



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 05:56 AM GMT

PDB ID : 3A11  
Title : Crystal structure of ribose-1,5-bisphosphate isomerase from *Thermococcus kodakaraensis* KOD1  
Authors : Nakamura, A.; Fujihashi, M.; Nishiba, Y.; Yoshida, S.; Yano, A.; Atomi, H.; Imanaka, T.; Miki, K.  
Deposited on : 2009-03-25  
Resolution : 2.50 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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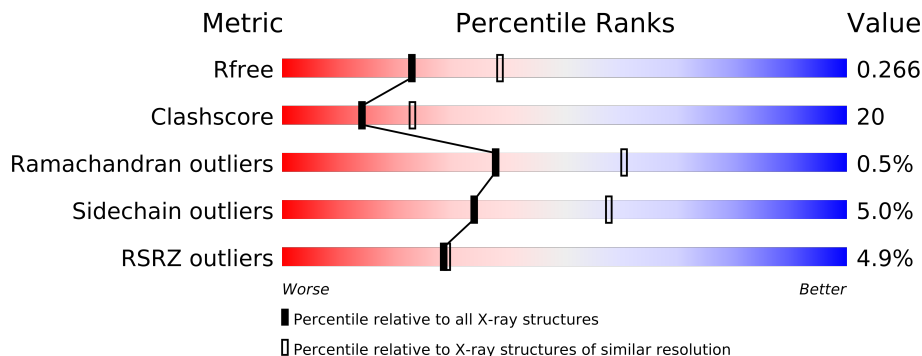
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	338	
1	B	338	
1	C	338	
1	D	338	
1	E	338	
1	F	338	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	PEG	A	401	-	X
2	PEG	B	401	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	PEG	C	401	-	X
2	PEG	D	401	-	X
2	PEG	E	401	-	X
3	MG	B	411	-	X
3	MG	E	411	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15535 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 Translation initiation factor eIF-2B, delta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2541	1631	428	470	12			
1	B	322	Total	C	N	O	S	0	0	0
			2556	1636	435	472	13			
1	C	317	Total	C	N	O	S	0	0	0
			2513	1613	424	464	12			
1	D	320	Total	C	N	O	S	0	0	0
			2531	1623	428	468	12			
1	E	317	Total	C	N	O	S	0	0	0
			2513	1613	424	464	12			
1	F	319	Total	C	N	O	S	0	0	0
			2529	1623	426	468	12			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	EXPRESSION TAG	UNP Q5JFM9
A	-14	ASN	-	EXPRESSION TAG	UNP Q5JFM9
A	-13	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	-12	LYS	-	EXPRESSION TAG	UNP Q5JFM9
A	-11	VAL	-	EXPRESSION TAG	UNP Q5JFM9
A	-10	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	-9	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	-8	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	-7	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	-6	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	-5	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	-4	ILE	-	EXPRESSION TAG	UNP Q5JFM9
A	-3	GLU	-	EXPRESSION TAG	UNP Q5JFM9
A	-2	GLY	-	EXPRESSION TAG	UNP Q5JFM9
A	-1	ARG	-	EXPRESSION TAG	UNP Q5JFM9
A	0	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-15	MET	-	EXPRESSION TAG	UNP Q5JFM9

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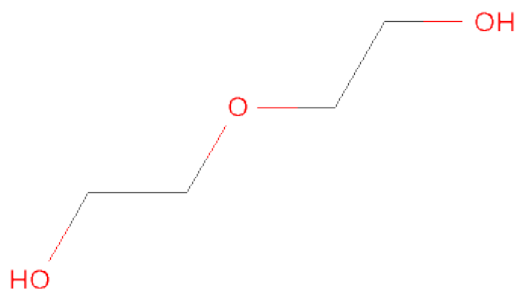
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	ASN	-	EXPRESSION TAG	UNP Q5JFM9
B	-13	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-12	LYS	-	EXPRESSION TAG	UNP Q5JFM9
B	-11	VAL	-	EXPRESSION TAG	UNP Q5JFM9
B	-10	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-9	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-8	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-7	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-6	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-5	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-4	ILE	-	EXPRESSION TAG	UNP Q5JFM9
B	-3	GLU	-	EXPRESSION TAG	UNP Q5JFM9
B	-2	GLY	-	EXPRESSION TAG	UNP Q5JFM9
B	-1	ARG	-	EXPRESSION TAG	UNP Q5JFM9
B	0	HIS	-	EXPRESSION TAG	UNP Q5JFM9
C	-15	MET	-	EXPRESSION TAG	UNP Q5JFM9
C	-14	ASN	-	EXPRESSION TAG	UNP Q5JFM9
C	-13	HIS	-	EXPRESSION TAG	UNP Q5JFM9
C	-12	LYS	-	EXPRESSION TAG	UNP Q5JFM9
C	-11	VAL	-	EXPRESSION TAG	UNP Q5JFM9
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C	-7	HIS	-	EXPRESSION TAG	UNP Q5JFM9
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C	-5	HIS	-	EXPRESSION TAG	UNP Q5JFM9
C	-4	ILE	-	EXPRESSION TAG	UNP Q5JFM9
C	-3	GLU	-	EXPRESSION TAG	UNP Q5JFM9
C	-2	GLY	-	EXPRESSION TAG	UNP Q5JFM9
C	-1	ARG	-	EXPRESSION TAG	UNP Q5JFM9
C	0	HIS	-	EXPRESSION TAG	UNP Q5JFM9
D	-15	MET	-	EXPRESSION TAG	UNP Q5JFM9
D	-14	ASN	-	EXPRESSION TAG	UNP Q5JFM9
D	-13	HIS	-	EXPRESSION TAG	UNP Q5JFM9
D	-12	LYS	-	EXPRESSION TAG	UNP Q5JFM9
D	-11	VAL	-	EXPRESSION TAG	UNP Q5JFM9
D	-10	HIS	-	EXPRESSION TAG	UNP Q5JFM9
D	-9	HIS	-	EXPRESSION TAG	UNP Q5JFM9
D	-8	HIS	-	EXPRESSION TAG	UNP Q5JFM9
D	-7	HIS	-	EXPRESSION TAG	UNP Q5JFM9
D	-6	HIS	-	EXPRESSION TAG	UNP Q5JFM9
D	-5	HIS	-	EXPRESSION TAG	UNP Q5JFM9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	ILE	-	EXPRESSION TAG	UNP Q5JFM9
D	-3	GLU	-	EXPRESSION TAG	UNP Q5JFM9
D	-2	GLY	-	EXPRESSION TAG	UNP Q5JFM9
D	-1	ARG	-	EXPRESSION TAG	UNP Q5JFM9
D	0	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-15	MET	-	EXPRESSION TAG	UNP Q5JFM9
E	-14	ASN	-	EXPRESSION TAG	UNP Q5JFM9
E	-13	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-12	LYS	-	EXPRESSION TAG	UNP Q5JFM9
E	-11	VAL	-	EXPRESSION TAG	UNP Q5JFM9
E	-10	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-9	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-8	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-7	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-6	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-5	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-4	ILE	-	EXPRESSION TAG	UNP Q5JFM9
E	-3	GLU	-	EXPRESSION TAG	UNP Q5JFM9
E	-2	GLY	-	EXPRESSION TAG	UNP Q5JFM9
E	-1	ARG	-	EXPRESSION TAG	UNP Q5JFM9
E	0	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-15	MET	-	EXPRESSION TAG	UNP Q5JFM9
F	-14	ASN	-	EXPRESSION TAG	UNP Q5JFM9
F	-13	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-12	LYS	-	EXPRESSION TAG	UNP Q5JFM9
F	-11	VAL	-	EXPRESSION TAG	UNP Q5JFM9
F	-10	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-9	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-8	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-7	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-6	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-5	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-4	ILE	-	EXPRESSION TAG	UNP Q5JFM9
F	-3	GLU	-	EXPRESSION TAG	UNP Q5JFM9
F	-2	GLY	-	EXPRESSION TAG	UNP Q5JFM9
F	-1	ARG	-	EXPRESSION TAG	UNP Q5JFM9
F	0	HIS	-	EXPRESSION TAG	UNP Q5JFM9

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		

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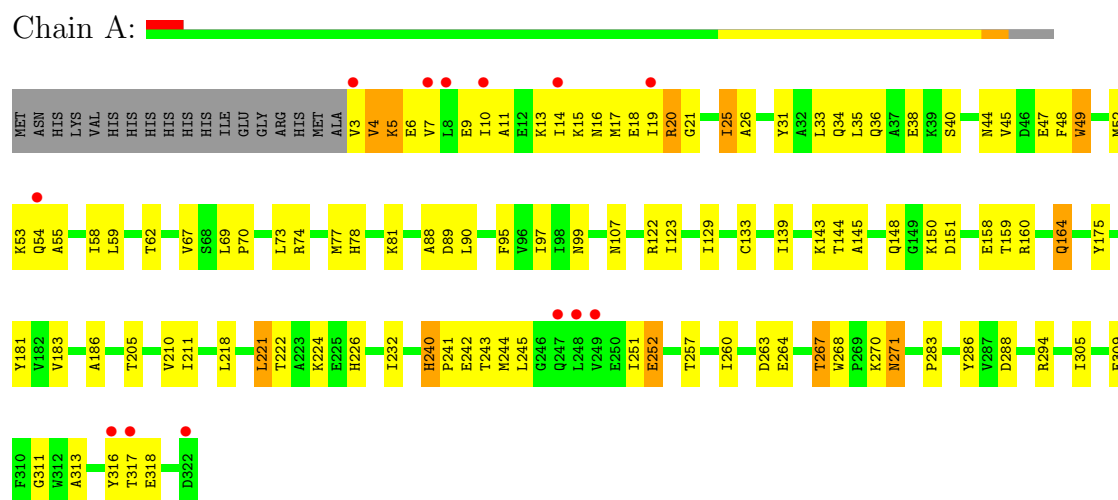
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	87	Total 87	O 87	0	0
4	C	34	Total 34	O 34	0	0
4	D	54	Total 54	O 54	0	0
4	E	46	Total 46	O 46	0	0
4	F	28	Total 28	O 28	0	0



