



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 11:36 AM EST

PDB ID : 5V12  
Title : Crystal structure of Carbon Sulfoxide lyase, Egt2 Y134F with sulfenic acid intermediate  
Authors : Irani, S.; Zhang, Y.  
Deposited on : 2017-03-01  
Resolution : 2.45 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

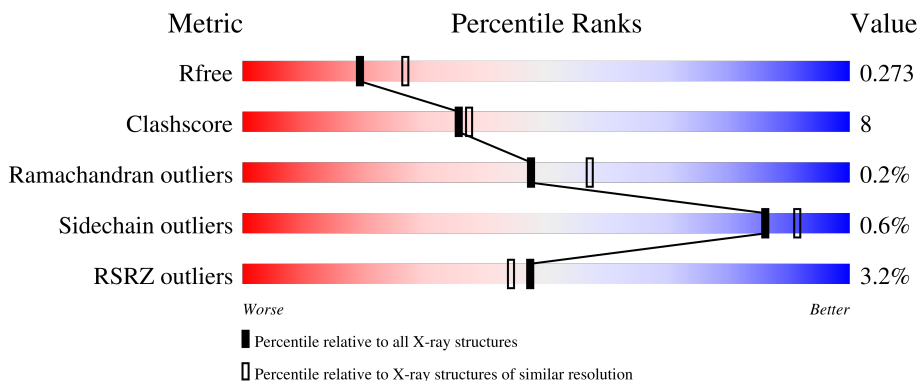
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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.



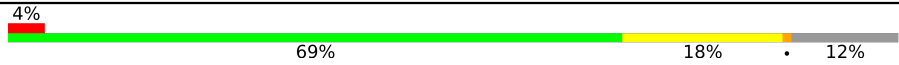

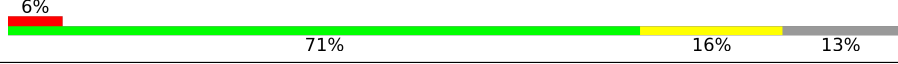
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	501	
1	B	501	
1	D	501	
1	E	501	
1	F	501	

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Mol	Chain	Length	Quality of chain
1	G	501	 4% 69% 18% 12%
1	H	501	 2% 72% 15% 13%
2	C	501	 6% 71% 16% 13%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 28363 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 Hercynylcysteine sulfoxide lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	E	436	3475	2226	586	642	1	20	0	0	0
1	G	441	3506	2244	592	649	1	20	0	0	0
1	F	440	3499	2239	591	648	1	20	0	0	0
1	H	435	3470	2222	585	642	1	20	0	0	0
1	D	438	3486	2233	588	644	1	20	0	0	0
1	A	439	3491	2236	589	645	1	20	0	0	0
1	B	437	3483	2230	588	644	1	20	0	0	0

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	MET	-	initiating methionine	UNP A7UX13
E	-5	GLY	-	expression tag	UNP A7UX13
E	-4	ASP	-	expression tag	UNP A7UX13
E	-3	ARG	-	expression tag	UNP A7UX13
E	-2	GLY	-	expression tag	UNP A7UX13
E	-1	PRO	-	expression tag	UNP A7UX13
E	0	GLU	-	expression tag	UNP A7UX13
E	1	PHE	-	expression tag	UNP A7UX13
E	134	PHE	TYR	conflict	UNP A7UX13
E	474	LEU	-	expression tag	UNP A7UX13
E	475	GLU	-	expression tag	UNP A7UX13
E	476	VAL	-	expression tag	UNP A7UX13
E	477	ASP	-	expression tag	UNP A7UX13
E	478	LEU	-	expression tag	UNP A7UX13
E	479	GLN	-	expression tag	UNP A7UX13

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Chain	Residue	Modelled	Actual	Comment	Reference
E	480	GLY	-	expression tag	UNP A7UX13
E	481	ASP	-	expression tag	UNP A7UX13
E	482	HIS	-	expression tag	UNP A7UX13
E	483	GLY	-	expression tag	UNP A7UX13
E	484	LEU	-	expression tag	UNP A7UX13
E	485	SER	-	expression tag	UNP A7UX13
E	486	ALA	-	expression tag	UNP A7UX13
E	487	TRP	-	expression tag	UNP A7UX13
E	488	SER	-	expression tag	UNP A7UX13
E	489	HIS	-	expression tag	UNP A7UX13
E	490	PRO	-	expression tag	UNP A7UX13
E	491	GLN	-	expression tag	UNP A7UX13
E	492	PHE	-	expression tag	UNP A7UX13
E	493	GLU	-	expression tag	UNP A7UX13
E	494	LYS	-	expression tag	UNP A7UX13
G	-6	MET	-	initiating methionine	UNP A7UX13
G	-5	GLY	-	expression tag	UNP A7UX13
G	-4	ASP	-	expression tag	UNP A7UX13
G	-3	ARG	-	expression tag	UNP A7UX13
G	-2	GLY	-	expression tag	UNP A7UX13
G	-1	PRO	-	expression tag	UNP A7UX13
G	0	GLU	-	expression tag	UNP A7UX13
G	1	PHE	-	expression tag	UNP A7UX13
G	134	PHE	TYR	conflict	UNP A7UX13
G	474	LEU	-	expression tag	UNP A7UX13
G	475	GLU	-	expression tag	UNP A7UX13
G	476	VAL	-	expression tag	UNP A7UX13
G	477	ASP	-	expression tag	UNP A7UX13
G	478	LEU	-	expression tag	UNP A7UX13
G	479	GLN	-	expression tag	UNP A7UX13
G	480	GLY	-	expression tag	UNP A7UX13
G	481	ASP	-	expression tag	UNP A7UX13
G	482	HIS	-	expression tag	UNP A7UX13
G	483	GLY	-	expression tag	UNP A7UX13
G	484	LEU	-	expression tag	UNP A7UX13
G	485	SER	-	expression tag	UNP A7UX13
G	486	ALA	-	expression tag	UNP A7UX13
G	487	TRP	-	expression tag	UNP A7UX13
G	488	SER	-	expression tag	UNP A7UX13
G	489	HIS	-	expression tag	UNP A7UX13
G	490	PRO	-	expression tag	UNP A7UX13
G	491	GLN	-	expression tag	UNP A7UX13

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Chain	Residue	Modelled	Actual	Comment	Reference
G	492	PHE	-	expression tag	UNP A7UX13
G	493	GLU	-	expression tag	UNP A7UX13
G	494	LYS	-	expression tag	UNP A7UX13
F	-6	MET	-	initiating methionine	UNP A7UX13
F	-5	GLY	-	expression tag	UNP A7UX13
F	-4	ASP	-	expression tag	UNP A7UX13
F	-3	ARG	-	expression tag	UNP A7UX13
F	-2	GLY	-	expression tag	UNP A7UX13
F	-1	PRO	-	expression tag	UNP A7UX13
F	0	GLU	-	expression tag	UNP A7UX13
F	1	PHE	-	expression tag	UNP A7UX13
F	134	PHE	TYR	conflict	UNP A7UX13
F	474	LEU	-	expression tag	UNP A7UX13
F	475	GLU	-	expression tag	UNP A7UX13
F	476	VAL	-	expression tag	UNP A7UX13
F	477	ASP	-	expression tag	UNP A7UX13
F	478	LEU	-	expression tag	UNP A7UX13
F	479	GLN	-	expression tag	UNP A7UX13
F	480	GLY	-	expression tag	UNP A7UX13
F	481	ASP	-	expression tag	UNP A7UX13
F	482	HIS	-	expression tag	UNP A7UX13
F	483	GLY	-	expression tag	UNP A7UX13
F	484	LEU	-	expression tag	UNP A7UX13
F	485	SER	-	expression tag	UNP A7UX13
F	486	ALA	-	expression tag	UNP A7UX13
F	487	TRP	-	expression tag	UNP A7UX13
F	488	SER	-	expression tag	UNP A7UX13
F	489	HIS	-	expression tag	UNP A7UX13
F	490	PRO	-	expression tag	UNP A7UX13
F	491	GLN	-	expression tag	UNP A7UX13
F	492	PHE	-	expression tag	UNP A7UX13
F	493	GLU	-	expression tag	UNP A7UX13
F	494	LYS	-	expression tag	UNP A7UX13
H	-6	MET	-	initiating methionine	UNP A7UX13
H	-5	GLY	-	expression tag	UNP A7UX13
H	-4	ASP	-	expression tag	UNP A7UX13
H	-3	ARG	-	expression tag	UNP A7UX13
H	-2	GLY	-	expression tag	UNP A7UX13
H	-1	PRO	-	expression tag	UNP A7UX13
H	0	GLU	-	expression tag	UNP A7UX13
H	1	PHE	-	expression tag	UNP A7UX13
H	134	PHE	TYR	conflict	UNP A7UX13

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Chain	Residue	Modelled	Actual	Comment	Reference
H	474	LEU	-	expression tag	UNP A7UX13
H	475	GLU	-	expression tag	UNP A7UX13
H	476	VAL	-	expression tag	UNP A7UX13
H	477	ASP	-	expression tag	UNP A7UX13
H	478	LEU	-	expression tag	UNP A7UX13
H	479	GLN	-	expression tag	UNP A7UX13
H	480	GLY	-	expression tag	UNP A7UX13
H	481	ASP	-	expression tag	UNP A7UX13
H	482	HIS	-	expression tag	UNP A7UX13
H	483	GLY	-	expression tag	UNP A7UX13
H	484	LEU	-	expression tag	UNP A7UX13
H	485	SER	-	expression tag	UNP A7UX13
H	486	ALA	-	expression tag	UNP A7UX13
H	487	TRP	-	expression tag	UNP A7UX13
H	488	SER	-	expression tag	UNP A7UX13
H	489	HIS	-	expression tag	UNP A7UX13
H	490	PRO	-	expression tag	UNP A7UX13
H	491	GLN	-	expression tag	UNP A7UX13
H	492	PHE	-	expression tag	UNP A7UX13
H	493	GLU	-	expression tag	UNP A7UX13
H	494	LYS	-	expression tag	UNP A7UX13
D	-6	MET	-	initiating methionine	UNP A7UX13
D	-5	GLY	-	expression tag	UNP A7UX13
D	-4	ASP	-	expression tag	UNP A7UX13
D	-3	ARG	-	expression tag	UNP A7UX13
D	-2	GLY	-	expression tag	UNP A7UX13
D	-1	PRO	-	expression tag	UNP A7UX13
D	0	GLU	-	expression tag	UNP A7UX13
D	1	PHE	-	expression tag	UNP A7UX13
D	134	PHE	TYR	conflict	UNP A7UX13
D	474	LEU	-	expression tag	UNP A7UX13
D	475	GLU	-	expression tag	UNP A7UX13
D	476	VAL	-	expression tag	UNP A7UX13
D	477	ASP	-	expression tag	UNP A7UX13
D	478	LEU	-	expression tag	UNP A7UX13
D	479	GLN	-	expression tag	UNP A7UX13
D	480	GLY	-	expression tag	UNP A7UX13
D	481	ASP	-	expression tag	UNP A7UX13
D	482	HIS	-	expression tag	UNP A7UX13
D	483	GLY	-	expression tag	UNP A7UX13
D	484	LEU	-	expression tag	UNP A7UX13
D	485	SER	-	expression tag	UNP A7UX13

