10-C11-C12	-2.00	116.77	121.54
1	G	255	LYR	C17-C11-C10	2.22	121.96	115.73
1	G	255	LYR	C8-C80-C9	2.26	121.70	118.10
1	B	255	LYR	C1-NZ-CE	3.44	118.90	113.46
1	E	255	LYR	C1-NZ-CE	3.88	119.61	113.46
1	C	255	LYR	C1-NZ-CE	3.95	119.72	113.46
1	F	255	LYR	C1-NZ-CE	4.24	120.17	113.46
1	G	255	LYR	C1-NZ-CE	4.34	120.34	113.46
1	A	255	LYR	C1-NZ-CE	4.35	120.34	113.46
1	I	255	LYR	C1-NZ-CE	4.37	120.37	113.46
1	J	255	LYR	C1-NZ-CE	4.51	120.60	113.46
1	D	255	LYR	C1-NZ-CE	4.53	120.63	113.46
1	H	255	LYR	C1-NZ-CE	4.55	120.66	113.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	255	LYR	5	0
1	B	255	LYR	8	0
1	C	255	LYR	7	0
1	D	255	LYR	6	0
1	E	255	LYR	7	0
1	F	255	LYR	6	0
1	G	255	LYR	3	0
1	H	255	LYR	8	0
1	I	255	LYR	4	0
1	J	255	LYR	6	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 138 ligands modelled in this entry, 10 are monoatomic - leaving 128 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	LFA	A	302	-	13,13,19	0.25	0	12,12,18	0.50	0
3	LFA	A	303	-	5,5,19	0.27	0	4,4,18	0.37	0
3	LFA	A	304	-	9,9,19	0.27	0	8,8,18	0.47	0
3	LFA	A	305	-	9,9,19	0.28	0	8,8,18	0.44	0
3	LFA	A	306	-	13,13,19	0.28	0	12,12,18	0.51	0
3	LFA	A	307	-	17,17,19	0.23	0	16,16,18	0.55	0
3	LFA	A	308	-	7,7,19	0.29	0	6,6,18	0.42	0
3	LFA	A	309	-	7,7,19	0.26	0	6,6,18	0.47	0
3	LFA	A	310	-	7,7,19	0.26	0	6,6,18	0.44	0
3	LFA	A	311	-	6,6,19	0.24	0	5,5,18	0.44	0
3	LFA	A	312	-	4,4,19	0.33	0	3,3,18	0.34	0
4	MPG	A	313	-	13,13,24	0.44	0	13,13,25	1.03	1 (7%)
3	LFA	B	302	-	6,6,19	0.26	0	5,5,18	0.40	0
3	LFA	B	303	-	6,6,19	0.25	0	5,5,18	0.45	0
3	LFA	B	304	-	13,13,19	0.29	0	12,12,18	0.49	0
3	LFA	B	305	-	5,5,19	0.30	0	4,4,18	0.29	0
3	LFA	B	306	-	7,7,19	0.31	0	6,6,18	0.41	0
3	LFA	B	307	-	15,15,19	0.26	0	14,14,18	0.56	0
3	LFA	B	308	-	17,17,19	0.28	0	16,16,18	0.50	0
3	LFA	B	309	-	12,12,19	0.31	0	11,11,18	0.44	0
3	LFA	B	310	-	10,10,19	0.27	0	9,9,18	0.48	0
3	LFA	B	311	-	7,7,19	0.27	0	6,6,18	0.43	0
4	MPG	B	312	-	13,13,24	0.44	0	13,13,25	1.00	1 (7%)
3	LFA	C	302	-	6,6,19	0.27	0	5,5,18	0.40	0
3	LFA	C	303	-	9,9,19	0.28	0	8,8,18	0.41	0
3	LFA	C	304	-	5,5,19	0.27	0	4,4,18	0.33	0
3	LFA	C	305	-	9,9,19	0.26	0	8,8,18	0.48	0
3	LFA	C	306	-	15,15,19	0.27	0	14,14,18	0.53	0
3	LFA	C	307	-	17,17,19	0.27	0	16,16,18	0.47	0
3	LFA	C	308	-	9,9,19	0.28	0	8,8,18	0.45	0
3	LFA	C	309	-	7,7,19	0.27	0	6,6,18	0.44	0
3	LFA	C	310	-	12,12,19	0.29	0	11,11,18	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LFA	C	311	-	7,7,19	0.27	0	6,6,18	0.44	0
3	LFA	C	312	-	3,3,19	0.45	0	2,2,18	0.64	0
4	MPG	C	313	-	12,12,24	0.42	0	12,12,25	1.00	1 (8%)
3	LFA	D	302	-	6,6,19	0.24	0	5,5,18	0.46	0
3	LFA	D	303	-	13,13,19	0.27	0	12,12,18	0.52	0
3	LFA	D	304	-	5,5,19	0.25	0	4,4,18	0.40	0
3	LFA	D	305	-	9,9,19	0.26	0	8,8,18	0.50	0
3	LFA	D	306	-	15,15,19	0.28	0	14,14,18	0.50	0
3	LFA	D	307	-	17,17,19	0.26	0	16,16,18	0.48	0
