



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 12:03 PM BST

PDB ID : 3KUM  
Title : Crystal structure of Dipeptide Epimerase from *Enterococcus faecalis* V583 complexed with Mg and dipeptide L-Arg-L-Tyr  
Authors : Fedorov, A.A.; Fedorov, E.V.; Sakai, A.; Gerlt, J.A.; Almo, S.C.  
Deposited on : 2009-11-27  
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

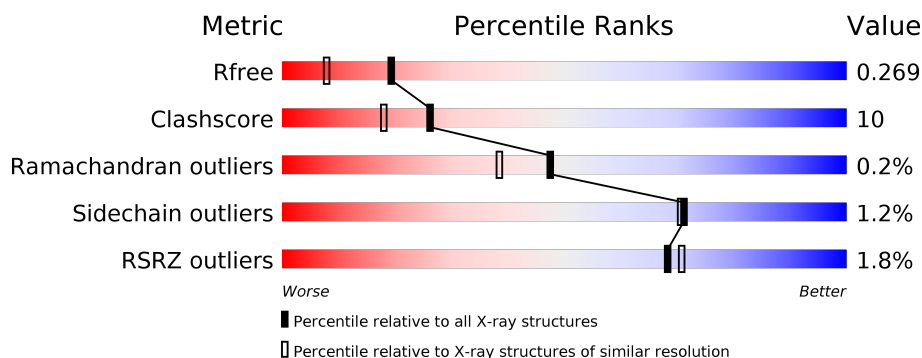
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	354	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>18%</div> </div> </div>
1	B	354	<div> <div></div> <div> <div>85%</div> <div>14%</div> </div> </div>
1	C	354	<div> <div></div> <div> <div>80%</div> <div>19%</div> </div> </div>
1	D	354	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>29%</div> </div> </div>
1	E	354	<div> <div></div> <div> <div>79%</div> <div>21%</div> </div> </div>
1	F	354	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>25%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	354	<div><div></div><div>2%</div><div>79%</div><div>21%</div><div></div></div>
1	H	354	<div><div></div><div>84%</div><div>14%</div><div></div></div>

## 2 Entry composition

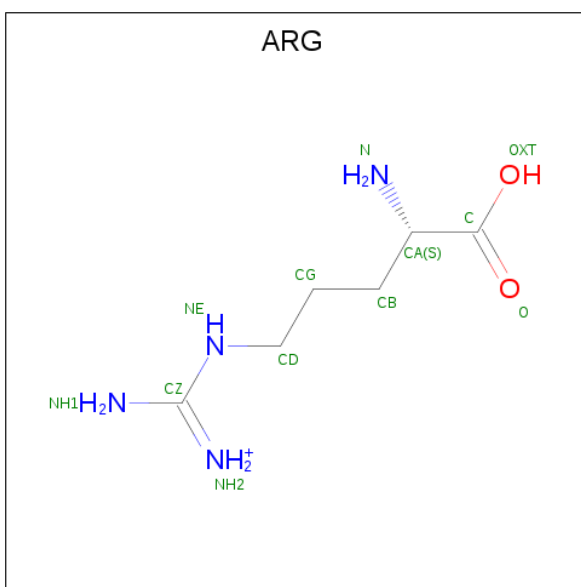
There are 5 unique types of molecules in this entry. The entry contains 22146 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dipeptide Epimerase.

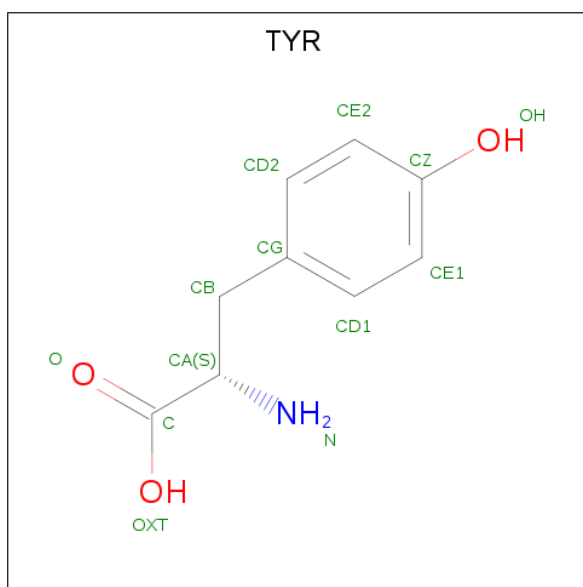
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2649	1680	437	518	14			
1	B	353	Total	C	N	O	S	0	0	0
			2638	1674	434	516	14			
1	C	354	Total	C	N	O	S	0	0	0
			2649	1680	437	518	14			
1	D	354	Total	C	N	O	S	0	0	0
			2649	1680	437	518	14			
1	E	354	Total	C	N	O	S	0	0	0
			2649	1680	437	518	14			
1	F	354	Total	C	N	O	S	0	0	0
			2649	1680	437	518	14			
1	G	354	Total	C	N	O	S	0	0	0
			2649	1680	437	518	14			
1	H	353	Total	C	N	O	S	0	0	0
			2638	1674	434	516	14			