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Chain	Residue	Modelled	Actual	Comment	Reference
D	486	ALA	-	expression tag	UNP A7UX13
D	487	TRP	-	expression tag	UNP A7UX13
D	488	SER	-	expression tag	UNP A7UX13
D	489	HIS	-	expression tag	UNP A7UX13
D	490	PRO	-	expression tag	UNP A7UX13
D	491	GLN	-	expression tag	UNP A7UX13
D	492	PHE	-	expression tag	UNP A7UX13
D	493	GLU	-	expression tag	UNP A7UX13
D	494	LYS	-	expression tag	UNP A7UX13
A	-6	MET	-	initiating methionine	UNP A7UX13
A	-5	GLY	-	expression tag	UNP A7UX13
A	-4	ASP	-	expression tag	UNP A7UX13
A	-3	ARG	-	expression tag	UNP A7UX13
A	-2	GLY	-	expression tag	UNP A7UX13
A	-1	PRO	-	expression tag	UNP A7UX13
A	0	GLU	-	expression tag	UNP A7UX13
A	1	PHE	-	expression tag	UNP A7UX13
A	134	PHE	TYR	conflict	UNP A7UX13
A	474	LEU	-	expression tag	UNP A7UX13
A	475	GLU	-	expression tag	UNP A7UX13
A	476	VAL	-	expression tag	UNP A7UX13
A	477	ASP	-	expression tag	UNP A7UX13
A	478	LEU	-	expression tag	UNP A7UX13
A	479	GLN	-	expression tag	UNP A7UX13
A	480	GLY	-	expression tag	UNP A7UX13
A	481	ASP	-	expression tag	UNP A7UX13
A	482	HIS	-	expression tag	UNP A7UX13
A	483	GLY	-	expression tag	UNP A7UX13
A	484	LEU	-	expression tag	UNP A7UX13
A	485	SER	-	expression tag	UNP A7UX13
A	486	ALA	-	expression tag	UNP A7UX13
A	487	TRP	-	expression tag	UNP A7UX13
A	488	SER	-	expression tag	UNP A7UX13
A	489	HIS	-	expression tag	UNP A7UX13
A	490	PRO	-	expression tag	UNP A7UX13
A	491	GLN	-	expression tag	UNP A7UX13
A	492	PHE	-	expression tag	UNP A7UX13
A	493	GLU	-	expression tag	UNP A7UX13
A	494	LYS	-	expression tag	UNP A7UX13
B	-6	MET	-	initiating methionine	UNP A7UX13
B	-5	GLY	-	expression tag	UNP A7UX13
B	-4	ASP	-	expression tag	UNP A7UX13

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	ARG	-	expression tag	UNP A7UX13
B	-2	GLY	-	expression tag	UNP A7UX13
B	-1	PRO	-	expression tag	UNP A7UX13
B	0	GLU	-	expression tag	UNP A7UX13
B	1	PHE	-	expression tag	UNP A7UX13
B	134	PHE	TYR	conflict	UNP A7UX13
B	474	LEU	-	expression tag	UNP A7UX13
B	475	GLU	-	expression tag	UNP A7UX13
B	476	VAL	-	expression tag	UNP A7UX13
B	477	ASP	-	expression tag	UNP A7UX13
B	478	LEU	-	expression tag	UNP A7UX13
B	479	GLN	-	expression tag	UNP A7UX13
B	480	GLY	-	expression tag	UNP A7UX13
B	481	ASP	-	expression tag	UNP A7UX13
B	482	HIS	-	expression tag	UNP A7UX13
B	483	GLY	-	expression tag	UNP A7UX13
B	484	LEU	-	expression tag	UNP A7UX13
B	485	SER	-	expression tag	UNP A7UX13
B	486	ALA	-	expression tag	UNP A7UX13
B	487	TRP	-	expression tag	UNP A7UX13
B	488	SER	-	expression tag	UNP A7UX13
B	489	HIS	-	expression tag	UNP A7UX13
B	490	PRO	-	expression tag	UNP A7UX13
B	491	GLN	-	expression tag	UNP A7UX13
B	492	PHE	-	expression tag	UNP A7UX13
B	493	GLU	-	expression tag	UNP A7UX13
B	494	LYS	-	expression tag	UNP A7UX13

- Molecule 2 is a protein called Hercynylcysteine sulfoxide lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
2	C	436	3485	2231	588	645	1	20	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

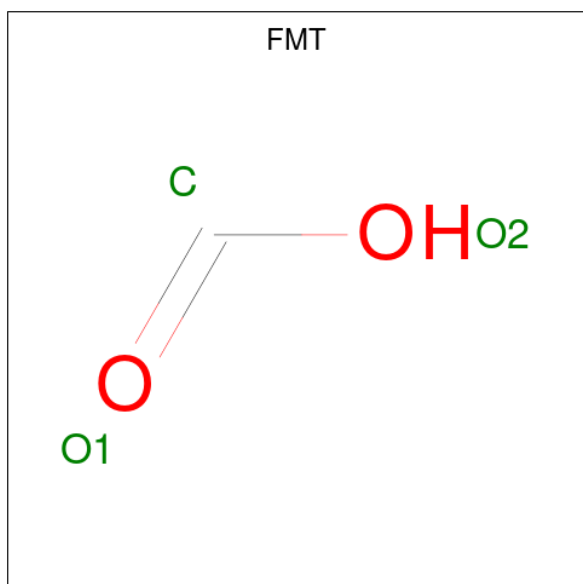
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	MET	-	initiating methionine	UNP A7UX13
C	-5	GLY	-	expression tag	UNP A7UX13
C	-4	ASP	-	expression tag	UNP A7UX13
C	-3	ARG	-	expression tag	UNP A7UX13
C	-2	GLY	-	expression tag	UNP A7UX13

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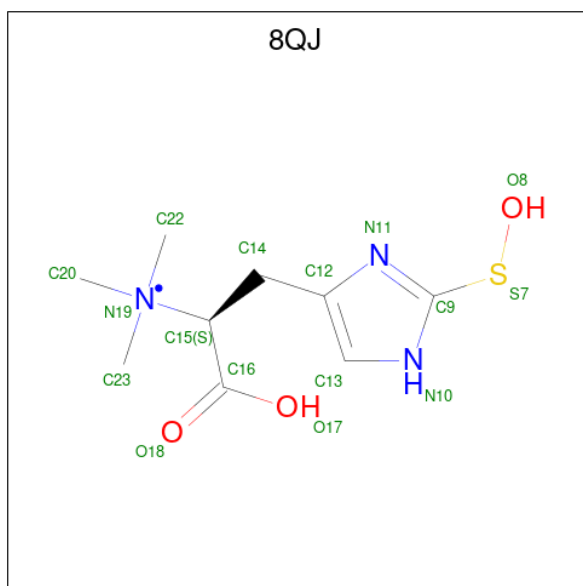
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	PRO	-	expression tag	UNP A7UX13
C	0	GLU	-	expression tag	UNP A7UX13
C	1	PHE	-	expression tag	UNP A7UX13
C	134	PHE	TYR	conflict	UNP A7UX13
C	474	LEU	-	expression tag	UNP A7UX13
C	475	GLU	-	expression tag	UNP A7UX13
C	476	VAL	-	expression tag	UNP A7UX13
C	477	ASP	-	expression tag	UNP A7UX13
C	478	LEU	-	expression tag	UNP A7UX13
C	479	GLN	-	expression tag	UNP A7UX13
C	480	GLY	-	expression tag	UNP A7UX13
C	481	ASP	-	expression tag	UNP A7UX13
C	482	HIS	-	expression tag	UNP A7UX13
C	483	GLY	-	expression tag	UNP A7UX13
C	484	LEU	-	expression tag	UNP A7UX13
C	485	SER	-	expression tag	UNP A7UX13
C	486	ALA	-	expression tag	UNP A7UX13
C	487	TRP	-	expression tag	UNP A7UX13
C	488	SER	-	expression tag	UNP A7UX13
C	489	HIS	-	expression tag	UNP A7UX13
C	490	PRO	-	expression tag	UNP A7UX13
C	491	GLN	-	expression tag	UNP A7UX13
C	492	PHE	-	expression tag	UNP A7UX13
C	493	GLU	-	expression tag	UNP A7UX13
C	494	LYS	-	expression tag	UNP A7UX13

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

- Molecule 4 is (2 {S})-3-(2-oxidanylsulfanyl-1 {H}-imidazol-4-yl)-2-(trimethyl- $\text{N}^{\oplus}$ {4}-azanyl)propanoic acid (three-letter code: 8QJ) (formula:  $\text{C}_9\text{H}_{16}\text{N}_3\text{O}_3\text{S}$ ).

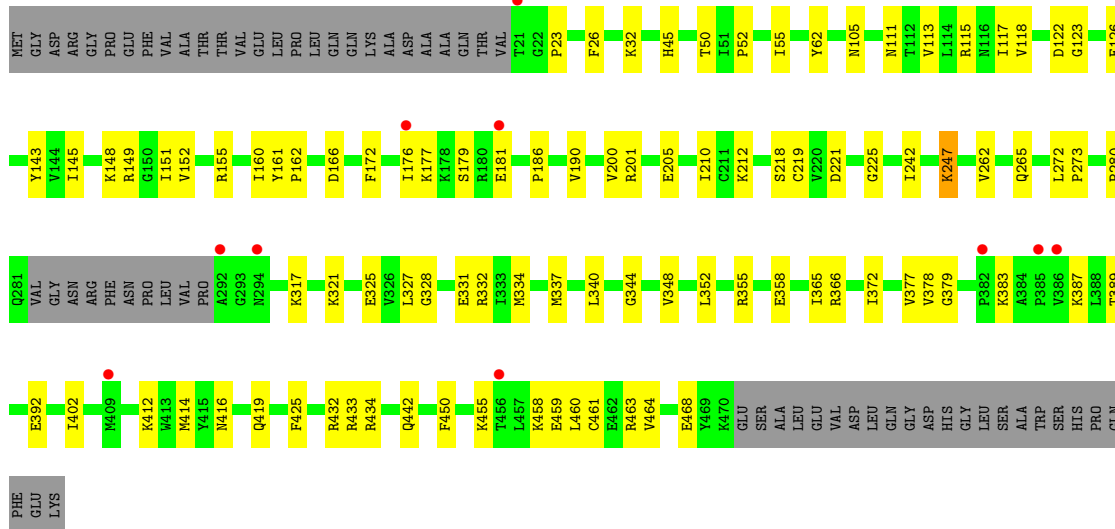


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C N O S 16 9 3 3 1	0	0
4	A	1	Total C N O S 16 9 3 3 1	0	0

