

# Full wwPDB X-ray Structure Validation Report (i)

#### Nov 5, 2023 – 09:20 AM EST

PDB ID	:	7U7H
Title	:	Cysteate acyl-ACP transferase from Alistipes finegoldii
Authors	:	Radka, C.D.; Miller, D.J.; Frank, M.W.; Rock, C.O.
Deposited on	:	2022-03-07
Resolution	:	2.90  Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
buster-report	:	1.1.7(2018)
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:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 2.90 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.



Motrie	Whole archive	Similar resolution		
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$		
R <sub>free</sub>	130704	1957 (2.90-2.90)		
Clashscore	141614	2172 (2.90-2.90)		
Ramachandran outliers	138981	2115 (2.90-2.90)		
Sidechain outliers	138945	2117 (2.90-2.90)		
RSRZ outliers	127900	1906 (2.90-2.90)		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	А	443	% • 70%	24%		• 5%
1	В	443	% 73%	21%		• 5%
1	С	443	% 64%	25%	•	10%
1	D	443	2% 65%	23%	•	9%
1	Е	443	9%	32%		• 5%



Mol	Chain	Length	Quality of cha	in	
			9%		
1	$\mathbf{F}$	443	65%	30%	• 5%



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18499 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.

Mol	Chain	Residues		A	Atoms	5			ZeroOcc	AltConf	Trace
1	Δ	193	Total	С	Ν	0	$\mathbf{S}$	Se	0	Ο	0
	Π	420	3236	2071	560	582	4	19	0	0	0
1	В	193	Total	С	Ν	Ο	S	Se	0	0	0
	D	420	3189	2040	551	575	4	19	0	0	0
1	С	400	Total	С	Ν	Ο	S	Se	0	0	0
	U	400	2975	1901	515	538	4	17	0	U	0
1	п	401	Total	С	Ν	Ο	S	Se	0	0	0
	D	401	2920	1863	505	532	4	16	0	0	0
1	F	499	Total	С	Ν	Ο	S	Se	0	0	0
L	Ľ	422	3036	1932	522	560	4	18	0	0	0
1	1 F	402	Total	С	Ν	0	S	Se	0	0	0
	Г	420	3113	1988	529	574	3	19		0	0

• Molecule 1 is a protein called 7-keto-8-aminopelargonate synthetase-like enzyme.

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-19	MSE	- initiating methionine U		UNP I3YKQ4
А	-18	GLY	-	expression tag	UNP I3YKQ4
А	-17	SER	-	expression tag	UNP I3YKQ4
А	-16	SER	-	expression tag	UNP I3YKQ4
А	-15	HIS	-	expression tag	UNP I3YKQ4
А	-14	HIS	-	expression tag	UNP I3YKQ4
А	-13	HIS	-	expression tag	UNP I3YKQ4
А	-12	HIS	-	expression tag	UNP I3YKQ4
А	-11	HIS	-	expression tag	UNP I3YKQ4
А	-10	HIS	-	expression tag	UNP I3YKQ4
А	-9	SER	-	expression tag	UNP I3YKQ4
А	-8	SER	-	expression tag	UNP I3YKQ4
А	-7	GLY	-	expression tag	UNP I3YKQ4
А	-6	LEU	-	expression tag	UNP I3YKQ4
A	-5	VAL	-	expression tag	UNP I3YKQ4
A	-4	PRO	-	expression tag	UNP I3YKQ4
A	-3	ARG	_	expression tag	UNP I3YKQ4



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Chain	Residue	Modelled	Actual	Reference		
А	-2	GLY	-	expression tag	UNP I3YKQ4	
А	-1	SER	-	expression tag	UNP I3YKQ4	
А	0	HIS	-	- expression tag U		
В	-19	MSE	-	initiating methionine	UNP I3YKQ4	
В	-18	GLY	-	expression tag	UNP I3YKQ4	
В	-17	SER	-	expression tag	UNP I3YKQ4	
В	-16	SER	-	expression tag	UNP I3YKQ4	
В	-15	HIS	-	expression tag	UNP I3YKQ4	
В	-14	HIS	-	expression tag	UNP I3YKQ4	
В	-13	HIS	-	expression tag	UNP I3YKQ4	
В	-12	HIS	-	expression tag	UNP I3YKQ4	
В	-11	HIS	-	expression tag	UNP I3YKQ4	
В	-10	HIS	-	expression tag	UNP I3YKQ4	
В	-9	SER	-	expression tag	UNP I3YKQ4	
В	-8	SER	-	expression tag	UNP I3YKQ4	
В	-7	GLY	-	expression tag	UNP I3YKQ4	
В	-6	LEU	-	expression tag	UNP I3YKQ4	
В	-5	VAL	-	expression tag	UNP I3YKQ4	
В	-4	PRO	-	expression tag	UNP I3YKQ4	
В	-3	ARG	-	expression tag	UNP I3YKQ4	
В	-2	GLY	-	expression tag	UNP I3YKQ4	
В	-1	SER	-	expression tag	UNP I3YKQ4	
В	0	HIS	-	expression tag	UNP I3YKQ4	
С	-19	MSE	-	initiating methionine	UNP I3YKQ4	
С	-18	GLY	-	expression tag	UNP I3YKQ4	
С	-17	SER	-	expression tag	UNP I3YKQ4	
С	-16	SER	-	expression tag	UNP I3YKQ4	
C	-15	HIS	-	expression tag	UNP I3YKQ4	
C	-14	HIS	-	expression tag	UNP I3YKQ4	
С	-13	HIS	-	expression tag	UNP I3YKQ4	
С	-12	HIS	-	expression tag	UNP I3YKQ4	
С	-11	HIS	-	expression tag	UNP I3YKQ4	
С	-10	HIS	-	expression tag	UNP I3YKQ4	
С	-9	SER	-	expression tag	UNP I3YKQ4	
С	-8	SER	-	expression tag	UNP I3YKQ4	
С	-7	GLY	-	expression tag	UNP I3YKQ4	
C	-6	LEU	-	expression tag	UNP I3YKQ4	
C	-5	VAL	-	expression tag	UNP I3YKQ4	
C	-4	PRO	-	expression tag	UNP I3YKQ4	
C	-3	ARG	-	expression tag	UNP I3YKQ4	
C	-2	GLY	-	expression tag	UNP I3YKQ4	
С	-1	SER	-	expression tag	UNP I3YKQ4	



Chain	Residue	Modelled	Actual	Comment	Reference	
С	0	HIS	-	- expression tag		
D	-19	MSE	-	initiating methionine	UNP I3YKQ4	
D	-18	GLY	- expression tag U		UNP I3YKQ4	
D	-17	SER	-	expression tag	UNP I3YKQ4	
D	-16	SER	-	expression tag	UNP I3YKQ4	
D	-15	HIS	-	expression tag	UNP I3YKQ4	
D	-14	HIS	-	expression tag	UNP I3YKQ4	
D	-13	HIS	-	expression tag	UNP I3YKQ4	
D	-12	HIS	-	expression tag	UNP I3YKQ4	
D	-11	HIS	-	expression tag	UNP I3YKQ4	
D	-10	HIS	-	expression tag	UNP I3YKQ4	
D	-9	SER	-	expression tag	UNP I3YKQ4	
D	-8	SER	-	expression tag	UNP I3YKQ4	
D	-7	GLY	-	expression tag	UNP I3YKQ4	
D	-6	LEU	-	expression tag	UNP I3YKQ4	
D	-5	VAL	-	expression tag	UNP I3YKQ4	
D	-4	PRO	-	expression tag	UNP I3YKQ4	
D	-3	ARG	-	expression tag	UNP I3YKQ4	
D	-2	GLY	-	expression tag	UNP I3YKQ4	
D	-1	SER	-	expression tag	UNP I3YKQ4	
D	0	HIS	-	expression tag	UNP I3YKQ4	
Е	-19	MSE	-	initiating methionine	UNP I3YKQ4	
Е	-18	GLY	-	expression tag	UNP I3YKQ4	
Е	-17	SER	-	expression tag	UNP I3YKQ4	
Ε	-16	SER	-	expression tag	UNP I3YKQ4	
Е	-15	HIS	-	expression tag	UNP I3YKQ4	
E	-14	HIS	-	expression tag	UNP I3YKQ4	
E	-13	HIS	-	expression tag	UNP I3YKQ4	
E	-12	HIS	-	expression tag	UNP I3YKQ4	
E	-11	HIS	-	expression tag	UNP I3YKQ4	
E	-10	HIS	-	expression tag	UNP I3YKQ4	
E	-9	SER	-	expression tag	UNP I3YKQ4	
E	-8	SER	-	expression tag	UNP I3YKQ4	
E	-7	GLY	-	expression tag	UNP I3YKQ4	
Е	-6	LEU	-	expression tag	UNP I3YKQ4	
E	-5	VAL	-	expression tag	UNP I3YKQ4	
E	-4	PRO	-	expression tag	UNP I3YKQ4	
E	-3	ARG	-	expression tag	UNP I3YKQ4	
E	-2	GLY	-	expression tag	UNP I3YKQ4	
E	-1	SER	-	expression tag	UNP I3YKQ4	
E	0	HIS	-	expression tag	UNP I3YKQ4	
F	-19	MSE	-	initiating methionine	UNP I3YKQ4	



