



# Full wwPDB X-ray Structure Validation Report

May 9, 2014 – 02:25 PM EDT

PDB ID : 4C8R  
Title : Human gamma-butyrobetaine dioxygenase (BBOX1) in complex with Ni(II) and N-(3-hydroxypicolinoyl)-S-(pyridin-2-ylmethyl)-L-cysteine(AR692B)  
Authors : Chowdhury, R.; Rydzik, A.M.; Kochan, G.T.; McDonough, M.A.; Schofield, C.J.  
Deposited on : 2013-10-01  
Resolution : 2.82 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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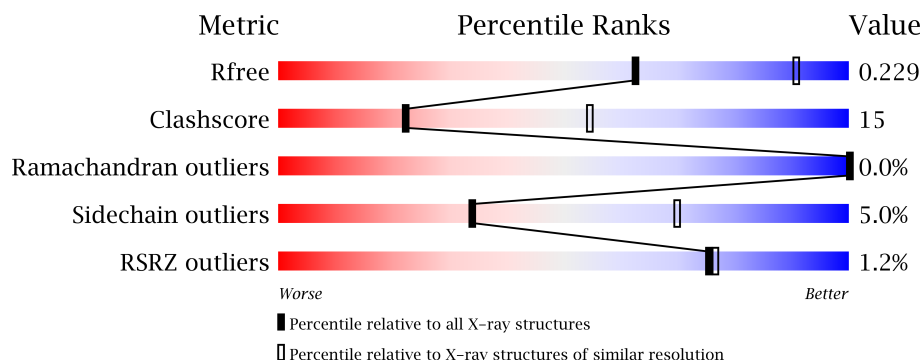
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 2.82 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))
$R_{free}$	66092	1963 (2.84-2.80)
Clashscore	79885	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)
RSRZ outliers	66119	1966 (2.84-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	388	
1	B	388	
1	C	388	
1	D	388	
1	E	388	
1	F	388	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	6YT	B	601	-	X
4	6YT	C	601	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	6YT	F	601	-	X
5	EDO	A	702	-	X
5	EDO	B	701	-	X
5	EDO	C	701	-	X
5	EDO	C	702	-	X
5	EDO	C	703	-	X
5	EDO	C	704	-	X
5	EDO	E	701	-	X
5	EDO	F	701	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19352 atoms, of which 0 are hydrogen and 0 are deuterium.

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 GAMMA-BUTYROBETAINE DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3116	1995	533	573	15			
1	B	384	Total	C	N	O	S	0	0	0
			3130	2006	535	574	15			
1	C	384	Total	C	N	O	S	0	0	0
			3117	1997	530	576	14			
1	D	384	Total	C	N	O	S	0	0	0
			3109	1995	535	565	14			
1	E	384	Total	C	N	O	S	0	0	0
			3097	1986	532	565	14			
1	F	384	Total	C	N	O	S	0	0	0
			3109	1997	531	567	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP O75936
B	0	SER	-	EXPRESSION TAG	UNP O75936
C	0	SER	-	EXPRESSION TAG	UNP O75936
D	0	SER	-	EXPRESSION TAG	UNP O75936
E	0	SER	-	EXPRESSION TAG	UNP O75936
F	0	SER	-	EXPRESSION TAG	UNP O75936

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Ni	0	0
			1	1		
2	E	1	Total	Ni	0	0
			1	1		
2	B	1	Total	Ni	0	0
			1	1		

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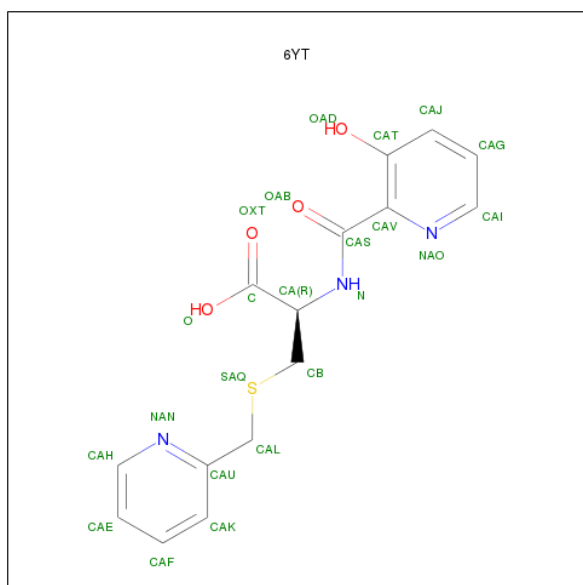
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Ni	0	0
			1	1		
2	A	1	Total	Ni	0	0
			1	1		
2	F	1	Total	Ni	0	0
			1	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

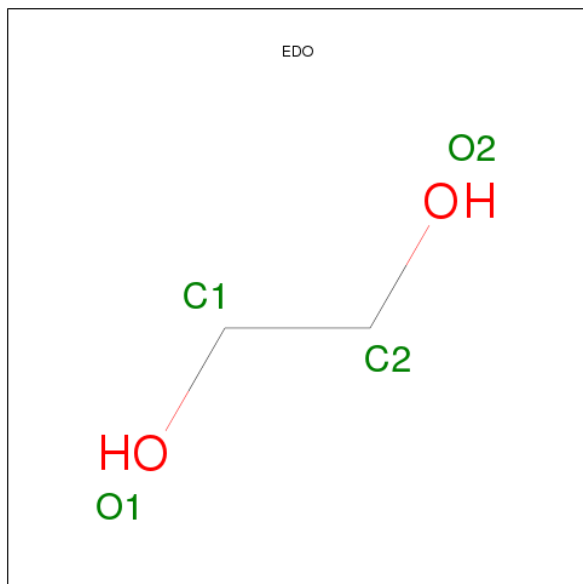
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is N-(3-HYDROXYPICOLINOYL)-S-(PYRIDIN-2-YLMETHYL)-L-CYSTEINE E (three-letter code: 6YT) (formula: C<sub>15</sub>H<sub>15</sub>N<sub>3</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			23	15	3	4	1		
4	B	1	Total	C	N	O	S	0	0
			23	15	3	4	1		
4	C	1	Total	C	N	O	S	0	0
			23	15	3	4	1		
4	D	1	Total	C	N	O	S	0	0
			23	15	3	4	1		
4	E	1	Total	C	N	O	S	0	0
			23	15	3	4	1		
4	F	1	Total	C	N	O	S	0	0
			23	15	3	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

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

- Molecule 6 is water.

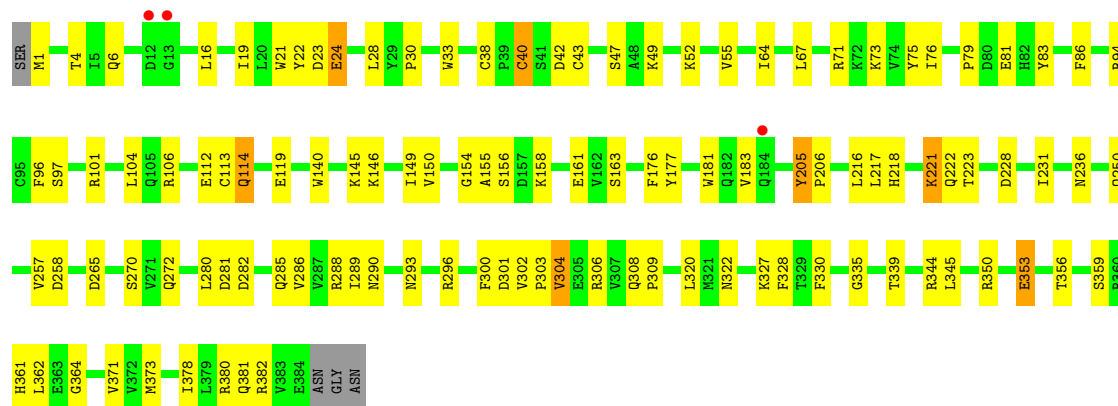
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	106	Total O 106 106	0	0
6	B	95	Total O 95 95	0	0
6	C	90	Total O 90 90	0	0
6	D	60	Total O 60 60	0	0
6	E	52	Total O 52 52	0	0
6	F	65	Total O 65 65	0	0

### 3 Residue-property plots

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

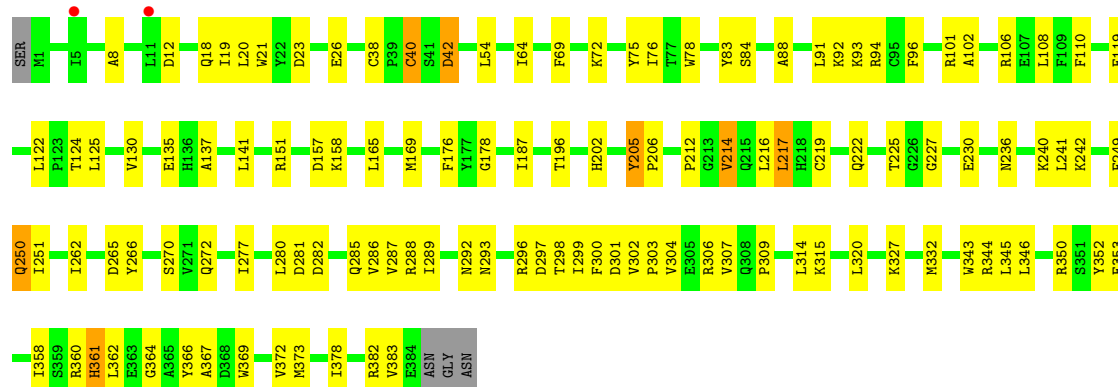
#### • Molecule 1: GAMMA-BUTYROBETAINE DIOXYGENASE

Chain A: 



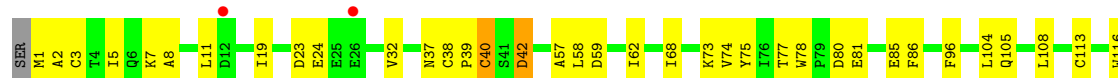
#### • Molecule 1: GAMMA-BUTYROBETAINE DIOXYGENASE

Chain B: 