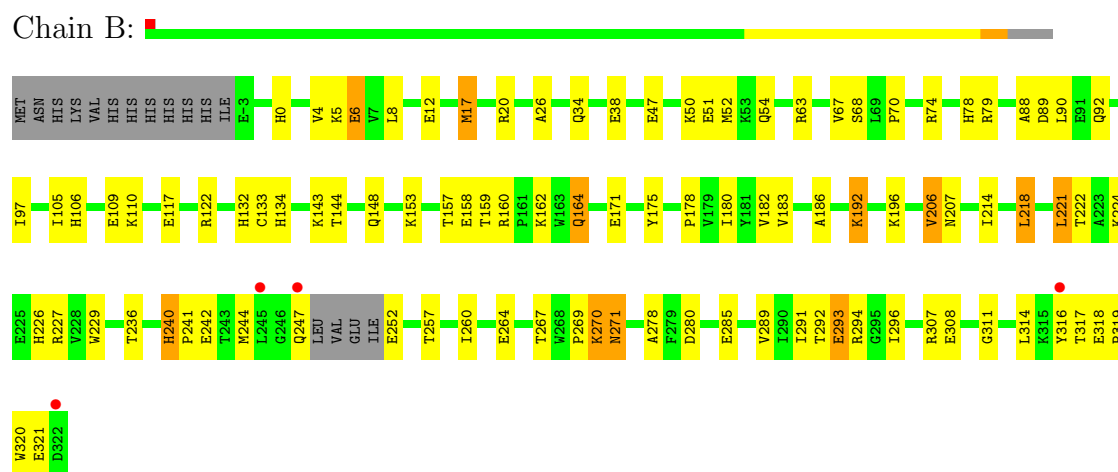
### 3 Residue-property plots

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.

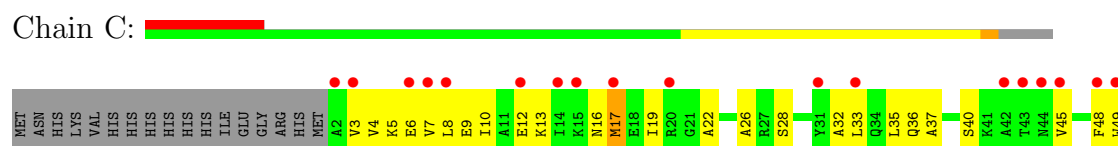
- Molecule 1: Translation initiation factor eIF-2B, delta subunit



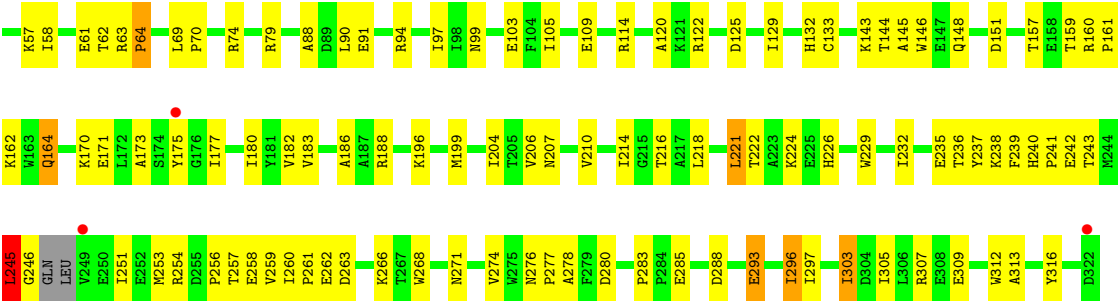
- Molecule 1: Translation initiation factor eIF-2B, delta subunit



- Molecule 1: Translation initiation factor eIF-2B, delta subunit







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.29Å 130.81Å 132.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.66 – 2.50 43.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.66-2.50) 99.9 (43.66-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.54 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.204 , 0.266 0.204 , 0.266	Depositor DCC
$R_{free}$ test set	3631 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 34.0	EDS
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 71397 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15535	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: MG, PEG

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	0.35	0/2595	0.60	0/3514
1	B	0.37	0/2610	0.61	0/3530
1	C	0.31	0/2566	0.57	0/3473
1	D	0.34	0/2584	0.57	0/3498
1	E	0.31	0/2566	0.56	0/3473
1	F	0.32	0/2582	0.55	0/3495
All	All	0.34	0/15503	0.58	0/20983

There are no bond length outliers.

There are no bond angle outliers.

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	2541	0	2583	112	0
1	B	2556	0	2591	106	0
1	C	2513	0	2553	115	0
1	D	2531	0	2566	97	0
1	E	2513	0	2553	95	0
1	F	2529	0	2568	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	7	0	10	2	0
2	B	7	0	10	2	0
2	C	7	0	10	0	0
2	D	7	0	10	2	0
2	E	7	0	10	1	0
2	F	7	0	10	2	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
4	A	59	0	0	1	0
4	B	87	0	0	2	0
4	C	34	0	0	3	0
4	D	54	0	0	2	0
4	E	46	0	0	2	0
4	F	28	0	0	0	0
All	All	15535	0	15474	605	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 20.

