



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:07 pm GMT

PDB ID : 3L7L  
Title : Structure of the Wall Teichoic Acid Polymerase TagF, H444N + CDPG (30 minute soak)  
Authors : Lovering, A.L.; Strynadka, N.C.J.  
Deposited on : 2009-12-28  
Resolution : 2.95 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28986

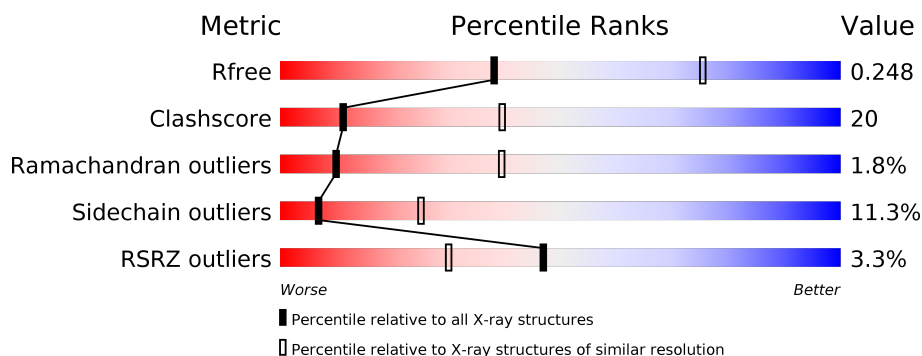
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	729	<div> <div>2%</div> <div>32% 22% 44%</div> </div>
1	B	729	<div> <div>2%</div> <div>33% 19% 44%</div> </div>
1	C	729	<div> <div>2%</div> <div>33% 20% 44%</div> </div>
1	D	729	<div> <div>2%</div> <div>31% 20% 45%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	734	-	-	X	-
3	CL	B	735	-	-	X	-
3	CL	D	732	-	-	X	-
5	EDO	D	734	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13868 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 Teichoic acid biosynthesis protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3462	2224	577	650	11			
1	B	411	Total	C	N	O	S	0	0	0
			3467	2227	578	651	11			
1	C	411	Total	C	N	O	S	0	0	0
			3467	2227	578	651	11			
1	D	401	Total	C	N	O	S	0	0	0
			3383	2169	568	635	11			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ASN	HIS	ENGINEERED	UNP Q5HLM5
A	722	LEU	-	EXPRESSION TAG	UNP Q5HLM5
A	723	GLU	-	EXPRESSION TAG	UNP Q5HLM5
A	724	HIS	-	EXPRESSION TAG	UNP Q5HLM5
A	725	HIS	-	EXPRESSION TAG	UNP Q5HLM5
A	726	HIS	-	EXPRESSION TAG	UNP Q5HLM5
A	727	HIS	-	EXPRESSION TAG	UNP Q5HLM5
A	728	HIS	-	EXPRESSION TAG	UNP Q5HLM5
A	729	HIS	-	EXPRESSION TAG	UNP Q5HLM5
B	444	ASN	HIS	ENGINEERED	UNP Q5HLM5
B	722	LEU	-	EXPRESSION TAG	UNP Q5HLM5
B	723	GLU	-	EXPRESSION TAG	UNP Q5HLM5
B	724	HIS	-	EXPRESSION TAG	UNP Q5HLM5
B	725	HIS	-	EXPRESSION TAG	UNP Q5HLM5
B	726	HIS	-	EXPRESSION TAG	UNP Q5HLM5
B	727	HIS	-	EXPRESSION TAG	UNP Q5HLM5
B	728	HIS	-	EXPRESSION TAG	UNP Q5HLM5
B	729	HIS	-	EXPRESSION TAG	UNP Q5HLM5
C	444	ASN	HIS	ENGINEERED	UNP Q5HLM5
C	722	LEU	-	EXPRESSION TAG	UNP Q5HLM5
C	723	GLU	-	EXPRESSION TAG	UNP Q5HLM5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	724	HIS	-	EXPRESSION TAG	UNP Q5HLM5
C	725	HIS	-	EXPRESSION TAG	UNP Q5HLM5
C	726	HIS	-	EXPRESSION TAG	UNP Q5HLM5
C	727	HIS	-	EXPRESSION TAG	UNP Q5HLM5
C	728	HIS	-	EXPRESSION TAG	UNP Q5HLM5
C	729	HIS	-	EXPRESSION TAG	UNP Q5HLM5
D	444	ASN	HIS	ENGINEERED	UNP Q5HLM5
D	722	LEU	-	EXPRESSION TAG	UNP Q5HLM5
D	723	GLU	-	EXPRESSION TAG	UNP Q5HLM5
D	724	HIS	-	EXPRESSION TAG	UNP Q5HLM5
D	725	HIS	-	EXPRESSION TAG	UNP Q5HLM5
D	726	HIS	-	EXPRESSION TAG	UNP Q5HLM5
D	727	HIS	-	EXPRESSION TAG	UNP Q5HLM5
D	728	HIS	-	EXPRESSION TAG	UNP Q5HLM5
D	729	HIS	-	EXPRESSION TAG	UNP Q5HLM5

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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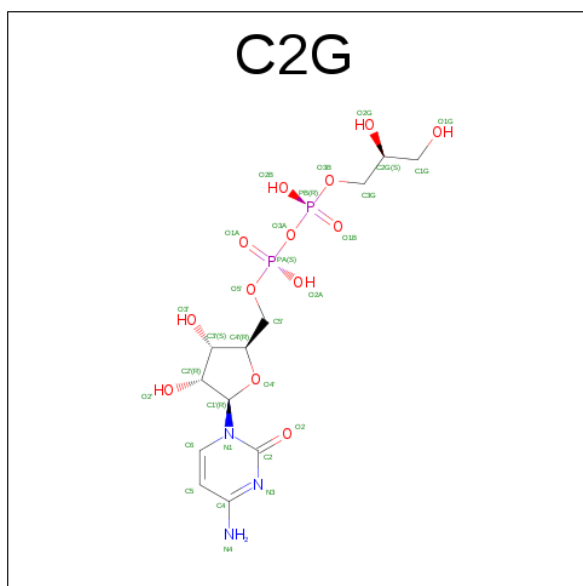
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	5	Total	Cl	0	0
			5	5		
3	A	8	Total	Cl	0	0
			8	8		
3	D	3	Total	Cl	0	0
			3	3		
3	C	5	Total	Cl	0	0
			5	5		

- Molecule 4 is [CYTIDINE-5'-PHOSPHATE] GLYCERYLPHOSPHORIC ACID ESTER (three-letter code: C2G) (formula: C<sub>12</sub>H<sub>21</sub>N<sub>3</sub>O<sub>13</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	
			30	12	3	13	2	
								0
								0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		

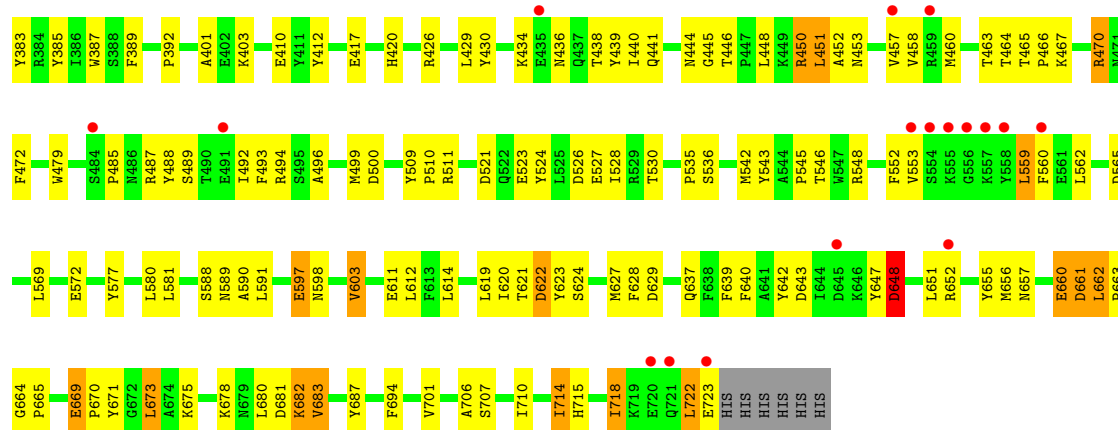
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	D	2	Total	O	0	0
			2	2		