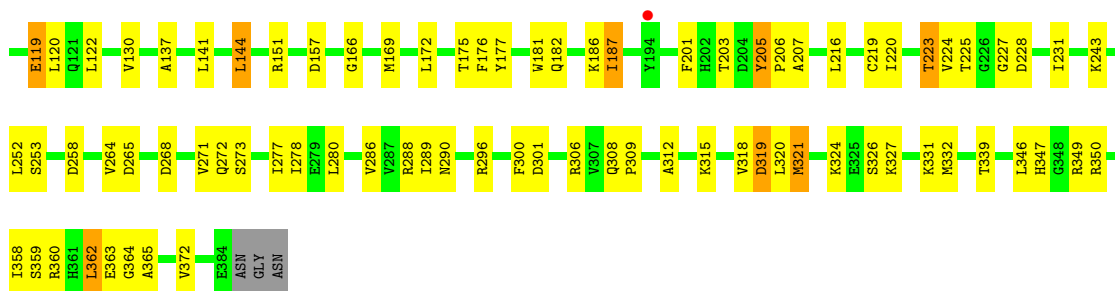


#### • Molecule 1: GAMMA-BUTYROBETAINE DIOXYGENASE

Chain C: 

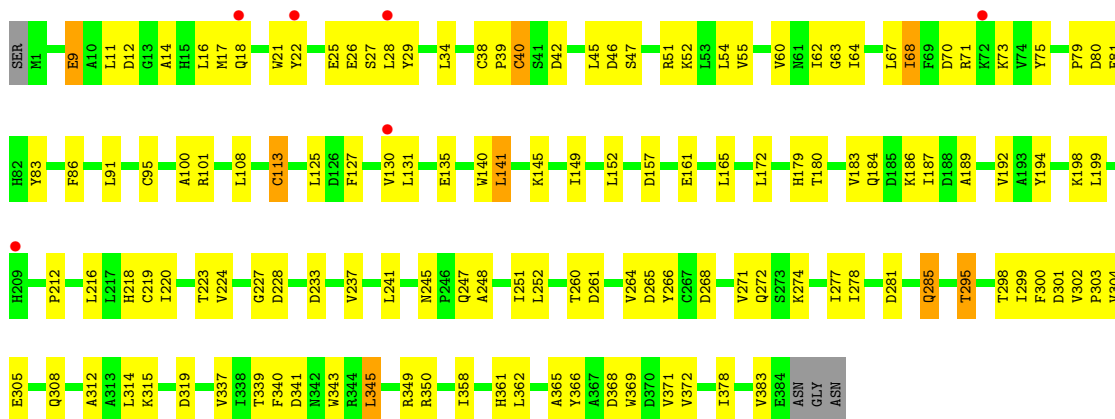






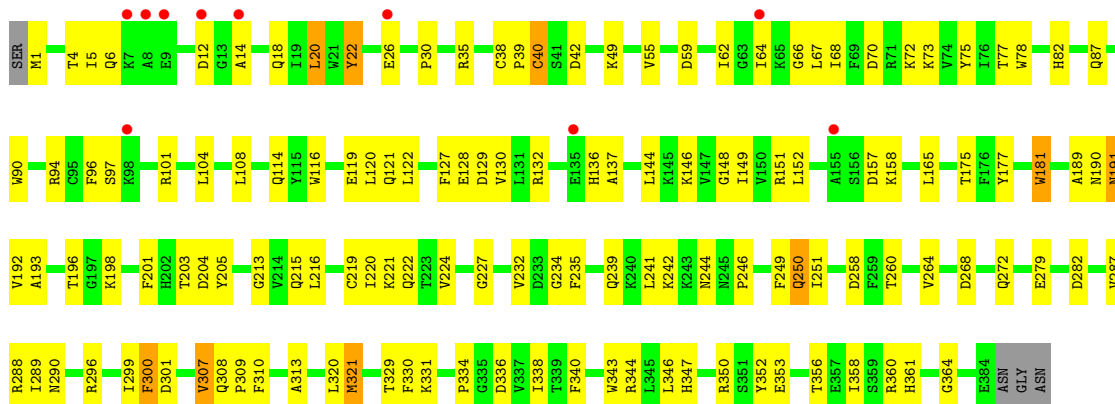
• Molecule 1: GAMMA-BUTYROBETAINE DIOXYGENASE

Chain D:



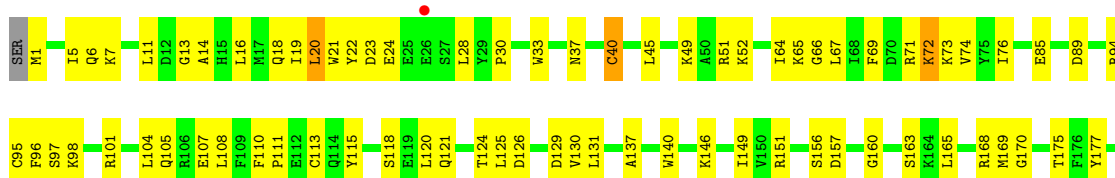
• Molecule 1: GAMMA-BUTYROBETAINE DIOXYGENASE

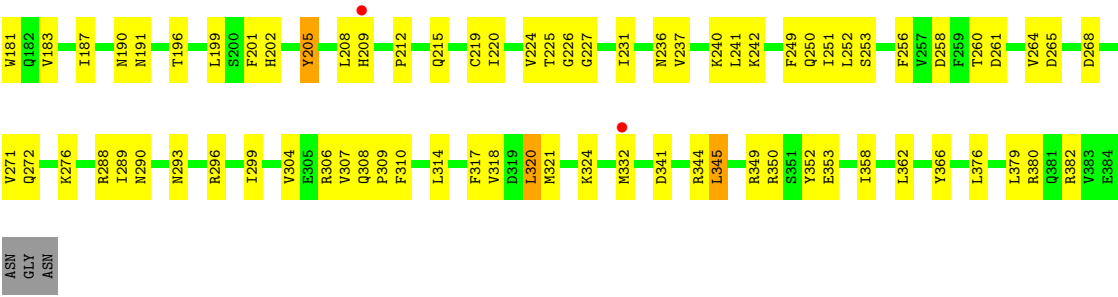
Chain E:



• Molecule 1: GAMMA-BUTYROBETAINE DIOXYGENASE

Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	195.74Å 91.66Å 167.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.42 – 2.82 48.94 – 2.82	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.42-2.82) 96.9 (48.94-2.82)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.81Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.215 , 0.244 0.226 , 0.229	Depositor DCC
$R_{free}$ test set	3576 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.8	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 32.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 70966 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19352	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.22 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.2781e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, ZN, EDO, 6YT