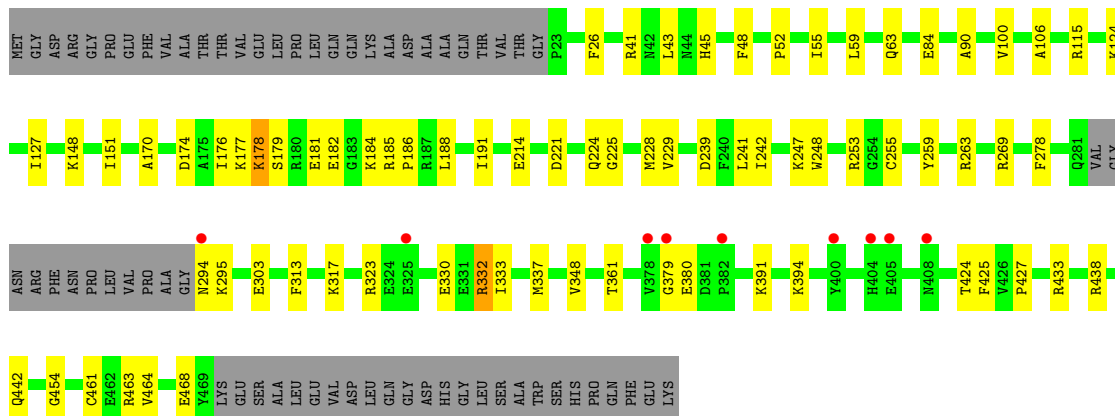
- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	E	54	Total O 54 54	0	0
5	G	48	Total O 48 48	0	0
5	F	40	Total O 40 40	0	0
5	H	65	Total O 65 65	0	0
5	C	21	Total O 21 21	0	0
5	D	54	Total O 54 54	0	0
5	A	71	Total O 71 71	0	0
5	B	59	Total O 59 59	0	0

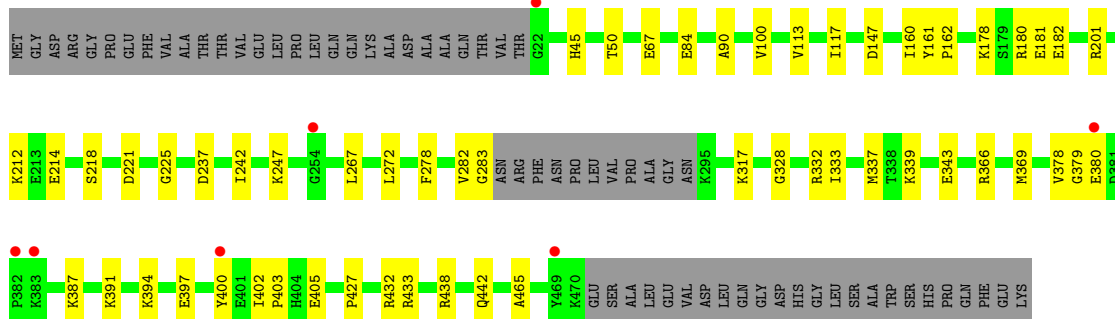
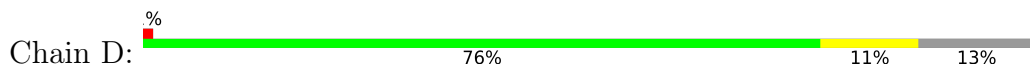




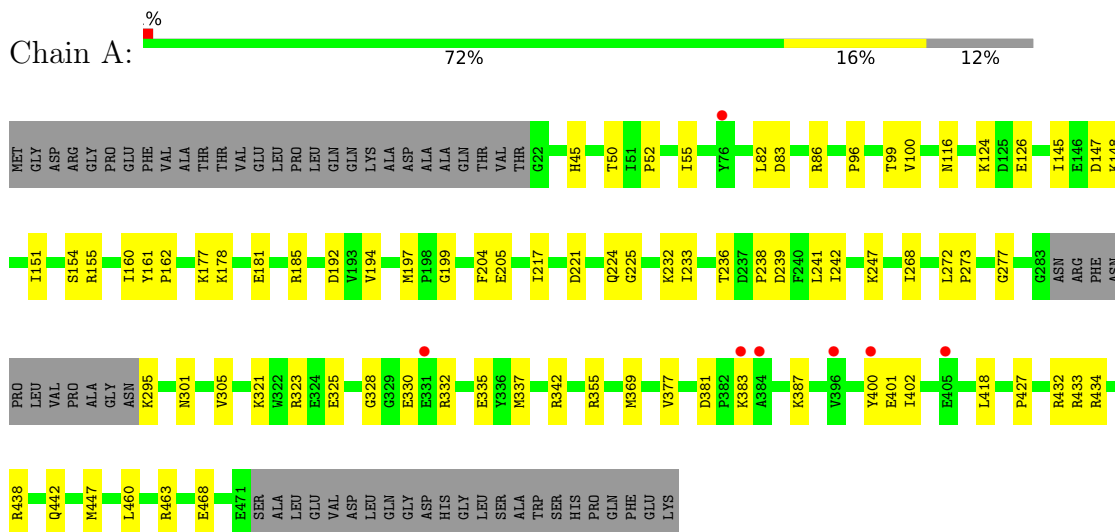
- Molecule 1: Hercynylcysteine sulfoxide lyase



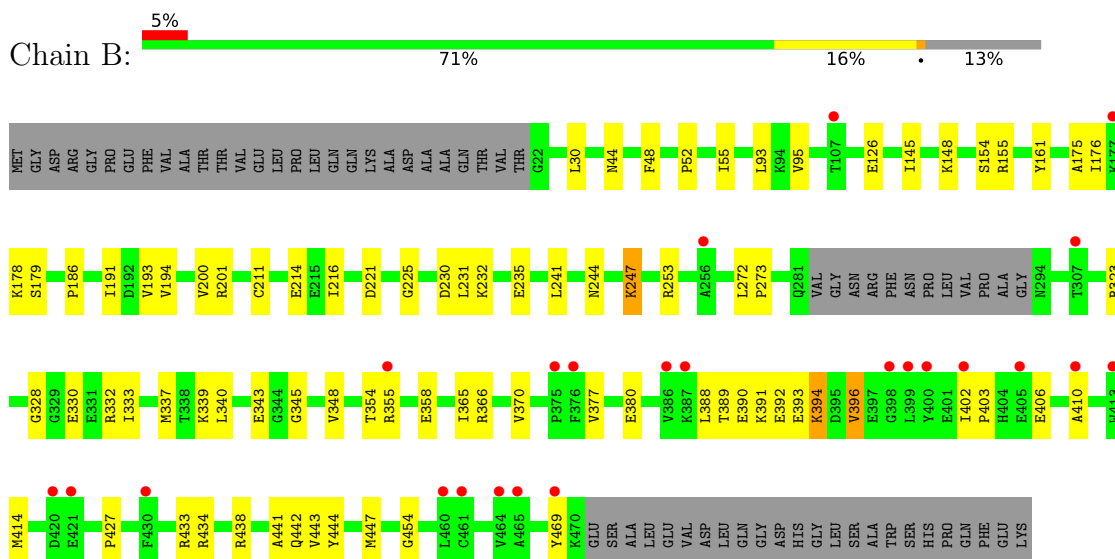
- Molecule 1: Hercynylcysteine sulfoxide lyase



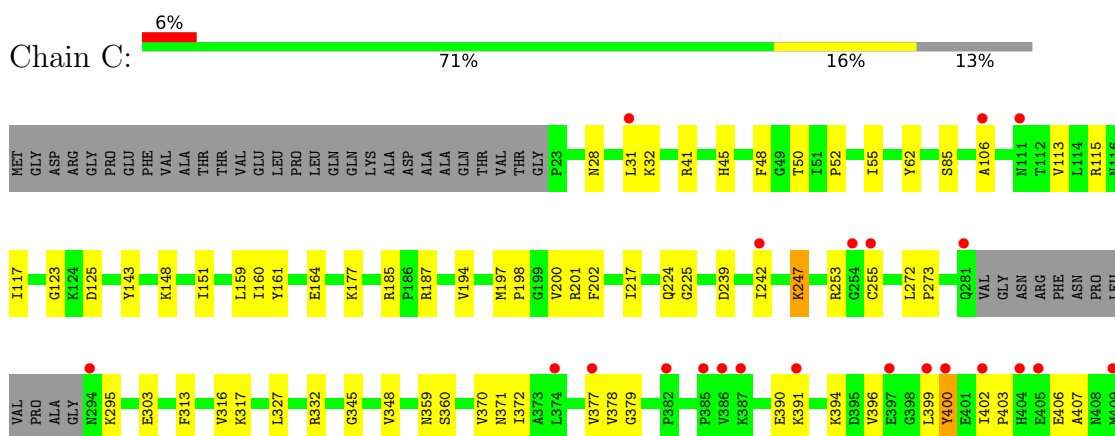
- Molecule 1: Hercynylcysteine sulfoxide lyase

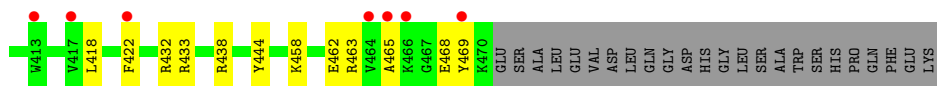


- Molecule 1: Hercynylcysteine sulfoxide lyase



- Molecule 2: Hercynylcysteine sulfoxide lyase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.02Å 195.16Å 110.10Å 90.00° 91.47° 90.00°	Depositor
Resolution (Å)	49.58 – 2.45 49.58 – 2.45	Depositor EDS
% Data completeness (in resolution range)	91.0 (49.58-2.45) 91.0 (49.58-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.45Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.222 , 0.272 0.223 , 0.273	Depositor DCC
$R_{free}$ test set	1988 reflections (1.36%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.6	Xtrriage
Anisotropy	1.058	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.084 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	28363	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, EXA, FMT, 8QJ

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	0.26	0/3544	0.41	0/4800
1	B	0.31	1/3536 (0.0%)	0.45	1/4789 (0.0%)
1	D	0.27	0/3539	0.43	0/4793
1	E	0.26	0/3528	0.41	0/4778
1	F	0.30	0/3552	0.44	0/4811
1	G	0.26	0/3560	0.42	0/4822
1	H	0.27	0/3523	0.43	1/4772 (0.0%)
2	C	0.30	0/3532	0.44	0/4783
All	All	0.28	1/28314 (0.0%)	0.43	2/38348 (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
2	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	394	LYS	CE-NZ	-5.99	1.34	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	178	LYS	CD-CE-NZ	-5.68	98.65	111.70
1	B	396	VAL	CA-CB-CG2	-5.47	102.69	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	247	EXA	Mainchain

## 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	3491	0	3475	49	0
1	B	3483	0	3467	76	0
1	D	3486	0	3473	40	0
1	E	3475	0	3460	53	0
1	F	3499	0	3481	74	0
1	G	3506	0	3490	61	0
1	H	3470	0	3452	55	0
2	C	3485	0	3447	60	0
3	A	3	0	1	0	0
3	B	3	0	1	0	0
3	C	3	0	1	0	0
3	D	3	0	1	0	0
3	E	3	0	1	0	0
3	F	3	0	1	0	0
3	G	3	0	1	0	0
3	H	3	0	1	1	0
4	A	16	0	0	0	0
4	F	16	0	0	2	0
5	A	71	0	0	0	0
5	B	59	0	0	0	0
5	C	21	0	0	0	0
5	D	54	0	0	0	0
5	E	54	0	0	0	0
5	F	40	0	0	0	0
5	G	48	0	0	1	0
5	H	65	0	0	1	0
All	All	28363	0	27753	450	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 8.

