



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:42 PM GMT

PDB ID : 4D41  
Title : Crystal structure of *S. aureus* FabI in complex with NADP and 5-hexyl- 2-(4-nitrophenoxy)phenol  
Authors : Schiebel, J.; Chang, A.; Tonge, P.J.; Sotriffer, C.A.; Kisker, C.  
Deposited on : 2014-10-26  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

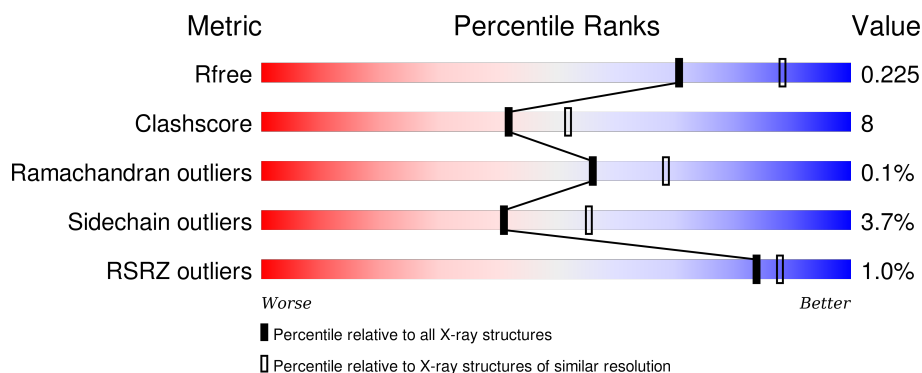
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	282	<div> <div></div> <div>75%15%10%</div> </div>
1	B	282	<div> <div></div> <div>77%12%10%</div> </div>
1	C	282	<div> <div>%</div> <div>70%18%10%</div> </div>
1	D	282	<div> <div>3%</div> <div>77%12%10%</div> </div>
1	E	282	<div> <div>%</div> <div>75%15%10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	282	
1	G	282	
1	H	282	

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	GLU	B	1001	-	-	-	X
2	GLU	C	1259	-	-	-	X
2	GLU	E	1259	-	-	-	X
2	GLU	F	1257	-	-	-	X
2	GLU	G	1258	-	-	X	-
3	MPD	A	1257	-	-	-	X
3	MPD	C	1260	-	-	-	X
3	MPD	D	1257	-	-	-	X
3	MPD	E	1260	-	-	X	X
3	MPD	F	1258	-	-	-	X
3	MPD	G	1259	-	-	-	X
3	MPD	H	1258	-	-	X	X
6	MRD	B	1258	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17716 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 ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	5	0
			1985	1250	343	388	4			
1	B	254	Total	C	N	O	S	0	1	0
			1963	1237	341	381	4			
1	C	254	Total	C	N	O	S	0	12	0
			2046	1285	359	397	5			
1	D	254	Total	C	N	O	S	0	11	0
			2033	1279	353	397	4			
1	E	254	Total	C	N	O	S	0	4	0
			1983	1250	344	385	4			
1	F	254	Total	C	N	O	S	0	9	0
			2024	1271	353	395	5			
1	G	255	Total	C	N	O	S	0	11	0
			2045	1285	357	398	5			
1	H	254	Total	C	N	O	S	0	9	0
			2026	1274	351	396	5			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	EXPRESSION TAG	UNP Q7A6D8
A	-24	LYS	-	EXPRESSION TAG	UNP Q7A6D8
A	-23	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-22	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-21	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-20	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-19	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-18	HIS	-	EXPRESSION TAG	UNP Q7A6D8
A	-17	PRO	-	EXPRESSION TAG	UNP Q7A6D8
A	-16	MET	-	EXPRESSION TAG	UNP Q7A6D8
A	-15	SER	-	EXPRESSION TAG	UNP Q7A6D8
A	-14	ASP	-	EXPRESSION TAG	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	TYR	-	EXPRESSION TAG	UNP Q7A6D8
A	-12	ASP	-	EXPRESSION TAG	UNP Q7A6D8
A	-11	ILE	-	EXPRESSION TAG	UNP Q7A6D8
A	-10	PRO	-	EXPRESSION TAG	UNP Q7A6D8
A	-9	THR	-	EXPRESSION TAG	UNP Q7A6D8
A	-8	THR	-	EXPRESSION TAG	UNP Q7A6D8
A	-7	GLU	-	EXPRESSION TAG	UNP Q7A6D8
A	-6	ASN	-	EXPRESSION TAG	UNP Q7A6D8
A	-5	LEU	-	EXPRESSION TAG	UNP Q7A6D8
A	-4	TYR	-	EXPRESSION TAG	UNP Q7A6D8
A	-3	PHE	-	EXPRESSION TAG	UNP Q7A6D8
A	-2	GLN	-	EXPRESSION TAG	UNP Q7A6D8
A	-1	GLY	-	EXPRESSION TAG	UNP Q7A6D8
A	0	ALA	-	EXPRESSION TAG	UNP Q7A6D8
A	2	VAL	LEU	ENGINEERED MUTATION	UNP Q7A6D8
B	-25	MET	-	EXPRESSION TAG	UNP Q7A6D8
B	-24	LYS	-	EXPRESSION TAG	UNP Q7A6D8
B	-23	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-22	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-21	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-20	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-19	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-18	HIS	-	EXPRESSION TAG	UNP Q7A6D8
B	-17	PRO	-	EXPRESSION TAG	UNP Q7A6D8
B	-16	MET	-	EXPRESSION TAG	UNP Q7A6D8
B	-15	SER	-	EXPRESSION TAG	UNP Q7A6D8
B	-14	ASP	-	EXPRESSION TAG	UNP Q7A6D8
B	-13	TYR	-	EXPRESSION TAG	UNP Q7A6D8
B	-12	ASP	-	EXPRESSION TAG	UNP Q7A6D8
B	-11	ILE	-	EXPRESSION TAG	UNP Q7A6D8
B	-10	PRO	-	EXPRESSION TAG	UNP Q7A6D8
B	-9	THR	-	EXPRESSION TAG	UNP Q7A6D8
B	-8	THR	-	EXPRESSION TAG	UNP Q7A6D8
B	-7	GLU	-	EXPRESSION TAG	UNP Q7A6D8
B	-6	ASN	-	EXPRESSION TAG	UNP Q7A6D8
B	-5	LEU	-	EXPRESSION TAG	UNP Q7A6D8
B	-4	TYR	-	EXPRESSION TAG	UNP Q7A6D8
B	-3	PHE	-	EXPRESSION TAG	UNP Q7A6D8
B	-2	GLN	-	EXPRESSION TAG	UNP Q7A6D8
B	-1	GLY	-	EXPRESSION TAG	UNP Q7A6D8
B	0	ALA	-	EXPRESSION TAG	UNP Q7A6D8
B	2	VAL	LEU	ENGINEERED MUTATION	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-25	MET	-	EXPRESSION TAG	UNP Q7A6D8
C	-24	LYS	-	EXPRESSION TAG	UNP Q7A6D8
C	-23	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-22	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-21	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-20	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-19	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-18	HIS	-	EXPRESSION TAG	UNP Q7A6D8
C	-17	PRO	-	EXPRESSION TAG	UNP Q7A6D8
C	-16	MET	-	EXPRESSION TAG	UNP Q7A6D8
C	-15	SER	-	EXPRESSION TAG	UNP Q7A6D8
C	-14	ASP	-	EXPRESSION TAG	UNP Q7A6D8
C	-13	TYR	-	EXPRESSION TAG	UNP Q7A6D8
C	-12	ASP	-	EXPRESSION TAG	UNP Q7A6D8
C	-11	ILE	-	EXPRESSION TAG	UNP Q7A6D8
C	-10	PRO	-	EXPRESSION TAG	UNP Q7A6D8
C	-9	THR	-	EXPRESSION TAG	UNP Q7A6D8
C	-8	THR	-	EXPRESSION TAG	UNP Q7A6D8
C	-7	GLU	-	EXPRESSION TAG	UNP Q7A6D8
C	-6	ASN	-	EXPRESSION TAG	UNP Q7A6D8
C	-5	LEU	-	EXPRESSION TAG	UNP Q7A6D8
C	-4	TYR	-	EXPRESSION TAG	UNP Q7A6D8
C	-3	PHE	-	EXPRESSION TAG	UNP Q7A6D8
C	-2	GLN	-	EXPRESSION TAG	UNP Q7A6D8
C	-1	GLY	-	EXPRESSION TAG	UNP Q7A6D8
C	0	ALA	-	EXPRESSION TAG	UNP Q7A6D8
C	2	VAL	LEU	ENGINEERED MUTATION	UNP Q7A6D8
D	-25	MET	-	EXPRESSION TAG	UNP Q7A6D8
D	-24	LYS	-	EXPRESSION TAG	UNP Q7A6D8
D	-23	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-22	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-21	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-20	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-19	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-18	HIS	-	EXPRESSION TAG	UNP Q7A6D8
D	-17	PRO	-	EXPRESSION TAG	UNP Q7A6D8
D	-16	MET	-	EXPRESSION TAG	UNP Q7A6D8
D	-15	SER	-	EXPRESSION TAG	UNP Q7A6D8
D	-14	ASP	-	EXPRESSION TAG	UNP Q7A6D8
D	-13	TYR	-	EXPRESSION TAG	UNP Q7A6D8
D	-12	ASP	-	EXPRESSION TAG	UNP Q7A6D8
D	-11	ILE	-	EXPRESSION TAG	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	PRO	-	EXPRESSION TAG	UNP Q7A6D8
D	-9	THR	-	EXPRESSION TAG	UNP Q7A6D8
D	-8	THR	-	EXPRESSION TAG	UNP Q7A6D8
D	-7	GLU	-	EXPRESSION TAG	UNP Q7A6D8
D	-6	ASN	-	EXPRESSION TAG	UNP Q7A6D8
D	-5	LEU	-	EXPRESSION TAG	UNP Q7A6D8
D	-4	TYR	-	EXPRESSION TAG	UNP Q7A6D8
D	-3	PHE	-	EXPRESSION TAG	UNP Q7A6D8
D	-2	GLN	-	EXPRESSION TAG	UNP Q7A6D8
D	-1	GLY	-	EXPRESSION TAG	UNP Q7A6D8
D	0	ALA	-	EXPRESSION TAG	UNP Q7A6D8
D	2	VAL	LEU	ENGINEERED MUTATION	UNP Q7A6D8
E	-25	MET	-	EXPRESSION TAG	UNP Q7A6D8
E	-24	LYS	-	EXPRESSION TAG	UNP Q7A6D8
E	-23	HIS	-	EXPRESSION TAG	UNP Q7A6D8
E	-22	HIS	-	EXPRESSION TAG	UNP Q7A6D8
E	-21	HIS	-	EXPRESSION TAG	UNP Q7A6D8
E	-20	HIS	-	EXPRESSION TAG	UNP Q7A6D8
E	-19	HIS	-	EXPRESSION TAG	UNP Q7A6D8
E	-18	HIS	-	EXPRESSION TAG	UNP Q7A6D8
E	-17	PRO	-	EXPRESSION TAG	UNP Q7A6D8
E	-16	MET	-	EXPRESSION TAG	UNP Q7A6D8
E	-15	SER	-	EXPRESSION TAG	UNP Q7A6D8
E	-14	ASP	-	EXPRESSION TAG	UNP Q7A6D8
E	-13	TYR	-	EXPRESSION TAG	UNP Q7A6D8
E	-12	ASP	-	EXPRESSION TAG	UNP Q7A6D8
E	-11	ILE	-	EXPRESSION TAG	UNP Q7A6D8
E	-10	PRO	-	EXPRESSION TAG	UNP Q7A6D8
E	-9	THR	-	EXPRESSION TAG	UNP Q7A6D8
E	-8	THR	-	EXPRESSION TAG	UNP Q7A6D8
E	-7	GLU	-	EXPRESSION TAG	UNP Q7A6D8
E	-6	ASN	-	EXPRESSION TAG	UNP Q7A6D8
E	-5	LEU	-	EXPRESSION TAG	UNP Q7A6D8
E	-4	TYR	-	EXPRESSION TAG	UNP Q7A6D8
E	-3	PHE	-	EXPRESSION TAG	UNP Q7A6D8
E	-2	GLN	-	EXPRESSION TAG	UNP Q7A6D8
E	-1	GLY	-	EXPRESSION TAG	UNP Q7A6D8
E	0	ALA	-	EXPRESSION TAG	UNP Q7A6D8
E	2	VAL	LEU	ENGINEERED MUTATION	UNP Q7A6D8
F	-25	MET	-	EXPRESSION TAG	UNP Q7A6D8
F	-24	LYS	-	EXPRESSION TAG	UNP Q7A6D8
F	-23	HIS	-	EXPRESSION TAG	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-22	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-21	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-20	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-19	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-18	HIS	-	EXPRESSION TAG	UNP Q7A6D8
F	-17	PRO	-	EXPRESSION TAG	UNP Q7A6D8
F	-16	MET	-	EXPRESSION TAG	UNP Q7A6D8
F	-15	SER	-	EXPRESSION TAG	UNP Q7A6D8
F	-14	ASP	-	EXPRESSION TAG	UNP Q7A6D8
F	-13	TYR	-	EXPRESSION TAG	UNP Q7A6D8
F	-12	ASP	-	EXPRESSION TAG	UNP Q7A6D8
F	-11	ILE	-	EXPRESSION TAG	UNP Q7A6D8
F	-10	PRO	-	EXPRESSION TAG	UNP Q7A6D8
F	-9	THR	-	EXPRESSION TAG	UNP Q7A6D8
F	-8	THR	-	EXPRESSION TAG	UNP Q7A6D8
F	-7	GLU	-	EXPRESSION TAG	UNP Q7A6D8
F	-6	ASN	-	EXPRESSION TAG	UNP Q7A6D8
F	-5	LEU	-	EXPRESSION TAG	UNP Q7A6D8
F	-4	TYR	-	EXPRESSION TAG	UNP Q7A6D8
F	-3	PHE	-	EXPRESSION TAG	UNP Q7A6D8
F	-2	GLN	-	EXPRESSION TAG	UNP Q7A6D8
F	-1	GLY	-	EXPRESSION TAG	UNP Q7A6D8
F	0	ALA	-	EXPRESSION TAG	UNP Q7A6D8
F	2	VAL	LEU	ENGINEERED MUTATION	UNP Q7A6D8
G	-25	MET	-	EXPRESSION TAG	UNP Q7A6D8
G	-24	LYS	-	EXPRESSION TAG	UNP Q7A6D8
G	-23	HIS	-	EXPRESSION TAG	UNP Q7A6D8
G	-22	HIS	-	EXPRESSION TAG	UNP Q7A6D8
G	-21	HIS	-	EXPRESSION TAG	UNP Q7A6D8
G	-20	HIS	-	EXPRESSION TAG	UNP Q7A6D8
G	-19	HIS	-	EXPRESSION TAG	UNP Q7A6D8
G	-18	HIS	-	EXPRESSION TAG	UNP Q7A6D8
G	-17	PRO	-	EXPRESSION TAG	UNP Q7A6D8
G	-16	MET	-	EXPRESSION TAG	UNP Q7A6D8
G	-15	SER	-	EXPRESSION TAG	UNP Q7A6D8
G	-14	ASP	-	EXPRESSION TAG	UNP Q7A6D8
G	-13	TYR	-	EXPRESSION TAG	UNP Q7A6D8
G	-12	ASP	-	EXPRESSION TAG	UNP Q7A6D8
G	-11	ILE	-	EXPRESSION TAG	UNP Q7A6D8
G	-10	PRO	-	EXPRESSION TAG	UNP Q7A6D8
G	-9	THR	-	EXPRESSION TAG	UNP Q7A6D8
G	-8	THR	-	EXPRESSION TAG	UNP Q7A6D8