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	0.47	0/3193	0.65	1/4323 (0.0%)
1	B	0.48	0/3208	0.65	0/4341
1	C	0.45	0/3195	0.62	0/4327
1	D	0.44	0/3187	0.61	0/4315
1	E	0.43	0/3175	0.59	0/4302
1	F	0.43	0/3187	0.60	0/4315
All	All	0.45	0/19145	0.62	1/25923 (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	A	24	GLU	CB-CA-C	-6.00	98.40	110.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3116	0	3043	79	0
1	B	3130	0	3070	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3117	0	3031	91	0
1	D	3109	0	3042	104	0
1	E	3097	0	3012	110	0
1	F	3109	0	3042	120	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	23	0	0	2	0
4	B	23	0	0	3	0
4	C	23	0	0	0	0
4	D	23	0	0	1	0
4	E	23	0	0	0	0
4	F	23	0	0	1	0
5	A	12	0	18	0	0
5	B	8	0	12	0	0
5	C	16	0	24	1	0
5	E	12	0	18	2	0
5	F	8	0	12	0	0
6	A	106	0	0	5	0
6	B	95	0	0	2	0
6	C	90	0	0	5	0
6	D	60	0	0	4	0
6	E	52	0	0	2	0
6	F	65	0	0	5	0
All	All	19352	0	18324	556	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (556) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:199:LEU:HD21	1:F:349:ARG:HB3	1.34	1.09
1:B:93:LYS:HE2	1:B:94:ARG:HH12	1.32	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:224:VAL:HG12	1:F:358:ILE:HA	1.56	0.85
1:B:93:LYS:HE2	1:B:94:ARG:NH1	1.92	0.85
1:C:219:CYS:HB2	1:C:332:MET:HE2	1.59	0.84
1:F:175:THR:HG23	1:F:177:TYR:H	1.43	0.84
1:D:187:ILE:HG13	1:D:358:ILE:HB	1.60	0.83
1:A:228:ASP:HB2	1:A:350:ARG:HD3	1.58	0.83
1:F:199:LEU:CD2	1:F:349:ARG:HB3	2.09	0.83
1:E:59:ASP:HB3	1:E:62:ILE:HB	1.59	0.83
1:E:264:VAL:HG22	1:E:268:ASP:HA	1.60	0.82
1:C:104:LEU:HD21	1:D:299:ILE:HD12	1.62	0.82
1:E:353:GLU:O	1:E:356:THR:HG23	1.81	0.80
1:B:38:CYS:SG	1:B:40:CYS:HB3	2.23	0.78
1:F:175:THR:HG22	6:F:2030:HOH:O	1.83	0.78
1:E:38:CYS:SG	1:E:40:CYS:HB3	2.21	0.78
1:F:1:MET:O	1:F:22:TYR:HB2	1.86	0.75
1:B:369:TRP:O	1:B:373:MET:HB2	1.86	0.75
1:F:107:GLU:HG3	1:F:380:ARG:HH22	1.52	0.75
1:F:183:VAL:HG21	1:F:362:LEU:HD12	1.69	0.75
1:B:358:ILE:HG22	6:B:2073:HOH:O	1.86	0.75
1:C:105:GLN:NE2	1:D:274:LYS:HE2	2.01	0.74
1:F:5:ILE:HG12	1:F:19:ILE:HD11	1.69	0.73
1:F:45:LEU:HD21	1:F:52:LYS:HE3	1.71	0.72
1:B:222:GLN:HG3	1:B:360:ARG:HB3	1.70	0.72
1:F:7:LYS:HB3	1:F:20:LEU:HD23	1.72	0.71
1:C:40:CYS:SG	1:C:42:ASP:HB2	2.31	0.71
1:C:223:THR:HG23	1:C:359:SER:HB2	1.72	0.71
1:A:217:LEU:HD22	4:A:601:6YT:CAK	2.20	0.71
1:F:72:LYS:O	1:F:73:LYS:HG3	1.90	0.71
1:C:116:TRP:HH2	1:C:231:ILE:HG22	1.57	0.70
1:A:30:PRO:HG3	1:B:307:VAL:HG11	1.73	0.69
1:B:94:ARG:HG3	1:B:94:ARG:HH11	1.55	0.69
1:F:264:VAL:HG12	1:F:268:ASP:HA	1.74	0.69
1:E:4:THR:HG22	1:E:72:LYS:HD3	1.74	0.69
5:E:703:EDO:H11	1:F:209:HIS:NE2	2.08	0.69
1:D:16:LEU:HD12	1:D:28:LEU:HD23	1.75	0.69
1:F:227:GLY:HA2	1:F:350:ARG:O	1.93	0.68
1:E:129:ASP:HB3	1:E:136:HIS:ND1	2.08	0.68
1:F:67:LEU:HD13	1:F:76:ILE:HG12	1.76	0.68
1:B:344:ARG:HG2	1:B:345:LEU:HD12	1.74	0.68
1:C:175:THR:HG22	6:C:2048:HOH:O	1.94	0.68
1:A:75:TYR:HD2	1:A:83:TYR:HH	1.42	0.68
1:C:38:CYS:SG	1:C:40:CYS:HB3	2.35	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:67:LEU:HD11	1:F:74:VAL:HG13	1.75	0.67
1:C:228:ASP:OD1	1:C:331:LYS:HG2	1.95	0.67
1:E:157:ASP:O	1:E:220:ILE:HG23	1.93	0.67
1:A:23:ASP:O	1:A:24:GLU:HB2	1.94	0.67
1:A:97:SER:O	1:A:101:ARG:HG3	1.95	0.66
1:C:272:GLN:HG3	1:D:108:LEU:HD22	1.77	0.66
1:F:224:VAL:HG12	1:F:358:ILE:CA	2.26	0.66
1:D:264:VAL:HG23	1:D:264:VAL:O	1.96	0.65
1:B:75:TYR:HD1	1:B:83:TYR:HH	1.42	0.65
1:C:108:LEU:HD22	1:D:272:GLN:HG3	1.77	0.65
1:A:280:LEU:HD23	1:A:286:VAL:HA	1.77	0.65
1:A:94:ARG:HH11	1:A:94:ARG:HG3	1.61	0.65
1:E:347:HIS:H	1:E:347:HIS:HD1	1.44	0.65
1:D:341:ASP:OD1	1:D:343:TRP:HB2	1.97	0.64
1:F:183:VAL:HG22	1:F:362:LEU:HB2	1.79	0.64
1:A:304:VAL:HG22	1:B:96:PHE:HB3	1.80	0.64
1:D:187:ILE:CG1	1:D:358:ILE:HB	2.27	0.64
1:E:175:THR:HG23	1:E:177:TYR:H	1.62	0.64
1:E:288:ARG:HG2	1:E:289:ILE:N	2.12	0.64
1:F:256:PHE:CE2	1:F:276:LYS:HE3	2.33	0.64
1:E:14:ALA:HB1	1:E:64:ILE:H	1.64	0.63
1:F:40:CYS:HA	6:F:2004:HOH:O	1.99	0.63
1:C:288:ARG:HG2	1:C:289:ILE:N	2.14	0.63
1:C:253:SER:HB3	1:C:278:ILE:HG13	1.79	0.63
1:E:5:ILE:HD12	1:E:70:ASP:O	1.99	0.62
1:A:55:VAL:O	1:B:315:LYS:HE3	2.00	0.62
1:B:72:LYS:HE3	6:B:2019:HOH:O	1.98	0.62
1:F:212:PRO:HB3	1:F:366:TYR:HB3	1.81	0.62
1:A:301:ASP:OD1	1:B:101:ARG:HB3	1.99	0.62
1:E:288:ARG:HG2	1:E:289:ILE:H	1.65	0.62
1:D:140:TRP:CE3	1:D:141:LEU:HD13	2.35	0.61
1:A:21:TRP:HB2	1:A:23:ASP:OD1	2.00	0.61
1:C:308:GLN:HB3	1:C:309:PRO:HD3	1.83	0.61
1:C:306:ARG:O	1:C:309:PRO:HD2	2.01	0.61
1:E:149:ILE:HD11	1:E:338:ILE:HG23	1.83	0.61
1:B:75:TYR:HD1	1:B:83:TYR:OH	1.84	0.60
1:C:227:GLY:HA2	1:C:350:ARG:O	2.00	0.60
1:E:227:GLY:HA2	1:E:350:ARG:O	2.01	0.60
1:E:234:GLY:HA3	1:E:289:ILE:HD13	1.83	0.60
1:F:94:ARG:HG3	1:F:94:ARG:HH11	1.67	0.60
1:E:289:ILE:HG21	1:E:346:LEU:HD11	1.84	0.60
1:D:219:CYS:HA	1:D:362:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:122:LEU:HD23	1:B:151:ARG:CZ	2.31	0.60
1:E:104:LEU:HD21	1:F:299:ILE:HG21	1.84	0.60
1:F:225:THR:O	1:F:353:GLU:HG2	2.01	0.60
1:B:212:PRO:HB3	1:B:366:TYR:HB3	1.83	0.59
1:F:67:LEU:HD13	1:F:76:ILE:CG1	2.32	0.59
1:B:236:ASN:HD21	1:B:240:LYS:NZ	2.00	0.59
1:E:49:LYS:HD2	1:F:260:THR:HG21	1.83	0.59
1:E:308:GLN:HB3	1:E:309:PRO:HD3	1.85	0.59
1:D:21:TRP:O	1:D:22:TYR:HB3	2.01	0.59
1:B:135:GLU:OE2	1:B:383:VAL:HG13	2.03	0.59
1:E:191:ASN:ND2	1:E:193:ALA:H	2.00	0.59
1:A:304:VAL:HG22	1:B:96:PHE:CB	2.33	0.58
1:D:227:GLY:HA2	1:D:350:ARG:O	2.03	0.58
1:B:219:CYS:HB2	1:B:332:MET:HE1	1.84	0.58
1:C:122:LEU:HD23	1:C:151:ARG:CZ	2.34	0.58
1:C:224:VAL:HG12	1:C:358:ILE:HA	1.84	0.58
1:D:172:LEU:HD12	1:D:179:HIS:CE1	2.38	0.58
1:F:318:VAL:HA	1:F:321:MET:CE	2.33	0.58
1:C:96:PHE:HB3	1:D:304:VAL:HG22	1.86	0.58
1:D:80:ASP:O	1:D:81:GLU:HB2	2.03	0.58
1:B:214:VAL:HG22	1:B:367:ALA:HB3	1.85	0.58
1:D:67:LEU:HD12	1:D:68:ILE:N	2.18	0.58
1:D:68:ILE:HA	6:D:2009:HOH:O	2.02	0.58
1:C:130:VAL:HG13	1:C:137:ALA:HA	1.86	0.58
1:C:288:ARG:HD2	1:C:290:ASN:HD21	1.69	0.57
1:F:258:ASP:HB3	6:F:2047:HOH:O	2.04	0.57
1:F:187:ILE:HD12	1:F:358:ILE:HD11	1.86	0.57
1:C:216:LEU:O	1:C:364:GLY:HA2	2.05	0.57
1:D:302:VAL:HG23	1:D:303:PRO:HD2	1.87	0.57
1:C:8:ALA:HA	1:C:19:ILE:HG22	1.86	0.57
1:D:14:ALA:HB1	1:D:64:ILE:HB	1.86	0.57
1:E:301:ASP:HA	1:F:101:ARG:HD2	1.86	0.57
1:F:21:TRP:O	1:F:24:GLU:N	2.38	0.57
1:B:219:CYS:HB2	1:B:332:MET:CE	2.35	0.57
1:C:176:PHE:HB2	1:C:205:TYR:OH	2.05	0.57
1:F:196:THR:HG21	1:F:352:TYR:HD2	1.68	0.57
1:A:353:GLU:HB3	1:A:356:THR:HG21	1.87	0.57
1:A:64:ILE:HG23	1:A:76:ILE:HG23	1.86	0.57
1:F:7:LYS:HA	1:F:69:PHE:CZ	2.40	0.57
1:B:303:PRO:HG2	1:B:306:ARG:HG3	1.86	0.56
1:D:277:ILE:HD13	1:D:314:LEU:HD13	1.87	0.56
1:D:68:ILE:HG13	1:D:75:TYR:HB2	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:THR:HB	1:A:359:SER:HB3	1.87	0.56
1:F:6:GLN:OE1	1:F:20:LEU:HD11	2.05	0.56
1:C:318:VAL:HG21	1:D:55:VAL:HG11	1.87	0.56
1:A:38:CYS:SG	1:A:40:CYS:HB3	2.45	0.56
1:D:180:THR:HG22	1:D:365:ALA:HB2	1.86	0.56
1:E:12:ASP:C	1:E:14:ALA:H	2.09	0.56
1:E:127:PHE:CE1	1:E:165:LEU:HD13	2.41	0.56
1:A:30:PRO:HG2	1:A:33:TRP:HB3	1.87	0.56
1:D:140:TRP:CH2	1:D:165:LEU:HD22	2.41	0.56
1:E:307:VAL:HG11	1:F:30:PRO:HG2	1.87	0.56
1:E:191:ASN:HD22	1:E:193:ALA:H	1.52	0.56
1:F:64:ILE:HG23	1:F:76:ILE:HG23	1.88	0.56
1:C:104:LEU:CD2	1:D:299:ILE:HD12	2.35	0.56
1:E:68:ILE:HG13	1:E:75:TYR:HD2	1.69	0.56
1:E:127:PHE:HE1	1:E:165:LEU:HD13	1.70	0.55
1:D:315:LYS:HE2	1:D:319:ASP:OD2	2.05	0.55
1:F:157:ASP:O	1:F:220:ILE:HG23	2.05	0.55
1:A:43:CYS:O	1:A:52:LYS:HG2	2.06	0.55
1:B:94:ARG:NH1	1:B:94:ARG:HG3	2.22	0.55
1:A:30:PRO:HG2	1:A:33:TRP:CB	2.36	0.55
1:C:32:VAL:HG12	6:C:2001:HOH:O	2.06	0.55
1:E:122:LEU:HD23	1:E:151:ARG:CZ	2.37	0.55
1:B:157:ASP:O	1:B:158:LYS:HD3	2.06	0.55
1:C:141:LEU:HD22	1:C:372:VAL:HG13	1.89	0.55
1:E:78:TRP:HD1	1:E:82:HIS:HB3	1.71	0.55
1:B:206:PRO:HG2	1:B:292:ASN:HB2	1.88	0.55
1:C:301:ASP:HA	1:D:101:ARG:HD2	1.89	0.55
1:B:54:LEU:HD12	1:B:54:LEU:N	2.22	0.54
1:A:288:ARG:HG2	1:A:289:ILE:N	2.22	0.54
1:A:371:VAL:HG13	6:A:2047:HOH:O	2.08	0.54
1:B:262:ILE:HD12	1:B:262:ILE:C	2.28	0.54
1:D:345:LEU:HD23	1:D:345:LEU:N	2.22	0.54
1:A:4:THR:HG23	1:A:71:ARG:HB3	1.89	0.54
1:C:5:ILE:HD13	1:C:74:VAL:HG23	1.90	0.54
1:A:23:ASP:O	1:A:24:GLU:CB	2.56	0.54
1:A:281:ASP:OD2	1:A:285:GLN:HB2	2.07	0.54
1:A:106:ARG:NH1	6:A:2031:HOH:O	2.40	0.54
1:F:318:VAL:HA	1:F:321:MET:HE2	1.89	0.54
1:A:302:VAL:HG22	1:A:306:ARG:HB2	1.90	0.54
1:A:75:TYR:HD2	1:A:83:TYR:OH	1.90	0.54
1:A:101:ARG:HD2	1:B:301:ASP:HA	1.89	0.54
1:D:70:ASP:OD1	1:D:73:LYS:HB2	2.07	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:130:VAL:HG13	1:E:137:ALA:HA	1.90	0.53