All (450) 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:342:ARG:NH1	1:G:365:ILE:O	1.67	1.27
2:C:378:VAL:O	2:C:433:ARG:NH1	1.93	1.01
1:D:380:GLU:OE2	1:D:433:ARG:NE	1.95	1.00
1:A:369:MET:HE1	1:A:438:ARG:HE	1.33	0.92
1:F:378:VAL:HG12	1:F:402:ILE:HD11	1.52	0.91
1:H:295:LYS:NZ	1:H:303:GLU:OE1	2.04	0.89
2:C:400:TYR:HE1	2:C:465:ALA:HA	1.39	0.85
1:H:174:ASP:C	1:H:178:LYS:NZ	2.30	0.85
1:E:149:ARG:HH21	1:F:118:VAL:HG22	1.40	0.85
1:A:147:ASP:OD1	1:B:148:LYS:NZ	2.11	0.84
1:D:339:LYS:NZ	1:D:343:GLU:OE1	2.11	0.83
1:D:180:ARG:NH2	1:D:214:GLU:OE2	2.12	0.82
1:H:239:ASP:OD1	1:H:263:ARG:NH1	2.14	0.81
1:F:126:GLU:OE1	1:F:155:ARG:NH1	2.12	0.81
1:B:328:GLY:HA3	1:B:332:ARG:HD3	1.65	0.78
1:A:116:ASN:HD22	1:A:268:ILE:HA	1.48	0.78
1:D:380:GLU:OE2	1:D:433:ARG:CZ	2.33	0.77
1:D:328:GLY:HA3	1:D:332:ARG:HD3	1.66	0.76
1:F:328:GLY:HA3	1:F:332:ARG:HD3	1.67	0.76
2:C:377:VAL:HG21	2:C:396:VAL:CG2	2.16	0.76
1:H:84:GLU:OE1	1:H:317:LYS:NZ	2.18	0.76
1:A:335:GLU:OE1	1:A:335:GLU:N	2.17	0.74
1:F:212:LYS:HZ1	1:F:218:SER:CB	2.00	0.74
1:H:174:ASP:O	1:H:178:LYS:NZ	2.19	0.74
1:D:379:GLY:N	1:D:402:ILE:O	2.20	0.74
1:A:369:MET:HE1	1:A:438:ARG:NE	2.02	0.73
1:B:126:GLU:OE1	1:B:155:ARG:NH2	2.23	0.72
1:G:274:THR:HG23	1:H:115:ARG:HH21	1.55	0.72
1:H:48:PHE:O	1:H:253:ARG:NH2	2.23	0.71
1:B:155:ARG:HH22	1:B:179:SER:HA	1.55	0.71
2:C:406:GLU:OE1	2:C:469:TYR:OH	2.09	0.71
1:G:145:ILE:HG22	1:G:152:VAL:HG13	1.73	0.71
1:A:205:GLU:OE2	1:A:232:LYS:NZ	2.21	0.70
1:F:201:ARG:NH2	1:F:205:GLU:OE2	2.24	0.70
2:C:400:TYR:CE1	2:C:465:ALA:HA	2.23	0.70
2:C:463:ARG:NH2	2:C:468:GLU:OE2	2.19	0.70
1:F:148:LYS:O	1:F:149:ARG:HG3	1.92	0.69
1:E:96:PRO:O	1:E:99:THR:OG1	2.09	0.69
1:G:377:VAL:HG21	1:G:396:VAL:HG13	1.74	0.69
1:D:369:MET:HE3	1:D:438:ARG:HD3	1.75	0.69
1:E:146:GLU:O	1:E:149:ARG:NH1	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:148:LYS:NZ	1:D:147:ASP:OD2	2.25	0.69
1:E:147:ASP:HA	1:E:149:ARG:HH12	1.58	0.68
1:F:115:ARG:HD2	1:F:272:LEU:HD21	1.76	0.68
1:F:331:GLU:OE2	1:F:331:GLU:N	2.26	0.68
1:H:178:LYS:N	1:H:178:LYS:HD2	2.07	0.68
2:C:345:GLY:HA3	2:C:370:VAL:HG11	1.76	0.68
1:B:377:VAL:HG21	1:B:396:VAL:HG12	1.76	0.68
2:C:377:VAL:HG21	2:C:396:VAL:HG21	1.73	0.67
1:G:270:SER:OG	1:G:274:THR:HG22	1.94	0.66
1:B:348:VAL:HG23	1:B:454:GLY:HA2	1.77	0.66
1:A:236:THR:HG23	1:A:238:PRO:HD3	1.77	0.66
1:F:321:LYS:HE2	1:F:325:GLU:HG3	1.76	0.66
1:F:160:ILE:HD11	1:F:432:ARG:HH11	1.60	0.65
1:F:212:LYS:NZ	1:F:218:SER:HB3	2.11	0.65
1:G:62:TYR:OH	1:G:317:LYS:NZ	2.29	0.65
1:D:84:GLU:OE1	1:D:317:LYS:NZ	2.29	0.65
1:G:48:PHE:HB3	1:G:253:ARG:HD3	1.79	0.64
1:B:389:THR:HG22	1:B:392:GLU:HB2	1.77	0.64
1:B:442:GLN:HG3	1:B:443:VAL:H	1.61	0.64
1:F:379:GLY:HA2	1:F:433:ARG:HH11	1.62	0.64
1:B:155:ARG:HH12	1:B:179:SER:HB2	1.62	0.64
1:D:180:ARG:NH1	1:D:214:GLU:OE2	2.31	0.64
1:B:390:GLU:C	1:B:394:LYS:HZ3	2.01	0.63
1:E:323:ARG:NH2	1:E:330:GLU:OE2	2.27	0.63
1:H:174:ASP:C	1:H:178:LYS:HZ2	2.00	0.63
1:E:148:LYS:HB3	1:E:151:ILE:HG22	1.80	0.63
1:A:86:ARG:NH1	1:A:100:VAL:O	2.30	0.63
1:D:212:LYS:NZ	1:D:237:ASP:O	2.21	0.63
1:A:126:GLU:OE1	1:A:155:ARG:NH1	2.32	0.62
1:F:344:GLY:HA3	1:F:450:PHE:CD2	2.34	0.62
1:F:419:GLN:HE21	1:F:425:PHE:HD2	1.44	0.62
1:A:96:PRO:O	1:A:99:THR:OG1	2.17	0.62
1:B:389:THR:HG23	1:B:392:GLU:H	1.64	0.62
2:C:458:LYS:O	2:C:462:GLU:HG3	2.00	0.61
2:C:390:GLU:O	2:C:394:LYS:N	2.33	0.61
1:E:337:MET:HE3	1:E:442:GLN:HA	1.83	0.61
1:F:419:GLN:NE2	1:F:425:PHE:HD2	1.98	0.61
1:D:337:MET:HE3	1:D:442:GLN:HA	1.82	0.61
1:E:264:ASN:HB3	1:E:267:LEU:HD12	1.83	0.61
1:G:188:LEU:HD11	1:G:219:CYS:HB2	1.83	0.61
1:G:274:THR:HG23	1:H:115:ARG:NH2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:406:GLU:OE1	1:G:469:TYR:OH	2.18	0.61
1:H:177:LYS:HE2	1:H:181:GLU:OE2	2.01	0.61
1:E:274:THR:H	1:F:111:ASN:ND2	1.99	0.60
1:F:172:PHE:CE2	1:F:210:ILE:HD11	2.35	0.60
1:F:212:LYS:N	1:F:212:LYS:HD3	2.16	0.60
1:F:414:MET:HG2	1:F:460:LEU:HD21	1.83	0.60
1:B:337:MET:HE3	1:B:442:GLN:HA	1.83	0.60
1:B:390:GLU:C	1:B:394:LYS:NZ	2.55	0.60
1:G:52:PRO:HG2	1:G:55:ILE:HG12	1.84	0.59
1:D:387:LYS:O	1:D:432:ARG:NH2	2.35	0.59
2:C:377:VAL:HG21	2:C:396:VAL:HG23	1.84	0.59
2:C:164:GLU:OE2	2:C:359:ASN:HB2	2.03	0.59
2:C:123:GLY:HA2	2:C:151:ILE:HG13	1.85	0.58
2:C:160:ILE:HD11	2:C:432:ARG:NH1	2.17	0.58
1:B:232:LYS:HE2	1:B:235:GLU:OE2	2.03	0.58
1:F:177:LYS:NZ	1:F:181:GLU:OE1	2.31	0.58
2:C:272:LEU:HD22	1:D:272:LEU:HD21	1.85	0.58
1:D:180:ARG:CZ	1:D:214:GLU:OE2	2.52	0.58
1:H:323:ARG:NE	1:H:330:GLU:OE2	2.26	0.58
1:B:390:GLU:O	1:B:393:GLU:N	2.36	0.58
1:G:146:GLU:OE1	1:H:269:ARG:NH1	2.36	0.57
2:C:348:VAL:HG13	2:C:372:ILE:HG12	1.87	0.57
2:C:418:LEU:HA	2:C:422:PHE:CD2	2.40	0.57
1:A:116:ASN:ND2	1:A:268:ILE:HA	2.19	0.57
1:B:345:GLY:HA3	1:B:370:VAL:HG21	1.86	0.57
1:B:155:ARG:CZ	1:B:178:LYS:NZ	2.68	0.57
1:E:176:ILE:HD13	1:E:214:GLU:HG3	1.87	0.56
2:C:418:LEU:HA	2:C:422:PHE:HD2	1.69	0.56
1:A:321:LYS:HE2	1:A:325:GLU:OE2	2.05	0.56
1:B:155:ARG:HH12	1:B:179:SER:CA	2.19	0.56
1:E:30:LEU:HD23	1:E:443:VAL:HG13	1.87	0.56
1:E:147:ASP:O	1:E:149:ARG:NH1	2.39	0.56
1:F:212:LYS:NZ	1:F:218:SER:CB	2.67	0.56
1:H:148:LYS:HB3	1:H:151:ILE:HG22	1.86	0.56
1:E:263:ARG:HG3	1:E:264:ASN:OD1	2.05	0.56
1:G:120:SER:O	1:G:151:ILE:HD11	2.06	0.56
1:G:214:GLU:HB2	1:G:216:ILE:HD11	1.87	0.56
2:C:28:ASN:HA	2:C:31:LEU:HD23	1.88	0.56
1:H:178:LYS:HD2	1:H:178:LYS:H	1.71	0.56
2:C:143:TYR:HB2	1:D:278:PHE:CE2	2.40	0.56
1:E:143:TYR:O	1:E:147:ASP:N	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ARG:CZ	1:B:178:LYS:HZ2	2.19	0.55
1:A:332:ARG:HG2	1:A:332:ARG:O	2.06	0.55
1:G:405:GLU:N	1:G:405:GLU:OE1	2.35	0.55
1:G:172:PHE:CE2	1:G:210:ILE:HD11	2.42	0.55
1:F:26:PHE:HE1	1:F:327:LEU:HG	1.70	0.55
1:B:343:GLU:HB2	1:B:447:MET:HE1	1.88	0.55
1:B:155:ARG:HH12	1:B:179:SER:CB	2.19	0.55
1:H:337:MET:HE3	1:H:442:GLN:HA	1.89	0.55
1:G:214:GLU:HB2	1:G:216:ILE:CD1	2.36	0.55
1:B:339:LYS:O	1:B:343:GLU:HG3	2.07	0.55
2:C:62:TYR:OH	2:C:317:LYS:NZ	2.37	0.55
1:B:391:LYS:HA	1:B:394:LYS:CE	2.36	0.55
1:H:391:LYS:HD3	1:H:394:LYS:HE2	1.88	0.54
1:B:343:GLU:CB	1:B:447:MET:HE1	2.37	0.54
1:B:390:GLU:HG3	1:B:391:LYS:HD3	1.90	0.54
1:E:278:PHE:CZ	1:F:143:TYR:HB2	2.42	0.54
1:F:172:PHE:CD2	1:F:210:ILE:HD11	2.43	0.54
1:B:155:ARG:NH1	1:B:179:SER:HB2	2.22	0.54
1:G:244:ASN:HD22	1:G:247:LLP:HE2	1.73	0.54
1:B:52:PRO:HG2	1:B:55:ILE:HG12	1.90	0.54
1:D:378:VAL:O	1:D:433:ARG:NH2	2.41	0.54
1:F:463:ARG:NE	1:F:468:GLU:OE1	2.30	0.54
1:D:380:GLU:OE2	1:D:433:ARG:NH2	2.41	0.54
1:A:427:PRO:HG2	1:A:438:ARG:HD3	1.90	0.53
1:A:463:ARG:HB3	1:A:468:GLU:OE2	2.08	0.53
1:F:160:ILE:HD11	1:F:432:ARG:HD2	1.89	0.53
1:D:160:ILE:CG2	1:D:432:ARG:HH11	2.21	0.53
1:H:379:GLY:HA2	1:H:433:ARG:HH21	1.74	0.53
2:C:217:ILE:HA	2:C:239:ASP:OD2	2.07	0.53