Chain	Residue	Modelled	Actual Comment		Reference
F	-18	GLY	-	expression tag	UNP I3YKQ4
F	-17	SER	-	expression tag	UNP I3YKQ4
F	-16	SER	-	expression tag	UNP I3YKQ4
F	-15	HIS	-	expression tag	UNP I3YKQ4
F	-14	HIS	-	expression tag	UNP I3YKQ4
F	-13	HIS	-	expression tag	UNP I3YKQ4
F	-12	HIS	-	expression tag	UNP I3YKQ4
F	-11	HIS	-	expression tag	UNP I3YKQ4
F	-10	HIS	-	expression tag	UNP I3YKQ4
F	-9	SER	-	expression tag	UNP I3YKQ4
F	-8	SER	-	expression tag	UNP I3YKQ4
F	-7	GLY	-	expression tag	UNP I3YKQ4
F	-6	LEU	-	expression tag	UNP I3YKQ4
F	-5	VAL	-	expression tag	UNP I3YKQ4
F	-4	PRO	-	expression tag	UNP I3YKQ4
F	-3	ARG	-	expression tag	UNP I3YKQ4
F	-2	GLY	-	expression tag	UNP I3YKQ4
F	-1	SER	-	expression tag	UNP I3YKQ4
F	0	HIS	-	expression tag	UNP I3YKQ4

• Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	Λ	1	Total	С	Ν	0	Р	0	0
2 A	I	15	8	1	5	1	0	0	



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	В	1	Total	С	Ν	0	Р	0	Ο
Z D	D	1	15	8	1	5	1	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 7-keto-8-aminopelargonate synthetase-like enzyme













• Molecule 1: 7-keto-8-aminopelargonate synthetase-like enzyme



#### G340 G341 1267 3282 283 284 .292 (293 (294 .269 .270 .271 N330 S331 P332 V333 V333 T334 • Molecule 1: 7-keto-8-aminopelargonate synthetase-like enzyme 9% Chain F: 65% • 5% 30% MSE GLY SER HIS HIS HIS HIS HIS HIS HIS SER HIS SER VAL LLEU VAL LLEU VAL HIS SER RAG 5 V185 T106 F324 F325 G327 G327 C327 F329 N330 S331 F332 F333 F333 T334 335 **1313 N347** 351 352 312 L375 R376 1378 1378 7379 7380 A381 A381 A382 H383 H383 N388 V388 V388 V389 V389 V389 V389 V390 V389 V390 V382 V390 (396 (396 (398 1406 Y407 (401



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants	127.52Å 127.52Å 177.30Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	29.55 - 2.90	Depositor
Resolution (A)	29.55 - 2.90	EDS
% Data completeness	$99.7\ (29.55-2.90)$	Depositor
(in resolution range)	$99.8\ (29.55-2.90)$	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.84 (at 2.90 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
B B.	0.218 , $0.268$	Depositor
It, Itfree	0.224 , $0.246$	DCC
$R_{free}$ test set	3563 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	74.4	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29 , $48.9$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.51, < L^2>=0.34$	Xtriage
	0.008 for -h,-k,l	
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
	0.008 for -k,-h,-l	
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18499	wwPDB-VP
Average B, all atoms $(Å^2)$	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: PLP

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).

Mal	Chain	Bond lengths		Bond angles	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.31	0/3289	0.55	0/4416
1	В	0.30	0/3241	0.55	0/4357
1	С	0.34	0/3019	0.58	0/4060
1	D	0.32	0/2961	0.58	0/3990
1	Е	0.32	0/3080	0.59	0/4160
1	F	0.33	0/3164	0.59	0/4271
All	All	0.32	0/18754	0.57	0/25254

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3236	0	3182	91	0
1	В	3189	0	3097	85	0
1	С	2975	0	2871	103	0
1	D	2920	0	2761	97	0
1	Е	3036	0	2829	123	0
1	F	3113	0	2932	93	0
2	А	15	0	7	1	0



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	15	0	7	0	0
All	All	18499	0	17686	547	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 15.

All (547) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:266:LEU:CD2	1:C:270:LEU:HD11	1.65	1.25
1:B:197:LEU:HD13	1:B:330:ASN:CB	1.79	1.11
1:D:190:VAL:HG22	1:D:197:LEU:HD23	1.28	1.10
1:C:266:LEU:HD23	1:C:270:LEU:CD1	1.80	1.10
1:D:256:ILE:H	1:D:287:MSE:HE3	1.05	1.09
1:D:190:VAL:HG22	1:D:197:LEU:CD2	1.83	1.08
1:B:197:LEU:CD1	1:B:330:ASN:HB2	1.89	1.01
1:D:96:LEU:HD22	1:D:111:LEU:HD13	1.51	0.93
1:C:96:LEU:HD22	1:C:111:LEU:HD13	1.52	0.91
1:B:197:LEU:HD13	1:B:330:ASN:HB2	0.93	0.90
1:D:256:ILE:N	1:D:287:MSE:HE3	1.86	0.90
1:C:266:LEU:HD23	1:C:270:LEU:HD11	0.92	0.89
1:F:119:MSE:HE1	1:F:215:LEU:HD21	1.57	0.87
1:A:80:PRO:HD3	1:A:285:MSE:HG2	1.56	0.87
1:B:364:ILE:HG13	1:B:366:PRO:HD2	1.55	0.86
1:F:78:ALA:O	1:F:81:MSE:SE	2.42	0.86
1:E:197:LEU:HD13	1:E:330:ASN:HB2	1.57	0.85
1:A:37:GLY:H	1:A:40:MSE:HE2	1.39	0.85
1:A:380:THR:H	1:A:383:HIS:HD2	1.27	0.81
1:D:256:ILE:H	1:D:287:MSE:CE	1.89	0.81
1:C:313:ARG:O	1:C:317:ASN:HB2	1.80	0.81
1:A:117:GLN:HE21	1:B:117:GLN:H	1.31	0.79
1:F:336:VAL:HB	1:F:338:MSE:HE1	1.64	0.78
1:B:80:PRO:HG3	1:B:285:MSE:HG2	1.64	0.77
1:C:266:LEU:O	1:C:270:LEU:HD12	1.84	0.77
1:D:197:LEU:HD11	1:D:225:MSE:HE2	1.67	0.76
1:B:270:LEU:HB3	1:B:274:MSE:HE2	1.68	0.76
1:B:224:THR:HG22	1:B:225:MSE:HG2	1.68	0.75
$1:\overline{C:224:THR:HG22}$	1:C:225:MSE:HE2	1.66	0.75
1:C:96:LEU:HD21	1:C:100:LEU:HD11	1.68	0.75
1:A:79:ALA:HB1	1:A:80:PRO:HD2	1.69	0.75
1:E:190:VAL:HG21	1:E:225:MSE:HE3	1.68	0.75