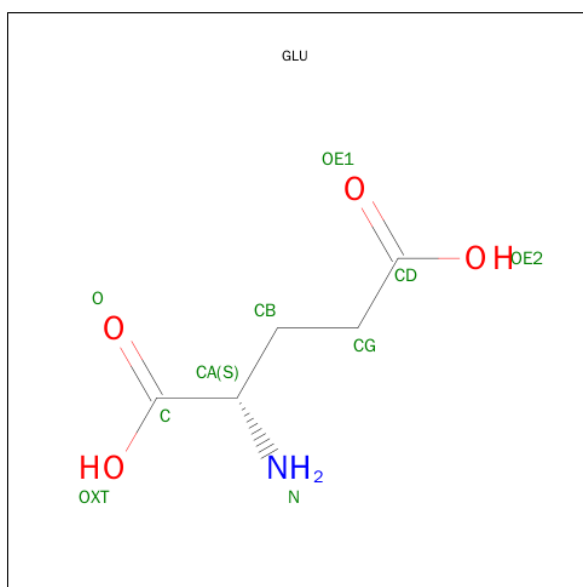
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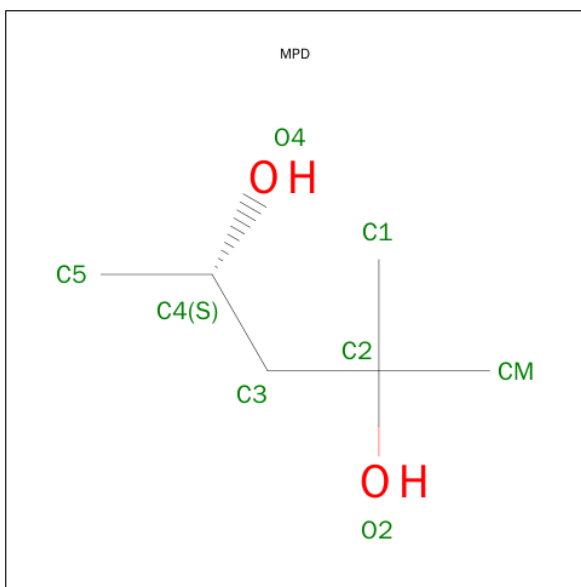
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	EXPRESSION TAG	UNP Q7A6D8
G	-6	ASN	-	EXPRESSION TAG	UNP Q7A6D8
G	-5	LEU	-	EXPRESSION TAG	UNP Q7A6D8
G	-4	TYR	-	EXPRESSION TAG	UNP Q7A6D8
G	-3	PHE	-	EXPRESSION TAG	UNP Q7A6D8
G	-2	GLN	-	EXPRESSION TAG	UNP Q7A6D8
G	-1	GLY	-	EXPRESSION TAG	UNP Q7A6D8
G	0	ALA	-	EXPRESSION TAG	UNP Q7A6D8
G	2	VAL	LEU	ENGINEERED MUTATION	UNP Q7A6D8
H	-25	MET	-	EXPRESSION TAG	UNP Q7A6D8
H	-24	LYS	-	EXPRESSION TAG	UNP Q7A6D8
H	-23	HIS	-	EXPRESSION TAG	UNP Q7A6D8
H	-22	HIS	-	EXPRESSION TAG	UNP Q7A6D8
H	-21	HIS	-	EXPRESSION TAG	UNP Q7A6D8
H	-20	HIS	-	EXPRESSION TAG	UNP Q7A6D8
H	-19	HIS	-	EXPRESSION TAG	UNP Q7A6D8
H	-18	HIS	-	EXPRESSION TAG	UNP Q7A6D8
H	-17	PRO	-	EXPRESSION TAG	UNP Q7A6D8
H	-16	MET	-	EXPRESSION TAG	UNP Q7A6D8
H	-15	SER	-	EXPRESSION TAG	UNP Q7A6D8
H	-14	ASP	-	EXPRESSION TAG	UNP Q7A6D8
H	-13	TYR	-	EXPRESSION TAG	UNP Q7A6D8
H	-12	ASP	-	EXPRESSION TAG	UNP Q7A6D8
H	-11	ILE	-	EXPRESSION TAG	UNP Q7A6D8
H	-10	PRO	-	EXPRESSION TAG	UNP Q7A6D8
H	-9	THR	-	EXPRESSION TAG	UNP Q7A6D8
H	-8	THR	-	EXPRESSION TAG	UNP Q7A6D8
H	-7	GLU	-	EXPRESSION TAG	UNP Q7A6D8
H	-6	ASN	-	EXPRESSION TAG	UNP Q7A6D8
H	-5	LEU	-	EXPRESSION TAG	UNP Q7A6D8
H	-4	TYR	-	EXPRESSION TAG	UNP Q7A6D8
H	-3	PHE	-	EXPRESSION TAG	UNP Q7A6D8
H	-2	GLN	-	EXPRESSION TAG	UNP Q7A6D8
H	-1	GLY	-	EXPRESSION TAG	UNP Q7A6D8
H	0	ALA	-	EXPRESSION TAG	UNP Q7A6D8
H	2	VAL	LEU	ENGINEERED MUTATION	UNP Q7A6D8