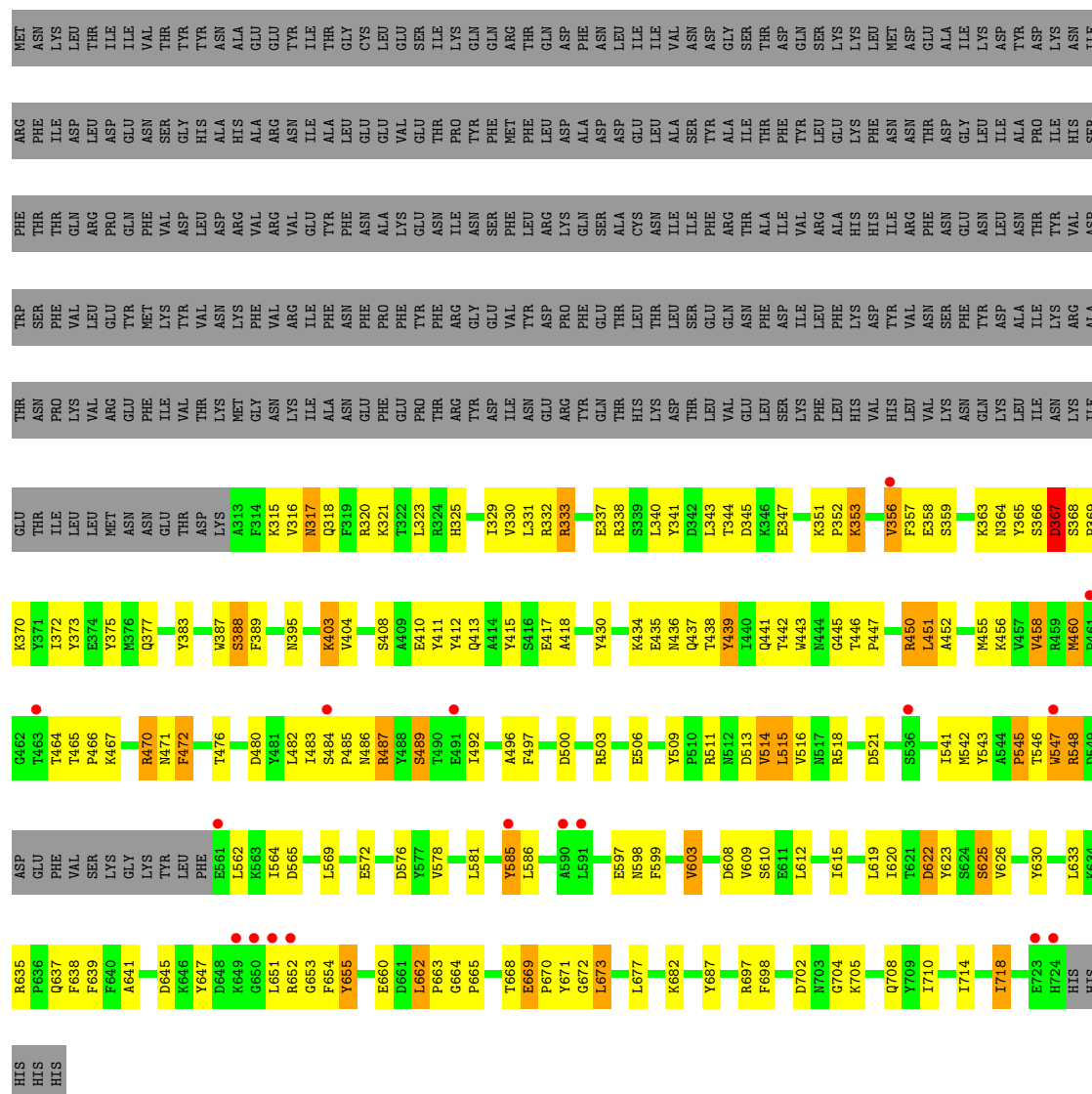




GLU	THR	THR	ASN	THR	TRP	PHE	ARG	MET
ILE	PRO	THR	ASN	THR	SER	THR	PHE	ASN
LEU	VAL	VAL	LYS	GLN	VAL	GLN	ASP	LYS
LEU	VAL	VAL	ARG	LEU	LEU	ARG	LEU	THR
MET	ARG	GLU	THR	GLU	GLU	PRO	ASP	ILE
ASN	GLU	THR	GLU	THR	TYR	GLN	ASN	ILE
ASN	PHE	PHE	ASN	VAL	MET	PHE	VAL	VAL
GLU	THR	VAL	VAL	THR	TYR	ASP	GLY	THR
ASP	THR	THR	LYS	VAL	VAL	LEU	HIS	TYR
LYS	THR	THR	THR	ASN	ASN	ASP	ALA	ASN
A313	MET	GLY	LYS	LYS	LYS	ARG	HIS	ALA
F314	GLY	ASN	PHE	PHE	VAL	VAL	ARG	GLU
K315	ASN	ASN	VAL	VAL	VAL	ARG	ARG	GLU
V316	LYS	LYS	ARG	ILE	ILE	GLU	ILE	TYR
N317	ILE	ILE	PHE	ASN	PHE	THR	ALA	THR
	ALA	ASN	ASN	ASN	ASN	PHE	ALA	GLY
K321	GLU	GLU	GLU	PHE	PHE	ASN	LEU	THR
T322	PHE	PHE	PRO	PRO	PRO	ALA	GLU	CYS
L323	GLU	PHE	GLU	PHE	PHE	LYS	VAL	LEU
R324	PRO	PRO	THR	THR	THR	GLU	GLU	GLU
H325	THR	THR	ARG	ARG	ARG	ILE	THR	SER
V326	ARG	ARG	GLY	GLY	GLY	ASN	PRO	LYS
	TYR	TYR	TYR	GLY	GLY	ASN	TYR	GLN
I329	ASP	ASP	ASP	GLU	VAL	PHE	PHE	GLN
V330	ILE	ILE	ASN	VAL	THR	LEU	THR	THR
L331	ASN	ASN	GLU	ASP	ASP	ARG	LEU	GLN
R332	GLU	ARG	THR	PRO	PRO	LYS	ASP	ASP
	THR	THR	THR	PHE	PHE	GLN	ALA	PHE
R338	THR	THR	THR	THR	THR	GLN	ALA	ASN
S339	GLN	GLN	GLN	GLU	GLU	SER	ASP	ASN
L340	THR	THR	THR	THR	THR	ALA	ASP	LEU
Y341	HIS	HIS	LEU	LEU	LEU	CYS	GLU	ILE
	LYS	LYS	THR	THR	THR	ASN	LEU	ILE
T344	ASP	ASP	LEU	LEU	LEU	ILE	ALA	VAL
D345	THR	THR	SER	SER	SER	ILE	SER	ASN
K346	LEU	LEU	GLU	GLU	GLU	PHE	TYR	ASP
E347	VAL	VAL	GLN	GLN	GLN	ARG	ALA	GLY
D348	GLU	GLU	ASN	ASN	ASN	THR	ILE	SER
R349	LEU	LEU	PHE	PHE	PHE	ALA	THR	THR
V350	SER	SER	ASP	ASP	ASP	ILE	PHE	ASP
K351	LYS	LYS	ILE	ILE	ILE	VAL	TYR	GLN
P352	PHE	PHE	LEU	LEU	LEU	ARG	LEU	SER
K353	LEU	LEU	LEU	LEU	PHE	ALA	GLU	LYS
	HIS	HIS	LYS	LYS	LYS	HIS	LYS	LYS
Y365	VAL	VAL	ASP	ASP	ASP	HIS	PHE	LEU
S366	HIS	HIS	TYR	TYR	TYR	ILE	ASN	MET
D367	VAL	VAL	VAL	VAL	VAL	ILE	ASN	MET
S368	VAL	VAL	ASN	ASN	ASN	PHE	THR	GLU
P369	LYS	LYS	SER	SER	SER	ALA	ASP	ALA
K370	ASN	ASN	PHE	PHE	PHE	GLU	GLY	ILE
Y371	GLN	GLN	THR	THR	THR	ASN	LEU	LYS
I372	LYS	LYS	ASP	ASP	ASP	ILE	ILE	ASP
	ILE	ILE	ILE	ILE	ILE	THR	PRO	TYR
Q377	ASN	ASN	ASN	ASN	ASN	VAL	THR	LYS
Y380	THR	THR	THR	THR	THR	THR	THR	ASN
	THR	THR	THR	THR	THR	THR	THR	THR
Y390	THR	THR	THR	THR	THR	THR	THR	THR
P391	THR	THR	THR	THR	THR	THR	THR	THR
R392	THR	THR	THR	THR	THR	THR	THR	THR



• Molecule 1: Teichoic acid biosynthesis protein F



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.88Å 222.88Å 100.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.01 – 2.95 20.01 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.01-2.95) 98.7 (20.01-2.95)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.93Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.193 , 0.254 0.186 , 0.248	Depositor DCC
$R_{free}$ test set	2646 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	88.4	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13868	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% 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: SO4, CL, C2G, EDO

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	0.52	0/3551	0.65	0/4798
1	B	0.52	0/3556	0.66	1/4805 (0.0%)
1	C	0.47	0/3556	0.64	0/4805
1	D	0.48	0/3469	0.62	0/4688
All	All	0.50	0/14132	0.64	1/19096 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	662	LEU	CA-CB-CG	5.66	128.32	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3462	0	3369	125	0
1	B	3467	0	3374	128	0
1	C	3467	0	3374	143	0
1	D	3383	0	3289	148	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10	0	0	0	0
3	A	8	0	0	2	0
3	B	5	0	0	5	0
3	C	5	0	0	2	0
3	D	3	0	0	5	0
4	D	30	0	19	3	0
5	D	4	0	6	0	0
6	A	2	0	0	0	0
6	D	2	0	0	0	0
All	All	13868	0	13431	542	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 20.