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:47:MSE:HE2	1:E:359:PHE:HB2	1.70	0.74
1:D:38:PRO:HB3	1:D:383:HIS:CE1	2.24	0.73
1:A:380:THR:H	1:A:383:HIS:CD2	2.06	0.73
1:E:294:ARG:HA	1:E:297:LEU:HD12	1.70	0.73
1:D:197:LEU:HD11	1:D:225:MSE:CE	2.19	0.72
1:A:177:GLU:HG2	1:B:1:MSE:HG3	1.71	0.72
1:E:108:ASP:OD1	1:E:109:ALA:N	2.22	0.72
1:C:197:LEU:HD13	1:C:330:ASN:HB2	1.71	0.71
1:D:190:VAL:CG2	1:D:197:LEU:CD2	2.64	0.71
1:B:110:PHE:HD2	1:B:274:MSE:HE3	1.57	0.70
1:C:380:THR:H	1:C:383:HIS:HD2	1.38	0.70
1:B:256:ILE:HB	1:B:287:MSE:HE3	1.73	0.70
1:C:201:ASP:OD1	1:C:202:GLU:N	2.25	0.69
1:C:380:THR:H	1:C:383:HIS:CD2	2.10	0.68
1:C:363:VAL:HB	1:C:374:ILE:HB	1.75	0.68
1:A:410:MSE:SE	1:A:411:PRO:HD2	2.43	0.68
1:F:312:VAL:HG21	1:F:332:PRO:HA	1.74	0.68
1:E:283:LEU:HD12	1:E:284:PRO:HD2	1.75	0.68
1:F:186:ILE:HG12	1:F:215:LEU:HD23	1.74	0.68
1:B:8:LEU:HA	1:B:12:ALA:HB3	1.76	0.67
1:F:309:TRP:HA	1:F:312:VAL:HG12	1.77	0.67
1:F:418:GLU:OE2	1:F:418:GLU:N	2.26	0.67
1:F:119:MSE:CE	1:F:215:LEU:HD21	2.25	0.66
1:C:338:MSE:HE1	1:C:399:ARG:HG3	1.76	0.66
1:E:201:ASP:H	1:E:236:PHE:HD2	1.41	0.66
1:F:380:THR:HG23	1:F:382:ALA:H	1.60	0.66
1:F:283:LEU:HD12	1:F:284:PRO:HD2	1.78	0.66
1:C:349:ILE:HD11	1:C:362:ILE:CG2	2.26	0.66
1:F:301:HIS:HB2	1:F:304:TYR:CE2	2.30	0.66
1:D:348:LEU:HD23	1:D:349:ILE:N	2.11	0.66
1:A:79:ALA:HB1	1:A:285:MSE:H	1.61	0.65
1:C:80:PRO:HG3	1:C:285:MSE:HG2	1.79	0.65
1:C:119:MSE:HE3	1:C:123:ILE:HD11	1.79	0.65
1:D:349:ILE:O	1:D:353:ARG:HG3	1.96	0.65
1:D:380:THR:H	1:D:383:HIS:CD2	2.15	0.65
1:F:224:THR:HG22	1:F:225:MSE:SE	2.47	0.65
1:C:119:MSE:HE1	1:C:215:LEU:HD21	1.80	0.64
1:E:113:ASN:H	1:E:277:GLN:HE22	1.44	0.64
1:C:364:ILE:HG23	1:C:366:PRO:HD2	1.80	0.64
1:B:385:LEU:HG	1:C:385:LEU:HD11	1.80	0.64
1:D:308:LEU:HD21	1:D:332:PRO:HG3	1.80	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:40:MSE:HB2	1:E:49:ASN:HD21	1.62	0.63
1:F:56:LEU:HG	1:F:252:SER:HB3	1.80	0.63
1:A:364:ILE:HG23	1:A:366:PRO:HD2	1.80	0.63
1:E:110:PHE:HB2	1:E:267:VAL:HG23	1.80	0.63
1:F:270:LEU:HB3	1:F:274:MSE:HE3	1.79	0.63
1:F:108:ASP:OD1	1:F:109:ALA:N	2.31	0.63
1:E:93:HIS:CE1	1:E:288:VAL:HG21	2.33	0.63
1:D:284:PRO:HD3	1:E:256:ILE:HD13	1.81	0.63
1:F:96:LEU:HD13	1:F:292:LEU:HG	1.81	0.63
1:F:329:THR:HG21	1:F:335:PRO:HD2	1.80	0.62
1:C:117:GLN:HB3	1:C:276:SER:HB2	1.81	0.62
1:D:38:PRO:HB3	1:D:383:HIS:ND1	2.15	0.62
1:A:85:MSE:HG3	1:B:28:ALA:O	2.00	0.62
1:B:207:LYS:NZ	1:B:241:GLY:O	2.28	0.62
1:A:116:TYR:HB3	1:B:117:GLN:NE2	2.15	0.61
1:B:352:LEU:HG	1:B:398:VAL:HG21	1.81	0.61
1:C:385:LEU:HD12	1:C:385:LEU:H	1.65	0.61
1:F:363:VAL:HB	1:F:374:ILE:HB	1.81	0.61
1:C:222:PHE:HE2	1:C:253:MSE:HE1	1.65	0.61
1:C:349:ILE:HD11	1:C:362:ILE:HG21	1.82	0.61
1:F:38:PRO:HB3	1:F:383:HIS:CD2	2.35	0.61
1:E:167:LEU:HG	1:E:171:HIS:HE1	1.66	0.61
1:F:319:LEU:HB3	1:F:324:PHE:HB2	1.82	0.61
1:C:108:ASP:HB3	1:C:267:VAL:HG21	1.81	0.61
1:A:119:MSE:SE	1:A:122:ILE:HD11	2.50	0.61
1:D:112:LEU:HD22	1:D:274:MSE:HE1	1.82	0.61
1:C:332:PRO:O	1:C:334:THR:HG23	2.00	0.60
1:F:35:GLU:OE1	1:F:60:ASN:ND2	2.33	0.60
1:E:235:HIS:HD1	1:E:236:PHE:HD1	1.48	0.60
1:C:96:LEU:CD2	1:C:100:LEU:CD1	2.80	0.60
1:D:96:LEU:CD2	1:D:111:LEU:HD13	2.28	0.60
1:A:89:GLN:HG3	1:B:29:PHE:HD2	1.66	0.60
1:C:96:LEU:CD2	1:C:100:LEU:HD11	2.31	0.60
1:F:351:ASP:OD1	1:F:355:ASN:ND2	2.35	0.60
1:D:197:LEU:HD21	1:D:225:MSE:HE2	1.84	0.60
1:E:93:HIS:HE1	1:E:288:VAL:HG21	1.67	0.60
1:A:256:ILE:HG13	1:B:284:PRO:HG3	1.85	0.59
1:B:201:ASP:OD1	1:B:202:GLU:N	2.35	0.59
1:C:93:HIS:O	1:C:97:GLU:HG3	2.01	0.59
1:D:134:VAL:HA	1:D:155:PHE:O	2.02	0.59
1:B:20:MSE:HE3	1:B:420:PHE:HZ	1.67	0.59



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:352:LEU:HG	1:A:398:VAL:HG21	1.85	0.59
1:B:113:ASN:OD1	1:B:277:GLN:NE2	2.36	0.59
1:F:116:TYR:O	1:F:120:ILE:HG12	2.03	0.59
1:C:122:ILE:HD11	1:C:260:VAL:HG11	1.85	0.59
1:A:73:ALA:O	1:B:65:ARG:NH2	2.36	0.58
1:D:96:LEU:HD23	1:D:100:LEU:HD23	1.84	0.58
1:D:138:GLU:OE1	1:D:193:MSE:SE	2.71	0.58
1:C:38:PRO:HB3	1:C:383:HIS:CE1	2.39	0.58
1:A:38:PRO:HB3	1:A:383:HIS:CE1	2.38	0.58
1:B:31:LYS:NZ	1:B:417:ASP:OD2	2.35	0.58
1:C:334:THR:OG1	1:C:377:VAL:HB	2.03	0.58
1:D:380:THR:HG22	1:D:383:HIS:CE1	2.39	0.58
1:A:326:ILE:HD12	1:A:334:THR:HG23	1.85	0.58
1:D:7:ARG:NH2	1:E:126:LEU:O	2.36	0.58
1:D:119:MSE:HE3	1:D:143:ILE:HG12	1.84	0.58
1:F:96:LEU:HD23	1:F:111:LEU:HD11	1.85	0.58
1:E:414:VAL:HG23	1:E:415:ARG:H	1.69	0.58
1:F:26:TYR:HD1	1:F:43:ARG:HH11	1.52	0.58
1:C:117:GLN:HB3	1:C:276:SER:CB	2.34	0.58
1:E:85:MSE:HB3	1:E:278:LEU:HD22	1.85	0.58
1:F:118:GLY:C	1:F:122:ILE:HD12	2.24	0.58
1:B:380:THR:HG23	1:B:382:ALA:H	1.69	0.57
1:D:275:ARG:NH1	1:E:145:ASP:OD1	2.36	0.57
1:F:309:TRP:O	1:F:313:ARG:HG2	2.03	0.57
1:F:225:MSE:HE1	1:F:309:TRP:HZ2	1.69	0.57
1:E:263:PRO:O	1:E:267:VAL:HG12	2.05	0.57
1:C:308:LEU:HD21	1:C:332:PRO:HG3	1.87	0.57
1:E:36:ILE:HD13	1:E:40:MSE:HE1	1.85	0.57
1:E:36:ILE:O	1:E:60:ASN:HB2	2.05	0.57
1:E:413:PRO:HB2	1:E:415:ARG:HG2	1.86	0.57
1:D:312:VAL:HG22	1:D:379:PRO:HG2	1.87	0.56
1:F:143:ILE:HG21	1:F:186:ILE:HG21	1.86	0.56
1:C:96:LEU:HD23	1:C:100:LEU:HD12	1.86	0.56
1:C:197:LEU:HD13	1:C:330:ASN:CB	2.34	0.56
1:D:54:ASN:HD21	1:D:59:ALA:CB	2.19	0.56
1:D:348:LEU:O	1:D:349:ILE:HB	2.05	0.56
1:E:61:HIS:CE1	1:E:63:GLU:HB2	2.40	0.56
1:A:106:LYS:NZ	1:A:242:VAL:O	2.36	0.56
1:B:75:PHE:HB3	1:B:79:ALA:HB2	1.86	0.56
1:B:159:HIS:NE2	1:B:196:ASP:OD2	2.37	0.56
1:F:199:LYS:O	1:F:203:ILE:HG13	2.06	0.56