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		
2	G	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



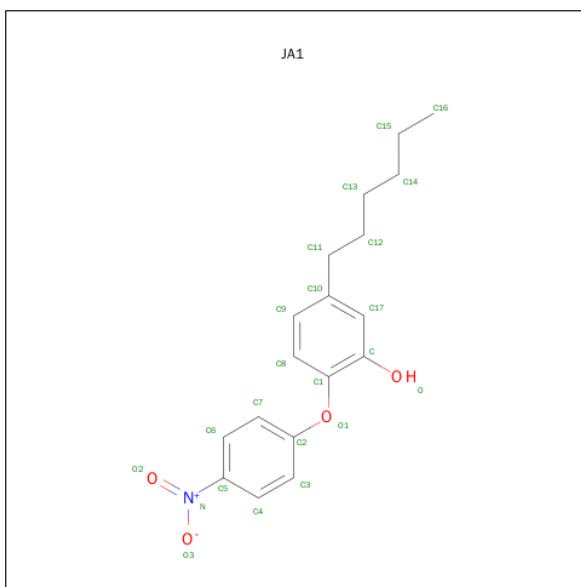
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is 5-HEXYL-2-(4-NITROPHENOXY)PHENOL (three-letter code: JA1) (formula: C<sub>18</sub>H<sub>21</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			23	18	1	4		
5	B	1	Total	C	N	O	0	0
			23	18	1	4		
5	C	1	Total	C	N	O	0	0
			23	18	1	4		
5	C	1	Total	C	N	O	0	0
			23	18	1	4		
5	E	1	Total	C	N	O	0	0
			23	18	1	4		
5	E	1	Total	C	N	O	0	0
			23	18	1	4		
5	G	1	Total	C	N	O	0	0
			23	18	1	4		
5	H	1	Total	C	N	O	0	0
			23	18	1	4		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	142	Total	O	0	0
			142	142		
7	B	113	Total	O	0	0
			113	113		
7	C	123	Total	O	0	0
			123	123		
7	D	82	Total	O	0	0
			82	82		
7	E	142	Total	O	0	0
			142	142		
7	F	115	Total	O	0	0
			115	115		
7	G	121	Total	O	0	0
			121	121		
7	H	85	Total	O	0	0
			85	85		
7	C	1	Total	O	0	0
			1	1		
7	A	1	Total	O	0	0
			1	1		
7	C	1	Total	O	0	0
			1	1		

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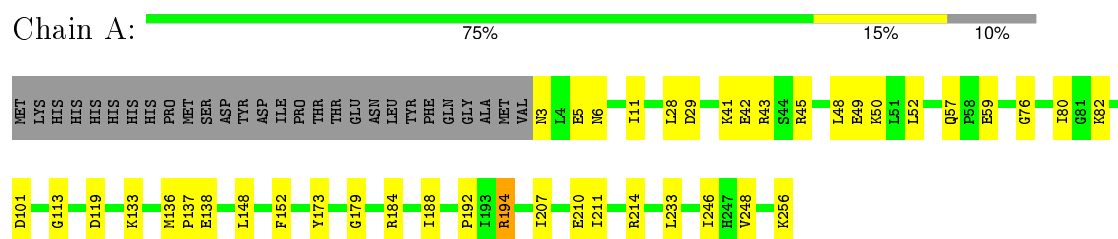
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	2	Total	O	0	0
			2	2		
7	A	1	Total	O	0	0
			1	1		

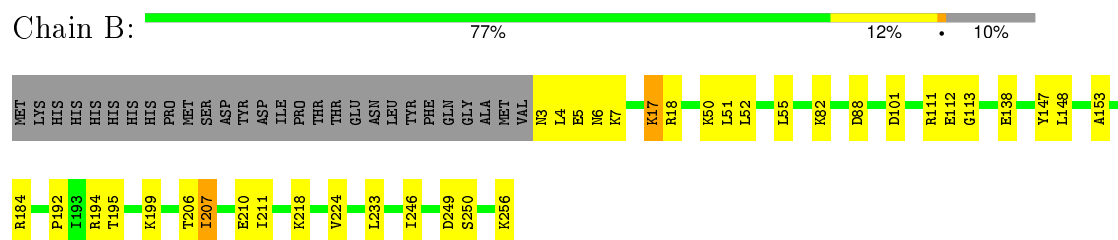
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

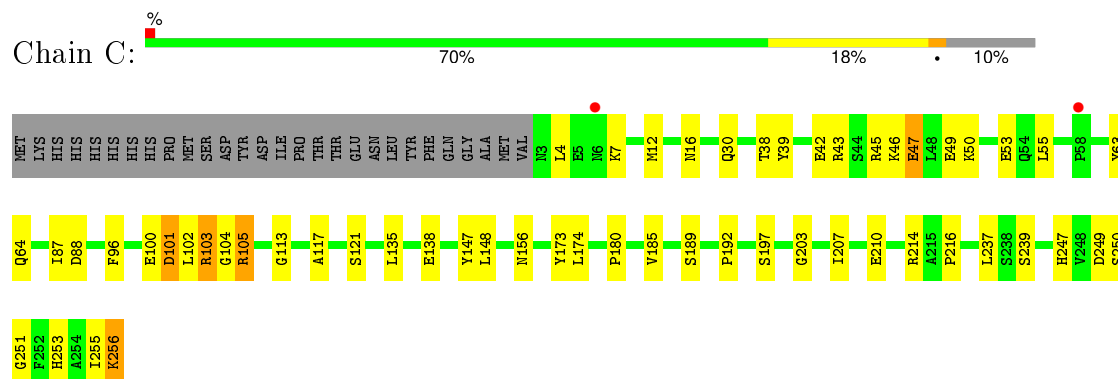
#### • Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



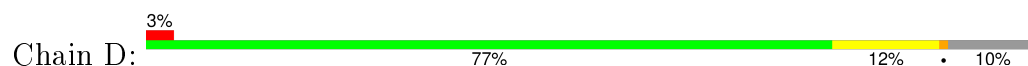
#### • Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



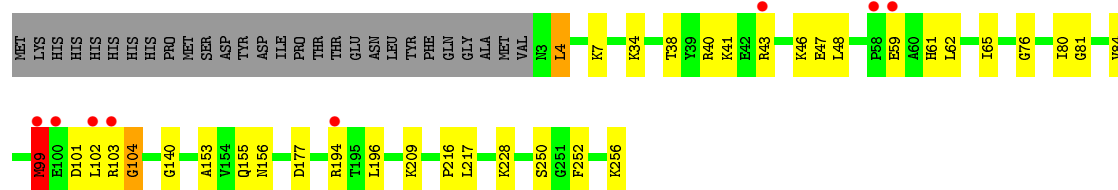
#### • Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



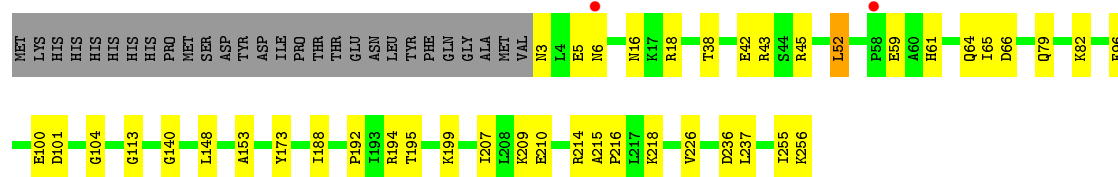
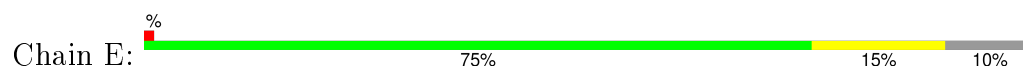
#### • Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



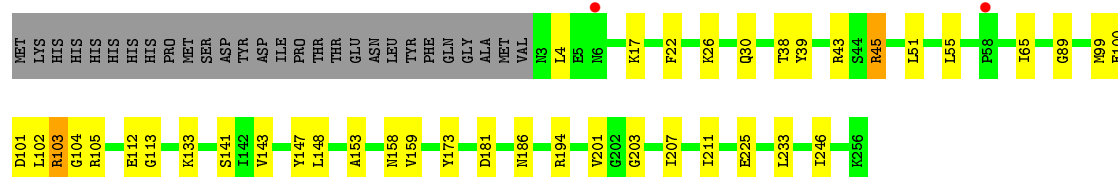
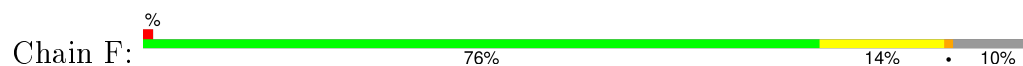