1:E:92:LEU:HD11	1:E:330:GLU:HG2	1.91	0.53
1:H:224:GLN:NE2	3:H:501:FMT:O2	2.39	0.53
1:B:176:ILE:HD13	1:B:214:GLU:HG3	1.91	0.53
1:F:160:ILE:CD1	1:F:432:ARG:HD2	2.38	0.52
1:F:45:HIS:CE1	1:F:50:THR:HG22	2.44	0.52
1:B:333:ILE:O	1:B:337:MET:HG3	2.10	0.52
1:B:391:LYS:HA	1:B:394:LYS:HE2	1.90	0.52
1:G:446:GLU:N	1:G:449:ASP:OD2	2.33	0.52
1:G:291:PRO:HB2	1:G:294:ASN:HD21	1.74	0.52
2:C:52:PRO:HG2	2:C:55:ILE:HG12	1.92	0.52
1:D:391:LYS:HA	1:D:394:LYS:HG2	1.91	0.52
1:A:323:ARG:NH2	1:A:330:GLU:OE1	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ARG:NH1	1:B:175:ALA:O	2.43	0.52
1:B:388:LEU:HD22	1:B:392:GLU:OE2	2.09	0.52
1:H:45:HIS:CD2	1:H:442:GLN:HE21	2.28	0.52
1:H:463:ARG:NH2	1:H:468:GLU:OE2	2.33	0.52
1:B:231:LEU:HD13	1:B:241:LEU:HD21	1.91	0.52
1:A:197:MET:SD	1:A:438:ARG:HD2	2.49	0.52
1:E:379:GLY:N	1:E:402:ILE:O	2.36	0.51
1:B:354:THR:OG1	1:B:355:ARG:N	2.42	0.51
1:B:402:ILE:HD12	1:B:403:PRO:HD2	1.92	0.51
1:F:455:LYS:O	1:F:459:GLU:N	2.33	0.51
1:D:160:ILE:HG21	1:D:432:ARG:HH11	1.75	0.51
1:A:272:LEU:HD11	1:B:272:LEU:HD11	1.93	0.51
1:E:149:ARG:NH2	1:F:118:VAL:HG22	2.16	0.51
1:F:62:TYR:OH	1:F:317:LYS:NZ	2.43	0.51
1:H:255:CYS:HA	1:H:313:PHE:HE1	1.75	0.51
1:E:427:PRO:HG2	1:E:438:ARG:HB3	1.92	0.51
2:C:115:ARG:HD2	2:C:272:LEU:HD11	1.93	0.51
1:A:381:ASP:OD2	1:A:383:LYS:HB2	2.11	0.51
1:F:412:LYS:O	1:F:416:ASN:ND2	2.43	0.51
1:D:160:ILE:HD13	1:D:432:ARG:NH1	2.25	0.51
1:E:377:VAL:HG11	1:E:396:VAL:HB	1.92	0.51
1:E:147:ASP:CA	1:E:149:ARG:HH12	2.23	0.50
2:C:143:TYR:HB2	1:D:278:PHE:CZ	2.46	0.50
1:G:139:LYS:HB3	1:H:278:PHE:HD1	1.76	0.50
2:C:48:PHE:HB3	2:C:253:ARG:HD3	1.92	0.50
1:B:390:GLU:HG2	1:B:391:LYS:NZ	2.27	0.50
1:B:244:ASN:HD22	1:B:247:LLP:HE2	1.76	0.50
1:B:442:GLN:HG3	1:B:443:VAL:N	2.26	0.50
1:E:142:ASP:HB3	1:F:280:PRO:HB3	1.93	0.50
1:G:208:VAL:HG21	1:G:236:THR:HB	1.93	0.50
1:H:41:ARG:O	1:H:424:THR:HG23	2.12	0.50
2:C:255:CYS:HA	2:C:313:PHE:HE1	1.76	0.50
1:D:45:HIS:CD2	1:D:442:GLN:HE21	2.30	0.50
1:D:178:LYS:O	1:D:181:GLU:N	2.44	0.50
1:G:240:PHE:HE1	1:G:268:ILE:HD11	1.77	0.50
1:H:176:ILE:HG23	1:H:186:PRO:HG2	1.94	0.50
1:A:277:GLY:HA3	1:A:301:ASN:HB3	1.93	0.50
1:A:52:PRO:HG2	1:A:55:ILE:HG12	1.94	0.50
1:F:123:GLY:HA2	1:F:151:ILE:HD12	1.94	0.49
1:H:174:ASP:CG	1:H:178:LYS:NZ	2.65	0.49
1:H:461:CYS:HA	1:H:464:VAL:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:HB	1:A:224:GLN:HB2	1.94	0.49
1:H:191:ILE:O	1:H:221:ASP:N	2.45	0.49
1:B:323:ARG:NH1	1:B:330:GLU:OE1	2.46	0.49
2:C:406:GLU:HB3	2:C:469:TYR:CE2	2.48	0.49
1:A:83:ASP:OD2	1:A:295:LYS:NZ	2.35	0.49
1:A:177:LYS:O	1:A:181:GLU:HG3	2.13	0.49
1:F:221:ASP:HA	1:F:242:ILE:HG22	1.95	0.49
1:F:334:MET:HA	1:F:337:MET:HE2	1.94	0.49
2:C:379:GLY:N	2:C:402:ILE:O	2.45	0.49
1:G:172:PHE:CD2	1:G:210:ILE:HD11	2.48	0.49
1:A:377:VAL:HG13	1:A:401:GLU:HG3	1.94	0.49
1:H:127:ILE:HG23	1:H:188:LEU:HD12	1.93	0.49
1:E:244:ASN:ND2	1:E:247:LLP:OP3	2.45	0.49
1:F:52:PRO:HG2	1:F:55:ILE:HG12	1.93	0.49
2:C:396:VAL:HG22	2:C:396:VAL:O	2.13	0.48
1:B:155:ARG:NE	1:B:178:LYS:HZ1	2.11	0.48
1:B:393:GLU:HA	1:B:396:VAL:CG2	2.42	0.48
1:G:120:SER:N	1:G:125:ASP:OD2	2.27	0.48
1:B:155:ARG:NH2	1:B:178:LYS:HZ2	2.11	0.48
2:C:378:VAL:HG12	2:C:433:ARG:HA	1.94	0.48
1:A:328:GLY:HA3	1:A:332:ARG:HH11	1.78	0.48
1:B:377:VAL:CG2	1:B:396:VAL:HG12	2.43	0.48
1:H:26:PHE:CE2	1:H:332:ARG:NH1	2.82	0.48
1:F:379:GLY:HA2	1:F:433:ARG:NH1	2.28	0.48
1:H:333:ILE:O	1:H:337:MET:HG3	2.13	0.48
1:D:182:GLU:N	1:D:182:GLU:OE1	2.46	0.48
1:E:380:GLU:HB2	1:E:433:ARG:NH1	2.29	0.48
1:F:340:LEU:HG	1:F:450:PHE:HE2	1.79	0.48
1:H:48:PHE:HB3	1:H:253:ARG:NH2	2.29	0.48
2:C:402:ILE:HD11	2:C:469:TYR:OH	2.14	0.48
1:E:58:LYS:HE2	1:E:318:ASP:OD2	2.13	0.47
1:E:394:LYS:HD3	1:E:394:LYS:N	2.29	0.47
1:F:201:ARG:HG2	1:F:366:ARG:HB2	1.95	0.47
1:F:461:CYS:HA	1:F:464:VAL:HG22	1.96	0.47
1:G:194:VAL:HB	1:G:224:GLN:HB2	1.97	0.47
1:F:145:ILE:HG23	1:F:152:VAL:O	2.14	0.47
1:H:241:LEU:HB3	1:H:259:TYR:HB3	1.95	0.47
1:D:221:ASP:HA	1:D:242:ILE:HG22	1.95	0.47
1:E:44:ASN:HD21	1:E:427:PRO:HG3	1.80	0.47
1:D:113:VAL:O	1:D:117:ILE:HG12	2.15	0.47
1:G:60:ARG:O	1:G:64:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:PRO:HB2	1:F:332:ARG:NH1	2.30	0.47
1:F:155:ARG:NH1	1:F:179:SER:HB2	2.30	0.47
1:H:224:GLN:OE1	1:H:248:TRP:NE1	2.39	0.47
1:A:273:PRO:HD2	1:A:305:VAL:HG12	1.96	0.47
1:G:178:LYS:NZ	1:G:182:GLU:OE2	2.33	0.47
1:F:161:TYR:HE2	1:F:200:VAL:HG11	1.78	0.47
1:E:340:LEU:HD12	1:E:441:ALA:HB1	1.97	0.47
1:F:328:GLY:N	1:F:332:ARG:HH11	2.12	0.47
2:C:194:VAL:HB	2:C:224:GLN:HB2	1.97	0.47
1:B:427:PRO:HG2	1:B:438:ARG:HB3	1.96	0.47
1:E:240:PHE:HD1	1:E:260:VAL:HG22	1.80	0.46
1:G:124:LYS:HB2	1:G:185:ARG:NH1	2.30	0.46
1:A:221:ASP:HA	1:A:242:ILE:HG22	1.96	0.46
1:F:105:ASN:HB2	1:F:247:LLP:OP2	2.15	0.46
2:C:31:LEU:HD22	2:C:444:TYR:HB2	1.98	0.46
1:G:21:THR:N	5:G:601:HOH:O	2.49	0.46
1:D:394:LYS:HA	1:D:397:GLU:HG3	1.97	0.46
1:E:247:LLP:H4'1	4:F:501:8QJ:S7	2.55	0.46
1:B:48:PHE:HB3	1:B:253:ARG:HE	1.80	0.46
1:F:23:PRO:HB2	1:F:332:ARG:HH12	1.81	0.46
1:B:230:ASP:OD1	1:B:232:LYS:N	2.47	0.46
1:B:442:GLN:HG2	1:B:444:TYR:CE2	2.51	0.46
1:E:48:PHE:HB3	1:E:253:ARG:HE	1.81	0.46
1:H:380:GLU:HG3	1:H:433:ARG:CZ	2.45	0.46
1:E:93:LEU:HB3	1:E:233:ILE:HD13	1.98	0.45
1:E:194:VAL:HB	1:E:224:GLN:HB2	1.97	0.45
1:E:247:LLP:OP1	4:F:501:8QJ:O8	2.34	0.45
1:F:352:LEU:HA	1:F:458:LYS:HE3	1.98	0.45
1:H:427:PRO:HG2	1:H:438:ARG:HB3	1.98	0.45
1:H:59:LEU:O	1:H:63:GLN:HG3	2.16	0.45
1:E:191:ILE:O	1:E:221:ASP:N	2.49	0.45
1:H:90:ALA:HB2	1:H:100:VAL:HG21	1.99	0.45
1:B:191:ILE:O	1:B:221:ASP:N	2.47	0.45
1:E:387:LYS:HA	1:E:387:LYS:HD3	1.58	0.45
1:E:44:ASN:ND2	1:E:427:PRO:HD3	2.32	0.45
1:E:273:PRO:HD2	1:E:305:VAL:HG12	1.98	0.45
1:F:272:LEU:HA	1:F:273:PRO:HA	1.80	0.45
1:H:176:ILE:HD13	1:H:214:GLU:HG3	1.99	0.45
1:H:178:LYS:N	1:H:178:LYS:CD	2.78	0.45
1:E:190:VAL:HA	1:E:219:CYS:O	2.17	0.45
1:H:52:PRO:HG2	1:H:55:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:LYS:O	1:F:151:ILE:HG22	2.16	0.45
1:D:282:VAL:O	1:D:283:GLY:C	2.56	0.45
1:E:314:PHE:O	1:E:317:LYS:HE3	2.17	0.45
1:F:377:VAL:HG12	1:F:434:ARG:HD2	1.99	0.45
1:H:178:LYS:O	1:H:182:GLU:N	2.48	0.45
1:A:337:MET:HE3	1:A:442:GLN:HA	1.98	0.45
1:A:418:LEU:HD21	1:A:460:LEU:HD22	1.98	0.45
1:B:390:GLU:HG3	1:B:391:LYS:N	2.32	0.45
2:C:160:ILE:HD11	2:C:432:ARG:CZ	2.47	0.44
2:C:377:VAL:O	2:C:402:ILE:N	2.31	0.44
1:H:43:LEU:HD12	1:H:424:THR:HG21	2.00	0.44
1:E:269:ARG:HA	1:E:269:ARG:HH11	1.83	0.44
1:G:247:LLP:NZ	1:G:247:LLP:O3	2.45	0.44
1:F:387:LYS:O	1:F:432:ARG:NH2	2.50	0.44
2:C:378:VAL:HG21	2:C:407:ALA:HB2	1.99	0.44
1:G:388:LEU:HA	1:G:432:ARG:NH2	2.33	0.44
1:E:93:LEU:HD22	1:E:233:ILE:HD11	2.00	0.44
1:G:336:TYR:CE2	1:G:340:LEU:HD12	2.53	0.44
1:H:106:ALA:HA	1:H:242:ILE:HG12	1.99	0.44
1:B:44:ASN:OD1	1:B:438:ARG:NH2	2.39	0.44