All (605) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:292:THR:HG22	1:E:294:ARG:H	1.13	1.09
1:C:164:GLN:HE21	1:C:164:GLN:H	1.06	1.02
1:B:270:LYS:H	1:B:270:LYS:HE3	1.21	0.99
1:C:218:LEU:HD22	1:D:218:LEU:HD22	1.46	0.97
1:B:292:THR:HG22	1:B:294:ARG:H	1.29	0.96
1:F:214:ILE:HD12	1:F:277:PRO:HG2	1.46	0.95
1:B:318:GLU:HG3	1:B:319:PRO:HD2	1.49	0.94
1:E:181:TYR:HB3	1:F:274:VAL:HG12	1.52	0.91
1:B:270:LYS:H	1:B:270:LYS:CE	1.84	0.91
1:E:186:ALA:HB2	1:F:214:ILE:HD11	1.53	0.91
1:D:164:GLN:HE21	1:D:164:GLN:H	1.14	0.88
1:E:211:ILE:HD11	1:E:244:MET:HG3	1.53	0.88
1:C:164:GLN:NE2	1:C:164:GLN:H	1.72	0.87
1:A:164:GLN:HE21	1:A:164:GLN:H	1.17	0.87
1:E:318:GLU:HG3	1:E:319:PRO:HD2	1.55	0.86
1:D:264:GLU:O	1:D:267:THR:HG22	1.74	0.86
1:F:199:MET:HE1	1:F:216:THR:HG23	1.59	0.84
1:E:164:GLN:HE21	1:E:164:GLN:H	1.26	0.84
1:D:288:ASP:OD2	2:D:401:PEG:H21	1.77	0.83
1:E:187:ALA:HB3	1:F:218:LEU:HD11	1.62	0.81
1:A:294:ARG:HH21	1:C:315:LYS:HD2	1.47	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:69:LEU:HB3	1:D:70:PRO:HD3	1.65	0.79
1:D:224:LYS:HA	2:D:401:PEG:H12	1.65	0.78
1:C:8:LEU:HD12	1:C:8:LEU:H	1.48	0.77
1:A:313:ALA:HB3	1:A:316:TYR:HB2	1.66	0.77
1:F:3:VAL:HG21	1:F:58:ILE:HD12	1.68	0.76
1:C:10:ILE:HD12	1:C:32:ALA:HB2	1.67	0.76
1:A:271:ASN:H	1:A:271:ASN:HD22	1.31	0.76
1:A:243:THR:HG22	1:A:245:LEU:H	1.48	0.76
1:B:244:MET:HB2	1:D:122:ARG:HH12	1.51	0.76
1:A:52:MET:HE1	1:A:97:ILE:HG21	1.67	0.76
1:C:164:GLN:HE21	1:C:164:GLN:N	1.84	0.76
1:F:256:PRO:HB3	1:F:274:VAL:HG23	1.68	0.76
1:B:227:ARG:HE	1:E:227:ARG:HG2	1.51	0.76
1:F:259:VAL:HG12	1:F:260:ILE:HG13	1.68	0.75
1:A:251:ILE:HG22	1:A:252:GLU:N	2.01	0.75
1:A:33:LEU:HD11	1:A:73:LEU:HD12	1.69	0.74
1:D:318:GLU:HG2	1:D:320:TRP:CZ2	2.22	0.74
1:D:247:GLN:CD	1:F:122:ARG:HG3	2.08	0.74
1:E:254:ARG:HB2	1:E:276:ASN:ND2	2.02	0.74
1:B:89:ASP:OD2	1:B:92:GLN:HG3	1.88	0.74
1:D:164:GLN:NE2	1:D:164:GLN:H	1.85	0.74
1:A:164:GLN:HE21	1:A:164:GLN:N	1.86	0.74
1:B:318:GLU:HG2	1:B:320:TRP:CH2	2.23	0.73
1:A:251:ILE:HG22	1:A:252:GLU:H	1.53	0.73
1:A:183:VAL:HG21	1:B:160:ARG:HB3	1.69	0.73
1:A:5:LYS:HD3	1:A:5:LYS:N	2.03	0.73
1:F:164:GLN:H	1:F:164:GLN:HE21	1.36	0.73
1:B:270:LYS:N	1:B:270:LYS:HE3	2.01	0.73
1:A:224:LYS:HA	2:A:401:PEG:H41	1.70	0.73
1:C:297:ILE:HD13	1:C:305:ILE:HD11	1.70	0.72
1:A:139:ILE:HG22	1:A:143:LYS:HE2	1.71	0.72
1:A:221:LEU:HD13	1:B:221:LEU:HD13	1.71	0.71
1:D:297:ILE:HD13	1:D:305:ILE:HD11	1.71	0.71
1:B:318:GLU:HG2	1:B:320:TRP:CZ2	2.25	0.71
1:E:318:GLU:HG2	1:E:320:TRP:CH2	2.24	0.71
1:F:260:ILE:HD13	1:F:268:TRP:CH2	2.26	0.70
1:C:93:LEU:O	1:C:97:ILE:HG12	1.91	0.70
1:F:288:ASP:OD2	2:F:401:PEG:H32	1.91	0.70
1:E:69:LEU:HB3	1:E:70:PRO:HD3	1.74	0.70
1:F:251:ILE:HD12	1:F:251:ILE:H	1.55	0.70
1:F:171:GLU:HG2	1:F:175:TYR:HE2	1.56	0.70
1:F:224:LYS:HA	2:F:401:PEG:H41	1.74	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:160:ARG:HD2	1:F:161:PRO:HA	1.74	0.70
1:E:186:ALA:CB	1:F:214:ILE:HD11	2.20	0.70
1:B:264:GLU:O	1:B:267:THR:HB	1.92	0.70
1:C:257:THR:HA	1:C:260:ILE:O	1.92	0.70
1:E:211:ILE:CD1	1:E:244:MET:HG3	2.22	0.69
1:B:47:GLU:O	1:B:51:GLU:HG3	1.91	0.69
1:F:307:ARG:HD3	1:F:312:TRP:O	1.90	0.69
1:A:143:LYS:HD3	1:A:175:TYR:CE2	2.27	0.69
1:F:164:GLN:H	1:F:164:GLN:NE2	1.89	0.69
1:E:143:LYS:HE2	1:E:147:GLU:HG3	1.73	0.69
1:A:160:ARG:HD3	1:B:158:GLU:OE2	1.93	0.69
1:F:199:MET:CE	1:F:216:THR:HG23	2.23	0.68
1:C:242:GLU:HG2	1:C:243:THR:H	1.58	0.68
1:C:76:VAL:HG23	1:C:77:MET:N	2.08	0.68
1:D:247:GLN:OE1	1:F:122:ARG:HG3	1.92	0.68
1:D:182:VAL:CG1	1:D:186:ALA:HB3	2.24	0.68
1:A:144:THR:O	1:A:148:GLN:HG3	1.93	0.68
1:C:221:LEU:HD13	1:D:221:LEU:HD13	1.74	0.68
4:C:603:HOH:O	1:D:183:VAL:HG13	1.93	0.68
1:C:211:ILE:HD11	1:C:244:MET:HG2	1.77	0.67
1:F:114:ARG:HH11	1:F:114:ARG:HG3	1.59	0.67
1:C:270:LYS:H	1:C:270:LYS:HE3	1.60	0.67
1:D:243:THR:HG22	1:D:247:GLN:HG2	1.75	0.67
1:E:183:VAL:HG13	4:E:617:HOH:O	1.94	0.66
1:D:52:MET:HE2	1:D:97:ILE:HD13	1.78	0.66
1:A:305:ILE:HD11	1:C:314:LEU:HD12	1.76	0.66
1:A:210:VAL:HG21	1:A:232:ILE:HG13	1.78	0.66
1:C:144:THR:O	1:C:148:GLN:HG3	1.95	0.66
1:A:45:VAL:HG22	1:A:90:LEU:N	2.10	0.66
1:B:122:ARG:HE	1:F:246:GLY:HA2	1.61	0.66
1:E:255:ASP:OD2	1:E:257:THR:HB	1.96	0.66
1:C:145:ALA:O	1:C:150:LYS:HB2	1.95	0.65
1:C:270:LYS:H	1:C:270:LYS:CE	2.09	0.65
1:B:132:HIS:HD2	1:B:157:THR:OG1	1.80	0.65
1:E:160:ARG:HB3	1:F:183:VAL:HG21	1.79	0.65
1:B:17:MET:CE	1:B:63:ARG:HD2	2.25	0.65
1:B:247:GLN:HE22	1:B:252:GLU:HB2	1.60	0.65
1:B:236:THR:HG23	1:B:292:THR:HG23	1.79	0.65
1:F:13:LYS:HB3	1:F:19:ILE:HG13	1.79	0.65
1:C:13:LYS:HB3	1:C:19:ILE:HG12	1.79	0.65
1:C:195:ASP:O	1:C:196:LYS:HD2	1.97	0.64
1:B:164:GLN:H	1:B:164:GLN:HE21	1.45	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:235:GLU:OE1	1:F:238:LYS:HE3	1.97	0.64
1:D:89:ASP:H	1:D:92:GLN:NE2	1.96	0.64
1:C:4:VAL:HG22	1:C:6:GLU:H	1.61	0.64
1:B:182:VAL:HG13	1:B:186:ALA:HB3	1.80	0.64
1:E:133:CYS:HA	1:E:159:THR:HG21	1.79	0.64
1:D:164:GLN:HE21	1:D:164:GLN:N	1.92	0.63
1:D:44:ASN:O	1:D:90:LEU:HD13	1.98	0.63
1:F:49:TRP:NE1	1:F:53:LYS:HD3	2.12	0.63
1:E:236:THR:HG23	1:E:292:THR:HG23	1.80	0.63
1:F:256:PRO:HB3	1:F:274:VAL:CG2	2.28	0.63
1:A:164:GLN:NE2	1:A:164:GLN:H	1.94	0.63
1:B:196:LYS:HD3	1:B:229:TRP:HB3	1.79	0.63
1:A:317:THR:HG22	1:A:318:GLU:H	1.61	0.63
1:B:247:GLN:NE2	1:B:252:GLU:HB2	2.13	0.63
1:F:3:VAL:HG21	1:F:58:ILE:CD1	2.28	0.63
1:E:160:ARG:CB	1:F:183:VAL:HG21	2.29	0.63
1:C:6:GLU:HB3	1:C:35:LEU:HD13	1.81	0.63
1:D:6:GLU:HB3	1:D:35:LEU:HD13	1.80	0.63
1:A:251:ILE:CG2	1:A:252:GLU:H	2.11	0.63
1:A:52:MET:HB3	1:A:77:MET:HE1	1.79	0.63
1:C:89:ASP:OD1	1:C:92:GLN:HB2	1.99	0.63
1:B:317:THR:HB	1:B:321:GLU:HB2	1.79	0.62
1:A:305:ILE:CD1	1:C:314:LEU:HD12	2.30	0.62
1:F:133:CYS:HA	1:F:159:THR:HG21	1.82	0.62
1:E:44:ASN:HD21	1:E:46:ASP:HB2	1.63	0.62
1:F:253:MET:HE2	1:F:277:PRO:HA	1.80	0.62
1:A:70:PRO:HB2	1:A:74:ARG:HH12	1.65	0.62
1:E:41:LYS:HE2	1:E:41:LYS:HA	1.81	0.62
1:D:4:VAL:HG12	1:D:6:GLU:H	1.63	0.62
1:B:5:LYS:HG3	1:B:6:GLU:OE1	2.00	0.62
1:E:318:GLU:HG2	1:E:320:TRP:CZ2	2.35	0.61
1:D:45:VAL:HG22	1:D:90:LEU:N	2.15	0.61
1:A:317:THR:HG22	1:A:318:GLU:N	2.15	0.61
1:F:50:LYS:O	1:F:54:GLN:HG3	2.00	0.61
1:B:34:GLN:O	1:B:38:GLU:HG3	1.99	0.61
1:E:214:ILE:HD12	1:E:280:ASP:HB3	1.82	0.61
1:D:314:LEU:HD11	1:F:297:ILE:CG2	2.30	0.61
1:E:292:THR:HG22	1:E:294:ARG:N	1.99	0.61
1:F:254:ARG:HG3	1:F:278:ALA:HB2	1.81	0.61
1:D:314:LEU:HD11	1:F:297:ILE:HG21	1.81	0.61
1:A:240:HIS:CD2	1:A:241:PRO:HD2	2.35	0.61
1:A:70:PRO:HB2	1:A:74:ARG:NH1	2.16	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:292:THR:HG21	1:E:294:ARG:HG3	1.83	0.61
1:A:264:GLU:O	1:A:267:THR:HB	2.01	0.61
1:D:144:THR:O	1:D:148:GLN:HG3	2.00	0.61
1:D:269:PRO:HD2	1:D:272:ILE:HD12	1.83	0.61
1:F:105:ILE:O	1:F:109:GLU:HG3	2.00	0.61
1:F:188:ARG:HA	1:F:222:THR:HG21	1.83	0.61
1:D:79:ARG:HH21	1:D:79:ARG:HG3	1.66	0.61
1:A:251:ILE:HG22	1:A:252:GLU:HG2	1.83	0.60
1:B:89:ASP:H	1:B:92:GLN:NE2	1.99	0.60
4:C:604:HOH:O	1:D:182:VAL:HG13	2.02	0.60
1:B:89:ASP:CG	1:B:92:GLN:HE21	2.05	0.60
1:E:144:THR:O	1:E:148:GLN:HG3	2.00	0.59
1:A:5:LYS:HG2	1:A:6:GLU:OE2	2.01	0.59
1:C:10:ILE:HG21	1:C:28:SER:HB3	1.84	0.59
1:C:211:ILE:CD1	1:C:244:MET:HG2	2.32	0.59
1:A:271:ASN:HD22	1:A:271:ASN:N	1.93	0.59
1:B:314:LEU:HB3	1:D:294:ARG:HB3	1.85	0.59
1:C:76:VAL:HG23	1:C:77:MET:H	1.67	0.59
1:F:129:ILE:CD1	1:F:196:LYS:HB2	2.33	0.59
1:F:144:THR:O	1:F:148:GLN:HG3	2.03	0.59
1:C:221:LEU:HD11	1:D:221:LEU:HD22	1.83	0.59
1:B:206:VAL:HG13	1:B:241:PRO:HA	1.84	0.59
1:A:5:LYS:H	1:A:5:LYS:HD3	1.66	0.58
1:B:79:ARG:HG3	1:B:79:ARG:HH11	1.68	0.58
1:B:244:MET:HB2	1:D:122:ARG:NH1	2.18	0.58
1:E:143:LYS:O	1:E:147:GLU:HG3	2.04	0.58
1:B:227:ARG:HG2	1:E:227:ARG:CG	2.34	0.58
1:F:307:ARG:HG3	1:F:307:ARG:HH21	1.68	0.58
1:A:52:MET:HE2	1:A:97:ILE:HD13	1.85	0.58
1:B:143:LYS:HD3	1:B:175:TYR:CE2	2.38	0.58
1:B:182:VAL:CG1	1:B:186:ALA:HB3	2.34	0.58
1:F:120:ALA:HB1	1:F:148:GLN:OE1	2.04	0.58
1:F:313:ALA:HB3	1:F:316:TYR:CD2	2.39	0.58
1:F:251:ILE:N	1:F:251:ILE:HD12	2.19	0.57
1:E:292:THR:CG2	1:E:293:GLU:N	2.67	0.57
1:C:49:TRP:NE1	1:C:53:LYS:HE3	2.19	0.57
1:F:235:GLU:HG2	1:F:237:TYR:CZ	2.39	0.57
1:E:206:VAL:CG1	1:E:243:THR:HG22	2.34	0.57
1:E:34:GLN:O	1:E:38:GLU:HG3	2.04	0.57
1:E:236:THR:HG23	1:E:292:THR:CG2	2.34	0.57
1:F:240:HIS:HD2	1:F:241:PRO:HD2	1.68	0.57
1:E:183:VAL:HG12	1:E:185:SER:H	1.69	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:67:VAL:HG23	1:B:240:HIS:CE1	2.40	0.57
1:A:70:PRO:O	1:A:74:ARG:HG3	2.04	0.57
1:A:294:ARG:NH2	1:C:315:LYS:HD2	2.19	0.57
1:B:164:GLN:H	1:B:164:GLN:NE2	2.01	0.57
1:E:171:GLU:O	1:E:174:SER:HB3	2.05	0.57
1:F:199:MET:HE1	1:F:216:THR:HA	1.87	0.57
1:A:251:ILE:CG2	1:A:252:GLU:N	2.66	0.57
1:A:31:TYR:CE2	1:A:35:LEU:HD11	2.39	0.57
1:C:54:GLN:O	1:C:58:ILE:HG13	2.05	0.57
1:E:211:ILE:HD11	1:E:244:MET:CG	2.30	0.57
1:B:143:LYS:HD3	1:B:175:TYR:CZ	2.40	0.56
1:B:285:GLU:H	1:B:285:GLU:CD	2.08	0.56