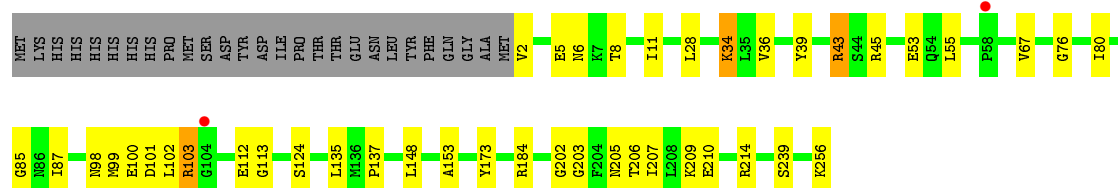
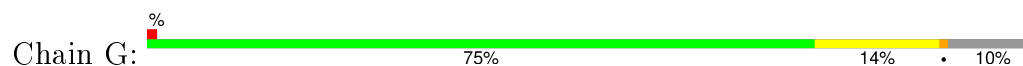
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



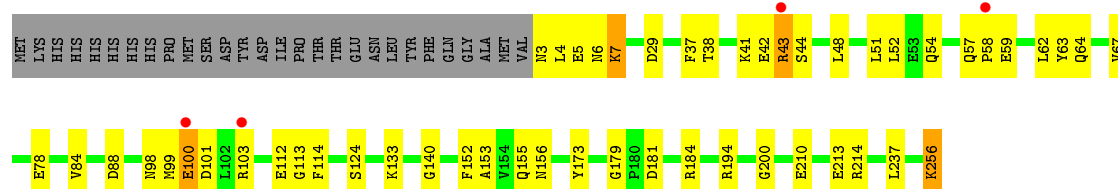
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.44Å 94.83Å 94.80Å 98.30° 111.35° 97.52°	Depositor
Resolution (Å)	40.82 – 2.30 40.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (40.82-2.30) 90.0 (40.82-2.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.152 , 0.213 0.167 , 0.225	Depositor DCC
$R_{free}$ test set	6135 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 120978 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17716	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MRD, NAP, MPD, JA1

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	0.53	0/2021	0.78	0/2722
1	B	0.54	0/1993	0.78	0/2685
1	C	0.50	0/2082	0.77	1/2801 (0.0%)
1	D	1.29	4/2067 (0.2%)	1.03	2/2783 (0.1%)
1	E	0.52	0/2022	0.78	1/2723 (0.0%)
1	F	0.53	0/2051	0.80	1/2761 (0.0%)
1	G	0.51	0/2078	0.77	0/2797
1	H	0.51	0/2059	0.76	0/2772
All	All	0.67	4/16373 (0.0%)	0.81	5/22044 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	99[A]	MET	CG-SD	27.98	2.53	1.81
1	D	99[B]	MET	CG-SD	27.98	2.53	1.81
1	D	99[A]	MET	SD-CE	26.73	3.27	1.77
1	D	99[B]	MET	SD-CE	26.73	3.27	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	99[A]	MET	CG-SD-CE	-27.30	56.53	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	99[B]	MET	CG-SD-CE	-27.30	56.53	100.20
1	F	45	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	E	43	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	C	88	ASP	CB-CG-OD1	-5.03	113.77	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	104[A]	GLY	Peptide

## 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	1985	0	2000	31	0
1	B	1963	0	1981	25	0
1	C	2046	0	2065	54	1
1	D	2033	0	2048	27	0
1	E	1983	0	2006	36	0
1	F	2024	0	2033	39	0
1	G	2045	0	2061	44	1
1	H	2026	0	2038	40	0
2	B	10	0	5	0	0
2	C	10	0	5	0	0
2	E	10	0	5	0	0
2	F	10	0	5	0	0
2	G	10	0	5	5	0
3	A	8	0	14	3	0
3	C	8	0	14	0	0
3	D	8	0	14	1	0
3	E	8	0	14	6	0
3	F	8	0	14	0	0
3	G	8	0	14	1	0
3	H	8	0	14	7	0
4	A	48	0	25	1	0
4	B	48	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	48	0	25	3	0
4	D	48	0	25	0	0
4	E	48	0	25	1	0
4	F	48	0	25	3	0
4	G	48	0	25	0	0
4	H	48	0	25	0	0
5	A	23	0	20	1	0
5	B	23	0	20	0	0
5	C	46	0	40	6	0
5	E	46	0	40	1	0
5	G	23	0	20	1	0
5	H	23	0	21	0	0
6	B	8	0	14	1	0
7	A	144	0	0	5	0
7	B	113	0	0	6	1
7	C	125	0	0	4	0
7	D	82	0	0	3	0
7	E	142	0	0	5	0
7	F	115	0	0	7	1
7	G	121	0	0	3	0
7	H	87	0	0	3	0
All	All	17716	0	16730	280	2

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 8.