1:A:16:LEU:HD21	1:A:28:LEU:HD13	1.90	0.53
1:F:177:TYR:HD1	1:F:265:ASP:OD2	1.91	0.53
1:C:1:MET:O	1:C:2:ALA:HB3	2.08	0.53
1:A:270:SER:HB2	1:B:378:ILE:HD11	1.89	0.53
1:B:281:ASP:HB3	1:B:287:VAL:HG11	1.90	0.53
1:C:360:ARG:HG2	1:C:362:LEU:HD13	1.90	0.53
1:F:107:GLU:CG	1:F:380:ARG:HH22	2.21	0.53
1:A:205:TYR:N	1:A:206:PRO:HD3	2.24	0.53
1:B:205:TYR:N	1:B:206:PRO:HD3	2.24	0.53
1:A:221:LYS:HE3	1:A:222:GLN:N	2.22	0.53
1:F:140:TRP:HH2	1:F:169:MET:HE2	1.73	0.53
1:D:247:GLN:O	1:D:251:ILE:HG13	2.09	0.53
1:D:345:LEU:HD23	1:D:345:LEU:H	1.73	0.53
5:E:703:EDO:C1	1:F:209:HIS:NE2	2.71	0.53
1:B:281:ASP:OD2	1:B:285:GLN:HB2	2.09	0.52
1:A:104:LEU:HD21	1:B:299:ILE:HD13	1.91	0.52
1:E:144:LEU:O	1:E:148:GLY:HA2	2.09	0.52
1:E:260:THR:HG21	1:F:49:LYS:HE3	1.90	0.52
1:A:288:ARG:HD3	1:A:290:ASN:OD1	2.09	0.52
1:A:380:ARG:HB3	1:A:380:ARG:CZ	2.38	0.52
1:C:268:ASP:OD2	1:D:378:ILE:HD13	2.09	0.52
1:E:251:ILE:HD13	1:E:310:PHE:HA	1.91	0.52
1:A:176:PHE:O	1:A:265:ASP:HB3	2.09	0.52
1:F:205:TYR:CD1	1:F:208:LEU:HG	2.44	0.52
1:A:183:VAL:O	1:A:361:HIS:HA	2.10	0.52
1:A:104:LEU:HD21	1:B:299:ILE:CD1	2.39	0.52
1:B:20:LEU:HG	1:B:26:GLU:HG2	1.92	0.52
1:D:187:ILE:O	1:D:187:ILE:HD12	2.10	0.52
1:D:264:VAL:HG12	1:D:268:ASP:HA	1.91	0.52
1:C:264:VAL:HG22	1:C:268:ASP:HB3	1.92	0.52
4:B:601:6YT:OAD	4:B:601:6YT:N	2.42	0.51
1:F:288:ARG:HG2	1:F:289:ILE:N	2.23	0.51
1:C:122:LEU:HD23	1:C:151:ARG:NH1	2.25	0.51
1:C:175:THR:HG23	1:C:177:TYR:H	1.75	0.51
1:C:201:PHE:HB2	1:C:321:MET:HE2	1.93	0.51
4:D:601:6YT:OAD	4:D:601:6YT:N	2.42	0.51
1:F:199:LEU:H	1:F:199:LEU:HD23	1.75	0.51
1:B:361:HIS:O	1:B:362:LEU:HD23	2.11	0.51
1:E:1:MET:N	1:E:22:TYR:HB3	2.25	0.51
1:E:264:VAL:HG22	1:E:268:ASP:CA	2.37	0.51
1:D:75:TYR:HD1	1:D:83:TYR:HH	1.55	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:144:LEU:HD23	1:E:144:LEU:O	2.10	0.51
1:B:217:LEU:HD22	4:B:601:6YT:CAK	2.40	0.51
1:C:296:ARG:HB3	1:D:51:ARG:HH12	1.75	0.51
1:C:96:PHE:CB	1:D:304:VAL:HG22	2.41	0.51
1:E:96:PHE:CB	1:F:304:VAL:HG22	2.40	0.51
1:B:178:GLY:HA2	1:B:266:TYR:CD2	2.46	0.51
1:E:1:MET:H2	1:E:22:TYR:HB3	1.76	0.51
1:F:131:LEU:HA	1:F:168:ARG:HD3	1.92	0.51
1:D:16:LEU:HD23	1:D:16:LEU:N	2.25	0.51
1:D:302:VAL:CG2	1:D:303:PRO:HD2	2.41	0.51
1:D:73:LYS:HD3	1:D:75:TYR:OH	2.11	0.51
1:E:191:ASN:HD22	1:E:192:VAL:N	2.09	0.51
1:A:155:ALA:HB3	1:A:335:GLY:O	2.11	0.50
1:D:199:LEU:HB2	1:D:349:ARG:HB3	1.92	0.50
1:F:237:VAL:HG13	1:F:320:LEU:HD13	1.93	0.50
1:B:187:ILE:HB	1:B:358:ILE:HG12	1.93	0.50
1:B:219:CYS:HA	1:B:362:LEU:HD22	1.92	0.50
1:E:55:VAL:HG23	6:E:2006:HOH:O	2.11	0.50
1:E:96:PHE:HB2	1:F:304:VAL:HG22	1.93	0.50
1:D:127:PHE:O	1:D:130:VAL:HG22	2.11	0.50
1:E:307:VAL:O	1:E:310:PHE:HB3	2.12	0.50
1:F:6:GLN:HB2	1:F:22:TYR:CD1	2.47	0.50
4:A:601:6YT:N	4:A:601:6YT:OAD	2.42	0.50
1:C:280:LEU:HD23	1:C:286:VAL:HA	1.92	0.50
1:D:260:THR:HB	1:D:272:GLN:NE2	2.27	0.50
1:E:67:LEU:HD23	1:E:68:ILE:N	2.27	0.50
1:C:264:VAL:HG22	1:C:268:ASP:CB	2.42	0.50
1:F:242:LYS:HD2	1:F:249:PHE:CE2	2.47	0.50
1:B:227:GLY:HA3	1:B:352:TYR:CE1	2.47	0.50
1:E:114:GLN:HG3	1:E:146:LYS:HE2	1.94	0.49
1:F:160:GLY:O	1:F:163:SER:HB2	2.12	0.49
1:F:314:LEU:O	1:F:318:VAL:HG23	2.12	0.49
1:A:16:LEU:HD12	1:A:30:PRO:HA	1.94	0.49
1:B:187:ILE:HD12	1:B:358:ILE:HD11	1.93	0.49
1:B:64:ILE:HG23	1:B:76:ILE:HG23	1.94	0.49
1:C:8:ALA:CB	1:C:19:ILE:HG22	2.42	0.49
1:B:302:VAL:CG2	1:B:303:PRO:HD2	2.42	0.49
1:C:187:ILE:HG13	1:C:358:ILE:HB	1.94	0.49
1:E:14:ALA:HB1	1:E:64:ILE:N	2.27	0.49
1:E:279:GLU:O	1:E:287:VAL:HG22	2.12	0.49
1:E:94:ARG:HG3	1:E:94:ARG:HH11	1.77	0.49
1:C:186:LYS:HA	1:C:358:ILE:O	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:93:LYS:CE	1:B:94:ARG:HH12	2.16	0.49
1:D:261:ASP:HB3	1:D:271:VAL:HG22	1.95	0.49
1:D:11:LEU:HD12	1:D:16:LEU:HD11	1.94	0.49
1:D:12:ASP:C	1:D:14:ALA:H	2.15	0.49
1:D:216:LEU:HD12	1:D:216:LEU:N	2.28	0.49
1:B:262:ILE:O	1:B:262:ILE:HD12	2.13	0.49
1:D:281:ASP:OD1	1:D:285:GLN:N	2.45	0.49
1:E:108:LEU:HD22	1:F:272:GLN:HG3	1.94	0.49
1:C:166:GLY:HA2	1:C:169:MET:HE2	1.95	0.49
1:E:353:GLU:O	1:E:356:THR:CG2	2.58	0.49
1:F:23:ASP:O	1:F:24:GLU:CB	2.59	0.48
1:B:21:TRP:CE2	1:B:92:LYS:HD3	2.48	0.48
1:C:252:LEU:HD22	1:C:277:ILE:HD12	1.94	0.48
1:C:347:HIS:ND1	1:C:347:HIS:N	2.61	0.48
1:F:253:SER:O	1:F:276:LYS:HD3	2.13	0.48
1:D:145:LYS:HG2	1:D:369:TRP:CZ3	2.48	0.48
1:D:312:ALA:O	1:D:315:LYS:HB3	2.12	0.48
1:C:3:CYS:SG	1:C:3:CYS:O	2.70	0.48
1:D:305:GLU:H	1:D:305:GLU:CD	2.17	0.48
1:A:380:ARG:HH11	1:A:380:ARG:HG2	1.78	0.48
1:E:220:ILE:HG21	1:E:361:HIS:HD2	1.77	0.48
1:F:115:TYR:HB3	1:F:236:ASN:HB2	1.96	0.48
1:F:288:ARG:HD3	1:F:290:ASN:OD1	2.14	0.48
1:F:293:ASN:OD1	1:F:296:ARG:NH2	2.47	0.48
1:B:230:GLU:OE2	1:B:350:ARG:HD3	2.13	0.48
1:E:251:ILE:HD11	1:E:313:ALA:HB3	1.96	0.48
1:B:262:ILE:HG22	1:B:270:SER:HA	1.96	0.48
1:B:288:ARG:HG3	1:B:343:TRP:CG	2.48	0.48
1:D:157:ASP:C	1:D:220:ILE:HG23	2.34	0.48
1:E:222:GLN:H	1:E:334:PRO:HG3	1.79	0.48
1:A:308:GLN:HB3	1:A:309:PRO:HD3	1.96	0.47
1:F:72:LYS:O	1:F:73:LYS:CG	2.61	0.47
1:D:127:PHE:CZ	1:D:161:GLU:HG3	2.50	0.47
1:E:235:PHE:CD2	1:E:344:ARG:HD2	2.49	0.47
1:B:358:ILE:HG13	1:B:358:ILE:O	2.15	0.47
1:C:116:TRP:CG	1:C:120:LEU:HD13	2.48	0.47
1:A:322:ASN:O	1:A:327:LYS:NZ	2.47	0.47
1:A:378:ILE:O	1:A:382:ARG:HG3	2.14	0.47
1:A:47:SER:HA	6:A:2014:HOH:O	2.14	0.47
1:C:312:ALA:HA	1:D:60:VAL:HG11	1.95	0.47
1:F:73:LYS:HZ1	1:F:85:GLU:HB3	1.78	0.47
1:B:176:PHE:HB2	1:B:205:TYR:OH	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:236:ASN:HD21	1:B:240:LYS:HZ2	1.62	0.47
1:E:251:ILE:CD1	1:E:310:PHE:HA	2.44	0.47
1:E:67:LEU:HD23	1:E:67:LEU:C	2.34	0.47
1:A:43:CYS:C	1:A:52:LYS:HG2	2.35	0.47
1:B:21:TRP:HB2	1:B:23:ASP:OD1	2.15	0.47
1:A:101:ARG:HB3	1:B:301:ASP:OD1	2.13	0.47
1:B:40:CYS:SG	1:B:42:ASP:HB2	2.55	0.47
1:E:213:GLY:HA2	1:E:343:TRP:NE1	2.30	0.47
1:E:40:CYS:SG	1:E:42:ASP:N	2.87	0.47
1:E:73:LYS:HB3	1:E:73:LYS:NZ	2.30	0.47
1:F:241:LEU:HD21	1:F:252:LEU:HD12	1.96	0.47
1:D:113:CYS:HB3	6:D:2017:HOH:O	2.15	0.47
1:F:251:ILE:HG21	1:F:310:PHE:HA	1.96	0.47
1:A:94:ARG:HG3	1:A:94:ARG:NH1	2.29	0.47
1:B:176:PHE:O	1:B:265:ASP:HB3	2.15	0.47
1:E:97:SER:O	1:E:101:ARG:HG3	2.14	0.47
1:B:72:LYS:HA	1:B:88:ALA:HB2	1.97	0.47
1:D:274:LYS:NZ	1:D:301:ASP:HB3	2.30	0.47
1:D:52:LYS:O	1:D:54:LEU:HD12	2.15	0.47
1:E:215:GLN:NE2	1:E:340:PHE:HZ	2.13	0.47
1:E:279:GLU:HG3	1:E:290:ASN:ND2	2.29	0.47
1:B:196:THR:HG21	1:B:352:TYR:HB2	1.97	0.47
1:C:7:LYS:O	1:C:19:ILE:HA	2.15	0.47
1:F:130:VAL:HG13	1:F:137:ALA:HA	1.97	0.47
1:A:79:PRO:C	1:A:81:GLU:H	2.18	0.46
1:E:94:ARG:HG2	1:F:299:ILE:HG22	1.97	0.46
1:A:302:VAL:HG23	1:A:303:PRO:HD2	1.97	0.46
1:E:260:THR:HB	1:E:272:GLN:NE2	2.30	0.46
1:F:181:TRP:HZ2	1:F:215:GLN:HE21	1.63	0.46
1:F:71:ARG:HH11	1:F:71:ARG:HG3	1.79	0.46
1:C:57:ALA:HB1	5:C:704:EDO:H21	1.97	0.46
1:C:5:ILE:CD1	1:C:74:VAL:HG23	2.46	0.46
1:F:113:CYS:HA	1:F:146:LYS:HG3	1.98	0.46
1:F:118:SER:HB3	1:F:324:LYS:O	2.15	0.46
1:F:94:ARG:HG3	1:F:94:ARG:NH1	2.29	0.46
1:D:21:TRP:HE1	1:D:27:SER:CB	2.28	0.46
1:D:368:ASP:O	1:D:371:VAL:HG22	2.14	0.46
1:D:79:PRO:C	1:D:81:GLU:H	2.19	0.46
1:E:299:ILE:HG12	1:F:104:LEU:HD21	1.98	0.46
1:A:181:TRP:CZ2	1:A:364:GLY:HA3	2.50	0.46
1:F:11:LEU:HD23	1:F:18:GLN:HB3	1.98	0.46
1:B:130:VAL:HG13	1:B:137:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:176:PHE:HB2	1:A:205:TYR:OH	2.16	0.46
1:C:315:LYS:NZ	1:C:319:ASP:OD2	2.46	0.46
1:D:45:LEU:HB2	1:D:52:LYS:HD2	1.96	0.46
1:D:71:ARG:HH11	1:D:71:ARG:HG3	1.80	0.46
1:B:18:GLN:HE21	1:B:26:GLU:HB3	1.81	0.46
1:C:207:ALA:O	1:C:273:SER:HB2	2.16	0.46
1:C:268:ASP:HB2	6:C:2073:HOH:O	2.15	0.46
1:A:177:TYR:HD1	1:A:265:ASP:OD2	1.99	0.46
1:E:272:GLN:HG3	1:F:108:LEU:HD22	1.98	0.46
1:E:216:LEU:O	1:E:364:GLY:HA2	2.15	0.46
1:F:33:TRP:NE1	1:F:37:ASN:ND2	2.64	0.46
1:C:264:VAL:HG22	1:C:268:ASP:HA	1.98	0.45
1:A:104:LEU:HD12	1:A:104:LEU:O	2.17	0.45
1:D:62:ILE:HG12	1:D:63:GLY:N	2.32	0.45
1:D:340:PHE:HE2	6:D:2060:HOH:O	1.98	0.45
1:E:241:LEU:HG	1:E:249:PHE:HB2	1.99	0.45
1:F:120:LEU:HD12	1:F:121:GLN:H	1.82	0.45
1:F:219:CYS:HA	1:F:362:LEU:HD23	1.99	0.45
1:E:30:PRO:HG2	1:F:307:VAL:HB	1.98	0.45
1:E:232:VAL:HG12	1:E:346:LEU:HB2	1.98	0.45
1:F:318:VAL:HA	1:F:321:MET:HE3	1.99	0.45
1:B:225:THR:HG21	1:B:353:GLU:OE1	2.17	0.45
1:C:59:ASP:HB3	1:C:62:ILE:HB	1.97	0.45
1:C:73:LYS:HD2	1:C:75:TYR:CE2	2.51	0.45
1:F:261:ASP:O	1:F:271:VAL:HG22	2.16	0.45
1:F:126:ASP:HB3	1:F:129:ASP:OD2	2.17	0.45
1:C:172:LEU:HD22	1:C:365:ALA:HB1	1.98	0.45
1:D:135:GLU:OE2	1:D:383:VAL:HG13	2.17	0.45
1:D:233:ASP:O	1:D:237:VAL:HG23	2.17	0.45
1:D:34:LEU:HD22	1:D:86:PHE:CE2	2.52	0.45
1:D:224:VAL:HG12	1:D:358:ILE:HA	1.98	0.45