3	LFA	D	308	-	9,9,19	0.28	0	8,8,18	0.46	0
3	LFA	D	309	-	7,7,19	0.25	0	6,6,18	0.45	0
3	LFA	D	310	-	7,7,19	0.27	0	6,6,18	0.45	0
3	LFA	D	311	-	6,6,19	0.25	0	5,5,18	0.43	0
3	LFA	D	312	-	5,5,19	0.26	0	4,4,18	0.36	0
3	LFA	D	313	-	5,5,19	0.26	0	4,4,18	0.34	0
3	LFA	D	314	-	6,6,19	0.26	0	5,5,18	0.40	0
4	MPG	D	315	-	13,13,24	0.42	0	13,13,25	1.05	2 (15%)
3	LFA	D	316	-	4,4,19	0.25	0	3,3,18	0.36	0
3	LFA	D	317	-	4,4,19	0.26	0	3,3,18	0.37	0
3	LFA	D	318	-	4,4,19	0.28	0	3,3,18	0.36	0
3	LFA	E	302	-	13,13,19	0.28	0	12,12,18	0.56	0
3	LFA	E	303	-	17,17,19	0.26	0	16,16,18	0.50	0
3	LFA	E	304	-	7,7,19	0.30	0	6,6,18	0.43	0
3	LFA	E	305	-	5,5,19	0.29	0	4,4,18	0.34	0
3	LFA	E	306	-	11,11,19	0.27	0	10,10,18	0.48	0
3	LFA	E	307	-	7,7,19	0.25	0	6,6,18	0.47	0
3	LFA	E	308	-	13,13,19	0.27	0	12,12,18	0.50	0
3	LFA	E	309	-	5,5,19	0.28	0	4,4,18	0.33	0
3	LFA	E	310	-	9,9,19	0.28	0	8,8,18	0.44	0
3	LFA	E	311	-	7,7,19	0.26	0	6,6,18	0.45	0
3	LFA	E	312	-	7,7,19	0.26	0	6,6,18	0.43	0
4	MPG	E	313	-	13,13,24	0.41	0	13,13,25	1.02	2 (15%)
3	LFA	F	302	-	6,6,19	0.23	0	5,5,18	0.46	0
3	LFA	F	303	-	13,13,19	0.27	0	12,12,18	0.50	0
3	LFA	F	304	-	9,9,19	0.28	0	8,8,18	0.46	0
3	LFA	F	305	-	5,5,19	0.26	0	4,4,18	0.34	0
3	LFA	F	306	-	9,9,19	0.26	0	8,8,18	0.49	0
3	LFA	F	307	-	5,5,19	0.29	0	4,4,18	0.31	0
3	LFA	F	308	-	7,7,19	0.29	0	6,6,18	0.40	0
3	LFA	F	309	-	9,9,19	0.31	0	8,8,18	0.40	0
3	LFA	F	310	-	17,17,19	0.27	0	16,16,18	0.48	0
3	LFA	F	311	-	9,9,19	0.29	0	8,8,18	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LFA	F	312	-	7,7,19	0.25	0	6,6,18	0.47	0
3	LFA	F	313	-	13,13,19	0.28	0	12,12,18	0.49	0
3	LFA	F	314	-	7,7,19	0.27	0	6,6,18	0.43	0
4	MPG	F	315	-	13,13,24	0.39	0	13,13,25	1.06	2 (15%)
3	LFA	G	302	-	15,15,19	0.25	0	14,14,18	0.57	0
3	LFA	G	303	-	6,6,19	0.26	0	5,5,18	0.41	0
3	LFA	G	304	-	13,13,19	0.30	0	12,12,18	0.47	0
3	LFA	G	305	-	5,5,19	0.27	0	4,4,18	0.34	0
3	LFA	G	306	-	9,9,19	0.28	0	8,8,18	0.43	0
3	LFA	G	307	-	15,15,19	0.26	0	14,14,18	0.58	0
3	LFA	G	308	-	17,17,19	0.27	0	16,16,18	0.48	0
3	LFA	G	309	-	7,7,19	0.26	0	6,6,18	0.45	0
3	LFA	G	310	-	9,9,19	0.30	0	8,8,18	0.43	0
3	LFA	G	311	-	7,7,19	0.25	0	6,6,18	0.47	0
4	MPG	G	312	-	13,13,24	0.42	0	13,13,25	1.06	1 (7%)
3	LFA	G	313	-	7,7,19	0.28	0	6,6,18	0.44	0
3	LFA	G	314	-	5,5,19	0.26	0	4,4,18	0.36	0
3	LFA	G	315	-	5,5,19	0.27	0	4,4,18	0.35	0
3	LFA	H	302	-	12,12,19	0.28	0	11,11,18	0.50	0
3	LFA	H	303	-	5,5,19	0.24	0	4,4,18	0.40	0
3	LFA	H	304	-	9,9,19	0.28	0	8,8,18	0.50	0
3	LFA	H	305	-	15,15,19	0.26	0	14,14,18	0.52	0
3	LFA	H	306	-	17,17,19	0.28	0	16,16,18	0.46	0
3	LFA	H	307	-	13,13,19	0.26	0	12,12,18	0.52	0
3	LFA	H	308	-	7,7,19	0.25	0	6,6,18	0.46	0
3	LFA	H	309	-	4,4,19	0.26	0	3,3,18	0.37	0
3	LFA	H	310	-	7,7,19	0.28	0	6,6,18	0.42	0
3	LFA	H	311	-	6,6,19	0.21	0	5,5,18	0.52	0
3	LFA	H	312	-	5,5,19	0.26	0	4,4,18	0.37	0
4	MPG	H	313	-	13,13,24	0.39	0	13,13,25	0.99	1 (7%)