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:138:GLU:HG3	1:F:159:HIS:CG	2.41	0.56
1:E:224:THR:HG23	1:E:308:LEU:HD21	1.87	0.56
1:A:8:LEU:HA	1:A:12:ALA:HB3	1.88	0.56
1:B:326:ILE:HD12	1:B:334:THR:HG23	1.88	0.56
1:A:349:ILE:HG13	1:A:362:ILE:HD13	1.87	0.55
1:A:36:ILE:HG21	1:B:81:MSE:HE3	1.87	0.55
1:C:96:LEU:HD23	1:C:100:LEU:CD1	2.35	0.55
1:E:288:VAL:O	1:E:292:LEU:HD12	2.06	0.55
1:D:280:ALA:HB1	1:E:114:PHE:HE1	1.72	0.55
1:B:75:PHE:HB3	1:B:79:ALA:CB	2.36	0.55
1:E:40:MSE:HB2	1:E:49:ASN:ND2	2.20	0.55
1:F:133:VAL:HG11	1:F:147:LEU:HD21	1.88	0.55
1:B:196:ASP:HB3	1:B:328:VAL:HG23	1.89	0.55
1:D:338:MSE:HB2	1:D:373:ILE:HG23	1.89	0.55
1:A:40:MSE:CE	1:A:52:LEU:HD21	2.37	0.55
1:D:358:ILE:HD13	1:D:391:THR:HG23	1.89	0.55
1:F:380:THR:HG22	1:F:383:HIS:ND1	2.22	0.55
1:A:251:LYS:NZ	2:A:501:PLP:O3	2.40	0.55
1:D:248:THR:HG23	1:D:250:ALA:H	1.71	0.55
1:F:407:TYR:HD1	1:F:410:MSE:HE1	1.72	0.54
1:A:117:GLN:HE22	1:B:114:PHE:HB3	1.71	0.54
1:D:197:LEU:CD1	1:D:225:MSE:HE2	2.36	0.54
1:F:55:TYR:HD2	1:F:224:THR:HG1	1.56	0.54
1:F:74:LYS:HD2	1:F:75:PHE:CE1	2.43	0.54
1:C:319:LEU:HB3	1:C:324:PHE:HB2	1.89	0.54
1:F:342:ILE:O	1:F:346:THR:HG22	2.08	0.54
1:F:407:TYR:HA	1:F:410:MSE:HE1	1.90	0.54
1:F:119:MSE:HE2	1:F:123:ILE:HG13	1.89	0.54
1:C:197:LEU:HD21	1:C:225:MSE:SE	2.58	0.54
1:D:385:LEU:HD12	1:D:385:LEU:H	1.72	0.54
1:C:225:MSE:HE1	1:C:331:SER:HA	1.90	0.54
1:C:54:ASN:HD21	1:C:57:GLY:HA2	1.73	0.54
1:C:116:TYR:CD1	1:C:142:CYS:HB3	2.42	0.54
1:F:227:GLU:O	1:F:230:ARG:HG3	2.08	0.54
1:D:224:THR:HG22	1:D:225:MSE:SE	2.58	0.54
1:E:275:ARG:HH11	1:E:275:ARG:HG3	1.73	0.54
1:F:97:GLU:CD	1:F:271:ARG:HH22	2.11	0.53
1:F:288:VAL:O	1:F:292:LEU:HD12	2.08	0.53
1:B:78:ALA:HB1	1:B:81:MSE:HE1	1.89	0.53
1:E:64:VAL:HG22	1:E:294:ARG:HG2	1.89	0.53
1:E:270:LEU:HD22	1:E:274:MSE:HE2	1.90	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:140:HIS:HD2	1:C:142:CYS:H	1.57	0.53
1:C:289:MSE:HE3	1:C:289:MSE:HA	1.89	0.53
1:E:127:LEU:HD21	1:E:133:VAL:CG2	2.38	0.53
1:C:77:MSE:HA	1:C:286:PRO:HG2	1.90	0.53
1:E:342:ILE:O	1:E:346:THR:HG22	2.09	0.53
1:A:306:GLN:O	1:A:310:GLU:HG3	2.09	0.53
1:E:201:ASP:OD1	1:E:202:GLU:N	2.41	0.53
1:F:51:SER:HA	1:F:378:ILE:HD12	1.91	0.53
1:C:266:LEU:HD21	1:C:270:LEU:HD11	1.79	0.52
1:C:348:LEU:HG	1:C:398:VAL:HG13	1.91	0.52
1:D:317:ASN:O	1:D:321:GLU:HG2	2.08	0.52
1:E:168:GLN:HA	1:E:171:HIS:HD1	1.73	0.52
1:E:270:LEU:HB3	1:E:274:MSE:HE3	1.92	0.52
1:F:7:ARG:HH11	1:F:8:LEU:HD21	1.74	0.52
1:F:114:PHE:HD1	1:F:115:GLY:H	1.57	0.52
1:E:388:VAL:O	1:E:392:ILE:HG12	2.10	0.52
1:D:53:ASN:HB3	1:D:251:LYS:HG3	1.91	0.52
1:D:93:HIS:O	1:D:97:GLU:HG3	2.10	0.52
1:D:348:LEU:CD2	1:D:349:ILE:HD12	2.40	0.52
1:E:47:MSE:HE3	1:E:48:LEU:H	1.74	0.52
1:C:96:LEU:CD2	1:C:111:LEU:HD13	2.33	0.52
1:C:122:ILE:HD11	1:C:260:VAL:HG21	1.92	0.52
1:C:348:LEU:HG	1:C:398:VAL:CG1	2.40	0.52
1:E:109:ALA:HA	1:E:260:VAL:O	2.10	0.52
1:F:334:THR:O	1:F:334:THR:OG1	2.26	0.52
1:F:340:GLY:HA3	1:F:373:ILE:HD11	1.92	0.52
1:C:112:LEU:HD13	1:C:118:GLY:HA3	1.92	0.52
1:F:36:ILE:HA	1:F:40:MSE:SE	2.60	0.52
1:A:284:PRO:HG3	1:B:256:ILE:HG13	1.93	0.51
1:B:114:PHE:CE1	1:B:256:ILE:HD12	2.45	0.51
1:E:255:GLY:C	1:E:256:ILE:HG13	2.31	0.51
1:C:84:ARG:HH12	1:C:111:LEU:HB3	1.75	0.51
1:C:204:VAL:O	1:C:207:LYS:HB2	2.09	0.51
1:D:14:GLY:HA2	1:E:269:LEU:HD23	1.93	0.51
1:C:93:HIS:CE1	1:C:288:VAL:HG21	2.45	0.51
1:C:140:HIS:CD2	1:C:142:CYS:H	2.28	0.51
1:E:346:THR:O	1:E:350:VAL:HG23	2.10	0.51
1:E:197:LEU:HD13	1:E:330:ASN:CB	2.36	0.51
1:B:214:LEU:HD23	1:B:242:VAL:HA	1.92	0.51
1:C:153:LYS:HD2	1:C:154:ARG:H	1.76	0.51
1:D:114:PHE:CZ	1:E:113:ASN:HB2	2.46	0.51