1:B:102:ALA:O	1:B:106:ARG:HG3	2.17	0.45
1:C:205:TYR:N	1:C:206:PRO:HD3	2.32	0.45
1:E:232:VAL:CG1	1:E:346:LEU:HB2	2.47	0.45
1:F:110:PHE:N	1:F:111:PRO:HD3	2.32	0.45
1:F:131:LEU:HD21	1:F:165:LEU:HD23	1.98	0.45
1:C:105:GLN:HE22	1:D:274:LYS:HE2	1.76	0.44
1:E:347:HIS:ND1	1:E:347:HIS:N	2.65	0.44
1:F:149:ILE:HD13	1:F:231:ILE:CD1	2.47	0.44
1:E:242:LYS:O	1:E:246:PRO:HG3	2.17	0.44
1:E:288:ARG:HG3	1:E:343:TRP:HB3	1.98	0.44
1:A:328:PHE:CE2	1:A:330:PHE:HB3	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:23:ASP:O	1:C:24:GLU:HB2	2.17	0.44
1:B:302:VAL:HG22	1:B:303:PRO:HD2	1.99	0.44
1:E:272:GLN:NE2	6:E:2037:HOH:O	2.50	0.44
1:C:39:PRO:HD3	1:C:86:PHE:CE1	2.53	0.44
1:D:165:LEU:HA	1:D:165:LEU:HD23	1.89	0.44
1:D:21:TRP:O	1:D:22:TYR:CB	2.64	0.44
1:D:245:ASN:HB3	1:D:248:ALA:HB3	2.00	0.44
1:D:25:GLU:O	1:D:26:GLU:CG	2.66	0.44
1:B:378:ILE:O	1:B:382:ARG:HG3	2.18	0.44
1:C:288:ARG:HG2	1:C:289:ILE:H	1.82	0.44
1:D:261:ASP:HB3	1:D:271:VAL:CG2	2.47	0.44
1:F:219:CYS:HB2	1:F:332:MET:CE	2.47	0.44
1:A:49:LYS:HB3	1:A:49:LYS:HE2	1.76	0.44
1:D:125:LEU:O	1:D:152:LEU:HA	2.18	0.44
1:D:9:GLU:OE2	1:D:18:GLN:HB3	2.17	0.44
1:B:280:LEU:HD23	1:B:286:VAL:HA	1.99	0.44
1:B:216:LEU:O	1:B:364:GLY:HA2	2.18	0.44
1:C:116:TRP:CH2	1:C:231:ILE:HG22	2.46	0.44
1:D:25:GLU:O	1:D:26:GLU:HG3	2.18	0.44
1:D:265:ASP:HB3	1:D:266:TYR:H	1.73	0.44
1:F:124:THR:O	1:F:125:LEU:HG	2.18	0.44
1:F:124:THR:HG22	1:F:125:LEU:N	2.32	0.44
1:F:199:LEU:HD23	1:F:199:LEU:N	2.33	0.44
1:F:98:LYS:HA	1:F:98:LYS:HD2	1.74	0.44
1:B:202:HIS:O	1:B:346:LEU:HA	2.18	0.43
1:C:77:THR:HG22	1:C:78:TRP:N	2.33	0.43
1:D:70:ASP:OD1	1:D:73:LYS:N	2.50	0.43
1:F:16:LEU:HD21	1:F:28:LEU:HD13	2.00	0.43
1:A:344:ARG:HG2	1:A:345:LEU:HD23	1.99	0.43
1:A:362:LEU:HD12	1:A:362:LEU:N	2.34	0.43
1:A:73:LYS:HG3	1:A:86:PHE:O	2.19	0.43
1:E:189:ALA:O	1:E:190:ASN:HB2	2.18	0.43
1:E:203:THR:HG21	1:E:289:ILE:O	2.17	0.43
1:E:329:THR:HG22	1:E:330:PHE:N	2.34	0.43
1:C:157:ASP:O	1:C:220:ILE:HG23	2.18	0.43
1:C:37:ASN:OD1	1:D:298:THR:HG22	2.18	0.43
1:D:218:HIS:HB2	1:D:337:VAL:HG22	2.00	0.43
1:E:6:GLN:HB3	1:E:20:LEU:O	2.18	0.43
1:B:277:ILE:HD13	1:B:314:LEU:HD13	2.00	0.43
1:B:241:LEU:HD23	1:B:320:LEU:HD22	2.01	0.43
1:C:288:ARG:HD2	1:C:290:ASN:ND2	2.31	0.43
1:E:18:GLN:NE2	1:E:26:GLU:CG	2.81	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:221:LYS:O	1:E:360:ARG:HA	2.18	0.43
1:F:124:THR:HA	1:F:151:ARG:O	2.19	0.43
1:B:306:ARG:O	1:B:309:PRO:HG2	2.19	0.43
1:E:152:LEU:O	1:E:336:ASP:HA	2.18	0.43
1:E:158:LYS:HD2	1:E:158:LYS:N	2.33	0.43
1:E:68:ILE:HG13	1:E:75:TYR:CD2	2.52	0.43
1:A:156:SER:OG	1:A:158:LYS:HG2	2.19	0.43
1:A:308:GLN:N	1:A:309:PRO:CD	2.82	0.43
1:B:293:ASN:OD1	1:B:296:ARG:NH2	2.47	0.43
1:D:62:ILE:HG12	1:D:63:GLY:H	1.83	0.43
1:E:87:GLN:HB2	1:E:90:TRP:HB2	2.00	0.43
1:C:201:PHE:CB	1:C:321:MET:HE2	2.49	0.43
1:F:126:ASP:HB3	1:F:129:ASP:HB2	1.99	0.43
1:C:265:ASP:OD1	1:C:265:ASP:C	2.56	0.43
1:F:345:LEU:N	1:F:345:LEU:HD23	2.34	0.43
1:D:38:CYS:SG	1:D:40:CYS:HB3	2.58	0.43
1:E:181:TRP:CH2	1:E:364:GLY:HA3	2.54	0.43
1:A:114:GLN:HG2	1:A:146:LYS:HE2	2.01	0.43
1:E:196:THR:HG21	1:E:352:TYR:HD2	1.83	0.43
1:A:145:LYS:HD3	1:A:373:MET:HE3	2.01	0.42
1:A:154:GLY:HA3	6:A:2037:HOH:O	2.19	0.42
1:B:110:PHE:CD1	1:B:110:PHE:N	2.87	0.42
1:B:250:GLN:HG3	1:B:251:ILE:N	2.33	0.42
1:E:116:TRP:CE3	1:E:120:LEU:HD22	2.54	0.42
1:E:244:ASN:C	1:E:246:PRO:HD3	2.39	0.42
1:A:286:VAL:HG23	6:A:2085:HOH:O	2.20	0.42
1:A:293:ASN:OD1	1:A:296:ARG:NH2	2.50	0.42
1:B:141:LEU:HD22	1:B:372:VAL:HG13	2.01	0.42
1:C:203:THR:HG23	1:C:346:LEU:HG	2.01	0.42
1:E:213:GLY:HA2	1:E:343:TRP:CD1	2.53	0.42
1:B:165:LEU:O	1:B:169:MET:HG3	2.19	0.42
1:C:11:LEU:HD12	1:C:11:LEU:O	2.19	0.42
1:E:288:ARG:HG3	1:E:343:TRP:CB	2.49	0.42
1:C:119:GLU:HA	1:E:331:LYS:HD2	2.02	0.42
1:E:66:GLY:HA3	1:E:77:THR:OG1	2.19	0.42
1:F:110:PHE:CE2	1:F:380:ARG:HD3	2.54	0.42
1:F:382:ARG:HG2	6:F:2064:HOH:O	2.18	0.42
1:C:105:GLN:HB3	6:C:2026:HOH:O	2.19	0.42
1:C:216:LEU:CD2	1:C:339:THR:HG22	2.50	0.42
1:D:183:VAL:HG13	1:D:183:VAL:O	2.19	0.42
1:D:212:PRO:HB3	1:D:366:TYR:HB3	2.02	0.42
1:F:308:GLN:CB	1:F:309:PRO:HD3	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:72:LYS:C	1:F:73:LYS:HG3	2.39	0.42
1:A:149:ILE:HD13	1:A:231:ILE:HD13	2.02	0.42
1:C:278:ILE:HG13	1:C:278:ILE:O	2.19	0.42
1:F:65:LYS:HG3	1:F:66:GLY:N	2.34	0.42
1:A:6:GLN:HG3	1:A:22:TYR:CZ	2.55	0.42
1:C:80:ASP:O	1:C:81:GLU:HB3	2.19	0.42
1:D:252:LEU:HB2	1:D:278:ILE:HD12	2.01	0.42
1:E:191:ASN:HD22	1:E:191:ASN:C	2.23	0.42
1:F:358:ILE:O	1:F:358:ILE:HG13	2.20	0.42
1:A:272:GLN:HG2	1:B:108:LEU:HD22	2.02	0.42
1:D:165:LEU:HD13	1:D:216:LEU:HD23	2.02	0.42
1:F:130:VAL:O	1:F:168:ARG:NE	2.51	0.42
1:F:21:TRP:C	1:F:24:GLU:H	2.22	0.42
1:B:124:THR:O	1:B:125:LEU:HG	2.20	0.42
1:D:219:CYS:HA	1:D:362:LEU:CD2	2.47	0.42
1:E:165:LEU:HD23	1:E:216:LEU:HD22	2.01	0.42
1:F:264:VAL:HG12	1:F:268:ASP:CA	2.46	0.42
1:F:95:CYS:SG	1:F:97:SER:HB3	2.60	0.42
1:B:196:THR:HG21	1:B:352:TYR:HD2	1.84	0.42
1:B:242:LYS:HB3	1:B:249:PHE:CG	2.55	0.42
1:D:184:GLN:HG2	1:D:361:HIS:CD2	2.55	0.42
1:D:21:TRP:HE1	1:D:27:SER:HB2	1.85	0.42
1:E:38:CYS:HA	1:E:39:PRO:HD3	1.85	0.42
1:E:78:TRP:CD1	1:E:82:HIS:HB3	2.54	0.42
1:A:302:VAL:CG2	1:A:303:PRO:HD2	2.50	0.41
1:F:140:TRP:HH2	1:F:169:MET:CE	2.32	0.41
1:F:190:ASN:O	1:F:191:ASN:HB2	2.20	0.41
1:A:155:ALA:N	1:A:335:GLY:O	2.53	0.41
1:C:8:ALA:CA	1:C:19:ILE:HG22	2.49	0.41
1:C:324:LYS:HA	1:C:327:LYS:HZ3	1.85	0.41
1:D:17:MET:O	1:D:28:LEU:HA	2.20	0.41
1:E:260:THR:OG1	1:E:272:GLN:NE2	2.53	0.41
1:F:20:LEU:HD12	1:F:21:TRP:O	2.20	0.41
1:A:140:TRP:HD1	1:A:150:VAL:HG11	1.86	0.41
1:F:13:GLY:O	1:F:14:ALA:HB3	2.20	0.41
1:A:161:GLU:HG3	1:A:218:HIS:CE1	2.55	0.41
1:B:8:ALA:HB3	1:B:69:PHE:CD1	2.55	0.41
1:E:250:GLN:HG3	1:E:251:ILE:N	2.35	0.41
1:E:73:LYS:HB3	1:E:73:LYS:HZ3	1.85	0.41
1:F:252:LEU:CD1	1:F:317:PHE:HB2	2.51	0.41
1:E:35:ARG:HD2	1:E:35:ARG:HA	1.85	0.41
1:F:156:SER:HB2	6:F:2025:HOH:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:308:GLN:HB3	1:F:309:PRO:HD3	2.01	0.41
1:E:296:ARG:O	1:F:51:ARG:NH2	2.54	0.41
1:B:288:ARG:HG2	1:B:289:ILE:N	2.36	0.41
1:C:104:LEU:HD21	1:D:299:ILE:CD1	2.42	0.41
1:C:144:LEU:HD22	1:C:144:LEU:O	2.20	0.41
1:E:198:LYS:HB2	1:E:198:LYS:HE3	1.85	0.41
1:F:219:CYS:HB2	1:F:332:MET:HE1	2.03	0.41
1:C:113:CYS:HB3	6:C:2029:HOH:O	2.21	0.41
1:D:218:HIS:HD2	6:D:2029:HOH:O	2.04	0.41
1:D:241:LEU:HD12	1:D:245:ASN:HB2	2.03	0.41
1:D:264:VAL:CG2	1:D:264:VAL:O	2.67	0.41
1:A:216:LEU:HD22	1:A:339:THR:HG22	2.03	0.41
1:C:207:ALA:HB1	1:C:271:VAL:HG23	2.03	0.41
1:C:73:LYS:HD3	1:C:85:GLU:OE1	2.20	0.41
1:D:260:THR:O	1:D:295:THR:HG22	2.21	0.41
1:B:202:HIS:CE1	4:B:601:6YT:OAB	2.74	0.41
1:B:297:ASP:OD1	1:B:298:THR:N	2.54	0.41
1:C:58:LEU:HD12	1:C:59:ASP:N	2.35	0.41
1:D:95:CYS:HB3	1:D:100:ALA:CB	2.51	0.41
1:D:149:ILE:HA	1:D:339:THR:O	2.21	0.41
1:E:18:GLN:NE2	1:E:26:GLU:HB2	2.35	0.41
4:F:601:6YT:N	4:F:601:6YT:OAD	2.52	0.41
1:C:68:ILE:CG1	1:C:75:TYR:HB2	2.51	0.41
1:D:187:ILE:HD13	1:D:194:TYR:CE1	2.56	0.41
1:E:244:ASN:O	1:E:246:PRO:HD3	2.20	0.41
1:F:201:PHE:O	1:F:202:HIS:HB3	2.20	0.41
1:E:224:VAL:HG12	1:E:358:ILE:HA	2.03	0.41
1:C:278:ILE:HG22	1:C:289:ILE:HD12	2.03	0.40
1:D:14:ALA:HB1	1:D:64:ILE:H	1.86	0.40
1:D:29:TYR:CE1	1:D:91:LEU:HD22	2.56	0.40
1:F:226:GLY:HA3	1:F:353:GLU:OE2	2.20	0.40
1:E:300:PHE:HB3	1:F:96:PHE:HE1	1.85	0.40
1:B:272:GLN:HE21	1:B:272:GLN:HB3	1.68	0.40
1:C:1:MET:C	1:C:3:CYS:H	2.24	0.40
1:F:240:LYS:HB3	1:F:320:LEU:HD11	2.03	0.40
1:A:181:TRP:CE2	1:A:364:GLY:HA3	2.57	0.40
1:A:30:PRO:HD2	1:A:96:PHE:CE2	2.56	0.40
1:A:353:GLU:HB3	1:A:356:THR:CG2	2.50	0.40
1:B:19:ILE:CD1	1:B:91:LEU:HD13	2.52	0.40
1:C:38:CYS:HA	1:C:39:PRO:HD3	1.88	0.40
1:D:189:ALA:CB	1:D:192:VAL:HG22	2.51	0.40
1:E:128:GLU:O	1:E:132:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:101:ARG:O	1:F:105:GLN:HG2	2.21	0.40
1:F:187:ILE:HB	1:F:358:ILE:CG1	2.52	0.40
1:A:112:GLU:HG2	1:A:113:CYS:N	2.35	0.40
1:E:219:CYS:SG	1:E:222:GLN:HB2	2.61	0.40
1:F:341:ASP:HB3	1:F:344:ARG:HB3	2.02	0.40
1:B:78:TRP:HZ3	1:B:84:SER:HB3	1.86	0.40
1:D:38:CYS:HA	1:D:39:PRO:HD3	1.92	0.40
1:E:201:PHE:HB2	1:E:321:MET:CE	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	382/388 (98%)	353 (92%)	29 (8%)	0	100	100
1	B	382/388 (98%)	349 (91%)	33 (9%)	0	100	100
1	C	382/388 (98%)	341 (89%)	41 (11%)	0	100	100
1	D	382/388 (98%)	356 (93%)	26 (7%)	0	100	100
1	E	382/388 (98%)	349 (91%)	33 (9%)	0	100	100
1	F	382/388 (98%)	355 (93%)	26 (7%)	1 (0%)	50	83
All	All	2292/2328 (98%)	2103 (92%)	188 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	170	GLY