All (542) 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:A:333:ARG:HH11	1:A:333:ARG:HG2	1.13	1.13
1:D:333:ARG:HH11	1:D:333:ARG:HG2	1.16	1.08
1:D:470:ARG:HG2	1:D:470:ARG:HH11	1.07	1.08
1:B:470:ARG:HG2	1:B:470:ARG:HH11	1.24	1.01
1:B:333:ARG:HH11	1:B:333:ARG:HG2	1.24	1.00
1:B:382:ASN:ND2	1:B:382:ASN:H	1.66	0.92
1:D:353:LYS:HG3	3:D:732:CL:CL	2.06	0.91
1:D:450:ARG:HA	1:D:655:TYR:CE2	2.06	0.90
1:C:367:ASP:HB2	1:C:511:ARG:HD3	1.54	0.89
1:C:383:TYR:CE2	1:C:718:ILE:HD11	2.08	0.88
1:B:722:LEU:O	1:B:723:GLU:HG3	1.75	0.87
1:B:561:GLU:HB2	3:B:734:CL:CL	2.12	0.85
1:B:451:LEU:H	1:B:451:LEU:HD12	1.42	0.84
1:C:383:TYR:CZ	1:C:718:ILE:HD11	2.11	0.84
1:B:714:ILE:O	1:B:718:ILE:HG22	1.77	0.84
1:D:470:ARG:HG2	1:D:470:ARG:NH1	1.86	0.84
1:A:333:ARG:HH11	1:A:333:ARG:CG	1.92	0.82
1:B:413:GLN:O	1:B:417:GLU:HG3	1.79	0.82
1:C:648:ASP:HB2	1:C:651:LEU:HB3	1.62	0.81
1:D:585:TYR:CZ	1:D:586:LEU:HG	2.15	0.81
1:B:403:LYS:HE2	3:B:735:CL:CL	2.18	0.81
1:A:485:PRO:HG3	1:A:509:TYR:CE2	2.16	0.80
1:D:543:TYR:CZ	1:D:545:PRO:HG3	2.15	0.80
1:C:662:LEU:H	1:C:662:LEU:CD2	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:LYS:HE3	1:B:349:ASN:HD21	1.46	0.79
1:D:442:THR:HG22	1:D:483:ILE:HD12	1.62	0.79
1:A:333:ARG:NH1	1:A:333:ARG:HG2	1.91	0.79
1:D:447:PRO:HA	4:D:730:C2G:H1G2	1.65	0.79
1:A:648:ASP:HB2	1:A:651:LEU:HB2	1.65	0.78
1:B:333:ARG:HH11	1:B:333:ARG:CG	1.95	0.78
1:A:451:LEU:HD12	1:A:451:LEU:H	1.50	0.77
1:A:383:TYR:CZ	1:A:718:ILE:HD11	2.20	0.77
1:D:451:LEU:HD12	1:D:451:LEU:H	1.48	0.77
1:C:662:LEU:H	1:C:662:LEU:HD23	1.51	0.76
1:C:316:VAL:HG23	1:D:331:LEU:HD22	1.66	0.75
1:B:465:THR:HB	1:B:466:PRO:HD3	1.68	0.75
1:D:363:LYS:HE2	1:D:364:ASN:OD1	1.85	0.75
1:D:670:PRO:HD2	1:D:671:TYR:CD2	2.22	0.75
1:A:662:LEU:HD23	1:A:662:LEU:H	1.52	0.75
1:D:465:THR:HB	1:D:466:PRO:HD3	1.67	0.75
1:B:458:VAL:HA	1:B:460:MET:HE1	1.68	0.74
1:A:345:ASP:OD1	1:A:434:LYS:HE3	1.87	0.74
1:B:347:GLU:O	1:B:436:ASN:ND2	2.20	0.74
1:C:458:VAL:CG1	1:C:460:MET:HG2	2.17	0.74
1:C:470:ARG:HG2	1:C:470:ARG:HH11	1.51	0.74
1:A:338:ARG:HD2	1:A:430:TYR:CD1	2.23	0.73
1:D:434:LYS:HG3	1:D:437:GLN:OE1	1.88	0.73
1:C:485:PRO:HG3	1:C:509:TYR:CE2	2.25	0.72
1:B:372:ILE:HD13	1:B:710:ILE:HG21	1.72	0.71
1:B:624:SER:OG	1:B:626:VAL:HG22	1.90	0.70
1:D:333:ARG:CG	1:D:333:ARG:HH11	1.98	0.70
1:D:697:ARG:HD3	1:D:698:PHE:CZ	2.27	0.70
1:B:663:PRO:HG3	1:B:694:PHE:CG	2.27	0.69
1:C:470:ARG:CG	1:C:470:ARG:HH11	2.05	0.69
1:A:486:ASN:HA	1:A:701:VAL:HG21	1.74	0.69
1:B:470:ARG:NH1	1:B:470:ARG:HG2	2.00	0.69
1:B:333:ARG:NH1	1:B:333:ARG:HG2	2.01	0.69
1:A:341:TYR:CD1	1:A:412:TYR:HB3	2.28	0.69
1:C:546:THR:HG23	1:C:624:SER:HB2	1.75	0.69
1:C:523:GLU:O	1:C:527:GLU:HG3	1.93	0.68
1:C:670:PRO:HD2	1:C:671:TYR:CD2	2.29	0.68
1:D:547:TRP:CD1	1:D:547:TRP:N	2.59	0.68
1:D:438:THR:HA	1:D:480:ASP:OD2	1.93	0.68
1:A:470:ARG:HD2	1:A:474:ARG:HH21	1.58	0.67
1:A:514:VAL:HG12	1:A:518:ARG:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:GLU:O	1:C:598:ASN:HB2	1.95	0.66
1:B:446:THR:O	1:B:625:SER:HB2	1.95	0.66
1:C:543:TYR:CZ	1:C:545:PRO:HG3	2.30	0.66
1:C:714:ILE:O	1:C:718:ILE:HG23	1.96	0.66
1:C:718:ILE:HG13	1:C:718:ILE:O	1.94	0.66
1:B:543:TYR:CZ	1:B:545:PRO:HG3	2.31	0.65
1:C:420:HIS:CD2	1:C:438:THR:HB	2.32	0.65
1:D:669:GLU:HG2	1:D:671:TYR:H	1.60	0.65
1:C:722:LEU:O	1:C:723:GLU:HG3	1.96	0.65
1:D:338:ARG:HD3	1:D:412:TYR:OH	1.97	0.65
1:D:365:TYR:CZ	1:D:370:LYS:HG3	2.32	0.64
1:D:714:ILE:O	1:D:718:ILE:HG23	1.98	0.64
1:B:563:LYS:HD2	1:B:563:LYS:H	1.62	0.64
1:D:480:ASP:O	1:D:503:ARG:HG2	1.98	0.64
1:B:470:ARG:CG	1:B:470:ARG:HH11	2.05	0.64
1:D:434:LYS:C	1:D:436:ASN:H	2.00	0.64
1:D:597:GLU:O	1:D:598:ASN:HB2	1.96	0.64
1:D:485:PRO:HB2	1:D:486:ASN:ND2	2.13	0.64
1:B:679:ASN:HD22	1:B:682:LYS:HE3	1.63	0.64
1:C:662:LEU:CD2	1:C:662:LEU:N	2.61	0.64
1:C:347:GLU:HG3	1:C:436:ASN:HB2	1.79	0.63
1:D:619:LEU:HD23	1:D:620:ILE:N	2.13	0.63
1:A:426:ARG:HG2	1:A:475:GLU:HG2	1.79	0.63
1:B:619:LEU:HD21	1:B:621:THR:HB	1.81	0.63
1:B:703:ASN:HD22	1:B:705:LYS:H	1.45	0.63
1:B:548:ARG:HD3	1:B:643:ASP:OD2	1.99	0.63
1:A:648:ASP:OD2	1:A:651:LEU:HD12	1.99	0.63
1:B:329:ILE:HD12	1:B:336:LYS:HB2	1.81	0.63
1:C:448:LEU:HD13	1:C:627:MET:HE1	1.81	0.63
1:B:380:TYR:N	1:B:381:PRO:HD3	2.14	0.63
1:B:648:ASP:HB2	1:B:651:LEU:HB3	1.81	0.63
1:A:470:ARG:HD2	1:A:474:ARG:NH2	2.14	0.62
1:D:317:ASN:ND2	1:D:320:ARG:HH21	1.97	0.62
1:D:325:HIS:CE1	1:D:329:ILE:CD1	2.81	0.62
1:B:352:PRO:O	1:B:718:ILE:HD12	1.99	0.62
1:B:513:ASP:HA	1:B:704:GLY:HA2	1.80	0.62
1:D:367:ASP:CG	1:D:368:SER:H	2.03	0.62
1:A:662:LEU:HB2	1:A:663:PRO:HD3	1.82	0.62
1:D:651:LEU:HD21	1:D:654:PHE:CD1	2.34	0.62
1:A:383:TYR:CE2	1:A:718:ILE:HD11	2.35	0.62
1:D:542:MET:HE1	1:D:612:LEU:HD13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:PRO:HB2	1:B:667:TYR:CE2	2.35	0.62
1:C:470:ARG:HG2	1:C:470:ARG:NH1	2.13	0.61
1:D:333:ARG:HG2	1:D:333:ARG:NH1	1.97	0.61
1:D:338:ARG:HD2	1:D:430:TYR:CD1	2.35	0.61
1:D:352:PRO:HD2	3:D:732:CL:CL	2.38	0.61
1:B:461:PRO:O	1:B:463:THR:HG22	1.99	0.61
1:B:485:PRO:HB2	1:B:486:ASN:ND2	2.15	0.61
1:D:451:LEU:HA	1:D:455:MET:CE	2.31	0.61
1:A:662:LEU:H	1:A:662:LEU:CD2	2.13	0.60
1:B:382:ASN:HD22	1:B:382:ASN:H	1.44	0.60
1:B:633:LEU:HB3	1:B:635:ARG:HD3	1.83	0.60
1:C:340:LEU:O	1:C:344:THR:HG23	2.02	0.60
1:A:679:ASN:ND2	1:A:682:LYS:HE3	2.17	0.59
1:C:322:THR:O	1:C:326:VAL:HG23	2.03	0.59
1:C:387:TRP:HB3	1:C:389:PHE:CE2	2.37	0.59
1:C:316:VAL:CG2	1:D:331:LEU:HD22	2.31	0.59
1:D:325:HIS:CE1	1:D:329:ILE:HD11	2.38	0.59
1:A:651:LEU:HD21	1:A:654:PHE:CD1	2.38	0.59
1:C:338:ARG:HD2	1:C:430:TYR:CD1	2.37	0.59
1:D:633:LEU:HB3	1:D:635:ARG:HD3	1.84	0.59
1:B:382:ASN:ND2	1:B:382:ASN:N	2.46	0.59
1:A:485:PRO:HG3	1:A:509:TYR:CZ	2.38	0.58
1:D:331:LEU:HB2	1:D:333:ARG:HD3	1.85	0.58
1:B:679:ASN:ND2	1:B:682:LYS:HB2	2.18	0.58
1:A:353:LYS:HB2	1:A:383:TYR:HD2	1.69	0.58
1:A:546:THR:HG21	1:A:623:TYR:O	2.04	0.58
1:A:662:LEU:N	1:A:662:LEU:CD2	2.66	0.58
1:D:434:LYS:HB2	1:D:436:ASN:HB3	1.85	0.58
1:C:458:VAL:HG13	1:C:460:MET:HG2	1.84	0.57
1:C:648:ASP:HB2	1:C:651:LEU:CB	2.31	0.57
1:A:325:HIS:CE1	1:A:340:LEU:HB2	2.39	0.57
1:C:543:TYR:CE2	1:C:545:PRO:HG3	2.39	0.57
1:A:515:LEU:HD12	1:A:632:ILE:HD12	1.86	0.57
1:B:450:ARG:HA	1:B:655:TYR:CE2	2.38	0.57
1:C:346:LYS:C	1:C:348:ASP:H	2.08	0.57
1:D:451:LEU:HD12	1:D:451:LEU:N	2.18	0.57
1:D:652:ARG:C	1:D:654:PHE:H	2.07	0.57
1:B:540:VAL:HG22	1:B:578:VAL:HG12	1.86	0.57
1:B:491:GLU:OE2	1:B:491:GLU:HA	2.05	0.57
1:D:347:GLU:CG	1:D:436:ASN:HD22	2.17	0.57
1:D:546:THR:HG23	1:D:547:TRP:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:653:GLY:O	1:D:654:PHE:HD1	1.86	0.57
1:A:492:ILE:HD13	1:A:655:TYR:CD2	2.39	0.57
1:A:368:SER:OG	1:A:511:ARG:HG2	2.05	0.57
1:B:475:GLU:OE1	1:B:478:ARG:NH1	2.38	0.57
1:C:492:ILE:HD13	1:C:655:TYR:CD2	2.40	0.57
1:C:494:ARG:HA	1:C:499:MET:HB2	1.86	0.57
1:A:543:TYR:CZ	1:A:545:PRO:HG3	2.40	0.56
1:A:358:GLU:HB2	1:A:388:SER:HB3	1.88	0.56
1:B:345:ASP:OD1	1:B:434:LYS:HE3	2.05	0.56
1:B:563:LYS:CD	1:B:563:LYS:H	2.18	0.56
1:C:392:PRO:HD2	3:C:733:CL:CL	2.42	0.56
1:C:372:ILE:HD13	1:C:710:ILE:HG21	1.86	0.56
1:B:451:LEU:N	1:B:451:LEU:HD12	2.14	0.56
1:C:467:LYS:NZ	1:C:470:ARG:HH22	2.03	0.56
1:A:638:PHE:HE1	1:A:676:GLU:HG2	1.71	0.56
1:C:325:HIS:ND1	1:C:339:SER:HB2	2.20	0.56
1:C:434:LYS:C	1:C:436:ASN:H	2.09	0.56
1:C:367:ASP:HB2	1:C:511:ARG:CD	2.32	0.56
1:C:511:ARG:HH22	1:C:629:ASP:CG	2.09	0.56
1:D:439:TYR:N	1:D:480:ASP:OD2	2.33	0.56
1:C:663:PRO:HG3	1:C:694:PHE:CG	2.40	0.56
1:A:353:LYS:HB2	1:A:383:TYR:CD2	2.40	0.56
1:C:382:ASN:ND2	1:C:382:ASN:H	2.01	0.56
1:C:640:PHE:CE2	1:C:642:TYR:HB3	2.41	0.56
1:C:657:ASN:O	1:C:661:ASP:OD1	2.24	0.56
1:A:450:ARG:HD2	1:A:653:GLY:HA2	1.87	0.55
1:A:548:ARG:NH2	1:A:622:ASP:OD1	2.33	0.55
1:A:722:LEU:O	1:A:723:GLU:HG3	2.07	0.55
1:D:464:THR:OG1	1:D:466:PRO:HD2	2.07	0.55
1:A:448:LEU:HD13	1:A:627:MET:HE1	1.88	0.55
1:A:510:PRO:HB3	1:A:707:SER:HB3	1.88	0.55
1:B:662:LEU:HB2	1:B:663:PRO:CD	2.37	0.55
1:D:564:ILE:HG12	1:D:569:LEU:HD11	1.88	0.55
1:A:652:ARG:C	1:A:654:PHE:H	2.11	0.54