3	LFA	I	302	-	6,6,19	0.26	0	5,5,18	0.41	0
3	LFA	I	303	-	6,6,19	0.26	0	5,5,18	0.41	0
3	LFA	I	304	-	13,13,19	0.28	0	12,12,18	0.50	0
3	LFA	I	305	-	5,5,19	0.28	0	4,4,18	0.31	0
3	LFA	I	306	-	9,9,19	0.25	0	8,8,18	0.51	0
3	LFA	I	307	-	5,5,19	0.27	0	4,4,18	0.32	0
3	LFA	I	308	-	15,15,19	0.23	0	14,14,18	0.59	0
3	LFA	I	309	-	17,17,19	0.29	0	16,16,18	0.45	0
3	LFA	I	310	-	13,13,19	0.26	0	12,12,18	0.54	0
3	LFA	I	311	-	7,7,19	0.26	0	6,6,18	0.46	0
3	LFA	I	312	-	6,6,19	0.23	0	5,5,18	0.45	0
3	LFA	I	313	-	3,3,19	0.47	0	2,2,18	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MPG	I	314	-	13,13,24	0.32	0	13,13,25	0.98	1 (7%)
3	LFA	J	302	-	15,15,19	0.26	0	14,14,18	0.54	0
3	LFA	J	303	-	17,17,19	0.27	0	16,16,18	0.49	0
3	LFA	J	304	-	7,7,19	0.27	0	6,6,18	0.43	0
3	LFA	J	305	-	13,13,19	0.30	0	12,12,18	0.46	0
3	LFA	J	306	-	7,7,19	0.26	0	6,6,18	0.47	0
3	LFA	J	307	-	6,6,19	0.26	0	5,5,18	0.41	0
3	LFA	J	308	-	13,13,19	0.31	0	12,12,18	0.42	0
3	LFA	J	309	-	9,9,19	0.24	0	8,8,18	0.50	0
3	LFA	J	310	-	9,9,19	0.26	0	8,8,18	0.47	0
3	LFA	J	311	-	3,3,19	0.46	0	2,2,18	0.65	0
4	MPG	J	312	-	13,13,24	0.42	0	13,13,25	1.07	1 (7%)

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	LFA	A	302	-	-	0/11/11/17	0/0/0/0
3	LFA	A	303	-	-	0/3/3/17	0/0/0/0
3	LFA	A	304	-	-	0/7/7/17	0/0/0/0
3	LFA	A	305	-	-	0/7/7/17	0/0/0/0
3	LFA	A	306	-	-	0/11/11/17	0/0/0/0
3	LFA	A	307	-	-	0/15/15/17	0/0/0/0
3	LFA	A	308	-	-	0/5/5/17	0/0/0/0
3	LFA	A	309	-	-	0/5/5/17	0/0/0/0
3	LFA	A	310	-	-	0/5/5/17	0/0/0/0
3	LFA	A	311	-	-	0/4/4/17	0/0/0/0
3	LFA	A	312	-	-	0/2/2/17	0/0/0/0
4	MPG	A	313	-	-	0/12/12/25	0/0/0/0
3	LFA	B	302	-	-	0/4/4/17	0/0/0/0
3	LFA	B	303	-	-	0/4/4/17	0/0/0/0
3	LFA	B	304	-	-	0/11/11/17	0/0/0/0
3	LFA	B	305	-	-	0/3/3/17	0/0/0/0
3	LFA	B	306	-	-	0/5/5/17	0/0/0/0
3	LFA	B	307	-	-	0/13/13/17	0/0/0/0
3	LFA	B	308	-	-	0/15/15/17	0/0/0/0
3	LFA	B	309	-	-	0/10/10/17	0/0/0/0
3	LFA	B	310	-	-	0/8/8/17	0/0/0/0
3	LFA	B	311	-	-	0/5/5/17	0/0/0/0
4	MPG	B	312	-	-	0/12/12/25	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	C	302	-	-	0/4/4/17	0/0/0/0
3	LFA	C	303	-	-	0/7/7/17	0/0/0/0
3	LFA	C	304	-	-	0/3/3/17	0/0/0/0
3	LFA	C	305	-	-	0/7/7/17	0/0/0/0
3	LFA	C	306	-	-	0/13/13/17	0/0/0/0
3	LFA	C	307	-	-	0/15/15/17	0/0/0/0
3	LFA	C	308	-	-	0/7/7/17	0/0/0/0
3	LFA	C	309	-	-	0/5/5/17	0/0/0/0
3	LFA	C	310	-	-	0/10/10/17	0/0/0/0
3	LFA	C	311	-	-	0/5/5/17	0/0/0/0
3	LFA	C	312	-	-	0/1/1/17	0/0/0/0
4	MPG	C	313	-	-	0/11/11/25	0/0/0/0
3	LFA	D	302	-	-	0/4/4/17	0/0/0/0
3	LFA	D	303	-	-	0/11/11/17	0/0/0/0
3	LFA	D	304	-	-	0/3/3/17	0/0/0/0
3	LFA	D	305	-	-	0/7/7/17	0/0/0/0
3	LFA	D	306	-	-	0/13/13/17	0/0/0/0
3	LFA	D	307	-	-	0/15/15/17	0/0/0/0
3	LFA	D	308	-	-	0/7/7/17	0/0/0/0
3	LFA	D	309	-	-	0/5/5/17	0/0/0/0
3	LFA	D	310	-	-	0/5/5/17	0/0/0/0
3	LFA	D	311	-	-	0/4/4/17	0/0/0/0
3	LFA	D	312	-	-	0/3/3/17	0/0/0/0