1:B:358:GLU:OE2	1:B:365:ILE:HG13	2.18	0.44
1:G:188:LEU:HD12	1:G:217:ILE:O	2.17	0.44
1:F:419:GLN:NE2	1:F:425:PHE:CD2	2.84	0.44
1:B:145:ILE:HD11	1:B:154:SER:HB3	2.00	0.44
1:G:321:LYS:HA	1:G:321:LYS:HD2	1.65	0.44
1:F:45:HIS:CD2	1:F:442:GLN:HE21	2.36	0.44
1:E:333:ILE:O	1:E:337:MET:HG3	2.17	0.44
1:G:272:LEU:HA	1:G:273:PRO:HA	1.89	0.44
1:G:402:ILE:HG13	1:G:403:PRO:HD2	2.00	0.44
1:H:124:LYS:HB2	1:H:185:ARG:HH12	1.83	0.44
1:D:333:ILE:O	1:D:337:MET:HG3	2.18	0.44
1:A:369:MET:HE2	1:A:369:MET:HB3	1.51	0.44
1:D:90:ALA:HB2	1:D:100:VAL:HG21	1.99	0.43
1:A:160:ILE:HD13	1:A:432:ARG:NH1	2.33	0.43
1:B:391:LYS:HD3	1:B:391:LYS:N	2.32	0.43
1:F:161:TYR:HA	1:F:162:PRO:C	2.39	0.43
1:A:199:GLY:HA3	1:A:369:MET:HE2	1.99	0.43
1:A:217:ILE:HA	1:A:239:ASP:OD2	2.18	0.43
1:B:230:ASP:OD1	1:B:230:ASP:C	2.56	0.43
1:A:233:ILE:HG12	1:A:241:LEU:HD13	2.00	0.43
1:G:113:VAL:O	1:G:117:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:ASP:C	1:E:149:ARG:NH1	2.71	0.43
1:G:90:ALA:HB2	1:G:100:VAL:HG21	2.00	0.43
1:G:186:PRO:HB2	1:G:216:ILE:HG12	2.00	0.43
1:H:179:SER:HB3	1:H:186:PRO:HG3	2.00	0.43
1:B:390:GLU:HG2	1:B:391:LYS:HZ2	1.82	0.43
2:C:106:ALA:HA	2:C:242:ILE:HG12	1.99	0.43
1:G:241:LEU:HD21	1:G:243:SER:HB2	2.00	0.43
1:H:348:VAL:HG13	1:H:454:GLY:HA2	2.00	0.43
2:C:272:LEU:HA	2:C:273:PRO:HA	1.85	0.43
1:B:272:LEU:HA	1:B:273:PRO:HA	1.88	0.43
1:B:391:LYS:HZ2	1:B:391:LYS:H	1.67	0.43
1:E:228:MET:HG2	1:E:229:VAL:HG13	1.99	0.43
2:C:32:LYS:HB2	2:C:32:LYS:NZ	2.34	0.43
1:D:45:HIS:CE1	1:D:50:THR:HG22	2.54	0.43
1:H:179:SER:O	1:H:184:LYS:N	2.52	0.43
2:C:378:VAL:CG2	2:C:407:ALA:HB2	2.49	0.43
1:A:178:LYS:HE3	1:A:178:LYS:HB2	1.82	0.43
1:A:447:MET:HB2	1:A:447:MET:HE2	1.81	0.43
1:H:424:THR:HG22	1:H:425:PHE:H	1.84	0.43
1:E:380:GLU:N	1:E:433:ARG:HH11	2.17	0.42
1:F:190:VAL:HA	1:F:219:CYS:O	2.19	0.42
1:F:455:LYS:O	1:F:458:LYS:N	2.52	0.42
1:F:113:VAL:O	1:F:117:ILE:HG12	2.19	0.42
1:B:161:TYR:CE1	1:B:200:VAL:HG21	2.55	0.42
2:C:159:LEU:HD23	2:C:159:LEU:HA	1.88	0.42
2:C:253:ARG:NH2	1:D:67:GLU:OE2	2.52	0.42
1:B:211:CYS:HB3	1:B:216:ILE:O	2.20	0.42
2:C:377:VAL:O	2:C:402:ILE:HG22	2.19	0.42
1:F:148:LYS:HA	1:F:148:LYS:HD3	1.83	0.42
1:F:402:ILE:H	1:F:402:ILE:HG13	1.59	0.42
1:D:400:TYR:CE2	1:D:465:ALA:HA	2.55	0.42
1:B:155:ARG:HH12	1:B:179:SER:N	2.16	0.42
1:G:187:ARG:HA	1:G:187:ARG:HD2	1.71	0.42
1:G:188:LEU:CD1	1:G:217:ILE:HG13	2.50	0.42
1:G:209:LYS:HE2	1:G:209:LYS:HB3	1.87	0.42
1:F:344:GLY:HA3	1:F:450:PHE:CE2	2.54	0.42
1:F:389:THR:HG23	1:F:392:GLU:H	1.84	0.42
1:F:262:VAL:HA	1:F:265:GLN:HG3	2.01	0.42
2:C:201:ARG:NH1	2:C:202:PHE:O	2.51	0.42
2:C:391:LYS:HA	2:C:394:LYS:HB3	2.01	0.42
1:D:201:ARG:HG2	1:D:366:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:HG12	1:B:194:VAL:HG23	2.01	0.42
1:B:201:ARG:HG2	1:B:366:ARG:HB2	2.00	0.42
1:G:85:SER:HB3	1:G:316:VAL:HB	2.02	0.42
1:G:375:PRO:HD2	1:G:461:CYS:SG	2.59	0.42
1:F:166:ASP:OD1	1:F:166:ASP:N	2.52	0.42
1:H:178:LYS:H	1:H:178:LYS:CD	2.32	0.42
2:C:295:LYS:NZ	2:C:303:GLU:OE2	2.44	0.42
2:C:371:ASN:ND2	2:C:438:ARG:HG3	2.35	0.42
1:B:389:THR:HG22	1:B:392:GLU:CD	2.40	0.42
1:F:328:GLY:CA	1:F:332:ARG:HH11	2.33	0.42
1:F:463:ARG:HB3	1:F:468:GLU:OE1	2.20	0.42
2:C:187:ARG:O	2:C:217:ILE:HG12	2.20	0.42
2:C:197:MET:HA	2:C:198:PRO:HA	1.93	0.42
1:G:427:PRO:HG3	1:G:438:ARG:HH21	1.85	0.42
1:F:32:LYS:HE3	1:F:32:LYS:HB2	1.80	0.42
1:F:358:GLU:OE2	1:F:365:ILE:HG13	2.20	0.42
2:C:327:LEU:O	2:C:332:ARG:NH1	2.51	0.42
1:B:393:GLU:HG3	1:B:396:VAL:HG21	2.02	0.42
1:G:161:TYR:CE2	1:G:200:VAL:HG21	2.55	0.41
1:B:179:SER:HB3	1:B:186:PRO:HG3	2.02	0.41
1:B:406:GLU:OE1	1:B:469:TYR:OH	2.22	0.41
1:E:37:ASP:OD1	1:E:38:PRO:HD2	2.20	0.41
1:E:380:GLU:CA	1:E:433:ARG:HH11	2.32	0.41
1:G:31:LEU:HD23	1:G:444:TYR:HB2	2.00	0.41
1:F:176:ILE:HG23	1:F:186:PRO:HG3	2.03	0.41
1:B:380:GLU:HG3	1:B:433:ARG:NH1	2.35	0.41
1:B:390:GLU:CG	1:B:391:LYS:HZ2	2.32	0.41
1:B:410:ALA:O	1:B:414:MET:HG3	2.19	0.41
1:G:467:GLY:O	1:G:470:LYS:HG2	2.21	0.41
1:H:228:MET:HG2	1:H:229:VAL:HG13	2.03	0.41
1:B:340:LEU:HD23	1:B:441:ALA:HB1	2.02	0.41
1:E:331:GLU:CD	1:E:331:GLU:H	2.23	0.41
1:G:291:PRO:HB2	1:G:294:ASN:ND2	2.35	0.41
2:C:125:ASP:OD1	2:C:185:ARG:HD2	2.21	0.41
1:B:389:THR:HG22	1:B:392:GLU:CB	2.46	0.41
1:F:348:VAL:HG13	1:F:372:ILE:HG12	2.02	0.41
2:C:161:TYR:CE2	2:C:200:VAL:HG11	2.55	0.41
1:A:82:LEU:O	1:A:86:ARG:HG3	2.20	0.41
1:A:232:LYS:O	1:A:236:THR:HG22	2.21	0.41
1:E:259:TYR:CE2	1:E:261:PRO:HD3	2.55	0.41
1:H:170:ALA:O	1:H:174:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:45:HIS:CE1	2:C:50:THR:HG22	2.55	0.41
1:A:433:ARG:C	1:A:434:ARG:HG2	2.40	0.41
1:G:45:HIS:CD2	1:G:442:GLN:HE21	2.39	0.41
1:F:45:HIS:HE1	1:F:50:THR:HG22	1.84	0.41
1:H:253:ARG:N	5:H:603:HOH:O	2.52	0.41
1:H:391:LYS:HA	1:H:394:LYS:HE2	2.01	0.41
2:C:85:SER:HB3	2:C:316:VAL:HB	2.02	0.41
1:A:45:HIS:CE1	1:A:50:THR:HG22	2.56	0.41
1:A:145:ILE:HD11	1:A:154:SER:HB3	2.03	0.41
1:G:180:ARG:HE	1:G:186:PRO:HG3	1.86	0.41
1:G:204:PHE:O	1:G:208:VAL:HG13	2.20	0.41
1:G:237:ASP:OD2	1:G:263:ARG:NH2	2.54	0.41
1:G:331:GLU:CD	1:G:331:GLU:H	2.24	0.41
1:G:378:VAL:HG11	1:G:430:PHE:CE1	2.56	0.41
1:D:161:TYR:HA	1:D:162:PRO:C	2.41	0.41
1:A:124:LYS:HB2	1:A:185:ARG:HH12	1.86	0.41
1:A:148:LYS:HB3	1:A:151:ILE:HG22	2.03	0.41
1:A:161:TYR:HA	1:A:162:PRO:C	2.42	0.41
1:B:377:VAL:HG22	1:B:434:ARG:HD3	2.03	0.41
1:B:389:THR:CG2	1:B:392:GLU:H	2.30	0.41
1:E:180:ARG:NH2	1:E:214:GLU:OE2	2.47	0.41
1:E:274:THR:H	1:F:111:ASN:HD21	1.68	0.41
1:D:403:PRO:HB2	1:D:405:GLU:OE2	2.21	0.41
1:G:79:PRO:O	1:G:83:ASP:OD1	2.38	0.40
2:C:402:ILE:HG13	2:C:403:PRO:HD2	2.02	0.40
1:D:427:PRO:HG2	1:D:438:ARG:HB3	2.03	0.40
2:C:295:LYS:HB2	2:C:295:LYS:HE3	1.89	0.40
2:C:399:LEU:HD23	2:C:399:LEU:HA	1.92	0.40
1:D:160:ILE:HG21	1:D:432:ARG:NH1	2.37	0.40
2:C:113:VAL:O	2:C:117:ILE:HG12	2.22	0.40
1:A:192:ASP:O	1:A:204:PHE:HB3	2.22	0.40
1:A:387:LYS:HD2	1:A:387:LYS:HA	1.93	0.40
1:A:400:TYR:HE2	1:A:402:ILE:HG12	1.87	0.40
1:B:30:LEU:HD12	1:B:30:LEU:HA	1.92	0.40
1:E:329:GLY:O	1:E:333:ILE:HG13	2.22	0.40
1:G:149:ARG:HH22	1:H:148:LYS:HD2	1.85	0.40
1:G:201:ARG:HG2	1:G:366:ARG:HB2	2.04	0.40
1:G:209:LYS:HE3	1:G:213:GLU:OE2	2.22	0.40
1:A:400:TYR:CE2	1:A:402:ILE:HG12	2.57	0.40
1:B:93:LEU:HB2	1:B:95:VAL:HG22	2.03	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	434/501 (87%)	416 (96%)	17 (4%)	1 (0%)	47	57
1	B	432/501 (86%)	419 (97%)	12 (3%)	1 (0%)	47	57
1	D	433/501 (86%)	414 (96%)	18 (4%)	1 (0%)	47	57
1	E	431/501 (86%)	417 (97%)	14 (3%)	0	100	100
1	F	435/501 (87%)	415 (95%)	19 (4%)	1 (0%)	47	57
1	G	436/501 (87%)	415 (95%)	20 (5%)	1 (0%)	47	57
1	H	430/501 (86%)	414 (96%)	15 (4%)	1 (0%)	47	57
2	C	431/501 (86%)	410 (95%)	20 (5%)	1 (0%)	47	57
All	All	3462/4008 (86%)	3320 (96%)	135 (4%)	7 (0%)	47	57