1:F:242:GLU:HG2	1:F:243:THR:N	2.20	0.56
1:C:222:THR:O	1:C:226:HIS:HD2	1.87	0.56
1:E:292:THR:CG2	1:E:294:ARG:HG3	2.35	0.56
1:F:143:LYS:HZ3	1:F:143:LYS:HB2	1.69	0.56
1:D:6:GLU:HG3	1:D:39:LYS:HD2	1.86	0.56
1:F:70:PRO:O	1:F:74:ARG:HG3	2.04	0.56
1:C:3:VAL:CG1	1:C:8:LEU:HD11	2.35	0.56
1:B:17:MET:HE2	1:B:63:ARG:HD2	1.86	0.56
1:F:235:GLU:HA	1:F:293:GLU:OE1	2.06	0.56
4:D:636:HOH:O	1:F:296:ILE:HD13	2.06	0.56
1:A:34:GLN:O	1:A:38:GLU:HG3	2.05	0.56
1:A:271:ASN:ND2	1:A:271:ASN:H	2.03	0.56
1:F:114:ARG:HG3	1:F:114:ARG:NH1	2.21	0.56
1:E:138:ALA:HB1	1:E:198:VAL:HG12	1.87	0.56
1:B:70:PRO:HB2	1:B:74:ARG:NH1	2.20	0.56
1:F:260:ILE:HD12	1:F:274:VAL:HG11	1.88	0.55
1:C:82:ILE:HG23	1:C:83:ALA:N	2.21	0.55
1:D:40:SER:HB3	1:D:94:ARG:NH2	2.22	0.55
1:E:224:LYS:HE2	1:E:227:ARG:NH1	2.21	0.55
1:F:271:ASN:N	1:F:271:ASN:HD22	2.04	0.55
1:A:3:VAL:HG11	1:A:55:ALA:HA	1.88	0.55
1:E:195:ASP:O	1:E:196:LYS:HG3	2.06	0.55
1:D:297:ILE:HD13	1:D:305:ILE:CD1	2.37	0.55
1:F:44:ASN:C	1:F:44:ASN:HD22	2.08	0.55
1:A:218:LEU:HD22	1:B:218:LEU:HD22	1.89	0.55
1:C:4:VAL:HG12	1:C:36:GLN:OE1	2.07	0.55
1:D:133:CYS:HA	1:D:159:THR:HG21	1.88	0.55
1:C:270:LYS:H	1:C:270:LYS:CD	2.19	0.55
1:B:183:VAL:HG22	4:B:611:HOH:O	2.07	0.54
1:A:21:GLY:O	1:A:25:ILE:HG23	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:17:MET:HE1	1:B:63:ARG:HD2	1.89	0.54
1:B:17:MET:O	1:B:20:ARG:NH2	2.40	0.54
1:F:222:THR:O	1:F:226:HIS:HD2	1.89	0.54
1:D:145:ALA:O	1:D:150:LYS:HB2	2.07	0.54
1:A:107:ASN:HD21	1:C:315:LYS:HE2	1.72	0.54
1:D:313:ALA:HB3	1:D:315:LYS:HE3	1.90	0.54
1:F:99:ASN:O	1:F:103:GLU:HG3	2.07	0.54
1:A:243:THR:HG22	1:A:244:MET:N	2.23	0.54
1:A:67:VAL:HG13	1:A:240:HIS:CD2	2.42	0.54
1:E:4:VAL:HG22	1:E:36:GLN:OE1	2.07	0.54
1:F:20:ARG:O	1:F:24:LYS:HE3	2.08	0.54
1:F:305:ILE:O	1:F:309:GLU:HB2	2.07	0.54
1:A:49:TRP:HA	1:A:49:TRP:CE3	2.43	0.54
1:B:192:LYS:NZ	1:B:192:LYS:HB3	2.23	0.54
1:D:42:ALA:HB2	1:D:51:GLU:OE2	2.08	0.53
1:C:221:LEU:CD1	1:D:221:LEU:HD22	2.37	0.53
1:B:314:LEU:O	1:D:294:ARG:HD3	2.07	0.53
1:A:3:VAL:HG11	1:A:58:ILE:HD12	1.90	0.53
1:D:77:MET:HB3	1:D:319:PRO:HB2	1.90	0.53
1:A:158:GLU:HG3	1:A:181:TYR:OH	2.09	0.53
1:E:16:ASN:OD1	1:E:18:GLU:HG3	2.08	0.53
1:D:247:GLN:HG3	1:F:122:ARG:HE	1.74	0.53
1:C:213:LYS:HD3	1:C:214:ILE:H	1.74	0.53
1:C:8:LEU:HD12	1:C:8:LEU:N	2.21	0.53
1:F:6:GLU:O	1:F:9:GLU:HB3	2.08	0.53
1:A:52:MET:CE	1:A:97:ILE:HD13	2.39	0.53
1:E:143:LYS:NZ	1:E:175:TYR:HB3	2.23	0.53
1:C:4:VAL:CG1	1:C:7:VAL:HG23	2.39	0.53
1:A:15:LYS:C	1:A:17:MET:H	2.12	0.53
1:B:153:LYS:HD3	1:B:180:ILE:HD11	1.90	0.53
1:F:254:ARG:HB2	1:F:276:ASN:ND2	2.23	0.53
1:E:162:LYS:HZ3	1:E:258:GLU:HB3	1.74	0.53
1:F:146:TRP:CG	1:F:177:ILE:HG12	2.44	0.53
1:B:292:THR:HG22	1:B:293:GLU:N	2.24	0.52
1:F:132:HIS:CB	1:F:199:MET:HE3	2.38	0.52
1:C:242:GLU:HG2	1:C:243:THR:N	2.24	0.52
1:E:158:GLU:HG3	1:E:181:TYR:OH	2.09	0.52
1:D:318:GLU:CG	1:D:320:TRP:CZ2	2.93	0.52
1:F:307:ARG:NH2	1:F:307:ARG:HG3	2.25	0.52
1:B:133:CYS:HA	1:B:159:THR:HG21	1.90	0.52
1:D:143:LYS:HD2	1:D:175:TYR:CZ	2.45	0.52
1:A:160:ARG:HB3	1:B:183:VAL:HG21	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:79:ARG:NH2	1:D:79:ARG:HG3	2.25	0.52
1:F:4:VAL:HG12	1:F:5:LYS:N	2.25	0.52
1:B:67:VAL:HG23	1:B:240:HIS:ND1	2.25	0.52
1:D:254:ARG:HB2	1:D:276:ASN:ND2	2.25	0.52
1:E:254:ARG:HH11	1:E:254:ARG:HG3	1.75	0.52
1:B:50:LYS:O	1:B:54:GLN:HG3	2.10	0.52
1:C:164:GLN:NE2	1:C:164:GLN:N	2.51	0.52
1:A:294:ARG:HB2	1:C:314:LEU:HD13	1.92	0.52
1:E:196:LYS:HG2	1:E:229:TRP:HB3	1.92	0.52
1:D:227:ARG:HB3	1:D:227:ARG:HH11	1.75	0.52
1:A:54:GLN:O	1:A:58:ILE:HG13	2.10	0.52
1:D:222:THR:O	1:D:226:HIS:HD2	1.92	0.52
1:F:236:THR:N	1:F:293:GLU:OE1	2.34	0.52
1:C:161:PRO:HB3	1:C:259:VAL:HG22	1.92	0.52
1:A:183:VAL:HG21	1:B:160:ARG:CB	2.38	0.52
1:D:105:ILE:O	1:D:109:GLU:HG3	2.09	0.52
1:A:45:VAL:HG22	1:A:90:LEU:H	1.75	0.51
1:C:79:ARG:HH11	1:C:79:ARG:HG3	1.74	0.51
1:A:205:THR:HG21	1:A:244:MET:HG2	1.91	0.51
1:A:69:LEU:HB3	1:A:70:PRO:CD	2.41	0.51
1:C:287:VAL:HG13	1:C:299:PRO:HG2	1.93	0.51
1:C:235:GLU:HG3	1:C:237:TYR:CZ	2.46	0.51
1:B:224:LYS:HE3	1:B:227:ARG:HH12	1.76	0.51
1:A:6:GLU:HA	1:A:9:GLU:HG2	1.91	0.51
1:A:123:ILE:HD12	1:A:129:ILE:HD11	1.92	0.51
1:E:297:ILE:HD13	1:E:305:ILE:CD1	2.40	0.51
1:F:257:THR:HG23	1:F:261:PRO:HA	1.92	0.51
1:B:236:THR:HG23	1:B:292:THR:CG2	2.40	0.51
1:F:171:GLU:HG2	1:F:175:TYR:CE2	2.42	0.51
1:D:262:GLU:O	1:D:266:LYS:HG3	2.10	0.51
1:F:61:GLU:HA	1:F:64:PRO:HG3	1.92	0.51
1:C:8:LEU:CD1	1:C:8:LEU:H	2.20	0.51
1:A:49:TRP:HA	1:A:49:TRP:HE3	1.74	0.51
1:A:44:ASN:HB3	1:A:47:GLU:HB3	1.93	0.51
1:E:79:ARG:HH11	1:E:79:ARG:HG3	1.76	0.51
1:E:67:VAL:O	1:E:70:PRO:HD2	2.11	0.51
1:D:27:ARG:HD3	1:D:108:SER:OG	2.11	0.51
1:D:182:VAL:HG12	1:D:186:ALA:HB3	1.94	0.50
1:C:319:PRO:HG2	1:C:320:TRP:CE3	2.47	0.50
1:C:48:PHE:O	1:C:51:GLU:HB3	2.10	0.50
1:B:214:ILE:HD12	1:B:280:ASP:HB3	1.94	0.50
1:E:206:VAL:HG12	1:E:243:THR:HG22	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:44:ASN:ND2	1:F:47:GLU:H	2.09	0.50
1:E:292:THR:HG22	1:E:293:GLU:N	2.27	0.50
1:E:186:ALA:HB2	1:F:214:ILE:CD1	2.34	0.50
1:E:213:LYS:HD3	1:E:278:ALA:O	2.10	0.50
1:F:45:VAL:HG22	1:F:90:LEU:N	2.27	0.50
1:C:69:LEU:HB3	1:C:70:PRO:CD	2.42	0.50
1:C:49:TRP:CD1	1:C:53:LYS:HE3	2.47	0.50
1:F:45:VAL:HG11	1:F:88:ALA:O	2.12	0.50
1:A:44:ASN:HB3	1:A:47:GLU:CB	2.41	0.50
1:F:207:ASN:ND2	1:F:245:LEU:HD22	2.26	0.50
1:C:69:LEU:HB3	1:C:70:PRO:HD3	1.93	0.50
1:D:20:ARG:O	1:D:24:LYS:HE2	2.12	0.50
1:B:316:TYR:OH	1:D:107:ASN:ND2	2.44	0.50
1:C:13:LYS:CB	1:C:19:ILE:HG12	2.42	0.50
1:A:164:GLN:NE2	1:A:164:GLN:N	2.54	0.49
1:A:6:GLU:HA	1:A:9:GLU:OE2	2.12	0.49
1:B:314:LEU:HD11	1:D:297:ILE:CG2	2.42	0.49
1:C:76:VAL:CG2	1:C:77:MET:N	2.74	0.49
1:C:270:LYS:N	1:C:270:LYS:HD2	2.27	0.49
1:C:4:VAL:HG13	1:C:7:VAL:HG23	1.93	0.49
1:A:181:TYR:CE2	1:B:260:ILE:HD11	2.47	0.49
1:E:251:ILE:N	1:E:251:ILE:HD13	2.27	0.49
1:E:260:ILE:HG13	1:E:268:TRP:CH2	2.47	0.49
1:E:143:LYS:HZ2	1:E:175:TYR:HB3	1.76	0.49
1:F:293:GLU:CD	1:F:293:GLU:H	2.15	0.49
1:F:222:THR:HG22	1:F:226:HIS:CD2	2.47	0.49
1:A:17:MET:HG2	1:A:20:ARG:HD2	1.93	0.49
1:F:63:ARG:N	1:F:64:PRO:HD3	2.27	0.49
1:E:152:ILE:H	1:E:152:ILE:HD13	1.77	0.49
1:B:292:THR:CG2	1:B:293:GLU:N	2.75	0.49
1:A:243:THR:HG22	1:A:244:MET:H	1.77	0.49
1:D:45:VAL:HG11	1:D:88:ALA:O	2.13	0.49
1:B:285:GLU:HG3	4:D:604:HOH:O	2.12	0.49
1:E:251:ILE:HG12	1:E:252:GLU:N	2.27	0.49
1:F:196:LYS:HD3	1:F:229:TRP:HB3	1.94	0.49
1:C:10:ILE:CG2	1:C:28:SER:HB3	2.43	0.49
1:A:9:GLU:O	1:A:13:LYS:HG3	2.13	0.49
1:F:313:ALA:HB3	1:F:316:TYR:HD2	1.76	0.49
1:E:25:ILE:HD11	1:E:63:ARG:HH11	1.77	0.49
1:E:135:SER:OG	1:E:200:GLY:HA3	2.13	0.49
1:C:212:ASN:O	1:C:279:PHE:HB3	2.12	0.49
1:F:242:GLU:HG2	1:F:243:THR:H	1.77	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:4:VAL:HG13	1:A:36:GLN:OE1	2.12	0.48
1:D:182:VAL:HG11	1:D:186:ALA:HB3	1.95	0.48
1:A:267:THR:HG22	1:A:268:TRP:HD1	1.78	0.48
1:F:69:LEU:HB3	1:F:70:PRO:CD	2.43	0.48
1:A:10:ILE:O	1:A:14:ILE:HG13	2.13	0.48
1:C:255:ASP:O	1:C:258:GLU:HB2	2.12	0.48
1:B:314:LEU:HD22	1:D:294:ARG:O	2.13	0.48
1:C:76:VAL:CG2	1:C:77:MET:H	2.26	0.48
1:C:5:LYS:O	1:C:9:GLU:HB2	2.14	0.48
1:D:40:SER:HB3	1:D:94:ARG:HH21	1.79	0.48
1:F:23:GLY:HA3	1:F:27:ARG:HH12	1.78	0.48
1:B:162:LYS:HE2	1:B:164:GLN:OE1	2.13	0.48
1:A:211:ILE:HD13	1:A:251:ILE:HD11	1.95	0.48
1:F:162:LYS:HE2	1:F:164:GLN:OE1	2.13	0.48
1:D:4:VAL:HG12	1:D:6:GLU:HG2	1.96	0.48
1:C:133:CYS:HA	1:C:159:THR:HG21	1.95	0.48
1:A:145:ALA:O	1:A:150:LYS:HB2	2.13	0.48
1:B:78:HIS:CE1	1:B:311:GLY:HA3	2.48	0.48
1:C:102:LYS:O	1:C:102:LYS:HD3	2.14	0.48
1:C:314:LEU:O	1:C:316:TYR:N	2.46	0.48
1:E:314:LEU:HD23	1:E:314:LEU:H	1.77	0.48
1:C:101:ALA:O	1:C:105:ILE:HG13	2.14	0.48
1:D:4:VAL:CG1	1:D:6:GLU:HG2	2.43	0.47
1:C:269:PRO:HD2	1:C:272:ILE:HD12	1.95	0.47
1:C:307:ARG:HG2	1:C:312:TRP:O	2.13	0.47
1:A:159:THR:O	1:A:159:THR:HG22	2.12	0.47
1:E:156:VAL:HG23	1:E:179:VAL:HG13	1.96	0.47
1:F:253:MET:CE	1:F:277:PRO:HA	2.44	0.47
1:C:3:VAL:HG13	1:C:8:LEU:HD11	1.96	0.47
1:B:105:ILE:O	1:B:109:GLU:HG3	2.14	0.47
1:C:270:LYS:N	1:C:270:LYS:CD	2.77	0.47
1:A:186:ALA:HA	1:B:214:ILE:HD11	1.96	0.47
1:B:291:ILE:HD13	1:B:296:ILE:HG12	1.94	0.47
1:F:9:GLU:O	1:F:12:GLU:HB2	2.14	0.47
1:A:17:MET:C	1:A:19:ILE:H	2.16	0.47
1:D:182:VAL:HG12	1:D:183:VAL:N	2.29	0.47
1:D:52:MET:CE	1:D:97:ILE:HG21	2.45	0.47
1:B:79:ARG:HG3	1:B:79:ARG:NH1	2.30	0.47
1:A:257:THR:HA	1:A:260:ILE:O	2.14	0.47
1:B:278:ALA:HA	4:B:668:HOH:O	2.14	0.47
1:F:20:ARG:HA	1:F:25:ILE:HD11	1.97	0.47
1:F:199:MET:HE1	1:F:216:THR:CG2	2.39	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:VAL:HG11	1:A:88:ALA:O	2.15	0.47
1:B:70:PRO:HB2	1:B:74:ARG:HH12	1.80	0.47
1:A:122:ARG:CZ	1:C:243:THR:HG22	2.45	0.46
1:D:45:VAL:HG22	1:D:90:LEU:HB2	1.96	0.46
1:C:49:TRP:HA	1:C:49:TRP:CE3	2.50	0.46
1:F:271:ASN:ND2	1:F:271:ASN:N	2.62	0.46
1:C:65:THR:HG23	1:C:66:ALA:N	2.30	0.46
1:E:3:VAL:HG21	1:E:58:ILE:HD12	1.98	0.46