All (280) 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:G:101[A]:ASP:O	1:G:102[A]:LEU:HD23	1.46	1.14
1:C:103[A]:ARG:HH11	1:C:103[A]:ARG:HG3	1.00	1.11
1:G:103[A]:ARG:CG	1:G:103[A]:ARG:HH11	1.70	1.04
1:F:103[A]:ARG:NH1	1:F:103[A]:ARG:HG3	1.56	1.04
1:F:103[A]:ARG:CG	1:F:103[A]:ARG:HH11	1.72	1.01
1:G:103[A]:ARG:HG3	1:G:103[A]:ARG:NH1	1.61	0.98
1:F:103[A]:ARG:HH11	1:F:103[A]:ARG:HG3	0.81	0.97
1:F:103[A]:ARG:HG2	7:F:2060:HOH:O	1.64	0.94
1:C:103[A]:ARG:HH11	1:C:103[A]:ARG:CG	1.82	0.93
1:C:103[A]:ARG:NH1	1:C:103[A]:ARG:HG3	1.79	0.92
1:G:2:VAL:HG13	1:G:2:VAL:O	1.69	0.92
1:G:103[A]:ARG:HG3	1:G:103[A]:ARG:HH11	0.80	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD21	1:C:256:LYS:HD3	1.54	0.89
1:C:101[A]:ASP:O	1:C:102[A]:LEU:HD23	1.74	0.87
1:C:101[A]:ASP:O	1:C:102[A]:LEU:CD2	2.23	0.86
1:G:101[A]:ASP:O	1:G:102[A]:LEU:CD2	2.23	0.85
3:A:1257:MPD:H53	7:A:2133:HOH:O	1.76	0.85
1:F:101[A]:ASP:O	1:F:102[A]:LEU:HD23	1.78	0.83
1:H:184:ARG:HE	3:H:1258:MPD:H51	1.43	0.83
1:C:101[A]:ASP:O	1:C:102[A]:LEU:HG	1.81	0.80
1:G:205:ASN:H	2:G:1258:GLU:HG2	1.45	0.80
1:C:101[A]:ASP:O	1:C:102[A]:LEU:CG	2.31	0.79
1:D:34:LYS:HD3	1:D:84[A]:VAL:HG11	1.65	0.79
1:E:210:GLU:HG3	1:E:214[A]:ARG:HD2	1.63	0.79
1:A:48:LEU:O	1:A:52:LEU:HD23	1.83	0.78
1:D:99[A]:MET:CE	1:D:99[A]:MET:HG3	2.13	0.78
1:G:210:GLU:HG2	1:G:214[B]:ARG:HD2	1.66	0.77
1:D:40:ARG:HD3	1:D:41:LYS:HE3	1.68	0.75
1:D:140:GLY:HA2	3:D:1257:MPD:HM1	1.69	0.75
1:F:104[A]:GLY:N	7:F:2061:HOH:O	2.20	0.75
1:H:98:ASN:HB3	1:H:100[B]:GLU:HG2	1.70	0.74
1:H:99[B]:MET:CE	1:H:200:GLY:O	2.36	0.74
1:F:101[B]:ASP:OD2	1:F:113:GLY:HA3	1.88	0.73
3:E:1260:MPD:O4	7:E:2079:HOH:O	2.03	0.72
1:F:99[A]:MET:O	1:F:100[A]:GLU:C	2.26	0.72
1:F:103[A]:ARG:CG	1:F:103[A]:ARG:NH1	2.38	0.72
1:E:236:ASP:OD1	3:E:1260:MPD:H52	1.90	0.71
1:A:207:ILE:HG13	5:A:1259:JA1:H14A	1.70	0.71
1:E:256:LYS:HG2	1:G:148:LEU:HD21	1.73	0.71
1:F:112:GLU:HG3	7:F:2056:HOH:O	1.90	0.70
1:D:81:GLY:HA3	7:D:2035:HOH:O	1.92	0.70
1:C:207:ILE:HG13	5:C:1257:JA1:H15	1.74	0.69
1:H:99[B]:MET:HE2	1:H:103[B]:ARG:HE	1.57	0.68
1:A:256:LYS:HE2	1:C:255:ILE:O	1.92	0.68
1:G:2:VAL:CG1	1:G:2:VAL:O	2.43	0.67
1:C:101[B]:ASP:OD2	1:C:113:GLY:HA3	1.95	0.67
1:G:5:GLU:O	1:G:6:ASN:HB2	1.92	0.67
1:D:76:GLY:O	1:D:80:ILE:HG13	1.94	0.67
1:F:101[A]:ASP:O	1:F:102[A]:LEU:CD2	2.42	0.67
1:A:42[B]:GLU:OE1	1:A:45:ARG:NH2	2.15	0.67
1:H:194:ARG:NH2	7:H:2071:HOH:O	2.27	0.66
1:D:101[A]:ASP:O	1:D:102[A]:LEU:HD23	1.96	0.66
3:A:1257:MPD:C5	7:A:2133:HOH:O	2.40	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:HH12	1:E:104:GLY:HA3	1.61	0.65
1:E:140:GLY:HA2	3:E:1260:MPD:H13	1.78	0.65
1:E:64:GLN:HG2	7:E:2041:HOH:O	1.97	0.65
1:A:256:LYS:HG2	1:C:148:LEU:HD21	1.79	0.64
1:B:112:GLU:HG3	7:B:2049:HOH:O	1.96	0.64
1:G:103[A]:ARG:CG	1:G:103[A]:ARG:NH1	2.40	0.63
1:A:3:ASN:HD21	1:A:5:GLU:HB2	1.63	0.63
7:F:2114:HOH:O	1:H:152:PHE:HE1	1.81	0.63
1:H:29:ASP:HB3	7:H:2013:HOH:O	1.98	0.63
1:H:100[B]:GLU:CD	1:H:100[B]:GLU:H	2.02	0.63
1:G:101[B]:ASP:OD2	1:G:113:GLY:HA3	1.99	0.63
1:C:103[A]:ARG:NH1	1:C:103[A]:ARG:CG	2.46	0.62
1:H:99[B]:MET:CE	1:H:103[B]:ARG:HE	2.13	0.62
1:D:34:LYS:HD3	1:D:84[A]:VAL:CG1	2.30	0.62
1:D:41:LYS:HD3	1:D:43:ARG:CZ	2.29	0.62
1:A:101:ASP:OD2	1:A:113:GLY:HA3	2.00	0.62
1:C:253:HIS:HD2	7:C:2120:HOH:O	1.83	0.60
1:B:194[A]:ARG:NH2	7:B:2089:HOH:O	2.13	0.60
7:G:2047:HOH:O	1:H:112[A]:GLU:OE2	2.15	0.60
1:G:99[A]:MET:C	1:G:101[A]:ASP:H	2.04	0.60
3:E:1260:MPD:O4	3:E:1260:MPD:H11	2.02	0.60
1:C:39:TYR:CE1	1:C:64:GLN:HB2	2.38	0.59
1:F:99[A]:MET:O	1:F:101[A]:ASP:N	2.36	0.59
1:B:184:ARG:HH21	6:B:1258:MRD:H5C2	1.67	0.59
1:A:45:ARG:HD2	1:A:49:GLU:OE2	2.02	0.58
1:G:103[A]:ARG:HB3	1:G:202:GLY:HA3	1.86	0.58
1:F:101[A]:ASP:HB3	1:F:159:VAL:HG12	1.86	0.58
1:H:140:GLY:HA2	3:H:1258:MPD:H12	1.86	0.58
3:H:1258:MPD:H53	7:H:2078:HOH:O	2.04	0.57
1:D:99[A]:MET:CE	1:D:99[A]:MET:CG	2.82	0.56
1:C:173:TYR:CZ	1:D:153:ALA:HA	2.40	0.56
1:H:184:ARG:HH21	3:H:1258:MPD:C5	2.18	0.56
1:C:147:TYR:CZ	5:C:1257:JA1:H13	2.40	0.56
1:D:99[A]:MET:HE2	1:D:99[A]:MET:HG3	1.87	0.56
1:B:3:ASN:HB3	7:B:2001:HOH:O	2.05	0.56
1:C:50:LYS:O	1:C:53:GLU:HG3	2.06	0.56
1:D:4:LEU:O	1:D:7:LYS:HB2	2.06	0.56
1:H:99[B]:MET:HE2	1:H:200:GLY:O	2.05	0.56
1:F:233:LEU:HD21	1:F:246:ILE:HD12	1.87	0.55
1:A:41:LYS:HE2	1:E:100:GLU:OE1	2.07	0.55
1:D:99[A]:MET:C	1:D:101[A]:ASP:H	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:98:ASN:HB3	1:G:100[B]:GLU:HG3	1.89	0.54
1:F:45:ARG:HD3	7:F:2024:HOH:O	2.07	0.54
1:B:18:ARG:HH12	1:B:194[B]:ARG:HE	1.55	0.54
1:F:102[A]:LEU:HD13	1:F:201:VAL:HG22	1.88	0.54
1:F:233:LEU:HD21	1:F:246:ILE:CD1	2.38	0.54
1:G:85:GLY:HA2	7:G:2051:HOH:O	2.08	0.54
1:A:194:ARG:HG2	1:A:194:ARG:HH11	1.71	0.54
1:B:148:LEU:HD21	1:D:256:LYS:HG2	1.90	0.54
1:E:148:LEU:HD21	1:G:256:LYS:HE3	1.90	0.54
1:G:203:GLY:H	2:G:1258:GLU:N	2.05	0.54
1:H:184:ARG:NE	3:H:1258:MPD:H51	2.18	0.53
1:G:103[A]:ARG:HD2	1:G:103[A]:ARG:N	2.22	0.53
1:E:210:GLU:CG	1:E:214[A]:ARG:HD2	2.38	0.53
1:H:155:GLN:O	1:H:156:ASN:HB2	2.08	0.53
1:A:179:GLY:HA3	1:D:216:PRO:O	2.08	0.53
7:A:2120:HOH:O	1:C:256:LYS:HE2	2.07	0.53
1:C:30:GLN:OE1	1:C:30:GLN:HA	2.07	0.53
1:F:101[A]:ASP:HB3	1:F:159:VAL:CG1	2.39	0.53
1:E:153:ALA:HA	1:F:173:TYR:CZ	2.44	0.53
1:B:7:LYS:HA	1:B:88:ASP:OD2	2.09	0.53
1:C:101[A]:ASP:HB3	7:C:2055:HOH:O	2.09	0.52
1:B:192:PRO:HG3	1:B:207:ILE:HG22	1.92	0.52
1:G:203:GLY:N	2:G:1258:GLU:HB2	2.24	0.52
1:C:249:ASP:O	1:C:250:SER:HB2	2.10	0.52
1:F:38:THR:HG21	1:F:65:ILE:HD12	1.90	0.52
1:H:210:GLU:HG3	1:H:214:ARG:HD2	1.91	0.52
1:A:184:ARG:HE	3:A:1257:MPD:H51	1.75	0.52
1:E:18[A]:ARG:HH21	1:E:199:LYS:HZ3	1.58	0.52
1:E:194:ARG:HG3	7:E:2112:HOH:O	2.09	0.52
1:E:101:ASP:OD2	1:E:113:GLY:HA3	2.10	0.51
1:D:155:GLN:O	1:D:156:ASN:HB2	2.11	0.51
1:D:99[A]:MET:O	1:D:101[A]:ASP:N	2.43	0.51
1:A:76:GLY:O	1:A:80:ILE:HG13	2.11	0.51
1:E:18[A]:ARG:HH21	1:E:199:LYS:NZ	2.08	0.51
1:B:249:ASP:O	1:B:250:SER:HB2	2.11	0.51
1:H:3:ASN:HD21	1:H:5:GLU:HG3	1.75	0.51
4:F:1259:NAP:O1N	4:F:1259:NAP:H2N	2.11	0.51
1:D:104[B]:GLY:HA3	7:D:2040:HOH:O	2.09	0.51
1:G:203:GLY:H	2:G:1258:GLU:HB2	1.75	0.50
1:F:207:ILE:O	1:F:211:ILE:HG12	2.10	0.50
1:H:184:ARG:HH21	3:H:1258:MPD:H51	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101[A]:ASP:C	1:C:102[A]:LEU:HG	2.32	0.50
1:G:173:TYR:CZ	1:H:153:ALA:HA	2.47	0.50
1:C:210:GLU:HG3	1:C:214[B]:ARG:HD2	1.93	0.50