3	LFA	D	313	-	-	0/3/3/17	0/0/0/0
3	LFA	D	314	-	-	0/4/4/17	0/0/0/0
4	MPG	D	315	-	-	0/12/12/25	0/0/0/0
3	LFA	D	316	-	-	0/2/2/17	0/0/0/0
3	LFA	D	317	-	-	0/2/2/17	0/0/0/0
3	LFA	D	318	-	-	0/2/2/17	0/0/0/0
3	LFA	E	302	-	-	0/11/11/17	0/0/0/0
3	LFA	E	303	-	-	0/15/15/17	0/0/0/0
3	LFA	E	304	-	-	0/5/5/17	0/0/0/0
3	LFA	E	305	-	-	0/3/3/17	0/0/0/0
3	LFA	E	306	-	-	0/9/9/17	0/0/0/0
3	LFA	E	307	-	-	0/5/5/17	0/0/0/0
3	LFA	E	308	-	-	0/11/11/17	0/0/0/0
3	LFA	E	309	-	-	0/3/3/17	0/0/0/0
3	LFA	E	310	-	-	0/7/7/17	0/0/0/0
3	LFA	E	311	-	-	0/5/5/17	0/0/0/0
3	LFA	E	312	-	-	0/5/5/17	0/0/0/0
4	MPG	E	313	-	-	0/12/12/25	0/0/0/0
3	LFA	F	302	-	-	0/4/4/17	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	F	303	-	-	0/11/11/17	0/0/0/0
3	LFA	F	304	-	-	0/7/7/17	0/0/0/0
3	LFA	F	305	-	-	0/3/3/17	0/0/0/0
3	LFA	F	306	-	-	0/7/7/17	0/0/0/0
3	LFA	F	307	-	-	0/3/3/17	0/0/0/0
3	LFA	F	308	-	-	0/5/5/17	0/0/0/0
3	LFA	F	309	-	-	0/7/7/17	0/0/0/0
3	LFA	F	310	-	-	0/15/15/17	0/0/0/0
3	LFA	F	311	-	-	0/7/7/17	0/0/0/0
3	LFA	F	312	-	-	0/5/5/17	0/0/0/0
3	LFA	F	313	-	-	0/11/11/17	0/0/0/0
3	LFA	F	314	-	-	0/5/5/17	0/0/0/0
4	MPG	F	315	-	-	0/12/12/25	0/0/0/0
3	LFA	G	302	-	-	0/13/13/17	0/0/0/0
3	LFA	G	303	-	-	0/4/4/17	0/0/0/0
3	LFA	G	304	-	-	0/11/11/17	0/0/0/0
3	LFA	G	305	-	-	0/3/3/17	0/0/0/0
3	LFA	G	306	-	-	0/7/7/17	0/0/0/0
3	LFA	G	307	-	-	0/13/13/17	0/0/0/0
3	LFA	G	308	-	-	0/15/15/17	0/0/0/0
3	LFA	G	309	-	-	0/5/5/17	0/0/0/0
3	LFA	G	310	-	-	0/7/7/17	0/0/0/0
3	LFA	G	311	-	-	0/5/5/17	0/0/0/0
4	MPG	G	312	-	-	0/12/12/25	0/0/0/0
3	LFA	G	313	-	-	0/5/5/17	0/0/0/0
3	LFA	G	314	-	-	0/3/3/17	0/0/0/0
3	LFA	G	315	-	-	0/3/3/17	0/0/0/0
3	LFA	H	302	-	-	0/10/10/17	0/0/0/0
3	LFA	H	303	-	-	0/3/3/17	0/0/0/0
3	LFA	H	304	-	-	0/7/7/17	0/0/0/0
3	LFA	H	305	-	-	0/13/13/17	0/0/0/0
3	LFA	H	306	-	-	0/15/15/17	0/0/0/0
3	LFA	H	307	-	-	0/11/11/17	0/0/0/0
3	LFA	H	308	-	-	0/5/5/17	0/0/0/0
3	LFA	H	309	-	-	0/2/2/17	0/0/0/0
3	LFA	H	310	-	-	0/5/5/17	0/0/0/0
3	LFA	H	311	-	-	0/4/4/17	0/0/0/0
3	LFA	H	312	-	-	0/3/3/17	0/0/0/0
4	MPG	H	313	-	-	0/12/12/25	0/0/0/0
3	LFA	I	302	-	-	0/4/4/17	0/0/0/0
3	LFA	I	303	-	-	0/4/4/17	0/0/0/0
3	LFA	I	304	-	-	0/11/11/17	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	I	305	-	-	0/3/3/17	0/0/0/0
3	LFA	I	306	-	-	0/7/7/17	0/0/0/0
3	LFA	I	307	-	-	0/3/3/17	0/0/0/0
3	LFA	I	308	-	-	0/13/13/17	0/0/0/0
3	LFA	I	309	-	-	0/15/15/17	0/0/0/0
3	LFA	I	310	-	-	0/11/11/17	0/0/0/0
3	LFA	I	311	-	-	0/5/5/17	0/0/0/0
3	LFA	I	312	-	-	0/4/4/17	0/0/0/0
3	LFA	I	313	-	-	0/1/1/17	0/0/0/0
4	MPG	I	314	-	-	0/12/12/25	0/0/0/0
3	LFA	J	302	-	-	0/13/13/17	0/0/0/0
3	LFA	J	303	-	-	0/15/15/17	0/0/0/0
3	LFA	J	304	-	-	0/5/5/17	0/0/0/0
3	LFA	J	305	-	-	0/11/11/17	0/0/0/0
3	LFA	J	306	-	-	0/5/5/17	0/0/0/0
3	LFA	J	307	-	-	0/4/4/17	0/0/0/0
3	LFA	J	308	-	-	0/11/11/17	0/0/0/0
3	LFA	J	309	-	-	0/7/7/17	0/0/0/0