### 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	336/343 (98%)	316 (94%)	20 (6%)	27	61
1	B	339/343 (99%)	326 (96%)	13 (4%)	44	80
1	C	335/343 (98%)	315 (94%)	20 (6%)	27	61
1	D	333/343 (97%)	314 (94%)	19 (6%)	29	63
1	E	330/343 (96%)	313 (95%)	17 (5%)	32	68
1	F	333/343 (97%)	322 (97%)	11 (3%)	50	84
All	All	2006/2058 (98%)	1906 (95%)	100 (5%)	34	70

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	19	ILE
1	A	40	CYS
1	A	42	ASP
1	A	67	LEU
1	A	114	GLN
1	A	119	GLU
1	A	163	SER
1	A	205	TYR
1	A	221	LYS
1	A	236	ASN
1	A	250	GLN
1	A	257	VAL
1	A	258	ASP
1	A	282	ASP
1	A	300	PHE
1	A	304	VAL
1	A	320	LEU
1	A	353	GLU
1	A	381	GLN
1	B	12	ASP
1	B	40	CYS
1	B	42	ASP
1	B	119	GLU
1	B	205	TYR
1	B	214	VAL
1	B	217	LEU
1	B	250	GLN

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Mol	Chain	Res	Type
1	B	282	ASP
1	B	300	PHE
1	B	304	VAL
1	B	327	LYS
1	B	361	HIS
1	C	40	CYS
1	C	42	ASP
1	C	119	GLU
1	C	144	LEU
1	C	181	TRP
1	C	182	GLN
1	C	187	ILE
1	C	205	TYR
1	C	223	THR
1	C	225	THR
1	C	243	LYS
1	C	258	ASP
1	C	300	PHE
1	C	319	ASP
1	C	320	LEU
1	C	321	MET
1	C	326	SER
1	C	349	ARG
1	C	362	LEU
1	C	363	GLU
1	D	9	GLU
1	D	40	CYS
1	D	42	ASP
1	D	46	ASP
1	D	47	SER
1	D	68	ILE
1	D	113	CYS
1	D	131	LEU
1	D	141	LEU
1	D	186	LYS
1	D	198	LYS
1	D	223	THR
1	D	228	ASP
1	D	285	GLN
1	D	295	THR
1	D	300	PHE
1	D	308	GLN