1:H:7:LYS:HA	1:H:88:ASP:OD2	2.11	0.50
1:D:59:GLU:HG3	1:D:61:HIS:NE2	2.27	0.50
1:F:101[A]:ASP:O	1:F:102[A]:LEU:CG	2.59	0.50
1:H:100[A]:GLU:O	1:H:100[A]:GLU:HG3	2.11	0.50
1:C:4:LEU:O	1:C:7:LYS:HB2	2.11	0.50
1:F:104[A]:GLY:O	7:F:2061:HOH:O	2.20	0.49
1:H:5:GLU:O	1:H:6:ASN:HB2	2.11	0.49
1:F:225:GLU:OE2	1:G:239[B]:SER:OG	2.29	0.49
1:A:152:PHE:CG	1:C:256:LYS:HG3	2.46	0.49
1:A:207:ILE:O	1:A:211:ILE:HG12	2.12	0.49
1:A:41:LYS:HE2	1:E:100:GLU:CD	2.32	0.49
1:A:233:LEU:HD21	1:A:246:ILE:HD12	1.93	0.49
1:C:45[A]:ARG:NH1	1:C:49:GLU:OE2	2.45	0.49
1:B:101:ASP:OD2	1:B:113:GLY:HA3	2.13	0.49
1:A:5:GLU:O	1:A:6:ASN:HB2	2.12	0.49
1:E:18[A]:ARG:NH2	1:E:199:LYS:NZ	2.60	0.48
1:G:137:PRO:HD2	7:G:2075:HOH:O	2.12	0.48
1:B:233:LEU:HD21	1:B:246:ILE:HD12	1.94	0.48
1:H:133:LYS:HE3	1:H:181:ASP:OD2	2.13	0.48
1:C:147:TYR:CE2	5:C:1257:JA1:H13	2.49	0.48
1:H:213[B]:GLU:HG2	1:H:214:ARG:HG3	1.94	0.48
1:F:103[A]:ARG:N	1:F:103[A]:ARG:HD2	2.28	0.48
1:E:214[B]:ARG:NH2	7:E:2118:HOH:O	2.45	0.48
1:E:96:PHE:HA	5:E:1257:JA1:O3	2.14	0.48
1:E:192:PRO:HA	4:E:1261:NAP:O7N	2.13	0.48
1:F:147:TYR:HB2	4:F:1259:NAP:H5N	1.96	0.48
7:B:2096:HOH:O	1:C:239[B]:SER:O	2.20	0.47
1:H:99[B]:MET:HE1	1:H:200:GLY:O	2.13	0.47
1:F:133:LYS:HE2	1:F:181:ASP:OD2	2.14	0.47
1:F:43:ARG:HG3	1:F:43:ARG:O	2.14	0.47
1:A:29:ASP:OD1	1:A:57:GLN:NE2	2.39	0.47
1:F:147:TYR:HB2	4:F:1259:NAP:C5N	2.45	0.47
1:E:38:THR:HG21	1:E:65:ILE:HD12	1.96	0.47
1:C:12:MET:HG2	1:C:38:THR:OG1	2.14	0.47
1:C:197:SER:HB3	5:C:1257:JA1:C3	2.44	0.47
1:C:117:ALA:O	1:C:121:SER:HB2	2.15	0.47
1:A:173:TYR:CZ	1:B:153:ALA:HA	2.49	0.47
1:G:8:THR:HA	1:G:34:LYS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:TYR:CE1	1:G:45:ARG:HB2	2.50	0.47
1:C:46:LYS:HE2	7:C:2027:HOH:O	2.14	0.47
1:G:98:ASN:HB3	1:G:100[B]:GLU:CG	2.44	0.47
1:C:42:GLU:HB2	1:C:45[B]:ARG:NH1	2.29	0.47
1:H:37:PHE:CE2	1:H:52:LEU:HD11	2.49	0.47
1:D:41:LYS:HD3	1:D:43:ARG:NH1	2.29	0.46
1:F:101[A]:ASP:O	1:F:102[A]:LEU:HG	2.16	0.46
1:E:255:ILE:HG22	1:G:153:ALA:HB3	1.97	0.46
1:G:153:ALA:HA	1:H:173:TYR:CZ	2.50	0.46
1:G:99[A]:MET:O	1:G:101[A]:ASP:N	2.48	0.46
1:E:140:GLY:HA2	3:E:1260:MPD:C1	2.45	0.46
1:C:63:TYR:N	1:C:63:TYR:CD1	2.83	0.46
1:B:224:VAL:HG23	7:B:2098:HOH:O	2.15	0.46
1:F:89:GLY:HA2	1:F:141:SER:O	2.16	0.46
1:H:51:LEU:O	1:H:54:GLN:HB2	2.15	0.46
1:D:196:LEU:HD23	7:D:2082:HOH:O	2.16	0.45
1:C:39:TYR:CZ	1:C:64:GLN:HB2	2.50	0.45
1:E:52:LEU:HA	1:E:52:LEU:HD12	1.69	0.45
1:A:194:ARG:NH1	1:A:194:ARG:HG2	2.32	0.45
1:H:101[B]:ASP:OD2	1:H:113:GLY:HA3	2.17	0.45
1:E:256:LYS:HG2	1:G:148:LEU:CD2	2.44	0.45
1:B:194[A]:ARG:HG2	1:B:194[A]:ARG:HH11	1.81	0.45
1:D:38:THR:HG21	1:D:65:ILE:HD12	1.99	0.45
1:F:148:LEU:HD21	1:H:256:LYS:HE3	1.99	0.45
4:C:1261:NAP:H2N	4:C:1261:NAP:O1N	2.17	0.45
1:D:80:ILE:O	1:D:84[B]:VAL:HG22	2.17	0.45
1:A:82:LYS:HD2	7:A:2053:HOH:O	2.17	0.45
1:B:256:LYS:HE3	1:D:252:PHE:CE2	2.52	0.45
1:G:76:GLY:O	1:G:80:ILE:HG13	2.17	0.44
1:C:100[B]:GLU:H	1:C:100[B]:GLU:HG2	1.20	0.44
1:C:16:ASN:HA	1:C:47:GLU:HG3	1.98	0.44
1:B:207:ILE:O	1:B:211:ILE:HG12	2.16	0.44
1:B:233:LEU:HD21	1:B:246:ILE:CD1	2.47	0.44
1:H:67:VAL:HB	1:H:124:SER:HB2	1.99	0.44
1:F:17:LYS:HB3	1:F:51:LEU:HD21	1.99	0.44
1:C:105[A]:ARG:HD2	7:C:2059:HOH:O	2.18	0.44
1:E:5:GLU:O	1:E:6:ASN:HB2	2.18	0.44
1:H:38:THR:HA	1:H:63:TYR:O	2.18	0.44
1:D:217:LEU:HB2	1:D:250:SER:HB3	2.00	0.44
1:G:11:ILE:HD11	1:G:28:LEU:HD12	1.99	0.44
1:E:16:ASN:HB2	7:E:2011:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:GLU:OE2	1:C:50:LYS:CE	2.66	0.43
1:E:3:ASN:C	1:E:3:ASN:ND2	2.70	0.43
1:C:103[A]:ARG:HA	1:C:156:ASN:OD1	2.18	0.43
1:C:189:SER:HB3	1:C:247:HIS:HA	2.00	0.43
1:F:203:GLY:O	1:F:207:ILE:HG12	2.19	0.43
1:H:48:LEU:HD13	1:H:62:LEU:HD22	2.00	0.43
1:H:43:ARG:HG3	1:H:44:SER:N	2.32	0.43
1:C:87:ILE:HG12	1:C:135:LEU:HB2	2.01	0.43
1:G:100[B]:GLU:H	1:G:100[B]:GLU:HG2	1.27	0.43
1:E:215:ALA:O	1:E:218:LYS:HD3	2.19	0.43
1:B:218:LYS:HE2	1:C:180:PRO:HG3	2.01	0.43
1:B:52:LEU:HD23	1:B:55:LEU:HD12	2.00	0.43
1:G:184:ARG:HH21	3:G:1259:MPD:H4	1.84	0.42
1:C:103[A]:ARG:HG2	1:C:104[A]:GLY:N	2.34	0.42
1:A:188:ILE:HG23	1:A:248:VAL:HG23	2.01	0.42
1:G:101[A]:ASP:O	1:G:102[A]:LEU:CG	2.66	0.42
1:C:174:LEU:HB3	1:C:185:VAL:HG21	2.01	0.42
1:E:66:ASP:OD1	1:E:66:ASP:C	2.58	0.42
1:C:103[A]:ARG:HD2	1:C:103[A]:ARG:O	2.19	0.42
5:C:1257:JA1:O1	4:C:1261:NAP:H2D	2.20	0.42
1:G:87:ILE:HG12	1:G:135:LEU:HB2	2.02	0.42
1:A:133:LYS:HE3	7:B:2058:HOH:O	2.18	0.42
1:F:143:VAL:HA	1:F:186:ASN:O	2.20	0.42
1:A:192:PRO:HA	4:A:1258:NAP:O7N	2.20	0.42
1:A:11:ILE:HD11	1:A:28:LEU:HD12	2.02	0.42
1:H:37:PHE:HB2	1:H:62:LEU:HD23	2.01	0.42
1:C:216:PRO:HG2	1:C:251:GLY:HA3	2.01	0.42
3:H:1258:MPD:H4	3:H:1258:MPD:H11	1.81	0.41
1:G:36:VAL:HG11	1:G:80:ILE:HD13	2.02	0.41
1:B:17:LYS:CB	1:B:51:LEU:HD21	2.50	0.41
1:G:207:ILE:HG13	5:G:1257:JA1:H16B	2.01	0.41
1:A:119:ASP:OD1	1:B:111:ARG:NH1	2.51	0.41
1:A:214[A]:ARG:NH2	7:A:2120:HOH:O	2.54	0.41
1:C:203:GLY:O	1:C:207:ILE:HG12	2.21	0.41
1:H:57:GLN:HA	1:H:58:PRO:HD3	1.91	0.41
1:G:67:VAL:CG2	1:G:124:SER:HB3	2.51	0.41
1:G:206:THR:HG23	2:G:1258:GLU:OE2	2.20	0.41
3:E:1260:MPD:O4	3:E:1260:MPD:C1	2.69	0.41
1:F:39:TYR:OH	1:F:45:ARG:HD2	2.19	0.41
1:F:158:ASN:HB3	7:F:2059:HOH:O	2.20	0.41
1:E:188:ILE:HG21	1:E:226:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:TYR:CZ	1:F:153:ALA:HA	2.56	0.41
1:H:112[A]:GLU:H	1:H:112[A]:GLU:CD	2.23	0.41
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.90	0.41
1:B:5:GLU:O	1:B:6:ASN:HB2	2.21	0.41
1:H:114:PHE:C	1:H:114:PHE:CD1	2.94	0.41
1:F:22:PHE:CE2	1:F:26:LYS:HE2	2.55	0.41
1:B:147:TYR:HB2	4:B:1259:NAP:C5N	2.50	0.41
1:G:99[A]:MET:C	1:G:101[A]:ASP:N	2.71	0.41
1:C:103[A]:ARG:HD2	1:C:103[A]:ARG:C	2.41	0.41
1:E:209:LYS:HE2	1:E:209:LYS:HB3	1.93	0.41
1:E:59:GLU:HG3	1:E:61:HIS:CE1	2.56	0.41
1:C:38:THR:HA	1:C:63:TYR:O	2.21	0.41
1:C:105[B]:ARG:NH2	1:D:177:ASP:O	2.51	0.41
1:E:216:PRO:O	1:H:179:GLY:HA3	2.21	0.41
1:E:42[B]:GLU:OE1	1:E:45:ARG:NH1	2.46	0.40
1:H:3:ASN:ND2	1:H:5:GLU:HG3	2.37	0.40
1:C:96:PHE:HA	5:C:1257:JA1:O3	2.21	0.40
1:C:192:PRO:HA	4:C:1261:NAP:O7N	2.21	0.40
1:G:39:TYR:CZ	1:G:45:ARG:HB2	2.55	0.40
1:B:18:ARG:O	1:B:195:THR:HG22	2.22	0.40
1:A:136:MET:N	1:A:137:PRO:HD3	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:ARG:NH1	7:B:2051:HOH:O[1_554]	2.03	0.17
1:C:43:ARG:NH1	7:F:2058:HOH:O[1_545]	2.11	0.09