1:F:132:HIS:HB2	1:F:199:MET:HE3	1.97	0.46
1:B:247:GLN:HG3	1:B:247:GLN:O	2.15	0.46
1:B:78:HIS:CG	1:B:311:GLY:HA3	2.50	0.46
4:E:619:HOH:O	1:F:182:VAL:HG23	2.15	0.46
1:E:294:ARG:C	1:E:294:ARG:HE	2.19	0.46
1:B:206:VAL:CG1	1:B:241:PRO:HA	2.44	0.46
1:C:16:ASN:O	1:C:17:MET:HB2	2.16	0.46
1:C:318:GLU:HG3	1:C:319:PRO:HD2	1.97	0.46
1:F:129:ILE:HD12	1:F:196:LYS:HB2	1.98	0.46
1:F:31:TYR:CZ	1:F:35:LEU:HD21	2.51	0.46
1:C:241:PRO:HA	1:C:306:LEU:CD1	2.46	0.46
1:F:4:VAL:CG1	1:F:5:LYS:N	2.78	0.46
1:D:84:TYR:C	1:D:86:SER:H	2.19	0.46
1:F:162:LYS:HB2	1:F:164:GLN:HE22	1.81	0.46
1:C:262:GLU:O	1:C:266:LYS:HG2	2.16	0.46
1:F:260:ILE:HD13	1:F:268:TRP:CZ3	2.51	0.46
1:A:211:ILE:HG21	1:A:251:ILE:HD12	1.97	0.46
1:D:52:MET:HE1	1:D:97:ILE:HG21	1.98	0.45
1:D:42:ALA:HA	1:D:47:GLU:OE2	2.16	0.45
1:C:263:ASP:OD2	1:C:264:GLU:N	2.49	0.45
1:E:318:GLU:CG	1:E:319:PRO:HD2	2.36	0.45
1:E:254:ARG:HG3	1:E:254:ARG:NH1	2.31	0.45
1:D:36:GLN:O	1:D:40:SER:HB2	2.16	0.45
1:C:40:SER:HB2	1:C:51:GLU:OE2	2.16	0.45
1:D:236:THR:N	1:D:293:GLU:OE2	2.47	0.45
1:F:170:LYS:O	1:F:173:ALA:HB3	2.17	0.45
1:F:253:MET:HE2	1:F:277:PRO:CA	2.46	0.45
1:C:8:LEU:O	1:C:12:GLU:HG3	2.16	0.45
1:B:0:HIS:HE1	1:B:51:GLU:OE2	2.00	0.45
1:B:289:VAL:HB	1:B:296:ILE:HG23	1.98	0.45
1:D:16:ASN:O	1:D:17:MET:HB2	2.17	0.45
2:E:401:PEG:H21	2:E:401:PEG:H42	1.73	0.45
1:D:77:MET:CB	1:D:319:PRO:HB2	2.46	0.45
1:E:271:ASN:HD21	1:F:173:ALA:CA	2.30	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:195:ASP:C	1:E:196:LYS:HG3	2.37	0.45
1:A:95:PHE:O	1:A:99:ASN:HB2	2.17	0.45
1:A:25:ILE:HG13	1:A:26:ALA:N	2.27	0.45
1:A:25:ILE:HD11	1:A:69:LEU:HB2	1.99	0.45
1:F:57:LYS:O	1:F:61:GLU:HG3	2.17	0.45
1:C:45:VAL:HG11	1:C:88:ALA:O	2.16	0.45
1:B:89:ASP:H	1:B:92:GLN:HE21	1.63	0.45
1:C:49:TRP:HA	1:C:49:TRP:HE3	1.82	0.45
1:F:206:VAL:CG1	1:F:241:PRO:HA	2.46	0.45
1:A:11:ALA:HB1	1:A:62:THR:HG21	1.99	0.45
1:D:34:GLN:O	1:D:38:GLU:HG3	2.17	0.45
1:B:224:LYS:HD2	2:B:401:PEG:H31	1.98	0.45
1:C:214:ILE:HD11	1:D:186:ALA:HA	1.99	0.45
1:D:317:THR:O	1:D:317:THR:HG22	2.17	0.45
1:A:107:ASN:HD21	1:C:315:LYS:CE	2.30	0.45
1:F:6:GLU:N	1:F:6:GLU:OE1	2.49	0.45
1:D:307:ARG:HD2	1:D:308:GLU:OE1	2.17	0.45
1:F:91:GLU:OE1	1:F:94:ARG:NH1	2.50	0.45
1:E:262:GLU:O	1:E:266:LYS:HG3	2.17	0.45
1:E:143:LYS:HE2	1:E:147:GLU:CG	2.46	0.44
1:C:221:LEU:HD13	1:D:221:LEU:CD1	2.43	0.44
1:C:35:LEU:C	1:C:37:ALA:N	2.71	0.44
1:B:144:THR:O	1:B:148:GLN:HG3	2.17	0.44
1:F:210:VAL:HG21	1:F:232:ILE:HG13	1.99	0.44
1:C:26:ALA:HB2	1:C:68:SER:HB2	1.98	0.44
1:F:23:GLY:O	1:F:26:ALA:HB3	2.17	0.44
1:B:207:ASN:OD1	1:D:298:PRO:HB3	2.16	0.44
1:C:33:LEU:HD11	1:C:73:LEU:HG	1.98	0.44
1:B:70:PRO:O	1:B:74:ARG:HG3	2.18	0.44
1:B:78:HIS:CD2	1:B:311:GLY:HA3	2.53	0.44
1:D:206:VAL:HG13	1:D:241:PRO:HA	1.98	0.44
1:B:206:VAL:HG13	1:B:241:PRO:C	2.36	0.44
1:C:79:ARG:C	1:C:82:ILE:HG22	2.37	0.44
1:E:314:LEU:CD2	1:E:314:LEU:H	2.29	0.44
1:D:26:ALA:HB2	1:D:68:SER:HB2	1.99	0.44
1:F:239:PHE:CD2	1:F:239:PHE:N	2.84	0.44
1:E:164:GLN:N	1:E:164:GLN:HE21	2.05	0.44
1:B:153:LYS:HD3	1:B:180:ILE:CD1	2.47	0.44
1:B:26:ALA:HB2	1:B:68:SER:HB2	2.00	0.44
1:D:1:MET:HA	1:D:54:GLN:HE21	1.82	0.44
1:E:181:TYR:CE2	1:F:260:ILE:HD11	2.52	0.44
1:A:59:LEU:O	1:A:69:LEU:HD21	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:15:LYS:C	1:A:17:MET:N	2.71	0.44
1:E:177:ILE:O	1:E:179:VAL:HG23	2.18	0.44
1:F:15:LYS:HB2	1:F:62:THR:HB	1.99	0.44
1:D:45:VAL:O	1:D:45:VAL:HG12	2.18	0.44
1:F:182:VAL:HG22	1:F:186:ALA:HB3	1.98	0.44
1:E:159:THR:HG22	1:E:159:THR:O	2.18	0.44
1:F:297:ILE:HD13	1:F:305:ILE:CD1	2.48	0.44
1:C:241:PRO:HA	1:C:306:LEU:HD13	2.00	0.44
1:E:204:ILE:HD12	1:E:210:VAL:HG22	2.00	0.44
1:D:89:ASP:CG	1:D:90:LEU:N	2.72	0.43
1:A:133:CYS:HA	1:A:159:THR:HG21	2.00	0.43
1:C:114:ARG:O	1:C:117:GLU:HB3	2.18	0.43
1:E:160:ARG:HB2	1:F:183:VAL:HG21	2.01	0.43
1:B:50:LYS:HE3	1:B:50:LYS:HB2	1.86	0.43
1:C:135:SER:O	1:C:139:ILE:HG13	2.18	0.43
1:F:125:ASP:OD1	1:F:151:ASP:N	2.48	0.43
1:E:268:TRP:H	1:E:268:TRP:HD1	1.64	0.43
1:B:88:ALA:HB1	1:B:92:GLN:HB2	2.00	0.43
1:C:160:ARG:HB3	1:C:161:PRO:HA	2.00	0.43
1:E:297:ILE:HD13	1:E:305:ILE:HD11	2.00	0.43
1:C:158:GLU:HG3	1:C:181:TYR:OH	2.17	0.43
1:E:221:LEU:HD13	1:F:221:LEU:HD13	2.01	0.43
1:B:52:MET:HG2	1:B:97:ILE:CD1	2.48	0.43
1:A:6:GLU:HA	1:A:9:GLU:CG	2.48	0.43
1:A:16:ASN:HB2	1:A:18:GLU:HG3	2.00	0.43
1:A:224:LYS:HG3	1:A:286:TYR:CD1	2.54	0.43
1:C:35:LEU:C	1:C:37:ALA:H	2.22	0.43
1:F:283:PRO:HB3	1:F:285:GLU:OE2	2.19	0.43
1:C:153:LYS:HE2	1:C:180:ILE:HD11	1.99	0.43
1:E:313:ALA:HB3	1:E:315:LYS:HG2	2.00	0.43
1:F:52:MET:CE	1:F:97:ILE:HG21	2.49	0.43
1:F:263:ASP:HA	1:F:266:LYS:CD	2.48	0.43
1:C:40:SER:H	1:C:94:ARG:NH2	2.16	0.43
1:E:131:THR:OG1	1:E:132:HIS:N	2.52	0.43
1:B:307:ARG:HH11	1:B:307:ARG:HG3	1.83	0.43
1:B:292:THR:HG23	1:B:293:GLU:OE1	2.19	0.43
1:A:271:ASN:ND2	1:A:271:ASN:N	2.64	0.43
1:E:119:GLY:CA	1:E:291:ILE:HD13	2.48	0.43
1:A:288:ASP:OD1	2:A:401:PEG:H31	2.19	0.43
1:B:153:LYS:HA	1:B:178:PRO:HG2	1.99	0.43
1:F:204:ILE:HD12	1:F:210:VAL:HG22	2.01	0.43
1:D:46:ASP:O	1:D:50:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:69:LEU:O	1:A:73:LEU:HD22	2.19	0.43
1:C:319:PRO:HG2	1:C:320:TRP:HE3	1.84	0.43
1:D:65:THR:O	1:D:66:ALA:C	2.56	0.43
1:B:134:HIS:HE1	1:B:171:GLU:OE1	2.02	0.43
1:A:4:VAL:HG22	1:A:7:VAL:HG23	2.01	0.42
1:C:314:LEU:HA	1:C:314:LEU:HD23	1.82	0.42
1:D:318:GLU:HG3	1:D:320:TRP:CH2	2.54	0.42
1:E:146:TRP:HB2	1:E:152:ILE:HD11	2.01	0.42
1:A:48:PHE:HB2	1:A:90:LEU:CD1	2.49	0.42
1:D:4:VAL:HG12	1:D:5:LYS:N	2.33	0.42
1:C:318:GLU:HG2	1:C:320:TRP:CZ2	2.53	0.42
1:D:139:ILE:HA	1:D:142:MET:HE3	2.01	0.42
1:A:160:ARG:CB	1:B:183:VAL:HG21	2.49	0.42
1:A:17:MET:C	1:A:19:ILE:N	2.73	0.42
1:E:275:TRP:CH2	1:F:180:ILE:HD13	2.55	0.42
1:F:143:LYS:HD3	1:F:175:TYR:CE1	2.54	0.42
1:C:4:VAL:CG2	1:C:6:GLU:HG2	2.50	0.42
1:E:268:TRP:CD1	1:E:268:TRP:N	2.88	0.42
1:A:78:HIS:CG	1:A:311:GLY:HA3	2.54	0.42
1:C:313:ALA:O	1:C:316:TYR:HB2	2.18	0.42
1:C:268:TRP:HA	1:C:269:PRO:HD3	1.88	0.42
1:D:245:LEU:HA	1:D:281:VAL:HG11	2.02	0.42
1:C:211:ILE:HD11	1:C:244:MET:CG	2.48	0.42
1:C:270:LYS:H	1:C:270:LYS:HD2	1.85	0.42
1:A:49:TRP:NE1	1:A:53:LYS:HE3	2.34	0.42
1:E:152:ILE:N	1:E:152:ILE:HD13	2.34	0.42
1:D:182:VAL:CG1	1:D:183:VAL:N	2.83	0.42
1:B:257:THR:HA	1:B:260:ILE:O	2.20	0.42
1:A:36:GLN:O	1:A:40:SER:HB2	2.20	0.42
1:E:69:LEU:HB3	1:E:70:PRO:CD	2.46	0.42
1:F:303:ILE:O	1:F:307:ARG:HG2	2.19	0.42
1:A:267:THR:O	1:A:267:THR:CG2	2.67	0.42
1:B:222:THR:O	1:B:226:HIS:HD2	2.01	0.42
1:D:164:GLN:NE2	1:D:164:GLN:N	2.61	0.42
1:F:132:HIS:HA	1:F:157:THR:OG1	2.19	0.42
1:A:52:MET:HG3	1:A:97:ILE:CD1	2.50	0.42
1:F:162:LYS:HD3	1:F:258:GLU:OE2	2.20	0.42
1:D:44:ASN:C	1:D:90:LEU:HD13	2.40	0.42
1:D:11:ALA:HB1	1:D:62:THR:CG2	2.50	0.42
1:E:143:LYS:HZ2	1:E:175:TYR:CB	2.33	0.41
1:F:129:ILE:HD13	1:F:196:LYS:HB2	2.02	0.41
1:B:206:VAL:HG22	1:B:242:GLU:O	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:283:PRO:HD2	1:A:286:TYR:CD2	2.55	0.41
1:A:49:TRP:CZ2	1:A:81:LYS:HA	2.56	0.41
1:E:146:TRP:HE3	1:E:152:ILE:HD13	1.84	0.41
1:C:199:MET:CE	1:C:216:THR:HG23	2.51	0.41
1:F:44:ASN:ND2	1:F:44:ASN:C	2.74	0.41
1:E:288:ASP:O	1:E:299:PRO:HD3	2.20	0.41
1:D:67:VAL:O	1:D:70:PRO:HD2	2.20	0.41
1:D:318:GLU:HA	1:D:319:PRO:HD3	1.96	0.41
1:B:314:LEU:HB3	1:D:294:ARG:CB	2.48	0.41
1:B:8:LEU:O	1:B:12:GLU:HG2	2.20	0.41
1:A:222:THR:O	1:A:226:HIS:HD2	2.04	0.41
1:B:224:LYS:HA	2:B:401:PEG:H31	2.02	0.41
1:C:33:LEU:HD13	1:C:76:VAL:HG21	2.02	0.41
1:A:49:TRP:CE2	1:A:53:LYS:HE3	2.56	0.41
1:F:239:PHE:HD2	1:F:239:PHE:N	2.18	0.41
1:F:31:TYR:CE2	1:F:35:LEU:HD11	2.56	0.41
1:F:132:HIS:HB3	1:F:199:MET:CE	2.51	0.41
1:B:227:ARG:HG2	1:E:227:ARG:HG2	2.02	0.41
1:A:183:VAL:HG22	4:A:603:HOH:O	2.21	0.41
1:B:4:VAL:HG12	1:B:6:GLU:HG2	2.03	0.41
1:C:90:LEU:O	1:C:94:ARG:HB2	2.21	0.41
1:A:16:ASN:CB	1:A:18:GLU:HG3	2.50	0.41
1:B:269:PRO:C	1:B:271:ASN:N	2.74	0.41
1:C:210:VAL:HG21	1:C:232:ILE:HG13	2.03	0.41
1:F:206:VAL:HG22	1:F:242:GLU:O	2.21	0.41
1:F:31:TYR:O	1:F:34:GLN:N	2.54	0.41
1:F:235:GLU:HG2	1:F:237:TYR:OH	2.21	0.40
1:F:145:ALA:O	1:F:148:GLN:HB2	2.20	0.40
1:B:106:HIS:O	1:B:110:LYS:HG2	2.20	0.40
1:B:227:ARG:HE	1:E:227:ARG:CG	2.28	0.40
1:C:7:VAL:C	1:C:9:GLU:N	2.75	0.40
1:B:291:ILE:CD1	1:B:296:ILE:HG12	2.52	0.40
1:C:65:THR:HG23	1:C:66:ALA:H	1.85	0.40
1:D:160:ARG:HD2	1:D:161:PRO:HA	2.02	0.40
1:C:90:LEU:HD21	1:C:94:ARG:HH11	1.87	0.40
1:F:45:VAL:HG13	1:F:90:LEU:HA	2.03	0.40
1:E:101:ALA:O	1:E:105:ILE:HG13	2.22	0.40
1:C:22:ALA:HB2	4:C:625:HOH:O	2.20	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	318/338 (94%)	302 (95%)	14 (4%)	2 (1%)	33	55
1	B	318/338 (94%)	307 (96%)	11 (4%)	0	100	100
1	C	313/338 (93%)	287 (92%)	24 (8%)	2 (1%)	33	55
1	D	316/338 (94%)	296 (94%)	18 (6%)	2 (1%)	33	55
1	E	313/338 (93%)	301 (96%)	12 (4%)	0	100	100
1	F	315/338 (93%)	289 (92%)	23 (7%)	3 (1%)	22	38
All	All	1893/2028 (93%)	1782 (94%)	102 (5%)	9 (0%)	38	60