1:B:387:TRP:HB3	1:B:389:PHE:CE2	2.42	0.54
1:A:662:LEU:HB2	1:A:663:PRO:CD	2.37	0.54
1:A:641:ALA:HB1	1:A:644:ILE:HB	1.89	0.54
1:A:651:LEU:HD23	1:A:651:LEU:O	2.08	0.54
1:B:364:ASN:HB3	1:B:366:SER:OG	2.08	0.54
1:C:315:LYS:HD3	1:C:315:LYS:H	1.72	0.54
1:C:671:TYR:O	1:C:675:LYS:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:LYS:NZ	1:C:682:LYS:HB2	2.23	0.54
1:D:458:VAL:C	1:D:460:MET:H	2.10	0.54
1:A:553:VAL:O	1:A:554:SER:HB2	2.08	0.54
1:C:420:HIS:HD2	1:C:438:THR:HB	1.71	0.54
1:C:350:VAL:CG2	1:C:436:ASN:HD22	2.21	0.54
1:C:467:LYS:NZ	1:C:470:ARG:NH2	2.56	0.54
1:C:572:GLU:O	1:C:678:LYS:HE3	2.08	0.54
1:D:483:ILE:HD11	1:D:710:ILE:HD11	1.90	0.54
1:A:519:ALA:HA	1:A:614:LEU:HD22	1.90	0.53
1:C:542:MET:HE1	1:C:612:LEU:HB3	1.90	0.53
1:D:347:GLU:HG2	1:D:436:ASN:ND2	2.24	0.53
1:A:679:ASN:HD22	1:A:682:LYS:HE3	1.72	0.53
1:C:465:THR:HB	1:C:466:PRO:HD3	1.89	0.53
1:D:451:LEU:HA	1:D:455:MET:HE3	1.90	0.53
1:D:615:ILE:C	1:D:615:ILE:HD12	2.29	0.53
1:A:624:SER:OG	1:A:626:VAL:HG22	2.09	0.53
1:B:461:PRO:O	1:B:463:THR:N	2.41	0.53
1:D:697:ARG:HD3	1:D:698:PHE:CE2	2.44	0.53
1:A:350:VAL:HA	1:A:417:GLU:O	2.09	0.53
1:B:488:TYR:OH	1:B:655:TYR:HB2	2.09	0.53
1:B:663:PRO:HG3	1:B:694:PHE:CD2	2.44	0.53
1:C:450:ARG:NH1	1:C:652:ARG:O	2.41	0.53
1:D:639:PHE:CZ	1:D:663:PRO:HD2	2.44	0.53
1:C:441:GLN:HG2	1:C:479:TRP:CE2	2.44	0.53
3:A:735:CL:CL	1:C:313:ALA:HB2	2.46	0.53
1:A:380:TYR:N	1:A:381:PRO:HD3	2.24	0.52
1:C:347:GLU:HA	1:C:434:LYS:HD3	1.89	0.52
1:C:445:GLY:HA2	1:C:509:TYR:CE2	2.44	0.52
1:A:347:GLU:O	1:A:436:ASN:ND2	2.43	0.52
1:D:485:PRO:HD2	1:D:489:SER:CB	2.39	0.52
1:A:572:GLU:O	1:A:573:LEU:HD23	2.10	0.52
1:C:701:VAL:HG12	1:C:701:VAL:O	2.09	0.52
1:B:350:VAL:HA	1:B:417:GLU:O	2.10	0.52
1:C:350:VAL:HG21	1:C:436:ASN:ND2	2.24	0.52
1:C:581:LEU:O	1:C:603:VAL:HG12	2.10	0.52
1:C:665:PRO:HG3	1:C:687:TYR:CE1	2.44	0.52
1:C:380:TYR:CE1	1:C:715:HIS:ND1	2.77	0.52
1:D:548:ARG:NH2	1:D:622:ASP:OD1	2.42	0.52
1:A:458:VAL:HG13	1:A:460:MET:HE2	1.92	0.52
1:A:438:THR:HA	1:A:480:ASP:OD2	2.11	0.51
1:A:561:GLU:HA	3:A:738:CL:CL	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:LYS:HA	1:B:456:LYS:HE2	1.92	0.51
1:A:547:TRP:CG	1:A:548:ARG:N	2.78	0.51
1:D:413:GLN:O	1:D:417:GLU:HG3	2.10	0.51
1:D:458:VAL:HG12	1:D:460:MET:HB2	1.92	0.51
1:A:540:VAL:HG22	1:A:578:VAL:HG12	1.92	0.51
1:C:639:PHE:CZ	1:C:663:PRO:HD2	2.45	0.51
1:D:347:GLU:HG2	1:D:436:ASN:HD22	1.75	0.51
1:C:341:TYR:O	1:C:345:ASP:HB2	2.11	0.51
1:A:670:PRO:HG2	1:A:671:TYR:CE2	2.46	0.51
1:A:345:ASP:OD1	1:A:434:LYS:CE	2.58	0.50
1:A:467:LYS:HG3	1:A:470:ARG:NH2	2.26	0.50
1:C:559:LEU:HD12	1:C:559:LEU:C	2.30	0.50
1:B:325:HIS:CE1	1:B:329:ILE:HD13	2.45	0.50
1:D:458:VAL:O	1:D:458:VAL:HG12	2.11	0.50
1:D:340:LEU:O	1:D:344:THR:HG23	2.11	0.50
1:C:453:ASN:HB2	1:C:496:ALA:O	2.11	0.50
1:D:325:HIS:CE1	1:D:329:ILE:HD13	2.46	0.50
1:D:317:ASN:O	1:D:321:LYS:HG3	2.11	0.50
1:C:367:ASP:CB	1:C:511:ARG:HD3	2.34	0.50
1:A:665:PRO:HG3	1:A:687:TYR:CE1	2.47	0.50
1:C:683:VAL:O	1:C:687:TYR:HB2	2.11	0.50
1:D:581:LEU:O	1:D:603:VAL:HG12	2.12	0.49
1:B:675:LYS:O	1:B:678:LYS:HB2	2.12	0.49
1:D:467:LYS:HE3	1:D:470:ARG:HH22	1.77	0.49
1:A:485:PRO:HA	1:A:508:GLY:HA2	1.93	0.49
1:D:446:THR:O	1:D:625:SER:HB2	2.13	0.49
1:D:637:GLN:O	1:D:664:GLY:HA3	2.12	0.49
1:B:345:ASP:CG	1:B:434:LYS:HE3	2.32	0.49
1:D:585:TYR:CE2	1:D:586:LEU:HG	2.46	0.49
1:D:662:LEU:HB2	1:D:663:PRO:HD3	1.95	0.49
1:D:470:ARG:CG	1:D:470:ARG:HH11	1.99	0.49
1:C:467:LYS:CE	1:C:470:ARG:HH22	2.26	0.49
1:A:325:HIS:CE1	1:A:329:ILE:HD13	2.48	0.49
1:B:487:ARG:HH11	1:B:487:ARG:HB2	1.78	0.49
1:C:662:LEU:H	1:C:662:LEU:HD22	1.77	0.49
1:D:514:VAL:C	1:D:516:VAL:H	2.16	0.49
1:B:404:VAL:HG12	1:B:410:GLU:HB3	1.94	0.48
1:C:329:ILE:HG22	1:C:330:VAL:N	2.29	0.48
1:C:669:GLU:HG2	1:C:671:TYR:H	1.78	0.48
1:D:487:ARG:HD3	1:D:506:GLU:OE2	2.14	0.48
1:C:350:VAL:HG21	1:C:436:ASN:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:LYS:C	1:D:436:ASN:N	2.65	0.48
1:A:378:LYS:HD3	1:A:379:TYR:CE2	2.48	0.48
1:D:485:PRO:HG3	1:D:509:TYR:CE2	2.49	0.48
1:A:420:HIS:CD2	1:A:714:ILE:HG12	2.48	0.48
1:D:412:TYR:O	1:D:413:GLN:C	2.52	0.48
1:B:669:GLU:HG2	1:B:671:TYR:H	1.78	0.48
1:A:576:ASP:HB2	1:A:577:TYR:CD2	2.49	0.48
1:B:603:VAL:HG13	1:B:603:VAL:O	2.14	0.48
1:C:581:LEU:C	1:C:603:VAL:HG12	2.34	0.48
1:D:375:TYR:C	1:D:375:TYR:CD2	2.87	0.48
1:D:450:ARG:HA	1:D:655:TYR:HE2	1.73	0.48
1:A:621:THR:O	1:A:639:PHE:HA	2.13	0.48
1:D:541:ILE:HD13	1:D:677:LEU:HD21	1.95	0.48
1:A:521:ASP:O	1:A:525:LEU:HG	2.13	0.48
1:B:525:LEU:O	1:B:529:ARG:HG3	2.14	0.48
1:B:438:THR:HA	1:B:480:ASP:OD2	2.13	0.47
1:D:669:GLU:OE2	1:D:672:GLY:N	2.47	0.47
1:D:673:LEU:O	1:D:677:LEU:HB2	2.14	0.47
1:B:338:ARG:HD2	1:B:430:TYR:HB2	1.97	0.47
1:B:445:GLY:HA2	1:B:509:TYR:CE2	2.49	0.47
1:C:350:VAL:CG2	1:C:436:ASN:ND2	2.78	0.47
1:C:542:MET:HB3	1:C:619:LEU:HD23	1.96	0.47
1:C:559:LEU:HD12	1:C:559:LEU:O	2.14	0.47
1:D:451:LEU:HA	1:D:455:MET:HE2	1.96	0.47
1:A:363:LYS:HE3	1:A:364:ASN:ND2	2.29	0.47
1:B:451:LEU:HD13	1:B:496:ALA:HB1	1.96	0.47
1:C:521:ASP:HB3	1:C:524:TYR:HB3	1.97	0.47
1:A:547:TRP:CD1	1:A:548:ARG:N	2.82	0.47
1:D:351:LYS:HB3	3:D:732:CL:CL	2.52	0.47
1:D:357:PHE:CE1	1:D:373:TYR:HB2	2.50	0.47
1:A:319:PHE:HE1	1:D:330:VAL:HG21	1.80	0.47
1:A:542:MET:CE	1:A:612:LEU:HB3	2.45	0.47
1:B:379:TYR:C	1:B:381:PRO:HD3	2.35	0.47
1:C:353:LYS:HG2	3:C:732:CL:CL	2.51	0.47
1:D:546:THR:CG2	1:D:547:TRP:N	2.77	0.47
1:D:639:PHE:CE2	1:D:663:PRO:HD2	2.50	0.47
1:B:355:ILE:HG22	1:B:357:PHE:CE2	2.49	0.47
1:B:458:VAL:C	1:B:460:MET:H	2.18	0.47
1:C:559:LEU:HD13	1:C:560:PHE:C	2.35	0.47
1:D:353:LYS:CG	3:D:732:CL:CL	2.91	0.47
1:B:333:ARG:NH1	1:B:333:ARG:CG	2.64	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:TYR:CE1	1:B:415:TYR:HE2	2.33	0.47
1:C:559:LEU:CD1	1:C:559:LEU:C	2.83	0.47
1:D:619:LEU:HB2	1:D:630:TYR:CE2	2.50	0.47
1:A:509:TYR:HB3	1:A:511:ARG:HG3	1.96	0.47
1:A:662:LEU:HD23	1:A:662:LEU:N	2.21	0.47
1:A:701:VAL:O	1:A:701:VAL:HG12	2.14	0.47
1:D:411:TYR:CE1	1:D:415:TYR:HE2	2.33	0.47
1:A:329:ILE:HG22	1:A:330:VAL:N	2.30	0.47
1:A:665:PRO:HG3	1:A:687:TYR:CZ	2.50	0.47
1:B:461:PRO:C	1:B:463:THR:H	2.18	0.47
1:C:444:ASN:O	1:C:511:ARG:NH1	2.43	0.47
1:D:442:THR:O	1:D:509:TYR:HE1	1.98	0.47
1:A:378:LYS:HD3	1:A:379:TYR:HE2	1.80	0.46
1:B:560:PHE:O	1:B:561:GLU:C	2.53	0.46
1:B:670:PRO:HD2	1:B:671:TYR:CD2	2.49	0.46
1:A:663:PRO:HG3	1:A:694:PHE:CG	2.50	0.46
1:B:325:HIS:CE1	1:B:340:LEU:HB2	2.49	0.46
1:C:548:ARG:HD3	1:C:643:ASP:OD2	2.15	0.46
1:C:621:THR:OG1	1:C:622:ASP:N	2.48	0.46
1:A:385:TYR:O	1:A:401:ALA:HA	2.15	0.46
1:B:509:TYR:HB3	1:B:511:ARG:HG2	1.95	0.46
1:C:446:THR:HB	1:C:628:PHE:CD2	2.50	0.46
1:A:427:THR:HG23	1:A:439:TYR:OH	2.16	0.46
1:B:396:VAL:HA	3:B:735:CL:CL	2.52	0.46
1:D:452:ALA:HB2	1:D:497:PHE:CE2	2.51	0.46
1:A:559:LEU:O	1:A:559:LEU:HD12	2.16	0.46
1:C:510:PRO:HA	1:C:706:ALA:HB3	1.98	0.46
1:D:562:LEU:HD23	1:D:562:LEU:HA	1.74	0.46
1:A:481:TYR:CE2	1:A:713:LEU:HD21	2.51	0.46
1:D:608:ASP:OD2	1:D:610:SER:HB2	2.15	0.46
1:C:367:ASP:CG	1:C:368:SER:H	2.18	0.46
1:A:639:PHE:CD2	1:A:639:PHE:N	2.84	0.46
1:B:648:ASP:HB2	1:B:651:LEU:CB	2.45	0.46
1:C:385:TYR:O	1:C:401:ALA:HA	2.15	0.46
1:D:410:GLU:N	1:D:410:GLU:OE1	2.37	0.46
1:B:511:ARG:HH22	1:B:629:ASP:CG	2.19	0.45
1:C:365:TYR:CE2	1:C:370:LYS:HD2	2.50	0.45
1:C:429:LEU:HD23	1:C:429:LEU:HA	1.51	0.45
1:A:338:ARG:HD3	1:A:412:TYR:OH	2.17	0.45
1:A:543:TYR:CE2	1:A:545:PRO:HG3	2.52	0.45
1:B:403:LYS:CE	3:B:735:CL:CL	2.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:ILE:HD11	1:C:611:GLU:HG2	1.98	0.45
1:C:588:SER:C	1:C:590:ALA:H	2.18	0.45
1:C:562:LEU:H	1:C:562:LEU:HG	1.55	0.45
1:D:395:ASN:O	1:D:403:LYS:HE2	2.16	0.45
1:A:549:ASP:O	1:A:551:GLU:N	2.49	0.45
1:B:485:PRO:HD2	1:B:489:SER:HB2	1.98	0.45
1:C:627:MET:HE3	1:C:628:PHE:CZ	2.52	0.45
1:C:620:ILE:HD13	1:C:673:LEU:HD11	1.99	0.45
1:D:705:LYS:O	1:D:708:GLN:HB3	2.17	0.45
1:A:548:ARG:HD3	1:A:643:ASP:OD2	2.16	0.45
1:B:467:LYS:O	1:B:467:LYS:HG3	2.16	0.45
1:C:441:GLN:HG2	1:C:479:TRP:CZ2	2.52	0.45
1:C:485:PRO:HD2	1:C:489:SER:HB2	1.99	0.45