## 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	257/282 (91%)	244 (95%)	12 (5%)	1 (0%)	39	48
1	B	253/282 (90%)	243 (96%)	10 (4%)	0	100	100
1	C	264/282 (94%)	253 (96%)	11 (4%)	0	100	100
1	D	263/282 (93%)	250 (95%)	12 (5%)	1 (0%)	39	48
1	E	256/282 (91%)	246 (96%)	10 (4%)	0	100	100
1	F	261/282 (93%)	246 (94%)	14 (5%)	1 (0%)	39	48
1	G	264/282 (94%)	252 (96%)	12 (4%)	0	100	100
1	H	261/282 (93%)	243 (93%)	18 (7%)	0	100	100
All	All	2079/2256 (92%)	1977 (95%)	99 (5%)	3 (0%)	56	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	46	LYS
1	F	194	ARG
1	A	194	ARG

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/234 (91%)	208 (98%)	4 (2%)	65	81
1	B	209/234 (89%)	200 (96%)	9 (4%)	35	47
1	C	218/234 (93%)	207 (95%)	11 (5%)	30	41
1	D	217/234 (93%)	206 (95%)	11 (5%)	29	39
1	E	212/234 (91%)	207 (98%)	5 (2%)	57	74
1	F	215/234 (92%)	208 (97%)	7 (3%)	45	61
1	G	218/234 (93%)	210 (96%)	8 (4%)	41	55
1	H	216/234 (92%)	203 (94%)	13 (6%)	24	31
All	All	1717/1872 (92%)	1649 (96%)	68 (4%)	41	52

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	59	GLU
1	A	138	GLU
1	A	210	GLU
1	B	4	LEU
1	B	17	LYS
1	B	50	LYS
1	B	82	LYS
1	B	138	GLU
1	B	199	LYS
1	B	206	THR
1	B	207	ILE
1	B	210	GLU
1	C	47	GLU
1	C	55	LEU
1	C	101[A]	ASP
1	C	101[B]	ASP
1	C	103[A]	ARG
1	C	103[B]	ARG
1	C	105[A]	ARG
1	C	105[B]	ARG
1	C	138	GLU
1	C	237	LEU
1	C	256	LYS
1	D	4	LEU
1	D	47	GLU
1	D	48	LEU
1	D	62	LEU
1	D	99[A]	MET
1	D	99[B]	MET
1	D	103[A]	ARG
1	D	103[B]	ARG
1	D	194	ARG
1	D	209	LYS
1	D	228	LYS
1	E	52	LEU
1	E	79	GLN
1	E	82	LYS
1	E	207	ILE
1	E	237	LEU
1	F	4	LEU
1	F	30	GLN

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Mol	Chain	Res	Type
1	F	55	LEU
1	F	103[A]	ARG
1	F	103[B]	ARG
1	F	105[A]	ARG
1	F	105[B]	ARG
1	G	34	LYS
1	G	43	ARG
1	G	53	GLU
1	G	55	LEU
1	G	103[A]	ARG
1	G	103[B]	ARG
1	G	112	GLU
1	G	209	LYS
1	H	4	LEU
1	H	7	LYS
1	H	41	LYS
1	H	42	GLU
1	H	43	ARG
1	H	59	GLU
1	H	64	GLN
1	H	78	GLU
1	H	84	VAL
1	H	100[A]	GLU
1	H	100[B]	GLU
1	H	237	LEU
1	H	256	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	79	GLN
1	A	253	HIS
1	B	56	ASN
1	D	155	GLN
1	E	3	ASN
1	E	253	HIS
1	H	155	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

29 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	MPD	A	1257	-	6,7,7	0.38	0	7,10,10	0.35	0
4	NAP	A	1258	-	42,52,52	1.58	3 (7%)	54,80,80	2.10	8 (14%)
5	JA1	A	1259	-	22,24,24	0.19	0	29,31,31	0.68	0
2	GLU	B	1001	-	3,9,9	0.28	0	2,11,11	0.21	0
5	JA1	B	1257	-	22,24,24	0.21	0	29,31,31	0.69	0
6	MRD	B	1258	-	6,7,7	0.31	0	7,10,10	0.53	0
4	NAP	B	1259	-	42,52,52	1.41	3 (7%)	54,80,80	2.29	10 (18%)
5	JA1	C	1257	-	22,24,24	0.19	0	29,31,31	0.65	0
5	JA1	C	1258	-	22,24,24	0.17	0	29,31,31	0.62	0
2	GLU	C	1259	-	3,9,9	0.31	0	2,11,11	0.30	0
3	MPD	C	1260	-	6,7,7	0.37	0	7,10,10	0.43	0
4	NAP	C	1261	-	42,52,52	1.49	3 (7%)	54,80,80	2.08	6 (11%)
3	MPD	D	1257	-	6,7,7	0.44	0	7,10,10	0.66	0
4	NAP	D	1258	-	42,52,52	1.52	3 (7%)	54,80,80	2.28	8 (14%)
5	JA1	E	1257	-	22,24,24	0.21	0	29,31,31	0.64	0
5	JA1	E	1258	-	22,24,24	0.18	0	29,31,31	0.65	0
2	GLU	E	1259	-	3,9,9	0.23	0	2,11,11	1.30	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MPD	E	1260	-	6,7,7	0.46	0	7,10,10	0.65	0
4	NAP	E	1261	-	42,52,52	1.45	3 (7%)	54,80,80	2.54	12 (22%)
2	GLU	F	1257	-	3,9,9	0.30	0	2,11,11	0.17	0
3	MPD	F	1258	-	6,7,7	0.49	0	7,10,10	0.56	0
4	NAP	F	1259	-	42,52,52	1.48	3 (7%)	54,80,80	2.07	8 (14%)
5	JA1	G	1257	-	22,24,24	0.19	0	29,31,31	0.59	0
2	GLU	G	1258	-	3,9,9	0.43	0	2,11,11	0.39	0
3	MPD	G	1259	-	6,7,7	0.44	0	7,10,10	0.41	0
4	NAP	G	1260	-	42,52,52	1.50	3 (7%)	54,80,80	2.25	7 (12%)
5	JA1	H	1257	-	22,24,24	0.16	0	29,31,31	0.64	0
3	MPD	H	1258	-	6,7,7	0.41	0	7,10,10	0.54	0
4	NAP	H	1259	-	42,52,52	1.57	3 (7%)	54,80,80	2.24	6 (11%)

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	MPD	A	1257	-	-	0/5/5/5	0/0/0/0
4	NAP	A	1258	-	-	0/27/67/67	0/5/5/5
5	JA1	A	1259	-	-	0/14/14/14	0/2/2/2
2	GLU	B	1001	-	-	0/3/9/9	0/0/0/0
5	JA1	B	1257	-	-	0/14/14/14	0/2/2/2
6	MRD	B	1258	-	-	0/5/5/5	0/0/0/0
4	NAP	B	1259	-	-	0/27/67/67	0/5/5/5
5	JA1	C	1257	-	-	0/14/14/14	0/2/2/2
5	JA1	C	1258	-	-	0/14/14/14	0/2/2/2
2	GLU	C	1259	-	-	0/3/9/9	0/0/0/0
3	MPD	C	1260	-	-	0/5/5/5	0/0/0/0
4	NAP	C	1261	-	-	0/27/67/67	0/5/5/5
3	MPD	D	1257	-	-	0/5/5/5	0/0/0/0
4	NAP	D	1258	-	-	0/27/67/67	0/5/5/5
5	JA1	E	1257	-	-	0/14/14/14	0/2/2/2
5	JA1	E	1258	-	-	0/14/14/14	0/2/2/2
2	GLU	E	1259	-	-	0/3/9/9	0/0/0/0
3	MPD	E	1260	-	-	0/5/5/5	0/0/0/0
4	NAP	E	1261	-	-	0/27/67/67	0/5/5/5
2	GLU	F	1257	-	-	0/3/9/9	0/0/0/0
3	MPD	F	1258	-	-	0/5/5/5	0/0/0/0
4	NAP	F	1259	-	-	0/27/67/67	0/5/5/5
5	JA1	G	1257	-	-	0/14/14/14	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	G	1258	-	-	0/3/9/9	0/0/0/0
3	MPD	G	1259	-	-	0/5/5/5	0/0/0/0
4	NAP	G	1260	-	-	0/27/67/67	0/5/5/5
5	JA1	H	1257	-	-	0/14/14/14	0/2/2/2
3	MPD	H	1258	-	-	0/5/5/5	0/0/0/0
4	NAP	H	1259	-	-	0/27/67/67	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1258	NAP	C2A-N1A	2.00	1.37	1.33
4	F	1259	NAP	C2A-N1A	2.02	1.37	1.33
4	E	1261	NAP	C2A-N1A	2.10	1.37	1.33
4	B	1259	NAP	C2A-N1A	2.27	1.38	1.33
4	C	1261	NAP	C2A-N1A	2.41	1.38	1.33
4	G	1260	NAP	C2A-N1A	2.64	1.38	1.33
4	A	1258	NAP	C2A-N1A	2.68	1.39	1.33
4	H	1259	NAP	C2A-N1A	2.77	1.39	1.33
4	B	1259	NAP	C2A-N3A	2.79	1.37	1.32
4	G	1260	NAP	C2A-N3A	3.02	1.37	1.32
4	C	1261	NAP	C2A-N3A	3.02	1.37	1.32
4	E	1261	NAP	C2A-N3A	3.26	1.38	1.32
4	A	1258	NAP	C2A-N3A	3.40	1.38	1.32
4	F	1259	NAP	C2A-N3A	3.48	1.38	1.32
4	D	1258	NAP	C2A-N3A	3.50	1.38	1.32
4	H	1259	NAP	C2A-N3A	3.75	1.38	1.32
4	B	1259	NAP	O7N-C7N	6.93	1.38	1.24
4	E	1261	NAP	O7N-C7N	7.01	1.39	1.24
4	G	1260	NAP	O7N-C7N	7.21	1.39	1.24
4	F	1259	NAP	O7N-C7N	7.37	1.39	1.24
4	C	1261	NAP	O7N-C7N	7.46	1.40	1.24
4	H	1259	NAP	O7N-C7N	7.51	1.40	1.24
4	D	1258	NAP	O7N-C7N	7.59	1.40	1.24
4	A	1258	NAP	O7N-C7N	7.61	1.40	1.24