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	F	245	LEU
1	A	252	GLU
1	D	42	ALA
1	C	314	LEU
1	C	315	LYS
1	F	4	VAL
1	F	64	PRO
1	D	269	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	268/284 (94%)	253 (94%)	15 (6%)	30	51
1	B	268/284 (94%)	254 (95%)	14 (5%)	32	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	264/284 (93%)	255 (97%)	9 (3%)	49 75
1	D	265/284 (93%)	252 (95%)	13 (5%)	35 59
1	E	264/284 (93%)	248 (94%)	16 (6%)	26 46
1	F	266/284 (94%)	253 (95%)	13 (5%)	35 59
All	All	1595/1704 (94%)	1515 (95%)	80 (5%)	34 58

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	20	ARG
1	A	25	ILE
1	A	49	TRP
1	A	89	ASP
1	A	151	ASP
1	A	164	GLN
1	A	221	LEU
1	A	240	HIS
1	A	242	GLU
1	A	263	ASP
1	A	267	THR
1	A	270	LYS
1	A	271	ASN
1	A	309	GLU
1	B	6	GLU
1	B	17	MET
1	B	90	LEU
1	B	117	GLU
1	B	164	GLN
1	B	192	LYS
1	B	206	VAL
1	B	218	LEU
1	B	221	LEU
1	B	240	HIS
1	B	270	LYS
1	B	271	ASN
1	B	293	GLU
1	B	308	GLU
1	C	17	MET
1	C	91	GLU
1	C	164	GLN