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	225	GLY
2	C	225	GLY
1	B	225	GLY
1	F	225	GLY
1	D	225	GLY
1	A	225	GLY
1	H	225	GLY

### 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	377/428 (88%)	375 (100%)	2 (0%)	88	93
1	B	377/428 (88%)	377 (100%)	0	100	100
1	D	377/428 (88%)	375 (100%)	2 (0%)	88	93
1	E	376/428 (88%)	375 (100%)	1 (0%)	92	95
1	F	378/428 (88%)	375 (99%)	3 (1%)	81	88
1	G	379/428 (89%)	376 (99%)	3 (1%)	81	88
1	H	376/428 (88%)	373 (99%)	3 (1%)	81	88
2	C	377/428 (88%)	373 (99%)	4 (1%)	73	82
All	All	3017/3424 (88%)	2999 (99%)	18 (1%)	86	91

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	394	LYS
1	G	331	GLU
1	G	342	ARG
1	G	458	LYS
1	F	122	ASP
1	F	355	ARG
1	F	383	LYS
1	H	294	ASN
1	H	332	ARG
1	H	361	THR
2	C	41	ARG
2	C	177	LYS
2	C	360	SER
2	C	400	TYR
1	D	218	SER
1	D	267	LEU
1	A	342	ARG
1	A	355	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	419	GLN
1	G	44	ASN
1	F	111	ASN
1	F	419	GLN

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Mol	Chain	Res	Type
1	H	42	ASN
2	C	371	ASN
1	D	371	ASN
1	A	42	ASN
1	A	63	GLN
1	A	116	ASN
1	B	42	ASN
1	B	419	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 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	LLP	F	247	1	23,24,25	2.63	6 (26%)	25,32,34	1.28	3 (12%)
1	LLP	E	247	1	23,24,25	2.65	7 (30%)	25,32,34	1.20	3 (12%)
1	LLP	H	247	1	23,24,25	2.66	5 (21%)	25,32,34	1.17	3 (12%)
1	LLP	A	247	1	23,24,25	2.64	6 (26%)	25,32,34	1.36	2 (8%)
1	LLP	G	247	1	23,24,25	2.63	6 (26%)	25,32,34	1.30	3 (12%)
1	LLP	B	247	1	23,24,25	2.63	6 (26%)	25,32,34	1.29	2 (8%)
2	EXA	C	247	2	28,30,31	2.80	6 (21%)	28,41,43	1.57	3 (10%)
1	LLP	D	247	1	23,24,25	2.66	5 (21%)	25,32,34	1.26	3 (12%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	F	247	1	-	5/16/17/19	0/1/1/1
1	LLP	E	247	1	-	5/16/17/19	0/1/1/1
1	LLP	H	247	1	-	4/16/17/19	0/1/1/1
1	LLP	A	247	1	-	5/16/17/19	0/1/1/1
1	LLP	G	247	1	-	4/16/17/19	0/1/1/1
1	LLP	B	247	1	-	4/16/17/19	0/1/1/1
2	EXA	C	247	2	-	7/24/28/30	0/1/1/1
1	LLP	D	247	1	-	5/16/17/19	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	247	EXA	C9-C7	-9.10	1.32	1.49
1	H	247	LLP	C4-C4'	8.33	1.62	1.46
1	E	247	LLP	C4-C4'	8.28	1.62	1.46
1	B	247	LLP	C4-C4'	8.25	1.62	1.46
1	A	247	LLP	C4-C4'	8.21	1.62	1.46
1	F	247	LLP	C4-C4'	8.21	1.62	1.46
1	D	247	LLP	C4-C4'	8.19	1.62	1.46
1	G	247	LLP	C4-C4'	8.17	1.62	1.46
2	C	247	EXA	C3-C2	8.11	1.49	1.40
1	F	247	LLP	C4'-NZ	5.04	1.44	1.27
1	B	247	LLP	C4'-NZ	5.04	1.44	1.27
1	H	247	LLP	C4'-NZ	5.04	1.44	1.27
1	D	247	LLP	C4'-NZ	5.01	1.44	1.27
1	G	247	LLP	C4'-NZ	5.00	1.44	1.27
1	E	247	LLP	C4'-NZ	4.98	1.44	1.27
1	A	247	LLP	C4'-NZ	4.97	1.43	1.27
2	C	247	EXA	C3-C4	4.71	1.48	1.40
2	C	247	EXA	C4-C5	4.34	1.49	1.40
1	D	247	LLP	C4-C5	-4.20	1.36	1.42
1	H	247	LLP	C4-C5	-4.14	1.36	1.42
1	E	247	LLP	C4-C5	-4.02	1.36	1.42
1	F	247	LLP	C4-C5	-3.87	1.37	1.42
1	G	247	LLP	C4-C5	-3.84	1.37	1.42
1	A	247	LLP	C4-C5	-3.82	1.37	1.42
1	B	247	LLP	C4-C5	-3.71	1.37	1.42
1	D	247	LLP	C2'-C2	3.64	1.56	1.50
1	H	247	LLP	C2'-C2	3.59	1.56	1.50
1	A	247	LLP	C2'-C2	3.58	1.56	1.50
1	G	247	LLP	C2'-C2	3.58	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	247	LLP	C2'-C2	3.56	1.56	1.50
1	B	247	LLP	C2'-C2	3.52	1.56	1.50
1	E	247	LLP	C2'-C2	3.52	1.56	1.50
2	C	247	EXA	C7-N3	3.28	1.34	1.28
1	A	247	LLP	C6-N1	3.05	1.40	1.34
1	G	247	LLP	C6-N1	3.02	1.40	1.34
1	D	247	LLP	C6-N1	3.01	1.40	1.34
1	F	247	LLP	C6-N1	2.99	1.40	1.34
1	B	247	LLP	C6-N1	2.97	1.40	1.34
1	E	247	LLP	C6-N1	2.96	1.40	1.34
1	H	247	LLP	C6-N1	2.95	1.40	1.34
2	C	247	EXA	C8-C7	-2.62	1.46	1.49
1	A	247	LLP	C5'-C5	2.15	1.56	1.50
1	B	247	LLP	C5'-C5	2.15	1.56	1.50
1	G	247	LLP	C5'-C5	2.12	1.56	1.50
1	E	247	LLP	C3-C2	2.06	1.43	1.40
1	E	247	LLP	C5'-C5	2.05	1.56	1.50
1	F	247	LLP	C5'-C5	2.02	1.56	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	247	EXA	C8-C7-N3	5.66	121.03	114.53
1	A	247	LLP	C4-C4'-NZ	-3.86	106.60	124.31
1	D	247	LLP	C4-C4'-NZ	-3.82	106.77	124.31
1	F	247	LLP	C4-C4'-NZ	-3.68	107.44	124.31
1	G	247	LLP	C4-C4'-NZ	-3.60	107.77	124.31
1	B	247	LLP	C4-C4'-NZ	-3.55	108.01	124.31
1	E	247	LLP	C4-C4'-NZ	-3.49	108.31	124.31
1	H	247	LLP	C4-C4'-NZ	-3.32	109.05	124.31
2	C	247	EXA	C3-C4-C5	-2.83	115.96	119.18
1	G	247	LLP	CE-NZ-C4'	-2.54	111.09	118.90
1	B	247	LLP	CE-NZ-C4'	-2.38	111.58	118.90
1	H	247	LLP	CE-NZ-C4'	-2.29	111.87	118.90
1	F	247	LLP	CE-NZ-C4'	-2.28	111.90	118.90
1	H	247	LLP	C5-C6-N1	-2.22	120.11	123.82
1	F	247	LLP	C5-C6-N1	-2.14	120.25	123.82
1	E	247	LLP	C5-C6-N1	-2.14	120.26	123.82
1	A	247	LLP	CE-NZ-C4'	-2.11	112.41	118.90
1	E	247	LLP	CE-NZ-C4'	-2.11	112.41	118.90
1	G	247	LLP	C5-C6-N1	-2.11	120.31	123.82
1	D	247	LLP	C5-C6-N1	-2.10	120.33	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	247	LLP	CE-NZ-C4'	-2.04	112.63	118.90
2	C	247	EXA	C9-C7-N3	-2.00	120.50	125.30