- Molecule 2 is ARGinine (three-letter code: ARG) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	4	1		
2	B	1	Total	C	N	O	0	0
			11	6	4	1		
2	C	1	Total	C	N	O	0	0
			11	6	4	1		
2	D	1	Total	C	N	O	0	0
			11	6	4	1		
2	E	1	Total	C	N	O	0	0
			11	6	4	1		
2	F	1	Total	C	N	O	0	0
			11	6	4	1		
2	G	1	Total	C	N	O	0	0
			11	6	4	1		
2	H	1	Total	C	N	O	0	0
			11	6	4	1		

- Molecule 3 is TYROSINE (three-letter code: TYR) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	1	3		
3	B	1	Total	C	N	O	0	0
			13	9	1	3		
3	C	1	Total	C	N	O	0	0
			13	9	1	3		
3	D	1	Total	C	N	O	0	0
			13	9	1	3		
3	E	1	Total	C	N	O	0	0
			13	9	1	3		
3	F	1	Total	C	N	O	0	0
			13	9	1	3		
3	G	1	Total	C	N	O	0	0
			13	9	1	3		
3	H	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0

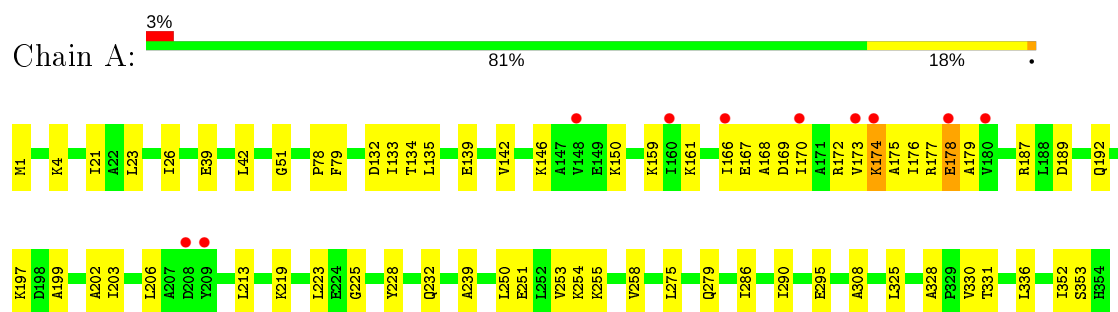
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total 110	O 110	0	0
5	B	138	Total 138	O 138	0	0
5	C	80	Total 80	O 80	0	0
5	D	63	Total 63	O 63	0	0
5	E	86	Total 86	O 86	0	0
5	F	71	Total 71	O 71	0	0
5	G	104	Total 104	O 104	0	0
5	H	124	Total 124	O 124	0	0

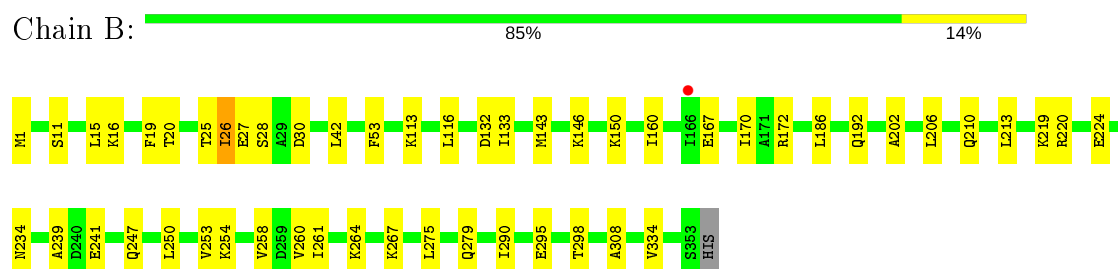
### 3 Residue-property plots [i](#)