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Mol	Chain	Res	Type
1	C	221	LEU
1	C	240	HIS
1	C	243	THR
1	C	270	LYS
1	C	309	GLU
1	C	314	LEU
1	D	50	LYS
1	D	117	GLU
1	D	164	GLN
1	D	206	VAL
1	D	214	ILE
1	D	221	LEU
1	D	227	ARG
1	D	254	ARG
1	D	293	GLU
1	D	308	GLU
1	D	316	TYR
1	D	317	THR
1	D	318	GLU
1	E	69	LEU
1	E	73	LEU
1	E	107	ASN
1	E	117	GLU
1	E	122	ARG
1	E	143	LYS
1	E	152	ILE
1	E	164	GLN
1	E	185	SER
1	E	218	LEU
1	E	221	LEU
1	E	224	LYS
1	E	251	ILE
1	E	287	VAL
1	E	294	ARG
1	E	316	TYR
1	F	6	GLU
1	F	39	LYS
1	F	44	ASN
1	F	45	VAL
1	F	79	ARG
1	F	164	GLN
1	F	221	LEU

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Mol	Chain	Res	Type
1	F	245	LEU
1	F	262	GLU
1	F	280	ASP
1	F	293	GLU
1	F	296	ILE
1	F	303	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	107	ASN
1	A	134	HIS
1	A	164	GLN
1	A	207	ASN
1	A	226	HIS
1	A	240	HIS
1	A	271	ASN
1	B	0	HIS
1	B	54	GLN
1	B	92	GLN
1	B	132	HIS
1	B	134	HIS
1	B	164	GLN
1	B	226	HIS
1	B	247	GLN
1	B	271	ASN
1	C	92	GLN
1	C	106	HIS
1	C	164	GLN
1	C	226	HIS
1	D	34	GLN
1	D	92	GLN
1	D	99	ASN
1	D	107	ASN
1	D	134	HIS
1	D	164	GLN
1	D	189	HIS
1	D	226	HIS
1	D	247	GLN
1	E	44	ASN
1	E	164	GLN