3	LFA	J	310	-	-	0/7/7/17	0/0/0/0
3	LFA	J	311	-	-	0/1/1/17	0/0/0/0
4	MPG	J	312	-	-	0/12/12/25	0/0/0/0

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	315	MPG	C1-O1-CX3	2.01	120.77	113.46
4	D	315	MPG	C1-O1-CX3	2.08	121.01	113.46
4	E	313	MPG	C1-O1-CX3	2.31	121.87	113.46
4	E	313	MPG	O1-CX3-CXD	2.57	118.34	109.55
4	C	313	MPG	O1-CX3-CXD	2.63	118.54	109.55
4	H	313	MPG	O1-CX3-CXD	2.75	118.94	109.55
4	I	314	MPG	O1-CX3-CXD	2.75	118.95	109.55
4	F	315	MPG	O1-CX3-CXD	2.83	119.23	109.55
4	B	312	MPG	O1-CX3-CXD	2.88	119.39	109.55
4	D	315	MPG	O1-CX3-CXD	2.93	119.56	109.55
4	J	312	MPG	O1-CX3-CXD	3.02	119.89	109.55
4	A	313	MPG	O1-CX3-CXD	3.03	119.91	109.55
4	G	312	MPG	O1-CX3-CXD	3.07	120.03	109.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

43 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	307	LFA	1	0
3	A	311	LFA	2	0
3	B	306	LFA	2	0
3	B	307	LFA	1	0
3	C	302	LFA	2	0
3	C	305	LFA	1	0
3	C	306	LFA	3	0
4	C	313	MPG	1	0
3	D	302	LFA	5	0
3	D	306	LFA	2	0
3	D	307	LFA	1	0
4	D	315	MPG	1	0
3	D	316	LFA	2	0
3	D	317	LFA	2	0
3	E	304	LFA	1	0
3	E	305	LFA	1	0
3	E	310	LFA	1	0
3	E	311	LFA	7	0
4	E	313	MPG	3	0
3	F	302	LFA	2	0
3	F	304	LFA	1	0
3	F	306	LFA	1	0
3	F	311	LFA	3	0
3	F	312	LFA	3	0
4	F	315	MPG	1	0
3	G	302	LFA	3	0
3	G	303	LFA	2	0
3	G	307	LFA	1	0
3	G	308	LFA	1	0
4	G	312	MPG	2	0
3	H	302	LFA	1	0
3	H	305	LFA	1	0
3	I	302	LFA	1	0
3	I	303	LFA	1	0
3	I	306	LFA	1	0
3	I	308	LFA	1	0
3	I	309	LFA	2	0
3	I	312	LFA	1	0
3	J	302	LFA	2	0
3	J	304	LFA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	307	LFA	1	0
3	J	311	LFA	1	0
4	J	312	MPG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	272/288 (94%)	-0.07	5 (1%) 69 66	24, 34, 52, 81	0
1	B	269/288 (93%)	0.15	18 (6%) 19 17	26, 39, 67, 90	0
1	C	270/288 (93%)	-0.04	7 (2%) 56 54	24, 34, 51, 74	0
1	D	270/288 (93%)	0.01	10 (3%) 42 40	22, 32, 49, 73	0
1	E	271/288 (94%)	0.01	8 (2%) 51 48	23, 34, 54, 69	0
1	F	270/288 (93%)	0.08	17 (6%) 21 19	25, 35, 56, 76	0
1	G	270/288 (93%)	-0.09	7 (2%) 56 54	23, 34, 51, 82	0
1	H	272/288 (94%)	-0.06	9 (3%) 47 44	23, 32, 51, 91	0
1	I	270/288 (93%)	-0.09	11 (4%) 38 36	21, 30, 49, 76	0
1	J	271/288 (94%)	0.11	16 (5%) 23 22	23, 32, 49, 76	0
All	All	2705/2880 (93%)	0.00	108 (3%) 39 37	21, 33, 54, 91	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	275	LEU	8.4
1	I	275	LEU	7.1
1	I	276	VAL	6.1
1	H	276	VAL	5.9
1	H	272	ASN	5.7
1	J	276	VAL	5.6
1	F	132	THR	5.1
1	B	195	GLY	5.1
1	B	3	GLN	5.0
1	G	276	VAL	4.9
1	A	132	THR	4.9
1	J	275	LEU	4.6
1	B	198	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	132	THR	4.3
1	H	3	GLN	4.3
1	F	195	GLY	4.2
1	J	233	PHE	4.1
1	F	196	ILE	4.1
1	B	196	ILE	4.0
1	D	276	VAL	3.9
1	B	129	SER	3.8
1	B	273	LYS	3.7
1	E	276	VAL	3.7
1	J	272	ASN	3.7
1	B	133	SER	3.6
1	C	233	PHE	3.4
1	A	276	VAL	3.4
1	B	197	SER	3.4
1	F	130	LEU	3.4
1	J	183	TRP	3.3
1	C	183	TRP	3.2