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

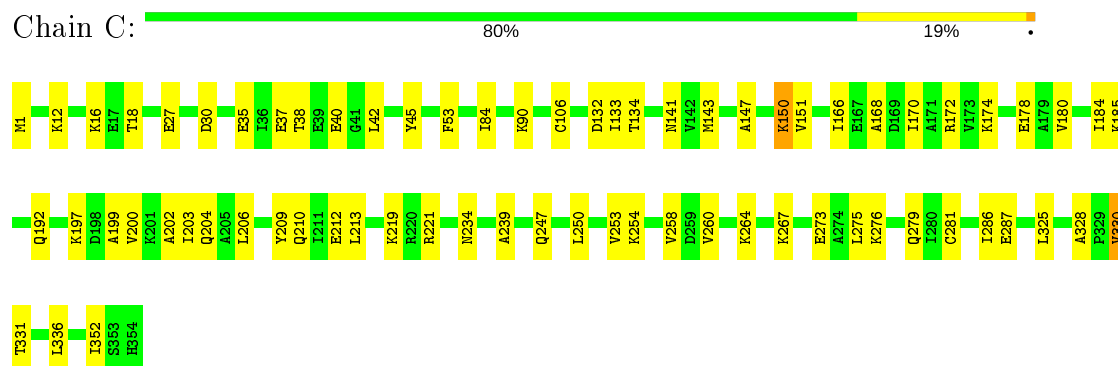
#### • Molecule 1: Dipeptide Epimerase



#### • Molecule 1: Dipeptide Epimerase



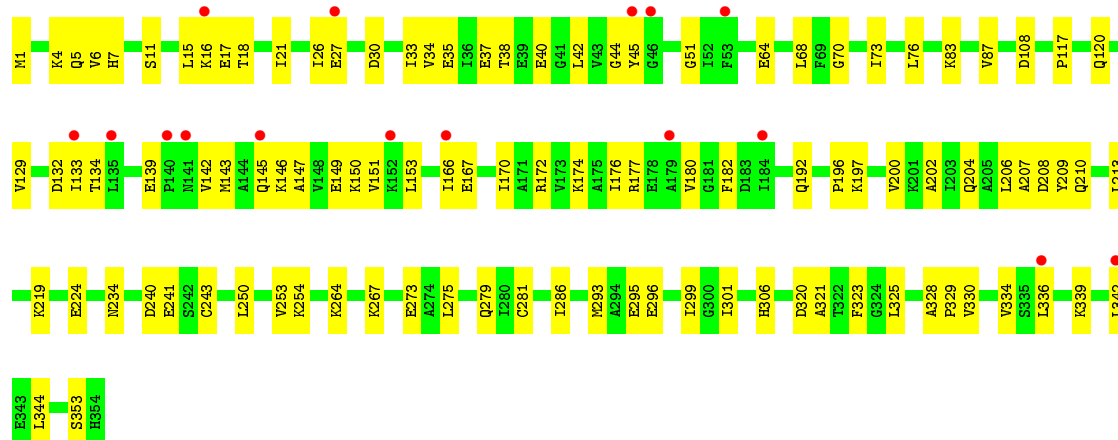
#### • Molecule 1: Dipeptide Epimerase



#### • Molecule 1: Dipeptide Epimerase

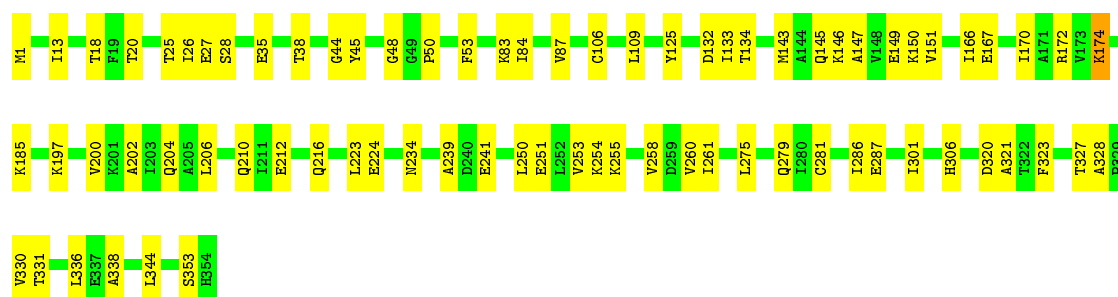






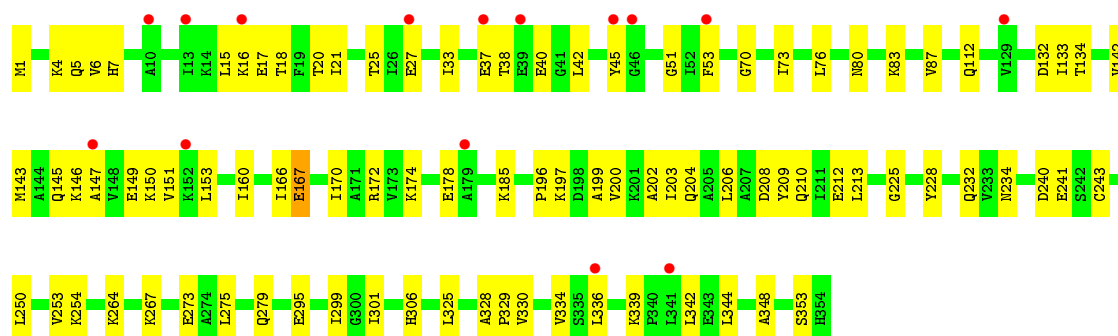
• Molecule 1: Dipeptide Epimerase

Chain E: 79% 21%



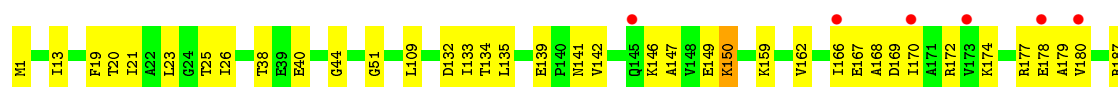
• Molecule 1: Dipeptide Epimerase