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Mol	Chain	Res	Type
1	E	226	HIS
1	F	44	ASN
1	F	54	GLN
1	F	164	GLN
1	F	189	HIS
1	F	207	ASN
1	F	226	HIS
1	F	240	HIS
1	F	271	ASN

### 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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	PEG	A	401	-	6,6,6	0.52	0	5,5,5	0.43	0
2	PEG	B	401	-	6,6,6	0.53	0	5,5,5	0.42	0
2	PEG	C	401	-	6,6,6	0.53	0	5,5,5	0.44	0
2	PEG	D	401	-	6,6,6	0.53	0	5,5,5	0.35	0
2	PEG	E	401	-	6,6,6	0.53	0	5,5,5	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PEG	F	401	-	6,6,6	0.52	0	5,5,5	0.47	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	PEG	A	401	-	-	0/4/4/4	0/0/0/0
2	PEG	B	401	-	-	0/4/4/4	0/0/0/0
2	PEG	C	401	-	-	0/4/4/4	0/0/0/0
2	PEG	D	401	-	-	0/4/4/4	0/0/0/0
2	PEG	E	401	-	-	0/4/4/4	0/0/0/0
2	PEG	F	401	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	320/338 (94%)	0.06	13 (4%) 35 36	14, 36, 87, 104	0
1	B	322/338 (95%)	-0.24	4 (1%) 75 77	12, 29, 56, 82	0
1	C	317/338 (93%)	0.50	44 (13%) 4 3	20, 51, 109, 122	0
1	D	320/338 (94%)	0.08	14 (4%) 33 34	16, 37, 78, 115	0
1	E	317/338 (93%)	-0.02	6 (1%) 64 66	24, 42, 68, 92	0
1	F	319/338 (94%)	0.21	11 (3%) 43 44	25, 48, 79, 111	0
All	All	1915/2028 (94%)	0.10	92 (4%) 28 30	12, 41, 86, 122	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	248	LEU	6.8
1	C	93	LEU	6.3
1	D	249	VAL	6.1
1	C	3	VAL	5.8
1	C	49	TRP	5.4
1	C	246	GLY	5.3
1	D	316	TYR	4.6
1	E	316	TYR	4.6
1	C	31	TYR	4.1
1	A	8	LEU	4.0
1	C	245	LEU	4.0
1	C	48	PHE	3.7
1	F	249	VAL	3.7
1	D	92	GLN	3.7
1	C	322	ASP	3.7
1	C	14	ILE	3.5
1	F	16	ASN	3.5
1	A	247	GLN	3.4
1	C	42	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	98	ILE	3.4
1	C	33	LEU	3.3
1	D	245	LEU	3.3
1	C	43	THR	3.3
1	C	94	ARG	3.3
1	C	90	LEU	3.2
1	A	10	ILE	3.2
1	C	96	VAL	3.2
1	F	322	ASP	3.1
1	C	100	ALA	3.0
1	A	248	LEU	3.0
1	C	2	ALA	3.0
1	A	14	ILE	3.0
1	C	65	THR	3.0
1	C	92	GLN	2.9
1	E	251	ILE	2.9
1	C	95	PHE	2.9
1	D	1	MET	2.8
1	C	17	MET	2.8
1	C	44	ASN	2.8
1	A	54	GLN	2.8
1	C	50	LYS	2.8
1	A	249	VAL	2.8
1	F	8	LEU	2.8
1	F	19	ILE	2.7
1	E	175	TYR	2.7
1	C	91	GLU	2.7
1	C	59	LEU	2.7
1	B	316	TYR	2.6
1	D	89	ASP	2.6
1	C	58	ILE	2.6
1	C	20	ARG	2.6
1	C	175	TYR	2.6
1	A	322	ASP	2.6
1	E	314	LEU	2.5
1	F	175	TYR	2.5
1	C	15	LYS	2.5
1	C	251	ILE	2.4
1	F	43	THR	2.4
1	D	322	ASP	2.4
1	D	270	LYS	2.4
1	E	246	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	245	LEU	2.4
1	F	12	GLU	2.3
1	C	56	ALA	2.3
1	A	3	VAL	2.3
1	C	54	GLN	2.3
1	C	7	VAL	2.3
1	D	49	TRP	2.3
1	D	2	ALA	2.3
1	D	84	TYR	2.3
1	A	316	TYR	2.2
1	C	45	VAL	2.2
1	F	2	ALA	2.2
1	C	99	ASN	2.2
1	C	8	LEU	2.2
1	C	66	ALA	2.2
1	D	247	GLN	2.2
1	C	84	TYR	2.2
1	F	54	GLN	2.1
1	C	240	HIS	2.1
1	D	90	LEU	2.1
1	C	6	GLU	2.1
1	A	7	VAL	2.1
1	A	317	THR	2.1
1	C	12	GLU	2.1
1	C	102	LYS	2.1
1	B	322	ASP	2.1
1	C	314	LEU	2.1
1	A	19	ILE	2.0
1	E	270	LYS	2.0
1	F	3	VAL	2.0
1	B	247	GLN	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
3	MG	E	411	1/1	0.43	19.23	56,56,56,56	0
3	MG	B	411	1/1	0.43	12.55	51,51,51,51	0
2	PEG	D	401	7/7	0.38	11.62	48,49,62,62	0
2	PEG	E	401	7/7	0.30	5.60	51,53,55,55	0
2	PEG	B	401	7/7	0.27	3.97	56,58,60,62	0
2	PEG	C	401	7/7	0.36	3.87	49,59,63,67	0
2	PEG	A	401	7/7	0.34	2.14	40,51,58,59	0
2	PEG	F	401	7/7	0.25	1.29	45,53,64,64	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.