1	B	131	THR	3.2
1	A	183	TRP	3.1
1	C	275	LEU	3.1
1	F	3	GLN	3.1
1	B	275	LEU	3.1
1	D	198	PRO	3.0
1	D	270	SER	3.0
1	F	233	PHE	3.0
1	B	134	LYS	2.9
1	B	233	PHE	2.9
1	F	274	GLU	2.9
1	J	69	VAL	2.9
1	A	272	ASN	2.9
1	G	233	PHE	2.9
1	C	232	GLY	2.9
1	H	195	GLY	2.9
1	B	130	LEU	2.9
1	B	190	ASN	2.8
1	F	198	PRO	2.8
1	J	133	SER	2.8
1	D	275	LEU	2.7
1	J	40	LEU	2.7
1	F	194	GLU	2.7
1	H	274	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	74[A]	LEU	2.6
1	I	40	LEU	2.6
1	F	197	SER	2.6
1	G	40	LEU	2.6
1	J	43	LEU	2.6
1	D	233	PHE	2.6
1	B	18	GLU	2.6
1	J	73	LEU	2.6
1	C	73	LEU	2.5
1	D	273	LYS	2.5
1	F	270	SER	2.5
1	I	274	GLU	2.5
1	E	76	TYR	2.5
1	F	275	LEU	2.5
1	D	73	LEU	2.4
1	J	72	PHE	2.4
1	D	269	LEU	2.4
1	F	131	THR	2.4
1	G	132	THR	2.3
1	I	92	VAL	2.3
1	I	73	LEU	2.3
1	H	92	VAL	2.3
1	E	73	LEU	2.3
1	D	274	GLU	2.3
1	E	129	SER	2.3
1	J	65	ALA	2.3
1	E	40	LEU	2.3
1	C	74[A]	LEU	2.2
1	I	75	LEU	2.2
1	G	183	TRP	2.2
1	H	233	PHE	2.2
1	F	92	VAL	2.2
1	B	40	LEU	2.2
1	F	269	LEU	2.2
1	H	40	LEU	2.2
1	G	195	GLY	2.2
1	C	72	PHE	2.2
1	D	40	LEU	2.2
1	J	269	LEU	2.1
1	I	43	LEU	2.1
1	I	74	LEU	2.1
1	J	132	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	201	GLN	2.1
1	E	4	GLU	2.1
1	F	55	LYS	2.1
1	I	76	TYR	2.1
1	G	164	LEU	2.1
1	F	133	SER	2.1
1	I	132	THR	2.0
1	E	72	PHE	2.0
1	E	228	THR	2.0
1	A	69	VAL	2.0
1	J	273	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	LYR	A	255	29/30	0.92	0.14	-	26,29,34,36	0
1	LYR	G	255	29/30	0.93	0.14	-	25,31,38,43	0
1	LYR	E	255	29/30	0.92	0.14	-	28,34,43,47	0
1	LYR	H	255	29/30	0.93	0.14	-	25,30,37,40	0
1	LYR	F	255	29/30	0.94	0.14	-	27,33,37,44	0
1	LYR	D	255	29/30	0.94	0.14	-	25,27,35,36	0
1	LYR	J	255	29/30	0.93	0.15	-	22,27,32,35	0
1	LYR	I	255	29/30	0.94	0.15	-	22,26,33,38	0
1	LYR	B	255	29/30	0.91	0.14	-	31,38,44,49	0
1	LYR	C	255	29/30	0.93	0.15	-	29,33,39,43	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	LFA	F	302	7/20	0.79	1.31	105.93	76,83,88,92	0
3	LFA	B	302	7/20	0.85	1.06	50.26	60,62,73,76	0
3	LFA	I	302	7/20	0.85	1.29	39.80	59,70,82,84	0
3	LFA	A	311	7/20	0.71	1.10	37.02	59,61,67,69	0
3	LFA	I	303	7/20	0.80	1.05	29.99	52,62,74,80	0
3	LFA	G	303	7/20	0.89	1.08	28.73	57,59,75,79	0
3	LFA	B	303	7/20	0.85	1.07	25.98	54,62,93,97	0
3	LFA	D	302	7/20	0.74	1.00	25.72	57,62,68,69	0
3	LFA	J	307	7/20	0.84	0.89	23.25	56,61,78,83	0
3	LFA	C	302	7/20	0.84	0.93	22.59	45,57,66,69	0
3	LFA	C	309	8/20	0.62	0.30	14.36	66,78,84,92	0
3	LFA	F	307	6/20	0.83	0.19	11.35	43,43,46,48	0
3	LFA	J	305	14/20	0.62	0.25	10.67	60,72,80,81	0
3	LFA	G	315	6/20	0.85	0.20	9.59	45,53,58,59	0
3	LFA	E	302	14/20	0.84	0.56	8.56	44,56,65,66	0
3	LFA	C	306	16/20	0.79	0.54	8.52	49,54,71,77	0
3	LFA	A	306	14/20	0.90	0.49	7.64	47,51,56,56	0
3	LFA	F	313	14/20	0.61	0.27	7.60	65,74,78,82	0
3	LFA	D	306	16/20	0.81	0.51	7.53	44,56,67,67	0
3	LFA	H	307	14/20	0.82	0.20	7.52	56,65,71,71	0