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	247	LLP	C-CA-CB-CG
1	G	247	LLP	C-CA-CB-CG
1	F	247	LLP	C-CA-CB-CG
1	H	247	LLP	C-CA-CB-CG
2	C	247	EXA	C-CA-CB-CG
2	C	247	EXA	C4-C4'-NZ-CE
2	C	247	EXA	C4-C4'-N3-C7
2	C	247	EXA	N3-C7-C8-O10
2	C	247	EXA	N3-C7-C8-O11
2	C	247	EXA	C9-C7-C8-O10
2	C	247	EXA	C9-C7-C8-O11
1	D	247	LLP	C-CA-CB-CG
1	A	247	LLP	C-CA-CB-CG
1	B	247	LLP	C-CA-CB-CG
1	G	247	LLP	C4-C4'-NZ-CE
1	H	247	LLP	C4-C4'-NZ-CE
1	B	247	LLP	C4-C4'-NZ-CE
1	F	247	LLP	C4-C4'-NZ-CE
1	E	247	LLP	C4-C4'-NZ-CE
1	A	247	LLP	CG-CD-CE-NZ
1	A	247	LLP	C3-C4-C4'-NZ
1	F	247	LLP	C5'-OP4-P-OP3
1	D	247	LLP	C4-C4'-NZ-CE
1	A	247	LLP	CD-CE-NZ-C4'
1	E	247	LLP	CD-CE-NZ-C4'
1	F	247	LLP	C3-C4-C4'-NZ
1	H	247	LLP	C3-C4-C4'-NZ
1	B	247	LLP	C3-C4-C4'-NZ
1	A	247	LLP	C5-C4-C4'-NZ
1	D	247	LLP	CD-CE-NZ-C4'
1	E	247	LLP	C3-C4-C4'-NZ
1	D	247	LLP	C3-C4-C4'-NZ
1	G	247	LLP	CD-CE-NZ-C4'
1	F	247	LLP	CD-CE-NZ-C4'
1	B	247	LLP	CD-CE-NZ-C4'

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Mol	Chain	Res	Type	Atoms
1	H	247	LLP	CD-CE-NZ-C4'
1	G	247	LLP	C3-C4-C4'-NZ
1	E	247	LLP	N-CA-CB-CG
1	D	247	LLP	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	247	LLP	1	0
1	E	247	LLP	3	0
1	G	247	LLP	2	0
1	B	247	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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	FMT	E	501	-	2,2,2	0.72	0	1,1,1	0.29	0
4	8QJ	F	501	-	9,16,16	1.01	0	10,23,23	1.16	1 (10%)
3	FMT	G	501	-	2,2,2	0.71	0	1,1,1	0.22	0
3	FMT	H	501	-	2,2,2	0.73	0	1,1,1	0.27	0
4	8QJ	A	501	-	9,16,16	0.96	0	10,23,23	0.97	1 (10%)
3	FMT	F	502	-	2,2,2	0.71	0	1,1,1	0.23	0
3	FMT	B	501	-	2,2,2	0.71	0	1,1,1	0.25	0
3	FMT	A	502	-	2,2,2	0.72	0	1,1,1	0.25	0
3	FMT	C	501	-	2,2,2	0.72	0	1,1,1	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FMT	D	501	-	2,2,2	0.70	0	1,1,1	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	8QJ	F	501	-	-	6/14/16/16	0/1/1/1
4	8QJ	A	501	-	-	5/14/16/16	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	501	8QJ	O17-C16-C15	3.20	119.47	111.87
4	A	501	8QJ	O17-C16-C15	2.13	116.94	111.87

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	501	8QJ	N11-C12-C14-C15
4	F	501	8QJ	C13-C12-C14-C15
4	F	501	8QJ	C12-C14-C15-C16
4	A	501	8QJ	C12-C14-C15-C16
4	A	501	8QJ	C12-C14-C15-N19
4	A	501	8QJ	N19-C15-C16-O18
4	F	501	8QJ	C12-C14-C15-N19
4	F	501	8QJ	C14-C15-N19-C23
4	A	501	8QJ	C14-C15-N19-C22
4	F	501	8QJ	N19-C15-C16-O17
4	A	501	8QJ	C13-C12-C14-C15

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	501	8QJ	2	0
3	H	501	FMT	1	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	438/501 (87%)	0.09	7 (1%) 72 69	25, 37, 52, 70	0
1	B	436/501 (87%)	0.39	24 (5%) 25 22	24, 39, 76, 89	0
1	D	437/501 (87%)	0.08	7 (1%) 72 69	22, 36, 52, 70	0
1	E	435/501 (86%)	0.08	7 (1%) 72 69	25, 36, 53, 71	0
1	F	439/501 (87%)	0.33	10 (2%) 60 56	21, 41, 62, 75	0
1	G	440/501 (87%)	0.36	20 (4%) 33 30	24, 44, 66, 78	0
1	H	434/501 (86%)	0.19	9 (2%) 63 60	26, 38, 57, 84	0
2	C	435/501 (86%)	0.45	29 (6%) 17 14	24, 40, 76, 92	0
All	All	3494/4008 (87%)	0.25	113 (3%) 47 44	21, 39, 64, 92	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	422	PHE	6.4
1	A	400	TYR	4.4
2	C	465	ALA	4.4
2	C	386	VAL	4.4
1	B	398	GLY	4.4
2	C	399	LEU	4.3
1	E	400	TYR	4.2
2	C	400	TYR	4.1
1	G	292	ALA	4.0
1	H	294	ASN	3.9
1	H	404	HIS	3.9
1	G	386	VAL	3.9
1	G	186	PRO	3.9
1	G	183	GLY	3.7
2	C	385	PRO	3.7
1	G	176	ILE	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	176	ILE	3.6
2	C	466	LYS	3.6
1	F	292	ALA	3.6
1	H	400	TYR	3.6
2	C	294	ASN	3.5
1	G	168	VAL	3.5
2	C	417	VAL	3.5
1	G	389	THR	3.4
2	C	397	GLU	3.4
1	D	383	LYS	3.3
1	G	293	GLY	3.3
1	B	465	ALA	3.3
1	D	400	TYR	3.2
1	H	378	VAL	3.2
1	B	402	ILE	3.1
1	B	460	LEU	3.1
1	A	396	VAL	3.1
1	E	404	HIS	3.0
1	B	400	TYR	3.0
1	A	331	GLU	3.0
1	F	386	VAL	3.0
2	C	405	GLU	2.9
1	B	376	PHE	2.9
1	E	382	PRO	2.9
2	C	469	TYR	2.9
1	B	387	LYS	2.8
1	B	386	VAL	2.8
1	F	385	PRO	2.8
1	F	456	THR	2.8
2	C	413	TRP	2.8
1	B	355	ARG	2.8
1	A	383	LYS	2.8
1	B	399	LEU	2.7
2	C	374	LEU	2.7
2	C	254	GLY	2.7
2	C	464	VAL	2.7
1	E	407	ALA	2.7
1	D	469	TYR	2.7
1	B	375	PRO	2.7
2	C	404	HIS	2.6
1	H	379	GLY	2.5
1	G	356	VAL	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	408	ASN	2.5
1	B	430	PHE	2.5
1	D	380	GLU	2.5
1	B	256	ALA	2.5
1	A	76	TYR	2.5
1	H	325	GLU	2.5
1	G	180	ARG	2.5
1	E	405	GLU	2.5
1	A	384	ALA	2.4
1	G	254	GLY	2.4
1	B	177	LYS	2.4
2	C	242	ILE	2.4
2	C	402	ILE	2.4
1	H	382	PRO	2.4
1	G	119	TRP	2.4
1	F	181	GLU	2.4
1	A	405	GLU	2.4
1	E	403	PRO	2.3
1	G	357	LEU	2.3
2	C	255	CYS	2.3
2	C	281	GLN	2.3
1	G	291	PRO	2.3
1	D	382	PRO	2.3
2	C	106	ALA	2.3
1	B	405	GLU	2.3
2	C	387	LYS	2.2
1	F	382	PRO	2.2
1	H	405	GLU	2.2
1	B	413	TRP	2.2
1	B	420	ASP	2.2
1	G	376	PHE	2.2
1	B	469	TYR	2.2
1	B	464	VAL	2.2
1	F	21	THR	2.1
2	C	31	LEU	2.1
1	D	22	GLY	2.1
1	B	461	CYS	2.1
1	G	172	PHE	2.1
1	F	409	MET	2.1
1	D	254	GLY	2.1
1	G	384	ALA	2.1
1	G	464	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	470	LYS	2.1
1	B	421	GLU	2.1
1	F	294	ASN	2.1
2	C	111	ASN	2.1
2	C	382	PRO	2.0
2	C	409	MET	2.0
1	B	410	ALA	2.0
1	B	107	THR	2.0
1	B	307	THR	2.0
2	C	391	LYS	2.0
2	C	377	VAL	2.0
1	G	217	ILE	2.0
1	G	383	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	EXA	C	247	30/31	0.91	0.22	30,43,58,62	0
1	LLP	G	247	24/25	0.94	0.20	31,42,48,50	0
1	LLP	B	247	24/25	0.94	0.19	31,39,44,46	0
1	LLP	D	247	24/25	0.95	0.17	26,35,42,47	0
1	LLP	F	247	24/25	0.95	0.17	25,38,43,45	0
1	LLP	H	247	24/25	0.96	0.16	30,38,41,44	0
1	LLP	A	247	24/25	0.96	0.18	29,36,41,50	0
1	LLP	E	247	24/25	0.96	0.18	24,33,41,43	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	8QJ	A	501	16/16	0.86	0.21	43,65,72,73	0
3	FMT	D	501	3/3	0.88	0.16	33,33,38,44	0
3	FMT	E	501	3/3	0.89	0.20	40,40,44,54	0
3	FMT	C	501	3/3	0.90	0.20	44,44,46,48	0
4	8QJ	F	501	16/16	0.91	0.29	49,64,79,98	0
3	FMT	B	501	3/3	0.92	0.15	45,45,48,51	0
3	FMT	F	502	3/3	0.95	0.12	36,36,39,40	0
3	FMT	G	501	3/3	0.95	0.17	37,37,41,42	0
3	FMT	A	502	3/3	0.96	0.16	37,37,39,40	0
3	FMT	H	501	3/3	0.97	0.13	32,32,36,37	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.