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:268:ASN:HB3	1:B:20:MSE:HE1	1.93	0.51
1:F:315:LEU:HD23	1:F:334:THR:HG21	1.93	0.51
1:E:47:MSE:HE1	1:E:358:ILE:C	2.32	0.51
1:A:107:GLU:OE2	1:A:264:ARG:NH2	2.44	0.50
1:D:54:ASN:HD21	1:D:59:ALA:HB3	1.75	0.50
1:C:190:VAL:HG22	1:C:197:LEU:HG	1.93	0.50
1:D:133:VAL:HG11	1:D:147:LEU:HD21	1.92	0.50
1:A:256:ILE:HB	1:A:287:MSE:HE3	1.94	0.50
1:B:270:LEU:HB3	1:B:274:MSE:CE	2.39	0.50
1:C:349:ILE:HG13	1:C:362:ILE:HD13	1.92	0.50
1:F:103:PHE:CE1	1:F:230:ARG:HG2	2.46	0.50
1:F:407:TYR:HA	1:F:410:MSE:CE	2.41	0.50
1:C:192:GLY:O	1:C:376:ARG:NH1	2.43	0.50
1:D:294:ARG:O	1:D:298:ILE:HD12	2.12	0.50
1:A:238:VAL:HG12	1:A:238:VAL:O	2.12	0.50
1:D:295:LEU:HD13	1:D:299:ARG:NE	2.27	0.50
1:E:113:ASN:OD1	1:E:113:ASN:N	2.45	0.50
1:F:159:HIS:NE2	1:F:196:ASP:OD2	2.42	0.50
1:C:113:ASN:HA	1:C:283:LEU:HD13	1.92	0.50
1:E:118:GLY:O	1:E:122:ILE:HG13	2.12	0.50
1:E:365:TYR:HA	1:E:368:ILE:O	2.11	0.50
1:E:401:LYS:HA	1:E:406:ILE:HD12	1.93	0.50
1:F:368:ILE:HG13	1:F:369:PRO:HD2	1.94	0.50
1:A:107:GLU:HB2	1:A:263:PRO:HA	1.93	0.50
1:E:351:ASP:OD1	1:E:355:ASN:ND2	2.45	0.49
1:C:54:ASN:ND2	1:C:57:GLY:HA2	2.27	0.49
1:D:97:GLU:OE2	1:D:110:PHE:HA	2.11	0.49
1:D:99:GLU:OE1	1:D:299:ARG:NH2	2.45	0.49
1:F:171:HIS:O	1:F:175:LEU:HD12	2.13	0.49
1:D:96:LEU:O	1:D:100:LEU:HD23	2.13	0.49
1:E:294:ARG:O	1:E:298:ILE:HG23	2.11	0.49
1:F:256:ILE:H	1:F:287:MSE:SE	2.44	0.49
1:A:354:GLU:OE1	1:A:415:ARG:NH2	2.43	0.49
1:C:134:VAL:HA	1:C:155:PHE:O	2.12	0.49
1:E:36:ILE:HA	1:E:40:MSE:CE	2.43	0.49
1:F:352:LEU:HD23	1:F:398:VAL:HG21	1.93	0.49
1:E:4:ILE:O	1:E:8:LEU:HD12	2.13	0.49
1:A:38:PRO:HB3	1:A:383:HIS:ND1	2.28	0.49
1:B:20:MSE:HE3	1:B:420:PHE:CZ	2.48	0.49
1:D:92:TYR:HB2	1:D:285:MSE:HE2	1.95	0.49
1:A:243:ASP:HB3	1:B:5:PHE:CZ	2.47	0.49



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:77:MSE:SE	1:C:286:PRO:HG2	2.63	0.49
1:C:100:LEU:HD13	1:C:259:PHE:CG	2.48	0.48
1:F:107:GLU:HB3	1:F:264:ARG:HB2	1.94	0.48
1:C:312:VAL:HG22	1:C:379:PRO:HG2	1.94	0.48
1:F:32:LEU:HB3	1:F:40:MSE:HE3	1.95	0.48
1:A:365:TYR:HA	1:A:368:ILE:O	2.13	0.48
1:D:131:ASP:OD2	1:E:7:ARG:NH2	2.46	0.48
1:D:387:ASP:O	1:D:391:THR:OG1	2.23	0.48
1:A:287:MSE:HE1	1:B:77:MSE:HB3	1.94	0.48
1:A:423:ARG:O	1:B:264:ARG:NH2	2.44	0.48
1:C:294:ARG:O	1:C:298:ILE:HD12	2.13	0.48
1:D:280:ALA:HB1	1:E:114:PHE:CE1	2.48	0.48
1:D:348:LEU:HD23	1:D:349:ILE:HD12	1.95	0.48
1:F:315:LEU:O	1:F:319:LEU:HD12	2.13	0.48
1:A:117:GLN:NE2	1:B:116:TYR:HB3	2.28	0.48
1:C:4:ILE:O	1:C:8:LEU:HG	2.14	0.48
1:A:264:ARG:NH1	1:B:423:ARG:O	2.47	0.48
1:D:222:PHE:HE2	1:D:253:MSE:HE2	1.79	0.48
1:E:342:ILE:HB	1:E:343:PRO:HD3	1.96	0.48
1:C:97:GLU:OE1	1:C:110:PHE:HA	2.13	0.48
1:D:61:HIS:CE1	1:D:63:GLU:HB2	2.48	0.48
1:D:144:ILE:O	1:D:148:ARG:HG3	2.13	0.48
1:A:201:ASP:OD1	1:A:202:GLU:N	2.47	0.48
1:B:319:LEU:HD13	1:B:326:ILE:HD11	1.96	0.48
1:C:126:LEU:HD21	1:C:266:LEU:HD11	1.96	0.48
1:E:218:ASP:HB3	1:E:247:ASN:ND2	2.29	0.47
1:E:290:GLY:O	1:E:294:ARG:HG3	2.14	0.47
1:F:55:TYR:OH	1:F:220:HIS:ND1	2.43	0.47
1:D:204:VAL:O	1:D:207:LYS:HB2	2.14	0.47
1:D:348:LEU:HD23	1:D:349:ILE:H	1.77	0.47
1:A:114:PHE:CE1	1:A:256:ILE:HD12	2.49	0.47
1:C:387:ASP:O	1:C:391:THR:OG1	2.28	0.47
1:D:269:LEU:CD2	1:E:8:LEU:HB3	2.44	0.47
1:E:253:MSE:HE3	1:E:253:MSE:HB3	1.78	0.47
1:F:37:GLY:H	1:F:40:MSE:SE	2.48	0.47
1:F:202:GLU:O	1:F:206:LEU:HG	2.14	0.47
1:E:108:ASP:CG	1:E:267:VAL:HG11	2.35	0.47
1:F:103:PHE:CE2	1:F:298:ILE:HD11	2.49	0.47
1:A:36:ILE:HD11	1:B:79:ALA:O	2.14	0.47
1:A:117:GLN:HG3	1:B:117:GLN:HB3	1.96	0.47
1:F:201:ASP:H	1:F:236:PHE:HD2	1.63	0.47