1:C:657:ASN:ND2	1:C:660:GLU:HB2	2.32	0.45
1:D:387:TRP:HB3	1:D:389:PHE:CE2	2.52	0.45
1:B:329:ILE:CG2	1:B:330:VAL:N	2.78	0.45
1:B:442:THR:HG22	1:B:483:ILE:HD12	1.99	0.45
1:B:487:ARG:HD3	1:B:487:ARG:HA	1.78	0.45
1:B:695:TYR:CD2	1:B:695:TYR:C	2.90	0.45
1:C:368:SER:HB2	1:C:369:PRO:HD3	1.99	0.45
1:C:569:LEU:N	1:C:569:LEU:HD23	2.31	0.45
1:C:612:LEU:HD23	1:C:612:LEU:HA	1.77	0.45
1:B:431:LEU:HA	1:B:431:LEU:HD23	1.63	0.45
1:D:343:LEU:HA	1:D:343:LEU:HD23	1.78	0.45
1:A:497:PHE:O	1:A:498:TRP:C	2.55	0.44
1:B:396:VAL:HG12	1:B:396:VAL:O	2.18	0.44
1:C:470:ARG:CB	1:C:470:ARG:HH11	2.30	0.44
1:C:440:ILE:HD12	1:C:714:ILE:HD11	1.99	0.44
1:D:367:ASP:CG	1:D:368:SER:N	2.65	0.44
1:B:684:GLN:O	1:B:688:GLN:HB2	2.16	0.44
1:C:377:GLN:O	1:C:381:PRO:HG3	2.16	0.44
1:C:450:ARG:HA	1:C:655:TYR:CZ	2.53	0.44
1:C:546:THR:CG2	1:C:624:SER:HB2	2.47	0.44
1:A:443:TRP:CG	1:A:444:ASN:N	2.85	0.44
1:D:446:THR:HA	1:D:447:PRO:HD3	1.88	0.44
1:D:483:ILE:HD11	1:D:710:ILE:CD1	2.47	0.44
1:A:421:TRP:CZ3	1:A:433:LYS:HG3	2.53	0.44
1:A:703:ASN:HB3	1:A:705:LYS:HB2	1.98	0.44
1:B:531:HIS:HD2	1:B:531:HIS:O	2.01	0.44
1:C:347:GLU:O	1:C:436:ASN:ND2	2.51	0.44
1:C:639:PHE:HZ	1:C:663:PRO:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:SER:HB3	1:D:369:PRO:HG2	2.00	0.44
1:D:651:LEU:HD23	1:D:651:LEU:O	2.18	0.44
1:A:420:HIS:HA	1:A:438:THR:O	2.17	0.44
1:A:451:LEU:HD12	1:A:451:LEU:N	2.16	0.44
1:A:638:PHE:CE1	1:A:676:GLU:HG2	2.52	0.44
1:C:316:VAL:HG13	1:C:317:ASN:N	2.33	0.44
1:C:552:PHE:O	1:C:553:VAL:HG13	2.18	0.44
1:D:458:VAL:CG1	1:D:460:MET:HB2	2.48	0.44
1:D:615:ILE:O	1:D:615:ILE:HD12	2.17	0.44
1:C:464:THR:HG23	1:C:467:LYS:H	1.83	0.43
1:C:661:ASP:N	1:C:661:ASP:OD1	2.50	0.43
1:A:624:SER:CB	1:A:626:VAL:HG22	2.48	0.43
1:D:383:TYR:CE2	1:D:718:ILE:HD11	2.52	0.43
1:A:458:VAL:HG12	1:A:458:VAL:O	2.18	0.43
1:A:444:ASN:O	1:A:511:ARG:NH1	2.50	0.43
1:C:458:VAL:HG13	1:C:460:MET:HE2	1.99	0.43
1:B:411:TYR:CE1	1:B:415:TYR:CE2	3.05	0.43
1:C:637:GLN:O	1:C:664:GLY:HA3	2.18	0.43
1:D:578:VAL:HG23	1:D:599:PHE:HA	2.00	0.43
1:A:458:VAL:HB	1:A:465:THR:OG1	2.18	0.43
1:A:572:GLU:C	1:A:573:LEU:HD23	2.38	0.43
1:D:445:GLY:HA2	1:D:509:TYR:CE2	2.53	0.43
1:C:426:ARG:HG3	1:C:426:ARG:H	1.65	0.43
1:C:470:ARG:HB3	1:C:470:ARG:HH11	1.82	0.43
1:C:488:TYR:OH	1:C:655:TYR:HB2	2.19	0.43
1:D:662:LEU:HB2	1:D:663:PRO:CD	2.48	0.43
1:A:357:PHE:N	1:A:357:PHE:CD2	2.87	0.43
1:B:329:ILE:HG22	1:B:330:VAL:N	2.34	0.43
1:B:347:GLU:HG2	1:B:436:ASN:ND2	2.34	0.43
1:D:351:LYS:HA	1:D:352:PRO:HD3	1.85	0.43
1:D:441:GLN:O	1:D:482:LEU:HA	2.18	0.43
1:A:528:ILE:HD13	1:A:611:GLU:HG2	2.01	0.43
1:B:642:TYR:N	1:B:642:TYR:CD1	2.87	0.43
1:B:718:ILE:O	1:B:718:ILE:CG1	2.67	0.43
1:C:670:PRO:HD2	1:C:671:TYR:CE2	2.53	0.43
1:D:356:VAL:HG22	1:D:418:ALA:CB	2.48	0.43
1:C:380:TYR:CE1	1:C:715:HIS:CE1	3.06	0.43
1:C:451:LEU:H	1:C:451:LEU:HD12	1.83	0.43
1:A:597:GLU:O	1:A:598:ASN:HB2	2.18	0.43
1:B:619:LEU:HD23	1:B:619:LEU:C	2.40	0.43
1:C:493:PHE:O	1:C:494:ARG:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:ASN:ND2	1:D:320:ARG:NH2	2.65	0.43
1:D:364:ASN:HD22	1:D:366:SER:HB3	1.84	0.43
1:D:373:TYR:CZ	1:D:377:GLN:HG3	2.54	0.43
1:D:641:ALA:O	1:D:668:THR:HG22	2.18	0.43
1:A:485:PRO:HD2	1:A:489:SER:HB2	2.00	0.42
1:B:457:VAL:HG11	1:B:459:ARG:NH2	2.34	0.42
1:B:597:GLU:O	1:B:598:ASN:HB2	2.19	0.42
1:C:718:ILE:O	1:C:722:LEU:HD22	2.18	0.42
1:D:452:ALA:HB2	1:D:497:PHE:HE2	1.82	0.42
1:D:318:GLN:HG2	3:D:731:CL:CL	2.55	0.42
1:B:662:LEU:HB2	1:B:663:PRO:HD3	2.01	0.42
1:B:713:LEU:HD12	1:B:713:LEU:O	2.19	0.42
1:C:346:LYS:C	1:C:348:ASP:N	2.73	0.42
1:D:404:VAL:HG23	1:D:404:VAL:O	2.18	0.42
1:D:626:VAL:HG12	4:D:730:C2G:HC2	2.00	0.42
4:D:730:C2G:HC6	4:D:730:C2G:O5'	2.19	0.42
1:A:450:ARG:HA	1:A:655:TYR:CZ	2.55	0.42
1:B:317:ASN:O	1:B:321:LYS:HG3	2.18	0.42
1:B:366:SER:HA	1:B:370:LYS:HD2	2.01	0.42
1:D:513:ASP:HA	1:D:704:GLY:HA2	2.00	0.42
1:A:333:ARG:NH1	1:A:333:ARG:CG	2.61	0.42
1:C:485:PRO:HG3	1:C:509:TYR:CZ	2.53	0.42
1:C:367:ASP:O	1:C:370:LYS:N	2.51	0.42
1:C:521:ASP:O	1:C:524:TYR:HB3	2.20	0.42
1:D:368:SER:O	1:D:372:ILE:HG13	2.19	0.42
1:D:408:SER:O	1:D:411:TYR:HB3	2.19	0.42
1:D:470:ARG:NH1	1:D:471:ASN:OD1	2.52	0.42
1:D:682:LYS:HB2	1:D:682:LYS:HE3	1.53	0.42
1:B:458:VAL:O	1:B:458:VAL:HG12	2.20	0.42
1:B:673:LEU:HD22	1:B:677:LEU:HD22	2.02	0.42
1:D:358:GLU:OE1	1:D:388:SER:HB3	2.20	0.42
1:B:531:HIS:O	1:B:531:HIS:CD2	2.72	0.42
1:A:578:VAL:HG22	1:A:599:PHE:O	2.19	0.42
1:B:446:THR:HA	1:B:447:PRO:HD3	1.76	0.42
1:B:455:MET:O	1:B:456:LYS:HE2	2.19	0.42
1:B:583:MET:HE2	1:B:587:ILE:HG21	2.01	0.42
1:D:670:PRO:HD2	1:D:671:TYR:CE2	2.55	0.42
1:A:329:ILE:HD12	1:A:336:LYS:HB2	2.01	0.42
1:A:446:THR:HA	1:A:447:PRO:HD3	1.91	0.42
1:B:434:LYS:C	1:B:436:ASN:N	2.74	0.42
1:D:387:TRP:O	1:D:404:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:PRO:HA	1:A:419:SER:HB3	2.02	0.41
1:A:442:THR:HG22	1:A:483:ILE:HD12	2.02	0.41
1:A:484:SER:HA	1:A:485:PRO:HD3	1.79	0.41
1:A:542:MET:HE2	1:A:612:LEU:HB3	2.01	0.41
1:B:697:ARG:HD3	1:B:698:PHE:CE2	2.55	0.41
1:C:580:LEU:HA	1:C:580:LEU:HD23	1.79	0.41
1:D:492:ILE:HD13	1:D:655:TYR:CG	2.55	0.41
1:A:346:LYS:HG3	1:A:349:ASN:HD21	1.85	0.41
1:A:431:LEU:HA	1:A:431:LEU:HD23	1.83	0.41
1:A:465:THR:N	1:A:466:PRO:CD	2.83	0.41
1:D:450:ARG:HA	1:D:655:TYR:CZ	2.54	0.41
1:B:338:ARG:HD2	1:B:430:TYR:CG	2.56	0.41
1:B:484:SER:HA	1:B:485:PRO:HD3	1.52	0.41
1:C:526:ASP:O	1:C:530:THR:HG23	2.20	0.41
1:D:718:ILE:HG13	1:D:718:ILE:O	2.09	0.41
1:A:584:HIS:HE1	1:A:586:LEU:HG	1.86	0.41
1:B:382:ASN:N	1:B:382:ASN:HD22	2.13	0.41
1:B:418:ALA:O	1:B:437:GLN:HG2	2.19	0.41
1:B:484:SER:O	1:B:506:GLU:HA	2.20	0.41
1:C:488:TYR:O	1:C:492:ILE:HG13	2.20	0.41
1:D:472:PHE:O	1:D:476:THR:HG23	2.21	0.41
1:A:406:ARG:O	1:A:407:ASN:HB2	2.21	0.41
1:A:542:MET:O	1:A:619:LEU:HD23	2.21	0.41
1:B:380:TYR:N	1:B:381:PRO:CD	2.83	0.41
1:B:528:ILE:HG22	1:B:615:ILE:HD13	2.03	0.41
1:C:321:LYS:O	1:C:322:THR:C	2.57	0.41
1:C:410:GLU:H	1:C:410:GLU:CD	2.24	0.41
1:C:509:TYR:HA	1:C:510:PRO:HD3	1.93	0.41
1:C:542:MET:CE	1:C:612:LEU:HB3	2.49	0.41
1:D:484:SER:HA	1:D:485:PRO:HD3	1.90	0.41
1:B:638:PHE:CD1	1:B:665:PRO:HG2	2.56	0.41
1:C:353:LYS:HA	1:C:718:ILE:HD12	2.02	0.41
1:C:380:TYR:N	1:C:381:PRO:HD3	2.35	0.41
1:C:341:TYR:CD1	1:C:412:TYR:HB3	2.56	0.41
1:A:325:HIS:HE1	1:A:340:LEU:HB2	1.82	0.41
1:B:675:LYS:HA	1:B:675:LYS:HD3	1.83	0.41
1:C:351:LYS:HD2	1:C:417:GLU:OE1	2.20	0.41
1:D:341:TYR:O	1:D:345:ASP:HB2	2.21	0.41
1:D:565:ASP:OD1	1:D:671:TYR:OH	2.26	0.41
1:D:586:LEU:HA	1:D:586:LEU:HD23	1.52	0.41
1:D:652:ARG:C	1:D:654:PHE:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:PRO:HD2	1:A:489:SER:CB	2.51	0.41
1:C:380:TYR:CE1	1:C:715:HIS:CG	3.09	0.41
1:C:577:TYR:OH	1:C:680:LEU:HG	2.21	0.41
1:B:316:VAL:O	1:B:320:ARG:HG3	2.21	0.41
1:D:446:THR:OG1	1:D:485:PRO:HG2	2.20	0.41
1:A:406:ARG:HA	1:A:411:TYR:CD1	2.56	0.41
1:B:670:PRO:HD2	1:B:671:TYR:CE2	2.55	0.41
1:D:485:PRO:HD2	1:D:489:SER:HB2	2.03	0.41
1:B:485:PRO:HG3	1:B:509:TYR:CZ	2.56	0.40
1:B:638:PHE:HE1	1:B:676:GLU:HG2	1.85	0.40
1:D:572:GLU:HA	1:D:572:GLU:OE1	2.21	0.40
1:A:509:TYR:HA	1:A:510:PRO:HD3	1.91	0.40
1:A:549:ASP:C	1:A:551:GLU:H	2.25	0.40
1:D:451:LEU:HD13	1:D:496:ALA:HB1	2.03	0.40
1:A:652:ARG:C	1:A:654:PHE:N	2.73	0.40
1:B:380:TYR:CE1	1:B:715:HIS:CG	3.10	0.40
1:B:458:VAL:HG13	1:B:460:MET:CE	2.51	0.40
1:D:638:PHE:CE2	1:D:677:LEU:CD1	3.04	0.40
1:B:323:LEU:HA	1:B:323:LEU:HD12	1.83	0.40
1:B:460:MET:HA	1:B:461:PRO:HD3	1.76	0.40
1:B:561:GLU:CB	3:B:734:CL:CL	2.97	0.40
1:D:515:LEU:HA	1:D:515:LEU:HD23	1.74	0.40
1:D:651:LEU:HG	1:D:653:GLY:H	1.87	0.40
1:A:639:PHE:CZ	1:A:663:PRO:HD2	2.57	0.40
1:C:316:VAL:CG1	1:C:317:ASN:N	2.84	0.40
1:D:665:PRO:HG3	1:D:687:TYR:OH	2.21	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	408/729 (56%)	376 (92%)	28 (7%)	4 (1%)	18	55
1	B	409/729 (56%)	362 (88%)	38 (9%)	9 (2%)	8	33
1	C	409/729 (56%)	356 (87%)	46 (11%)	7 (2%)	11	41
1	D	397/729 (54%)	346 (87%)	42 (11%)	9 (2%)	7	32
All	All	1623/2916 (56%)	1440 (89%)	154 (10%)	29 (2%)	10	39