3	LFA	B	309	13/20	0.75	0.26	7.08	50,69,76,80	0
3	LFA	D	309	8/20	0.83	0.26	6.93	56,70,81,82	0
3	LFA	B	307	16/20	0.81	0.53	6.79	46,57,66,66	0
3	LFA	C	310	13/20	0.69	0.27	6.69	58,69,79,81	0
3	LFA	B	304	14/20	0.76	0.24	6.57	50,61,77,78	0
3	LFA	J	302	16/20	0.79	0.52	5.94	45,53,60,61	0
3	LFA	G	309	8/20	0.75	0.18	5.92	53,59,62,62	0
3	LFA	F	308	8/20	0.68	0.20	5.77	47,59,64,65	0
3	LFA	G	304	14/20	0.82	0.25	5.69	39,54,62,62	0
3	LFA	I	304	14/20	0.77	0.22	5.62	41,54,62,65	0
3	LFA	C	312	4/20	0.81	0.15	5.62	44,46,47,47	0
3	LFA	E	305	6/20	0.79	0.18	5.61	54,59,67,68	0
3	LFA	G	302	16/20	0.76	0.46	5.46	46,51,57,58	0
3	LFA	G	310	10/20	0.65	0.20	5.34	53,66,73,74	0
3	LFA	J	304	8/20	0.71	0.20	5.14	46,54,63,63	0
3	LFA	H	302	13/20	0.83	0.20	4.92	41,52,61,61	0
3	LFA	B	310	11/20	0.75	0.22	4.85	50,60,67,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	LFA	H	304	10/20	0.68	0.18	4.81	56,62,64,65	0
3	LFA	H	309	5/20	0.90	0.17	4.79	41,42,45,47	0
3	LFA	H	305	16/20	0.89	0.44	4.77	40,51,56,59	0
3	LFA	I	308	16/20	0.88	0.49	4.71	42,53,68,72	0
3	LFA	G	307	16/20	0.79	0.43	4.66	48,54,59,59	0
3	LFA	F	303	14/20	0.88	0.27	4.57	54,61,66,70	0
3	LFA	H	311	7/20	0.93	0.18	4.53	44,44,53,57	0
3	LFA	D	303	14/20	0.84	0.25	4.40	40,67,73,73	0
3	LFA	A	305	10/20	0.77	0.14	4.36	45,52,58,58	0
3	LFA	E	311	8/20	0.86	0.37	4.13	40,45,48,50	0
3	LFA	I	309	18/20	0.88	0.29	4.01	32,42,64,75	0
3	LFA	A	302	14/20	0.86	0.24	3.93	49,55,63,65	0
3	LFA	A	309	8/20	0.90	0.17	3.90	55,61,70,73	0
3	LFA	C	307	18/20	0.89	0.31	3.73	42,48,57,57	0
3	LFA	I	310	14/20	0.80	0.19	3.40	47,55,63,64	0
3	LFA	E	303	18/20	0.91	0.29	3.39	35,46,62,66	0
3	LFA	E	312	8/20	0.87	0.15	3.34	47,52,55,57	0
3	LFA	J	308	14/20	0.87	0.23	3.30	39,52,59,60	0
3	LFA	F	310	18/20	0.89	0.29	3.24	39,51,65,66	0
3	LFA	B	308	18/20	0.78	0.29	2.83	44,58,74,77	0
4	MPG	D	315	14/25	0.83	0.19	2.49	49,54,63,68	0
3	LFA	A	304	10/20	0.87	0.16	2.42	47,50,55,57	0
3	LFA	F	312	8/20	0.81	0.17	2.30	48,64,82,84	0
3	LFA	D	312	6/20	0.94	0.14	2.24	40,45,49,52	0
2	NA	A	301	1/1	0.98	0.15	2.21	34,34,34,34	0
3	LFA	A	307	18/20	0.92	0.25	2.09	37,45,63,71	0
3	LFA	J	303	18/20	0.89	0.30	1.92	37,45,57,62	0
3	LFA	E	308	14/20	0.89	0.20	1.88	51,56,64,65	0
3	LFA	F	309	10/20	0.77	0.17	1.86	37,42,45,46	0
3	LFA	G	308	18/20	0.89	0.28	1.75	43,48,60,64	0
3	LFA	D	305	10/20	0.82	0.19	1.67	51,54,63,64	0
2	NA	G	301	1/1	0.99	0.17	1.44	26,26,26,26	0
3	LFA	D	307	18/20	0.93	0.26	1.37	34,39,50,60	0
3	LFA	I	306	10/20	0.91	0.12	1.25	37,39,41,42	0
4	MPG	C	313	13/25	0.89	0.12	1.12	46,53,64,74	0
3	LFA	I	312	7/20	0.95	0.12	1.03	30,34,45,48	0
3	LFA	E	310	10/20	0.75	0.16	0.87	42,48,60,60	0
2	NA	C	301	1/1	0.99	0.14	0.78	28,28,28,28	0
3	LFA	F	306	10/20	0.82	0.13	0.74	48,54,59,63	0
2	NA	F	301	1/1	0.98	0.12	0.69	29,29,29,29	0