	i agein	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:F:401:LYS:HA	1:F:406:ILE:HD12	1.96	0.47	
1:A:256:ILE:H	1:A:287:MSE:SE	2.48	0.47	
1:A:308:LEU:O	1:A:312:VAL:HG23	2.14	0.47	
1:A:319:LEU:HD13	1:A:326:ILE:HD11	1.96	0.47	
1:B:197:LEU:HD11	1:B:331:SER:HB3	1.96	0.47	
1:C:351:ASP:OD2	1:C:407:TYR:OH	2.25	0.47	
1:D:117:GLN:OE1	1:E:116:TYR:HB3	2.15	0.47	
1:E:333:VAL:HG12	1:E:335:PRO:HD3	1.95	0.47	
1:E:352:LEU:HG	1:E:398:VAL:HG21	1.96	0.47	
1:B:84:ARG:HG2	1:B:282:SER:HB2	1.97	0.47	
1:D:116:TYR:CD1	1:D:142:CYS:HB3	2.50	0.47	
1:E:283:LEU:HD11	1:E:287:MSE:HG2	1.96	0.47	
1:A:215:LEU:HD13	1:A:244:VAL:HB	1.97	0.47	
1:D:75:PHE:CG	1:D:285:MSE:HG2	2.48	0.47	
1:D:289:MSE:HE3	1:D:289:MSE:HA	1.97	0.47	
1:E:201:ASP:N	1:E:236:PHE:HD2	2.12	0.47	
1:A:138:GLU:HG3	1:A:159:HIS:CG	2.50	0.47	
1:B:157:TYR:CD2	1:B:165:LEU:HD13	2.50	0.47	
1:A:171:HIS:ND1	1:A:171:HIS:N	2.63	0.46	
1:C:162:MSE:HE1	1:C:203:ILE:HG12	1.96	0.46	
1:F:334:THR:OG1	1:F:377:VAL:HB	2.15	0.46	
1:C:66:LYS:NZ	1:C:70:GLU:OE1	2.30	0.46	
1:D:148:ARG:HH12	1:E:275:ARG:HH12	1.64	0.46	
1:D:338:MSE:HE2	1:D:375:LEU:HD11	1.96	0.46	
1:E:332:PRO:O	1:E:334:THR:HG23	2.15	0.46	
1:E:368:ILE:HG13	1:E:372:GLU:OE1	2.15	0.46	
1:B:38:PRO:HB3	1:B:383:HIS:CD2	2.51	0.46	
1:D:287:MSE:O	1:D:287:MSE:HG3	2.15	0.46	
1:E:301:HIS:ND1	1:E:303:GLU:OE2	2.49	0.46	
1:B:249:PHE:HA	1:B:253:MSE:HB2	1.98	0.46	
1:B:256:ILE:H	1:B:287:MSE:SE	2.48	0.46	
1:D:283:LEU:HD12	1:D:284:PRO:HD2	1.98	0.46	
1:F:351:ASP:OD2	1:F:407:TYR:OH	2.33	0.46	
1:A:36:ILE:HA	1:A:40:MSE:HE2	1.97	0.46	
1:D:351:ASP:HA	1:D:355:ASN:HB2	1.97	0.46	
1:D:267:VAL:HA	1:D:270:LEU:HD12	1.97	0.45	
1:A:159:HIS:NE2	1:A:196:ASP:OD2	2.49	0.45	
1:C:122:ILE:HD13	1:C:122:ILE:HA	1.87	0.45	
1:E:83:ALA:HB1	1:E:278:LEU:O	2.17	0.45	
1:F:118:GLY:O	1:F:122:ILE:HD12	2.16	0.45	
1:B:100:LEU:HD22	1:B:259:PHE:CZ	2.51	0.45	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:269:LEU:HD12	1:D:273:ASN:ND2	2.31	0.45
1:E:275:ARG:HG3	1:E:275:ARG:NH1	2.31	0.45
1:A:5:PHE:O	1:A:9:GLU:HB2	2.16	0.45
1:A:43:ARG:NH1	1:A:417:ASP:OD1	2.41	0.45
1:B:107:GLU:HB2	1:B:263:PRO:HA	1.99	0.45
1:B:346:THR:O	1:B:350:VAL:HG23	2.15	0.45
1:C:270:LEU:HB3	1:C:274:MSE:HG3	1.98	0.45
1:F:114:PHE:HD1	1:F:115:GLY:N	2.14	0.45
1:E:110:PHE:CE2	1:E:271:ARG:HA	2.51	0.45
1:E:167:LEU:HG	1:E:171:HIS:CE1	2.49	0.45
1:B:139:ALA:HB3	1:B:144:ILE:HD11	1.99	0.45
1:D:265:TRP:CE3	1:E:9:GLU:HA	2.52	0.45
1:E:140:HIS:HD2	1:E:141:ALA:N	2.15	0.45
1:E:204:VAL:HG21	1:E:238:VAL:HG11	1.98	0.45
1:C:114:PHE:HD1	1:C:115:GLY:H	1.64	0.45
1:C:119:MSE:HE1	1:C:215:LEU:CD2	2.45	0.45
1:C:267:VAL:HA	1:C:270:LEU:CD1	2.46	0.45
1:D:108:ASP:HB3	1:D:267:VAL:HG21	1.99	0.45
1:D:365:TYR:N	1:D:366:PRO:HD2	2.32	0.45
1:E:213:ARG:HD3	1:E:213:ARG:HA	1.65	0.45
1:A:89:GLN:HG3	1:B:29:PHE:CD2	2.50	0.45
1:A:342:ILE:HA	1:A:364:ILE:HD11	1.98	0.45
1:B:380:THR:CG2	1:B:382:ALA:H	2.28	0.45
1:D:380:THR:HG22	1:D:383:HIS:NE2	2.32	0.45
1:A:204:VAL:O	1:A:207:LYS:HB2	2.16	0.45
1:B:342:ILE:HD12	1:B:364:ILE:HD12	1.99	0.45
1:C:222:PHE:CE2	1:C:253:MSE:HE1	2.48	0.45
1:E:169:LEU:HD13	1:E:210:PHE:CD2	2.51	0.45
1:E:36:ILE:HA	1:E:40:MSE:HE3	1.98	0.45
1:E:351:ASP:OD2	1:E:407:TYR:OH	2.28	0.45
1:F:388:VAL:O	1:F:392:ILE:HG12	2.17	0.45
1:B:165:LEU:O	1:B:169:LEU:HD12	2.17	0.44
1:E:61:HIS:HB3	1:E:64:VAL:HB	1.99	0.44
1:E:143:ILE:O	1:E:147:LEU:HD13	2.17	0.44
1:D:37:GLY:H	1:D:40:MSE:SE	2.49	0.44
1:D:96:LEU:CD2	1:D:100:LEU:CD2	2.95	0.44
1:D:384:THR:O	1:D:387:ASP:HB2	2.17	0.44
1:E:168:GLN:HA	1:E:168:GLN:OE1	2.18	0.44
1:E:260:VAL:HG21	1:E:274:MSE:HE1	1.98	0.44
1:B:312:VAL:HG22	1:B:379:PRO:HG2	1.99	0.44
1:D:118:GLY:O	1:D:122:ILE:HG12	2.17	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:E:221:GLY:HA2	1:E:225:MSE:CE	2.48	0.44
1:E:342:ILE:HB	1:E:343:PRO:CD	2.48	0.44
1:A:80:PRO:HB2	1:A:88:GLY:HA2	1.99	0.44
1:D:75:PHE:HB3	1:D:79:ALA:HB2	1.99	0.44
1:E:167:LEU:O	1:E:171:HIS:ND1	2.51	0.44
1:E:284:PRO:O	1:E:288:VAL:HG23	2.18	0.44
1:A:415:ARG:HG2	1:A:415:ARG:HH11	1.83	0.44
1:C:80:PRO:HG2	1:C:283:LEU:O	2.18	0.44
1:C:293:LYS:HA	1:C:293:LYS:HD3	1.62	0.44
1:D:385:LEU:HD12	1:D:385:LEU:N	2.33	0.44
1:F:414:VAL:HG23	1:F:415:ARG:H	1.82	0.44
1:A:113:ASN:HB2	1:B:114:PHE:CZ	2.53	0.44
1:C:112:LEU:HD11	1:C:260:VAL:HG23	1.99	0.44
1:C:225:MSE:HE1	1:C:309:TRP:HZ2	1.83	0.44
1:E:238:VAL:O	1:E:242:VAL:HG23	2.17	0.44
1:A:20:MSE:HG2	1:B:272:TYR:CE1	2.52	0.44
1:C:189:GLY:HA3	1:C:218:ASP:OD1	2.17	0.44
1:E:39:HIS:HA	1:E:47:MSE:O	2.18	0.44
1:F:4:ILE:HD12	1:F:4:ILE:H	1.82	0.44
1:A:348:LEU:HG	1:A:398:VAL:HG13	1.99	0.43
1:B:5:PHE:O	1:B:9:GLU:HB2	2.17	0.43
1:C:263:PRO:O	1:C:267:VAL:HG23	2.18	0.43
1:D:100:LEU:HD12	1:D:259:PHE:CZ	2.52	0.43
1:E:197:LEU:HD11	1:E:331:SER:HB3	1.99	0.43
1:F:347:ASN:HA	1:F:350:VAL:HG22	1.99	0.43
1:A:60:ASN:OD1	1:A:65:ARG:NH1	2.51	0.43
1:A:80:PRO:HG3	1:A:93:HIS:CE1	2.53	0.43
1:B:110:PHE:CD2	1:B:274:MSE:HE3	2.43	0.43
1:B:165:LEU:HG	1:B:169:LEU:HD11	1.99	0.43
1:E:357:GLY:O	1:E:358:ILE:HD13	2.18	0.43
1:A:37:GLY:N	1:A:40:MSE:HE2	2.18	0.43
1:D:80:PRO:HG2	1:D:283:LEU:O	2.18	0.43
1:A:270:LEU:HB3	1:A:274:MSE:SE	2.69	0.43
1:A:117:GLN:NE2	1:B:114:PHE:HB3	2.34	0.43
1:C:112:LEU:HD11	1:C:260:VAL:CG2	2.48	0.43
1:C:283:LEU:HD12	1:C:283:LEU:HA	1.85	0.43
1:E:293:LYS:O	1:E:297:LEU:HG	2.19	0.43
1:A:79:ALA:HB1	1:A:80:PRO:CD	2.46	0.43
1:F:208:LYS:HA	1:F:208:LYS:HD2	1.71	0.43
1:F:263:PRO:HB2	1:F:265:TRP:HD1	1.84	0.43
1:A:364:ILE:O	1:A:368:ILE:HG22	2.18	0.43