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1261	NAP	N3A-C2A-N1A	-14.00	118.17	128.89
4	D	1258	NAP	N3A-C2A-N1A	-12.86	119.05	128.89
4	H	1259	NAP	N3A-C2A-N1A	-12.77	119.12	128.89
4	C	1261	NAP	N3A-C2A-N1A	-11.83	119.83	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1260	NAP	N3A-C2A-N1A	-11.73	119.91	128.89
4	A	1258	NAP	N3A-C2A-N1A	-11.56	120.04	128.89
4	B	1259	NAP	N3A-C2A-N1A	-10.78	120.64	128.89
4	F	1259	NAP	N3A-C2A-N1A	-10.03	121.22	128.89
4	B	1259	NAP	O7N-C7N-C3N	-6.17	112.85	119.59
4	A	1258	NAP	C4B-O4B-C1B	-5.37	103.82	109.72
4	F	1259	NAP	O7N-C7N-C3N	-5.23	113.87	119.59
4	B	1259	NAP	C4B-O4B-C1B	-5.17	104.04	109.72
4	D	1258	NAP	C4B-O4B-C1B	-4.56	104.71	109.72
4	G	1260	NAP	C4B-O4B-C1B	-4.11	105.20	109.72
4	E	1261	NAP	O7N-C7N-C3N	-3.75	115.49	119.59
4	G	1260	NAP	O7N-C7N-C3N	-3.61	115.64	119.59
4	H	1259	NAP	C4B-O4B-C1B	-3.46	105.91	109.72
4	C	1261	NAP	O7N-C7N-C3N	-3.21	116.08	119.59
4	F	1259	NAP	C4B-O4B-C1B	-3.13	106.28	109.72
4	F	1259	NAP	O4B-C1B-C2B	-3.02	101.14	106.60
4	G	1260	NAP	C4A-C5A-N7A	-2.99	106.73	109.48
4	H	1259	NAP	O7N-C7N-N7N	-2.90	118.52	122.59
4	F	1259	NAP	C4D-O4D-C1D	-2.79	106.65	109.72
4	H	1259	NAP	C1B-N9A-C4A	-2.72	122.84	126.94
4	D	1258	NAP	O4B-C1B-C2B	-2.71	101.69	106.60
4	C	1261	NAP	C4B-O4B-C1B	-2.69	106.76	109.72
4	A	1258	NAP	C1B-N9A-C4A	-2.66	122.92	126.94
4	E	1261	NAP	O4B-C1B-C2B	-2.58	101.93	106.60
4	E	1261	NAP	O7N-C7N-N7N	-2.55	119.01	122.59
4	E	1261	NAP	C1B-N9A-C4A	-2.48	123.20	126.94
4	A	1258	NAP	O7N-C7N-C3N	-2.47	116.89	119.59
4	E	1261	NAP	O5B-C5B-C4B	-2.37	100.37	109.12
4	D	1258	NAP	O7N-C7N-N7N	-2.35	119.29	122.59
4	C	1261	NAP	C4A-C5A-N7A	-2.34	107.32	109.48
4	E	1261	NAP	C4B-O4B-C1B	-2.34	107.15	109.72
4	C	1261	NAP	C1B-N9A-C4A	-2.33	123.42	126.94
4	D	1258	NAP	O5B-C5B-C4B	-2.32	100.56	109.12
4	B	1259	NAP	O5B-C5B-C4B	-2.29	100.69	109.12
4	A	1258	NAP	C4A-C5A-N7A	-2.27	107.39	109.48
4	B	1259	NAP	O4B-C1B-C2B	-2.19	102.65	106.60
4	B	1259	NAP	C3N-C2N-N1N	-2.14	117.89	120.36
4	H	1259	NAP	O2N-PN-O1N	2.02	123.47	112.53
4	A	1258	NAP	O4B-C1B-N9A	2.07	112.43	108.10
4	F	1259	NAP	O2N-PN-O1N	2.11	123.96	112.53
4	F	1259	NAP	O4B-C1B-N9A	2.12	112.53	108.10
4	E	1261	NAP	O2N-PN-O1N	2.13	124.07	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1259	NAP	O4B-C1B-N9A	2.23	112.77	108.10
4	E	1261	NAP	C2A-N1A-C6A	2.24	122.76	118.77
4	B	1259	NAP	O2N-PN-O1N	2.24	124.68	112.53
4	B	1259	NAP	C2N-C3N-C4N	2.31	120.86	118.29
4	D	1258	NAP	O4B-C1B-N9A	2.34	113.00	108.10
4	G	1260	NAP	O3-PA-O5B	2.41	109.33	102.94
4	A	1258	NAP	O2N-PN-O1N	2.45	125.81	112.53
4	E	1261	NAP	O4B-C1B-N9A	2.49	113.30	108.10
4	G	1260	NAP	O4B-C1B-N9A	2.63	113.59	108.10
4	D	1258	NAP	O4D-C1D-N1N	3.21	111.66	108.13
4	E	1261	NAP	O4D-C1D-N1N	4.17	112.72	108.13
4	C	1261	NAP	C3N-C7N-N7N	4.26	122.48	117.82
4	A	1258	NAP	C3N-C7N-N7N	4.31	122.53	117.82
4	D	1258	NAP	C3N-C7N-N7N	4.66	122.92	117.82
4	H	1259	NAP	C3N-C7N-N7N	5.43	123.76	117.82
4	G	1260	NAP	C3N-C7N-N7N	5.84	124.21	117.82
4	F	1259	NAP	C3N-C7N-N7N	5.90	124.27	117.82
4	B	1259	NAP	C3N-C7N-N7N	6.83	125.30	117.82
4	E	1261	NAP	C3N-C7N-N7N	7.02	125.50	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1257	MPD	3	0
4	A	1258	NAP	1	0
5	A	1259	JA1	1	0
6	B	1258	MRD	1	0
4	B	1259	NAP	1	0
5	C	1257	JA1	6	0
4	C	1261	NAP	3	0
3	D	1257	MPD	1	0
5	E	1257	JA1	1	0
3	E	1260	MPD	6	0
4	E	1261	NAP	1	0
4	F	1259	NAP	3	0
5	G	1257	JA1	1	0
2	G	1258	GLU	5	0
3	G	1259	MPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1258	MPD	7	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	254/282 (90%)	-0.40	0 100 100	22, 33, 54, 69	0
1	B	254/282 (90%)	-0.36	0 100 100	24, 35, 58, 69	0
1	C	254/282 (90%)	-0.33	2 (0%) 87 90	26, 36, 55, 68	0
1	D	254/282 (90%)	-0.10	8 (3%) 52 62	26, 39, 72, 87	0
1	E	254/282 (90%)	-0.42	2 (0%) 87 90	24, 33, 53, 67	0
1	F	254/282 (90%)	-0.50	2 (0%) 87 90	24, 34, 57, 64	0
1	G	255/282 (90%)	-0.30	2 (0%) 87 90	26, 35, 54, 71	0
1	H	254/282 (90%)	-0.33	4 (1%) 74 80	26, 38, 62, 83	0
All	All	2033/2256 (90%)	-0.34	20 (0%) 84 88	22, 36, 59, 87	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	58	PRO	4.2
1	C	58	PRO	3.7
1	D	100[A]	GLU	3.2
1	F	6	ASN	2.9
1	H	58	PRO	2.9
1	D	103[A]	ARG	2.8
1	D	58	PRO	2.7
1	C	6	ASN	2.6
1	F	58	PRO	2.4
1	D	99[A]	MET	2.4
1	E	6	ASN	2.4
1	E	58	PRO	2.3
1	H	100[A]	GLU	2.2
1	D	43	ARG	2.2
1	H	103[A]	ARG	2.1
1	D	59	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	104[A]	GLY	2.1
1	H	43	ARG	2.1
1	D	102[A]	LEU	2.0
1	D	194	ARG	2.0

## 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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	GLU	B	1001	10/10	0.42	0.36	10.66	96,99,105,106	0
3	MPD	D	1257	8/8	0.70	0.27	9.29	67,71,73,74	0
3	MPD	H	1258	8/8	0.82	0.24	9.27	56,64,66,67	0
6	MRD	B	1258	8/8	0.76	0.23	7.75	84,90,92,92	0
2	GLU	F	1257	10/10	0.37	0.42	7.57	115,116,118,118	0
2	GLU	E	1259	10/10	0.69	0.23	7.21	97,98,100,100	0
3	MPD	G	1259	8/8	0.79	0.21	6.04	54,65,68,68	0
3	MPD	E	1260	8/8	0.81	0.29	5.30	63,69,72,72	0
3	MPD	F	1258	8/8	0.79	0.22	4.30	51,58,60,61	0
2	GLU	C	1259	10/10	0.53	0.25	3.20	91,95,96,97	0
3	MPD	C	1260	8/8	0.84	0.19	3.08	60,68,71,71	0
3	MPD	A	1257	8/8	0.85	0.15	2.51	68,74,75,75	0
2	GLU	G	1258	10/10	0.72	0.17	1.45	78,79,82,84	0
5	JA1	A	1259	23/23	0.95	0.11	0.68	30,35,44,49	0
5	JA1	C	1257	23/23	0.95	0.12	0.60	33,39,48,52	0
5	JA1	C	1258	23/23	0.94	0.17	0.35	41,51,58,61	0
5	JA1	G	1257	23/23	0.95	0.13	0.35	36,40,46,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	JA1	H	1257	23/23	0.94	0.12	0.21	33,42,50,51	0
5	JA1	E	1257	23/23	0.97	0.11	0.04	30,32,38,40	0
5	JA1	E	1258	23/23	0.96	0.11	-0.14	30,37,44,47	0
4	NAP	E	1261	48/48	0.98	0.10	-0.31	26,32,36,40	0
4	NAP	G	1260	48/48	0.98	0.10	-0.35	27,34,38,40	0
4	NAP	A	1258	48/48	0.98	0.08	-0.37	27,31,35,42	0
4	NAP	F	1259	48/48	0.99	0.09	-0.55	29,34,38,43	0
4	NAP	H	1259	48/48	0.97	0.09	-0.56	28,38,59,61	0
4	NAP	C	1261	48/48	0.98	0.09	-0.57	28,37,41,43	0
4	NAP	D	1258	48/48	0.97	0.09	-0.61	31,42,62,67	0
5	JA1	B	1257	23/23	0.97	0.10	-0.66	27,37,42,48	0
4	NAP	B	1259	48/48	0.98	0.09	-0.81	25,34,38,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.