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Mol	Chain	Res	Type
1	D	345	LEU
1	D	372	VAL
1	E	20	LEU
1	E	22	TYR
1	E	40	CYS
1	E	119	GLU
1	E	121	GLN
1	E	181	TRP
1	E	191	ASN
1	E	204	ASP
1	E	205	TYR
1	E	239	GLN
1	E	250	GLN
1	E	258	ASP
1	E	282	ASP
1	E	300	PHE
1	E	307	VAL
1	E	320	LEU
1	E	321	MET
1	F	20	LEU
1	F	40	CYS
1	F	72	LYS
1	F	89	ASP
1	F	205	TYR
1	F	250	GLN
1	F	306	ARG
1	F	320	LEU
1	F	345	LEU
1	F	376	LEU
1	F	379	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	191	ASN
1	A	215	GLN
1	A	218	HIS
1	A	236	ASN
1	A	244	ASN
1	A	250	GLN
1	B	18	GLN

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Mol	Chain	Res	Type
1	B	136	HIS
1	B	236	ASN
1	B	250	GLN
1	B	333	ASN
1	C	61	ASN
1	C	105	GLN
1	C	250	GLN
1	C	272	GLN
1	D	179	HIS
1	D	182	GLN
1	D	272	GLN
1	D	285	GLN
1	D	308	GLN
1	D	322	ASN
1	E	18	GLN
1	E	87	GLN
1	E	191	ASN
1	E	215	GLN
1	E	239	GLN
1	E	250	GLN
1	E	272	GLN
1	E	333	ASN
1	E	361	HIS
1	F	114	GLN
1	F	182	GLN
1	F	184	GLN
1	F	215	GLN
1	F	222	GLN
1	F	250	GLN
1	F	347	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 32 ligands modelled in this entry, 12 are monoatomic - leaving 20 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	$\# Z  > 2$
4	6YT	A	601	2	24,24,24	2.23	4 (16%)	31,31,31	1.38	5 (16%)
5	EDO	A	701	-	3,3,3	0.67	0	2,2,2	0.28	0
5	EDO	A	702	-	3,3,3	0.59	0	2,2,2	0.32	0
5	EDO	A	703	-	3,3,3	0.57	0	2,2,2	0.34	0
4	6YT	B	601	2	24,24,24	2.23	4 (16%)	31,31,31	1.38	5 (16%)
5	EDO	B	701	-	3,3,3	0.56	0	2,2,2	0.36	0
5	EDO	B	702	-	3,3,3	0.52	0	2,2,2	0.41	0
4	6YT	C	601	2	24,24,24	2.11	4 (16%)	31,31,31	1.21	2 (6%)
5	EDO	C	701	-	3,3,3	0.57	0	2,2,2	0.38	0
5	EDO	C	702	-	3,3,3	0.59	0	2,2,2	0.31	0
5	EDO	C	703	-	3,3,3	0.58	0	2,2,2	0.35	0
5	EDO	C	704	-	3,3,3	0.52	0	2,2,2	0.43	0
4	6YT	D	601	2	24,24,24	2.11	4 (16%)	31,31,31	1.29	4 (12%)
4	6YT	E	601	2	24,24,24	2.08	4 (16%)	31,31,31	1.38	7 (22%)
5	EDO	E	701	-	3,3,3	0.55	0	2,2,2	0.35	0
5	EDO	E	702	-	3,3,3	0.62	0	2,2,2	0.33	0
5	EDO	E	703	-	3,3,3	0.56	0	2,2,2	0.32	0
4	6YT	F	601	2	24,24,24	2.13	4 (16%)	31,31,31	1.50	7 (22%)
5	EDO	F	701	-	3,3,3	0.54	0	2,2,2	0.38	0
5	EDO	F	702	-	3,3,3	0.58	0	2,2,2	0.37	0