	<b>A</b> + <b>O</b>	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:134:VAL:HA	1:B:155:PHE:O	2.18	0.43	
1:B:159:HIS:HE2	1:B:196:ASP:CG	2.21	0.43	
1:D:175:LEU:O	1:D:179:GLN:HG3	2.19	0.43	
1:E:130:ARG:HD3	1:E:179:GLN:O	2.19	0.43	
1:E:340:GLY:HA3	1:E:373:ILE:HD11	2.01	0.43	
1:F:247:ASN:HB2	1:F:259:PHE:CE1	2.54	0.43	
1:A:144:ILE:O	1:A:148:ARG:HG3	2.19	0.43	
1:B:348:LEU:HG	1:B:398:VAL:HG13	2.00	0.43	
1:C:119:MSE:HE2	1:C:143:ILE:HG12	2.00	0.43	
1:E:107:GLU:H	1:E:107:GLU:CD	2.21	0.43	
1:F:114:PHE:CE2	1:F:256:ILE:HD11	2.54	0.43	
1:F:256:ILE:HG22	1:F:287:MSE:HG2	2.01	0.43	
1:D:243:ASP:HB3	1:E:5:PHE:CZ	2.53	0.42	
1:E:313:ARG:O	1:E:317:ASN:HB2	2.19	0.42	
1:C:214:LEU:HD12	1:C:215:LEU:N	2.34	0.42	
1:C:364:ILE:HG13	1:C:365:TYR:H	1.84	0.42	
1:E:267:VAL:O	1:E:271:ARG:N	2.50	0.42	
1:D:77:MSE:HE2	1:E:287:MSE:HE2	2.01	0.42	
1:D:197:LEU:CD2	1:D:225:MSE:HE2	2.49	0.42	
1:D:296:GLU:HA	1:D:299:ARG:HH21	1.84	0.42	
1:E:47:MSE:HE1	1:E:359:PHE:N	2.34	0.42	
1:E:218:ASP:OD1	1:E:221:GLY:HA3	2.19	0.42	
1:A:40:MSE:HE1	1:A:52:LEU:HD21	2.01	0.42	
1:A:61:HIS:HB3	1:A:64:VAL:HB	2.01	0.42	
1:A:369:PRO:HG2	1:A:372:GLU:OE2	2.19	0.42	
1:E:224:THR:HG23	1:E:308:LEU:CD2	2.49	0.42	
1:A:5:PHE:CZ	1:B:243:ASP:HB3	2.55	0.42	
1:A:20:MSE:HG2	1:B:272:TYR:CZ	2.55	0.42	
1:A:342:ILE:HB	1:A:343:PRO:HD3	2.02	0.42	
1:B:201:ASP:HB3	1:B:236:PHE:HB3	2.02	0.42	
1:D:353:ARG:HD3	1:D:359:PHE:CE1	2.55	0.42	
1:E:266:LEU:O	1:E:270:LEU:N	2.48	0.42	
1:B:47:MSE:HE1	1:B:353:ARG:HB3	2.01	0.42	
1:D:207:LYS:HG3	1:D:212:PHE:CZ	2.55	0.42	
1:E:384:THR:O	1:E:388:VAL:HG23	2.19	0.42	
1:E:415:ARG:HA	1:E:415:ARG:HD3	1.88	0.42	
1:F:301:HIS:HB2	1:F:304:TYR:HE2	1.80	0.42	
1:C:112:LEU:O	$1:\overline{C:283:LEU:HD22}$	2.19	0.42	
1:C:197:LEU:HD11	1:C:331:SER:HB3	2.02	0.42	
1:C:342:ILE:HD13	1:C:342:ILE:HA	1.85	0.42	
1:D:148:ARG:NH1	1:E:275:ARG:HH12	2.17	0.42	



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:308:LEU:O	1:E:312:VAL:HG23	2.19	0.42
1:A:224:THR:CG2	1:A:225:MSE:HG2	2.50	0.42
1:E:134:VAL:HA	1:E:155:PHE:O	2.19	0.42
1:A:45:LYS:HD3	1:A:45:LYS:HA	1.77	0.42
1:A:196:ASP:HB3	1:A:328:VAL:O	2.20	0.42
1:A:420:PHE:O	1:A:421:LYS:HE2	2.19	0.42
1:B:363:VAL:HB	1:B:374:ILE:HG13	2.01	0.42
1:E:42:PHE:CE1	1:E:43:ARG:HD2	2.54	0.42
1:E:144:ILE:HD12	1:E:144:ILE:H	1.85	0.42
1:E:208:LYS:HA	1:E:208:LYS:HD2	1.70	0.42
1:E:227:GLU:O	1:E:227:GLU:HG2	2.20	0.42
1:F:119:MSE:HE2	1:F:123:ILE:CG1	2.50	0.42
1:F:194:LYS:O	1:F:329:THR:HG22	2.20	0.42
1:B:119:MSE:HA	1:B:122:ILE:HG12	2.01	0.41
1:B:284:PRO:O	1:B:288:VAL:HG23	2.20	0.41
1:D:79:ALA:HB3	1:D:285:MSE:HB2	2.02	0.41
1:F:134:VAL:HA	1:F:155:PHE:O	2.21	0.41
1:A:117:GLN:HE22	1:B:114:PHE:HD2	1.68	0.41
1:E:40:MSE:O	1:E:47:MSE:N	2.53	0.41
1:A:256:ILE:HG13	1:B:284:PRO:CG	2.50	0.41
1:D:319:LEU:HB3	1:D:324:PHE:HB2	2.03	0.41
1:A:333:VAL:HG12	1:A:335:PRO:HD3	2.02	0.41
1:B:384:THR:O	1:B:388:VAL:HG23	2.20	0.41
1:E:326:ILE:HD13	1:E:326:ILE:HA	1.95	0.41
1:A:29:PHE:N	1:A:30:PRO:HD3	2.36	0.41
1:A:112:LEU:HD13	1:A:118:GLY:HA3	2.02	0.41
1:E:168:GLN:HA	1:E:171:HIS:ND1	2.34	0.41
1:F:68:ASP:OD1	1:F:294:ARG:NH1	2.50	0.41
1:F:97:GLU:OE2	1:F:271:ARG:NH2	2.54	0.41
1:F:283:LEU:HD12	1:F:284:PRO:CD	2.49	0.41
1:C:145:ASP:OD1	1:C:148:ARG:NH1	2.54	0.41
1:D:347:ASN:HB2	1:D:407:TYR:HB3	2.03	0.41
1:E:267:VAL:HA	1:E:270:LEU:HB2	2.03	0.41
1:F:263:PRO:HB2	1:F:265:TRP:CD1	2.56	0.41
1:C:40:MSE:HE3	1:C:40:MSE:HB2	1.86	0.41
1:E:47:MSE:HE3	1:E:48:LEU:N	2.36	0.41
1:F:354:GLU:N	1:F:354:GLU:OE1	2.54	0.41
1:C:293:LYS:O	1:C:297:LEU:HD13	2.21	0.41
1:F:45:LYS:HD2	1:F:46:LYS:N	2.36	0.41
1:F:109:ALA:HA	1:F:260:VAL:O	2.21	0.41
1:F:307:LYS:HZ2	1:F:311:ILE:HG12	1.86	0.41



A + a 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:F:312:VAL:CG2	1:F:332:PRO:HA	2.49	0.41
1:B:75:PHE:O	1:B:79:ALA:HB2	2.20	0.40
1:C:61:HIS:CE1	1:C:63:GLU:HB2	2.56	0.40
1:E:96:LEU:O	1:E:100:LEU:HG	2.22	0.40
1:E:145:ASP:HA	1:E:148:ARG:HD3	2.02	0.40
1:C:218:ASP:HB3	1:C:247:ASN:OD1	2.21	0.40
1:F:108:ASP:OD2	1:F:264:ARG:HG3	2.21	0.40
1:F:116:TYR:CD2	1:F:142:CYS:HB3	2.56	0.40
1:A:265:TRP:CE2	1:B:9:GLU:HG2	2.56	0.40
1:C:349:ILE:CD1	1:C:362:ILE:CG2	2.97	0.40
1:D:222:PHE:HE2	1:D:253:MSE:CE	2.33	0.40
1:A:134:VAL:HA	1:A:155:PHE:O	2.22	0.40
1:C:364:ILE:HD12	1:C:364:ILE:HA	1.87	0.40
1:D:255:GLY:HA2	1:D:287:MSE:HE1	2.02	0.40
1:E:322:ASN:O	1:E:399:ARG:NH1	2.52	0.40
1:A:7:ARG:NH1	1:B:131:ASP:OD2	2.48	0.40
1:A:284:PRO:CG	1:B:256:ILE:HG13	2.51	0.40
1:A:342:ILE:H	1:A:342:ILE:HG12	1.75	0.40
1:C:122:ILE:HG23	1:C:122:ILE:HD12	1.80	0.40
1:C:201:ASP:HA	1:C:238:VAL:HG11	2.02	0.40
1:C:214:LEU:HD12	1:C:215:LEU:H	1.87	0.40
1:D:220:HIS:CE1	1:D:251:LYS:NZ	2.89	0.40
1:E:202:GLU:O	1:E:206:LEU:HG	2.22	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	А	421/443~(95%)	406 (96%)	14 (3%)	1 (0%)	47 78
1	В	421/443~(95%)	402 (96%)	18 (4%)	1 (0%)	47 78



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	С	396/443~(89%)	373~(94%)	21~(5%)	2~(0%)	29	61
1	D	397/443~(90%)	371~(94%)	26~(6%)	0	100	100
1	Ε	418/443~(94%)	395~(94%)	22~(5%)	1 (0%)	47	78
1	F	421/443~(95%)	394~(94%)	26~(6%)	1 (0%)	47	78
All	All	2474/2658~(93%)	2341~(95%)	127 (5%)	6~(0%)	47	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	79	ALA
1	С	251	LYS
1	F	79	ALA
1	В	80	PRO
1	Е	79	ALA
1	С	14	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	327/339~(96%)	311~(95%)	16 (5%)	25 57
1	В	316/339~(93%)	305~(96%)	11 (4%)	36 70
1	С	290/339~(86%)	283~(98%)	7~(2%)	49 79
1	D	276/339~(81%)	264~(96%)	12 (4%)	29 62
1	Ε	283/339~(84%)	268~(95%)	15~(5%)	22 54
1	F	299/339~(88%)	284~(95%)	15 (5%)	24 57
All	All	1791/2034 (88%)	1715 (96%)	76 (4%)	30 63