3	LFA	H	306	18/20	0.90	0.25	0.59	42,46,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	LFA	J	310	10/20	0.87	0.12	0.56	51,56,58,60	0
3	LFA	G	306	10/20	0.86	0.14	0.30	45,54,57,57	0
3	LFA	A	312	5/20	0.91	0.10	0.14	43,45,50,54	0
3	LFA	J	311	4/20	0.96	0.09	0.04	33,35,36,37	0
3	LFA	C	305	10/20	0.91	0.12	-0.05	41,47,51,52	0
3	LFA	B	306	8/20	0.81	0.14	-0.09	53,63,65,66	0
3	LFA	H	310	8/20	0.91	0.12	-0.28	39,46,48,50	0
2	NA	E	301	1/1	0.98	0.10	-0.47	27,27,27,27	0
2	NA	B	301	1/1	0.97	0.06	-1.30	29,29,29,29	0
2	NA	D	301	1/1	0.98	0.09	-1.98	29,29,29,29	0
2	NA	H	301	1/1	0.97	0.08	-3.39	30,30,30,30	0
2	NA	J	301	1/1	0.99	0.09	-4.61	28,28,28,28	0
2	NA	I	301	1/1	0.98	0.07	-8.32	23,23,23,23	0
3	LFA	I	311	8/20	0.92	0.12	-	45,54,56,59	0
3	LFA	D	311	7/20	0.88	0.14	-	51,53,55,57	0
3	LFA	D	308	10/20	0.77	0.29	-	56,61,70,70	0
3	LFA	E	307	8/20	0.85	0.19	-	61,68,70,73	0
3	LFA	C	303	10/20	0.49	0.24	-	61,77,88,94	0
3	LFA	F	304	10/20	0.73	0.21	-	58,61,73,73	0
3	LFA	A	303	6/20	0.83	0.18	-	52,54,59,63	0
3	LFA	G	313	8/20	0.81	0.20	-	48,55,59,65	0
3	LFA	D	314	7/20	0.88	0.12	-	50,55,59,60	0
3	LFA	E	306	12/20	0.65	0.27	-	66,78,86,89	0
4	MPG	I	314	14/25	0.91	0.16	-	35,42,60,72	0
3	LFA	E	309	6/20	0.70	0.27	-	60,66,70,70	0
3	LFA	D	317	5/20	0.77	0.18	-	56,64,69,70	0
3	LFA	F	314	8/20	0.73	0.17	-	61,71,76,76	0
3	LFA	B	311	8/20	0.68	0.22	-	57,70,73,82	0
4	MPG	E	313	14/25	0.81	0.18	-	48,53,68,72	0
3	LFA	H	308	8/20	0.84	0.20	-	64,70,71,72	0
3	LFA	E	304	8/20	0.62	0.22	-	60,64,68,72	0
3	LFA	I	305	6/20	0.81	0.22	-	48,57,60,61	0
4	MPG	J	312	14/25	0.85	0.22	-	51,59,67,68	0
3	LFA	D	316	5/20	0.88	0.11	-	50,52,53,54	0
3	LFA	C	311	8/20	0.88	0.24	-	59,64,67,71	0
3	LFA	J	306	8/20	0.77	0.20	-	60,73,81,81	0
3	LFA	D	310	8/20	0.73	0.22	-	56,69,70,74	0
3	LFA	F	311	10/20	0.71	0.20	-	64,77,86,87	0
4	MPG	B	312	14/25	0.90	0.23	-	50,62,71,72	0
4	MPG	H	313	14/25	0.91	0.21	-	49,62,72,75	0
3	LFA	G	311	8/20	0.83	0.20	-	51,62,68,69	0
3	LFA	I	307	6/20	0.90	0.15	-	38,41,44,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	LFA	C	304	6/20	0.74	0.22	-	60,63,65,68	0
3	LFA	H	312	6/20	0.88	0.13	-	51,53,54,56	0
4	MPG	A	313	14/25	0.82	0.25	-	54,60,66,70	0
3	LFA	J	309	10/20	0.84	0.15	-	49,52,58,58	0
4	MPG	F	315	14/25	0.90	0.18	-	41,51,57,62	0
3	LFA	F	305	6/20	0.83	0.24	-	54,56,58,58	0
3	LFA	C	308	10/20	0.65	0.25	-	67,74,85,88	0
3	LFA	A	310	8/20	0.75	0.25	-	54,62,70,72	0
3	LFA	D	313	6/20	0.79	0.12	-	44,51,57,57	0
3	LFA	B	305	6/20	0.69	0.20	-	50,58,59,64	0
3	LFA	G	314	6/20	0.90	0.22	-	50,54,54,55	0
4	MPG	G	312	14/25	0.90	0.20	-	48,54,62,64	0
3	LFA	H	303	6/20	0.88	0.18	-	54,55,57,63	0
3	LFA	G	305	6/20	0.83	0.21	-	55,56,58,64	0
3	LFA	I	313	4/20	0.92	0.09	-	38,42,43,44	0
3	LFA	D	304	6/20	0.86	0.19	-	47,51,52,57	0
3	LFA	A	308	8/20	0.73	0.18	-	55,61,65,72	0
3	LFA	D	318	5/20	0.66	0.23	-	63,66,66,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.