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	651	LEU
1	C	367	ASP
1	D	367	ASP
1	A	647	TYR
1	B	462	GLY
1	C	647	TYR
1	C	648	ASP
1	D	332	ARG
1	D	521	ASP
1	D	655	TYR
1	A	550	ASP
1	B	345	ASP
1	B	461	PRO
1	B	561	GLU
1	B	649	LYS
1	D	515	LEU
1	C	565	ASP
1	D	458	VAL
1	B	443	TRP
1	B	459	ARG
1	B	565	ASP
1	C	535	PRO
1	C	614	LEU
1	D	443	TRP
1	C	452	ALA
1	B	603	VAL
1	D	545	PRO
1	D	603	VAL
1	A	535	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	379/675 (56%)	339 (89%)	40 (11%)	8	28
1	B	379/675 (56%)	328 (86%)	51 (14%)	4	17
1	C	379/675 (56%)	341 (90%)	38 (10%)	9	31
1	D	370/675 (55%)	329 (89%)	41 (11%)	7	26
All	All	1507/2700 (56%)	1337 (89%)	170 (11%)	7	25

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	LEU
1	A	333	ARG
1	A	336	LYS
1	A	339	SER
1	A	341	TYR
1	A	346	LYS
1	A	356	VAL
1	A	359	SER
1	A	367	ASP
1	A	403	LYS
1	A	406	ARG
1	A	433	LYS
1	A	439	TYR
1	A	451	LEU
1	A	456	LYS
1	A	460	MET
1	A	472	PHE
1	A	488	TYR
1	A	494	ARG
1	A	495	SER
1	A	511	ARG
1	A	514	VAL
1	A	567	ASP
1	A	591	LEU