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	6YT	A	601	2	-	0/18/18/18	0/2/2/2
5	EDO	A	701	-	-	0/1/1/1	0/0/0/0
5	EDO	A	702	-	-	0/1/1/1	0/0/0/0
5	EDO	A	703	-	-	0/1/1/1	0/0/0/0
4	6YT	B	601	2	-	0/18/18/18	0/2/2/2
5	EDO	B	701	-	-	0/1/1/1	0/0/0/0
5	EDO	B	702	-	-	0/1/1/1	0/0/0/0
4	6YT	C	601	2	-	0/18/18/18	0/2/2/2
5	EDO	C	701	-	-	0/1/1/1	0/0/0/0
5	EDO	C	702	-	-	0/1/1/1	0/0/0/0
5	EDO	C	703	-	-	0/1/1/1	0/0/0/0
5	EDO	C	704	-	-	0/1/1/1	0/0/0/0
4	6YT	D	601	2	-	2/18/18/18	0/2/2/2
4	6YT	E	601	2	-	0/18/18/18	0/2/2/2
5	EDO	E	701	-	-	0/1/1/1	0/0/0/0
5	EDO	E	702	-	-	0/1/1/1	0/0/0/0
5	EDO	E	703	-	-	0/1/1/1	0/0/0/0
4	6YT	F	601	2	-	0/18/18/18	0/2/2/2
5	EDO	F	701	-	-	0/1/1/1	0/0/0/0
5	EDO	F	702	-	-	0/1/1/1	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	6YT	CAV-CAS	-6.99	1.38	1.50
4	A	601	6YT	CAV-CAS	-6.98	1.38	1.50
4	F	601	6YT	CAV-CAS	-6.75	1.39	1.50
4	E	601	6YT	OAB-CAS	6.39	1.35	1.23
4	C	601	6YT	OAB-CAS	6.26	1.35	1.23
4	D	601	6YT	OAB-CAS	6.20	1.35	1.23
4	D	601	6YT	CAV-CAS	-6.19	1.39	1.50
4	A	601	6YT	OAB-CAS	6.15	1.35	1.23
4	B	601	6YT	OAB-CAS	6.14	1.35	1.23
4	C	601	6YT	CAV-CAS	-6.09	1.40	1.50
4	E	601	6YT	CAV-CAS	-5.93	1.40	1.50
4	F	601	6YT	OAB-CAS	5.62	1.34	1.23
4	A	601	6YT	CAL-SAQ	-3.12	1.77	1.82
4	B	601	6YT	CAL-SAQ	-3.09	1.77	1.82
4	F	601	6YT	CAL-SAQ	-2.84	1.77	1.82
4	D	601	6YT	CAL-SAQ	-2.50	1.78	1.82
4	C	601	6YT	CAL-SAQ	-2.44	1.78	1.82
4	F	601	6YT	OAD-CAT	2.42	1.41	1.36
4	A	601	6YT	OAD-CAT	2.36	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	6YT	OAD-CAT	2.34	1.41	1.36
4	D	601	6YT	OAD-CAT	2.33	1.41	1.36
4	E	601	6YT	OAD-CAT	2.32	1.41	1.36
4	C	601	6YT	OAD-CAT	2.31	1.41	1.36
4	E	601	6YT	CAL-SAQ	-2.02	1.79	1.82

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	601	6YT	CAV-CAS-N	4.08	120.01	115.92
4	E	601	6YT	CAJ-CAT-CAV	3.23	120.24	118.11
4	C	601	6YT	CAJ-CAT-CAV	3.02	120.10	118.11
4	B	601	6YT	CAS-CAV-NAO	2.92	120.03	115.81
4	A	601	6YT	CAS-CAV-NAO	2.91	120.02	115.81
4	D	601	6YT	CAJ-CAT-CAV	2.78	119.94	118.11
4	D	601	6YT	CAS-CAV-NAO	2.72	119.74	115.81
4	F	601	6YT	CB-SAQ-CAL	-2.61	96.47	101.62
4	A	601	6YT	CAJ-CAT-CAV	2.46	119.73	118.11
4	F	601	6YT	OAB-CAS-CAV	-2.46	117.49	120.90
4	F	601	6YT	CAJ-CAT-CAV	2.45	119.72	118.11
4	B	601	6YT	CAJ-CAT-CAV	2.43	119.71	118.11
4	E	601	6YT	CAH-NAN-CAU	2.41	120.75	117.37
4	E	601	6YT	CAS-CAV-NAO	2.36	119.22	115.81
4	E	601	6YT	CAI-NAO-CAV	2.22	121.03	116.89
4	F	601	6YT	CAH-NAN-CAU	2.21	120.47	117.37
4	D	601	6YT	CAV-CAS-N	2.19	118.12	115.92
4	E	601	6YT	CAV-CAS-N	2.18	118.11	115.92
4	A	601	6YT	CAL-CAU-NAN	2.17	120.28	116.90
4	B	601	6YT	CAL-CAU-NAN	2.16	120.28	116.90
4	C	601	6YT	CAS-CAV-NAO	2.14	118.90	115.81
4	B	601	6YT	CAG-CAI-NAO	-2.14	119.82	123.42
4	A	601	6YT	CAG-CAI-NAO	-2.12	119.86	123.42
4	E	601	6YT	CAG-CAI-NAO	-2.10	119.88	123.42
4	F	601	6YT	CAE-CAH-NAN	-2.06	119.95	123.42
4	F	601	6YT	CAL-CAU-NAN	2.04	120.09	116.90
4	D	601	6YT	CAG-CAI-NAO	-2.04	119.98	123.42
4	E	601	6YT	CAE-CAH-NAN	-2.03	120.00	123.42
4	A	601	6YT	CB-SAQ-CAL	-2.01	97.65	101.62
4	B	601	6YT	CB-SAQ-CAL	-2.01	97.66	101.62

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	601	6YT	CAT-CAV-CAS-N
4	D	601	6YT	NAO-CAV-CAS-N

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	384/388 (98%)	-0.23	3 (0%)	83 84	36, 55, 80, 95	0
1	B	384/388 (98%)	-0.18	2 (0%)	88 90	34, 53, 76, 91	0
1	C	384/388 (98%)	-0.12	3 (0%)	83 84	27, 61, 82, 109	0
1	D	384/388 (98%)	-0.01	6 (1%)	68 69	37, 65, 98, 113	1 (0%)
1	E	384/388 (98%)	0.02	10 (2%)	53 54	43, 72, 103, 113	0
1	F	384/388 (98%)	-0.09	3 (0%)	83 84	41, 64, 85, 98	1 (0%)
All	All	2304/2328 (98%)	-0.10	27 (1%)	75 76	27, 61, 90, 113	2 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	72	LYS	3.9
1	A	12	ASP	3.6
1	E	64	ILE	3.5
1	E	98	LYS	3.2
1	E	8	ALA	3.1
1	E	155	ALA	2.9
1	E	7	LYS	2.9
1	D	209	HIS	2.8
1	D	28	LEU	2.8
1	E	9	GLU	2.6
1	B	5	ILE	2.6
1	F	332	MET	2.5
1	F	26	GLU	2.5
1	C	26	GLU	2.5
1	F	209	HIS	2.4
1	E	26	GLU	2.4
1	D	18	GLN	2.3
1	E	14	ALA	2.3
1	D	130	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	194	TYR	2.2
1	A	184	GLN	2.2
1	B	11	LEU	2.2
1	A	13	GLY	2.2
1	C	12	ASP	2.1
1	E	135	GLU	2.1
1	D	22	TYR	2.1
1	E	12	ASP	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	C	704	4/4	0.33	12.16	62,63,64,65	0
5	EDO	E	701	4/4	0.37	7.01	72,72,73,73	0
5	EDO	B	701	4/4	0.23	5.90	62,63,63,63	0
5	EDO	C	702	4/4	0.29	3.95	82,83,84,84	0
5	EDO	C	703	4/4	0.24	3.70	71,72,72,73	0
4	6YT	F	601	23/23	0.39	3.63	94,97,100,101	0
4	6YT	C	601	23/23	0.26	3.55	98,100,100,101	0
4	6YT	B	601	23/23	0.30	3.15	98,100,100,101	0
5	EDO	A	702	4/4	0.30	3.00	68,68,69,70	0
5	EDO	C	701	4/4	0.28	2.55	73,73,73,74	0
5	EDO	F	701	4/4	0.26	2.13	78,79,79,80	0
4	6YT	A	601	23/23	0.23	1.27	98,100,100,101	0
4	6YT	E	601	23/23	0.25	1.05	94,97,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	B	502	1/1	0.17	0.85	55,55,55,55	0
5	EDO	A	701	4/4	0.21	0.83	61,63,64,65	0
3	ZN	F	502	1/1	0.15	0.80	63,63,63,63	0
5	EDO	E	702	4/4	0.23	0.73	72,76,77,79	0
3	ZN	C	502	1/1	0.16	0.58	63,63,63,63	0
3	ZN	E	502	1/1	0.17	0.35	95,95,95,95	0
4	6YT	D	601	23/23	0.23	0.32	80,84,91,91	0
5	EDO	B	702	4/4	0.17	-0.03	62,64,64,65	0
2	NI	A	501	1/1	0.15	-0.53	76,76,76,76	0
2	NI	F	501	1/1	0.14	-0.68	49,49,49,49	0
2	NI	C	501	1/1	0.15	-0.69	67,67,67,67	0
2	NI	D	501	1/1	0.14	-0.73	54,54,54,54	0
3	ZN	A	502	1/1	0.14	-0.74	52,52,52,52	0
3	ZN	D	502	1/1	0.12	-0.79	67,67,67,67	0
5	EDO	E	703	4/4	0.16	-0.94	54,58,59,60	0
5	EDO	A	703	4/4	0.15	-1.12	60,62,62,63	0
5	EDO	F	702	4/4	0.14	-1.55	63,65,65,65	0
2	NI	B	501	1/1	0.15	-1.60	70,70,70,70	0
2	NI	E	501	1/1	0.09	-1.82	81,81,81,81	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.