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type	
1	А	51	SER	
Carting 1 and and a set				



Mol	Chain	Res	Type
1	А	62	PRO
1	А	66	LYS
1	А	114	PHE
1	А	119	MSE
1	А	149	LEU
1	А	171	HIS
1	А	177	GLU
1	А	209	ASP
1	А	224	THR
1	А	234	SER
1	А	276	SER
1	А	322	ASN
1	А	329	THR
1	A	330	ASN
1	А	350	VAL
1	В	51	SER
1	В	114	PHE
1	В	121	SER
1	В	125	CYS
1	В	224	THR
1	В	234	SER
1	В	252	SER
1	В	302	PRO
1	В	367	VAL
1	В	380	THR
1	В	423	ARG
1	С	90	THR
1	С	114	PHE
1	С	119	MSE
1	С	154	ARG
1	С	321	GLU
1	С	390	TYR
1	С	397	SER
1	D	114	PHE
1	D	119	MSE
1	D	121	SER
1	D	193	MSE
1	D	239	THR
1	D	251	LYS
1	D	313	ARG
1	D	329	THR
1	D	349	ILE



Mol	Chain	Res	Type
1	D	351	ASP
1	D	361	SER
1	D	385	LEU
1	Е	3	ASP
1	Е	4	ILE
1	Е	24	HIS
1	Е	42	PHE
1	Е	65	ARG
1	Е	68	ASP
1	Е	90	THR
1	Е	159	HIS
1	Е	230	ARG
1	Е	273	ASN
1	Е	282	SER
1	Е	317	ASN
1	Е	367	VAL
1	Е	386	ASP
1	Е	390	TYR
1	F	20	MSE
1	F	61	HIS
1	F	85	MSE
1	F	106	LYS
1	F	114	PHE
1	F	131	ASP
1	F	225	MSE
1	F	247	ASN
1	F	253	MSE
1	F	276	SER
1	F	331	SER
1	F	336	VAL
1	F	390	TYR
1	F	396	LYS
1	F	410	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	39	HIS
1	А	117	GLN
1	А	277	GLN
1	А	316	GLN
1	А	383	HIS



Mol	Chain	Res	Type
1	В	301	HIS
1	С	11	ASN
1	С	140	HIS
1	С	220	HIS
1	С	305	GLN
1	С	330	ASN
1	С	347	ASN
1	С	383	HIS
1	D	54	ASN
1	D	383	HIS
1	Е	24	HIS
1	Е	277	GLN
1	Е	305	GLN
1	F	268	ASN
1	F	277	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)

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

2 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).



Mal	Mal Truna Chain Bag		Dec	Tinle	Bo	Bond lengths			Bond angles		
INIOI	туре	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
2	PLP	А	501	1	15,15,16	1.06	1 (6%)	20,22,23	1.25	2 (10%)	
2	PLP	В	501	1	15,15,16	1.02	1 (6%)	20,22,23	1.33	3 (15%)	

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
2	PLP	А	501	1	-	3/6/6/8	0/1/1/1
2	PLP	В	501	1	-	3/6/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	А	501	PLP	C2-N1	2.42	1.38	1.33
2	В	501	PLP	C2-N1	2.42	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	501	PLP	O4P-C5A-C5	3.49	116.00	109.35
2	В	501	PLP	O4P-C5A-C5	3.42	115.87	109.35
2	В	501	PLP	C6-C5-C4	2.10	119.81	118.16
2	В	501	PLP	C4A-C4-C3	-2.07	116.99	120.50
2	А	501	PLP	O4P-P-O1P	2.02	112.15	106.47

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	501	PLP	C5A-O4P-P-O2P
2	А	501	PLP	C5A-O4P-P-O3P
2	В	501	PLP	C5A-O4P-P-O2P
2	В	501	PLP	C5A-O4P-P-O3P
2	А	501	PLP	C5A-O4P-P-O1P
2	В	501	PLP	C5A-O4P-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	501	PLP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	404/443~(91%)	0.01	3 (0%) 87 87	40, 71, 113, 142	0
1	В	404/443~(91%)	0.01	3 (0%) 87 87	39, 71, 112, 138	0
1	С	381/443~(86%)	0.04	5 (1%) 77 77	53, 89, 131, 158	0
1	D	382/443~(86%)	0.06	11 (2%) 51 47	50, 89, 131, 164	0
1	Е	403/443~(90%)	0.36	38 (9%) 8 6	59, 135, 185, 199	0
1	F	404/443 (91%)	0.38	41 (10%) 7 5	59, 139, 182, 197	0
All	All	2378/2658~(89%)	0.15	101 (4%) 36 32	39, 92, 167, 199	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	315	LEU	4.2
1	F	324	PHE	4.2
1	F	358	ILE	4.1
1	F	395	PHE	4.1
1	F	377	VAL	4.1
1	Е	89	GLN	4.1
1	Е	224	THR	4.0
1	F	104	VAL	4.0
1	Е	49	ASN	3.9
1	Е	391	THR	3.9
1	Е	256	ILE	3.9
1	Е	336	VAL	3.9
1	F	11	ASN	3.9
1	D	21	SER	3.9
1	С	228	GLY	3.8
1	F	373	ILE	3.8
1	Е	311	ILE	3.8
1	Е	316	GLN	3.7
1	F	315	LEU	3.7



Mol	Chain	Res	Type	RSRZ	
1	Е	223 GLY		3.7	
1	Е	373	ILE	3.6	
1	F	360	CYS	3.6	
1	Е	200	LEU	3.6	
1	F	224	224 THR 3		
1	F	363	VAL	3.4	
1	F	223	GLY	3.4	
1	Е	11	ASN	3.2	
1	D	79	ALA	3.2	
1	F	214	LEU	3.2	
1	Е	26	TYR	3.2	
1	С	11	ASN	3.1	
1	F	413	PRO	3.1	
1	Е	358	ILE	3.0	
1	В	211	GLN	3.0	
1	F	414	VAL	3.0	
1	С	34	GLY	3.0	
1	Е	259	PHE	3.0	
1	В	374	ILE	2.9	
1	F	311	ILE	2.9	
1	Е	22	TYR	2.9	
1	D	359	PHE	2.9	
1	F	36	ILE	2.9	
1	F	375	LEU	2.9	
1	F	259	PHE	2.8	
1	С	12	ALA	2.8	
1	D	360	CYS	2.8	
1	F	349	ILE	2.8	
1	Е	360	CYS	2.8	
1	Е	349	ILE	2.8	
1	Е	398	VAL	2.7	
1	Е	412	ILE	2.7	
1	F	200	LEU	2.6	
1	В	212	PHE	2.6	
1	F	314	ALA	2.6	
1	F	391	THR	2.6	
1	F	336	VAL	2.6	
1	Е	363	VAL	2.5	
1	Е	215	LEU	2.5	
1	F	334	THR	2.5	
1	А	10	LYS	2.5	
1	Е	420	PHE	2.5	



Mol	Chain	Res Type		RSRZ	
1	Е	298 ILE		2.5	
1	Е	369	PRO	2.4	
1	F	27	PHE	2.4	
1	D	19 TYR		2.4	
1	Е	324	324 PHE		
1	D	349	349 ILE		
1	Е	214	LEU	2.4	
1	D	11	ASN	2.4	
1	F	49	ASN	2.4	
1	Е	36	ILE	2.4	
1	F	326	ILE	2.4	
1	А	212	PHE	2.4	
1	Е	377	VAL	2.4	
1	Е	56	LEU	2.4	
1	Е	184	LEU	2.4	
1	F	242	VAL	2.3	
1	D	34	GLY	2.3	
1	D	76	GLY	2.3	
1	F	93	HIS	2.3	
1	Ε	242	VAL	2.3	
1	F	327	GLY	2.3	
1	F	359	PHE	2.3	
1	F	216	VAL	2.3	
1	F	283	LEU	2.3	
1	A	11	ASN	2.3	
1	F	92	TYR	2.2	
1	Е	104	VAL	2.2	
1	F	316	GLN	2.2	
1	F	50	TRP	2.2	
1	E	246	PHE	2.2	
1	F	333	VAL	2.2	
1	F	184	LEU	2.2	
1	F	319	LEU	2.2	
1	F	90	THR	2.2	
1	E	304	TYR	2.1	
1	C	126	LEU	2.1	
1	Е	185	VAL	2.0	
1	Е	312	VAL	2.0	
1	D	315	LEU	2.0	
1	D	4	ILE	2.0	

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### 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 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,  $95^{th}$  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	$B-factors(A^2)$	Q<0.9
2	PLP	А	501	15/16	0.94	0.24	43,65,71,71	8
2	PLP	В	501	15/16	0.95	0.29	45,62,70,71	10

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







## 6.5 Other polymers (i)

There are no such residues in this entry.