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Mol	Chain	Res	Type
1	A	594	SER
1	A	597	GLU
1	A	619	LEU
1	A	622	ASP
1	A	656	MET
1	A	659	MET
1	A	662	LEU
1	A	669	GLU
1	A	673	LEU
1	A	677	LEU
1	A	678	LYS
1	A	680	LEU
1	A	702	ASP
1	A	707	SER
1	A	717	ASP
1	A	720	GLU
1	B	316	VAL
1	B	323	LEU
1	B	329	ILE
1	B	333	ARG
1	B	343	LEU
1	B	356	VAL
1	B	367	ASP
1	B	382	ASN
1	B	402	GLU
1	B	404	VAL
1	B	407	ASN
1	B	433	LYS
1	B	439	TYR
1	B	449	LYS
1	B	450	ARG
1	B	451	LEU
1	B	456	LYS
1	B	470	ARG
1	B	472	PHE
1	B	477	SER
1	B	487	ARG
1	B	491	GLU
1	B	514	VAL
1	B	533	ASN
1	B	548	ARG
1	B	549	ASP

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Mol	Chain	Res	Type
1	B	559	LEU
1	B	563	LYS
1	B	578	VAL
1	B	579	ILE
1	B	582	ARG
1	B	589	ASN
1	B	597	GLU
1	B	603	VAL
1	B	607	ASN
1	B	609	VAL
1	B	622	ASP
1	B	645	ASP
1	B	647	TYR
1	B	651	LEU
1	B	661	ASP
1	B	662	LEU
1	B	668	THR
1	B	673	LEU
1	B	677	LEU
1	B	678	LYS
1	B	702	ASP
1	B	703	ASN
1	B	717	ASP
1	B	718	ILE
1	B	722	LEU
1	C	315	LYS
1	C	323	LEU
1	C	332	ARG
1	C	339	SER
1	C	367	ASP
1	C	382	ASN
1	C	403	LYS
1	C	439	TYR
1	C	450	ARG
1	C	451	LEU
1	C	457	VAL
1	C	463	THR
1	C	470	ARG
1	C	472	PHE
1	C	487	ARG
1	C	500	ASP
1	C	536	SER

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Mol	Chain	Res	Type
1	C	559	LEU
1	C	589	ASN
1	C	591	LEU
1	C	597	GLU
1	C	603	VAL
1	C	622	ASP
1	C	623	TYR
1	C	648	ASP
1	C	656	MET
1	C	660	GLU
1	C	661	ASP
1	C	662	LEU
1	C	669	GLU
1	C	673	LEU
1	C	681	ASP
1	C	682	LYS
1	C	683	VAL
1	C	707	SER
1	C	714	ILE
1	C	718	ILE
1	C	722	LEU
1	D	315	LYS
1	D	316	VAL
1	D	317	ASN
1	D	323	LEU
1	D	333	ARG
1	D	337	GLU
1	D	353	LYS
1	D	356	VAL
1	D	367	ASP
1	D	388	SER
1	D	403	LYS
1	D	435	GLU
1	D	439	TYR
1	D	450	ARG
1	D	451	LEU
1	D	456	LYS
1	D	460	MET
1	D	470	ARG
1	D	472	PHE
1	D	487	ARG
1	D	489	SER

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Mol	Chain	Res	Type
1	D	500	ASP
1	D	511	ARG
1	D	514	VAL
1	D	518	ARG
1	D	547	TRP
1	D	548	ARG
1	D	576	ASP
1	D	585	TYR
1	D	609	VAL
1	D	622	ASP
1	D	623	TYR
1	D	625	SER
1	D	645	ASP
1	D	647	TYR
1	D	660	GLU
1	D	662	LEU
1	D	669	GLU
1	D	673	LEU
1	D	702	ASP
1	D	718	ILE

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

Mol	Chain	Res	Type
1	A	325	HIS
1	A	349	ASN
1	A	708	GLN
1	B	349	ASN
1	B	377	GLN
1	B	382	ASN
1	B	407	ASN
1	B	531	HIS
1	B	679	ASN
1	B	686	GLN
1	B	703	ASN
1	C	349	ASN
1	C	382	ASN
1	C	420	HIS
1	C	436	ASN
1	C	686	GLN
1	D	317	ASN
1	D	349	ASN

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Mol	Chain	Res	Type
1	D	413	GLN
1	D	436	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 21 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	730	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	A	731	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	B	730	-	4,4,4	0.19	0	6,6,6	0.24	0
2	SO4	B	731	-	4,4,4	0.18	0	6,6,6	0.19	0
2	SO4	C	730	-	4,4,4	0.16	0	6,6,6	0.17	0
2	SO4	C	731	-	4,4,4	0.12	0	6,6,6	0.25	0
4	C2G	D	730	-	26,31,31	3.46	9 (34%)	26,46,46	1.06	2 (7%)
5	EDO	D	734	-	3,3,3	0.65	0	2,2,2	0.13	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
2	SO4	A	730	-	-	0/0/0/0	0/0/0/0
2	SO4	A	731	-	-	0/0/0/0	0/0/0/0
2	SO4	B	730	-	-	0/0/0/0	0/0/0/0
2	SO4	B	731	-	-	0/0/0/0	0/0/0/0
2	SO4	C	730	-	-	0/0/0/0	0/0/0/0
2	SO4	C	731	-	-	0/0/0/0	0/0/0/0
4	C2G	D	730	-	-	0/20/40/40	0/2/2/2
5	EDO	D	734	-	-	0/1/1/1	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	730	C2G	C4-N4	3.15	1.45	1.35
4	D	730	C2G	PA-O1A	3.99	1.65	1.50
4	D	730	C2G	C5-C4	4.01	1.51	1.41
4	D	730	C2G	PB-O1B	4.04	1.66	1.50
4	D	730	C2G	O4'-C1'	5.07	1.48	1.41
4	D	730	C2G	C2-N3	5.98	1.50	1.38
4	D	730	C2G	C6-C5	6.13	1.51	1.38
4	D	730	C2G	C4-N3	7.80	1.48	1.35
4	D	730	C2G	C6-N1	8.65	1.47	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	730	C2G	C6-N1-C2	-2.03	117.99	121.28
4	D	730	C2G	N4-C4-N3	3.18	122.00	116.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	730	C2G	3	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	410/729 (56%)	-0.17	7 (1%) 70 51	61, 83, 149, 220	0
1	B	411/729 (56%)	-0.12	13 (3%) 48 30	64, 85, 159, 242	0
1	C	411/729 (56%)	-0.08	17 (4%) 38 23	69, 94, 166, 263	0
1	D	401/729 (55%)	-0.04	17 (4%) 37 23	66, 92, 151, 279	0
All	All	1633/2916 (56%)	-0.10	54 (3%) 47 30	61, 88, 156, 279	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	652	ARG	7.2
1	C	558	TYR	5.5
1	D	590	ALA	5.4
1	D	724	HIS	5.0
1	D	649	LYS	4.8
1	A	649	LYS	4.4
1	D	652	ARG	4.2
1	C	652	ARG	4.1
1	C	555	LYS	4.0
1	D	650	GLY	4.0
1	B	555	LYS	3.7
1	D	723	GLU	3.6
1	C	554	SER	3.3
1	B	557	LYS	3.3
1	C	557	LYS	3.3
1	A	459	ARG	3.3
1	B	459	ARG	3.2
1	B	649	LYS	3.1
1	C	556	GLY	3.1
1	C	459	ARG	3.0
1	C	457	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	560	PHE	2.9
1	C	560	PHE	2.9
1	B	554	SER	2.8
1	D	585	TYR	2.7
1	C	491	GLU	2.6
1	B	720	GLU	2.6
1	D	491	GLU	2.5
1	B	313	ALA	2.5
1	C	435	GLU	2.5
1	C	553	VAL	2.5
1	A	458	VAL	2.3
1	B	558	TYR	2.3
1	C	720	GLU	2.3
1	D	484	SER	2.3
1	D	356	VAL	2.3
1	D	591	LEU	2.3
1	D	547	TRP	2.3
1	A	557	LYS	2.3
1	D	651	LEU	2.2
1	A	723	GLU	2.2
1	D	461	PRO	2.2
1	A	348	ASP	2.2
1	C	645	ASP	2.2
1	C	721	GLN	2.2
1	D	561	GLU	2.2
1	B	356	VAL	2.2
1	D	463	THR	2.1
1	A	314	PHE	2.1
1	C	484	SER	2.1
1	C	723	GLU	2.1
1	B	561	GLU	2.1
1	D	536	SER	2.1
1	B	457	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	D	734	4/4	0.81	0.35	13.98	90,90,90,90	0
2	SO4	B	731	5/5	0.76	0.26	1.80	171,171,171,171	0
3	CL	A	736	1/1	0.74	0.26	1.80	106,106,106,106	0
2	SO4	A	731	5/5	0.89	0.23	1.71	166,166,166,166	0
3	CL	A	739	1/1	0.96	0.21	1.71	88,88,88,88	0
3	CL	A	732	1/1	0.92	0.32	1.56	114,114,114,114	0
4	C2G	D	730	30/30	0.91	0.26	0.92	122,122,123,123	0
3	CL	C	735	1/1	0.83	0.20	0.81	118,118,118,118	0
3	CL	A	735	1/1	0.96	0.26	0.71	94,94,94,94	0
2	SO4	A	730	5/5	0.98	0.15	-0.37	103,104,105,107	0
2	SO4	B	730	5/5	0.98	0.09	-1.75	90,90,91,94	0
2	SO4	C	730	5/5	0.96	0.13	-1.80	129,129,131,132	0
3	CL	A	738	1/1	0.96	0.14	-2.52	97,97,97,97	0
3	CL	B	736	1/1	0.95	0.09	-2.52	83,83,83,83	0
3	CL	D	731	1/1	0.98	0.07	-2.90	68,68,68,68	0
2	SO4	C	731	5/5	0.95	0.14	-	124,125,127,128	0
3	CL	C	733	1/1	0.94	0.20	-	102,102,102,102	0
3	CL	C	736	1/1	0.86	0.23	-	106,106,106,106	0
3	CL	A	734	1/1	0.95	0.27	-	96,96,96,96	0
3	CL	A	737	1/1	0.87	0.18	-	108,108,108,108	0
3	CL	B	732	1/1	0.88	0.42	-	100,100,100,100	0
3	CL	B	735	1/1	0.92	0.56	-	127,127,127,127	0
3	CL	D	732	1/1	0.93	0.07	-	101,101,101,101	0
3	CL	A	733	1/1	0.84	0.65	-	130,130,130,130	0
3	CL	B	733	1/1	0.93	0.47	-	121,121,121,121	0
3	CL	B	734	1/1	0.90	0.20	-	111,111,111,111	0
3	CL	C	734	1/1	0.80	0.42	-	106,106,106,106	0
3	CL	C	732	1/1	0.88	0.20	-	107,107,107,107	0
3	CL	D	733	1/1	0.86	0.21	-	92,92,92,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.