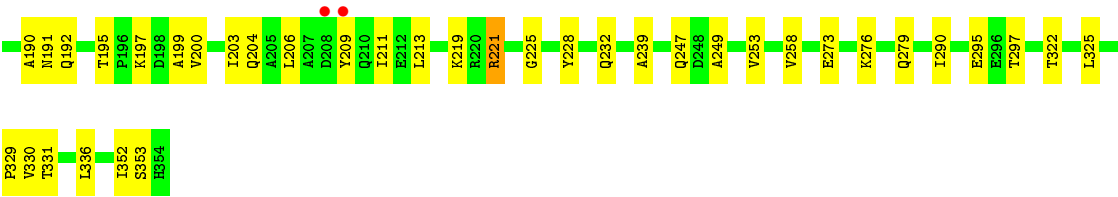
Chain F: 4% 74% 25%



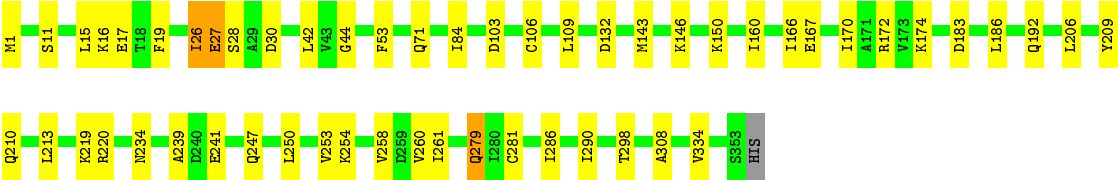
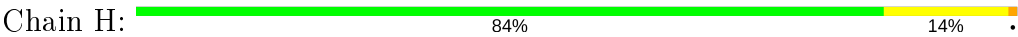
• Molecule 1: Dipeptide Epimerase

Chain G: 2% 79% 21%





● Molecule 1: Dipeptide Epimerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.30Å 163.30Å 317.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.69 – 1.90 32.33 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (24.69-1.90) 98.8 (32.33-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.236 , 0.270 0.236 , 0.269	Depositor DCC
$R_{free}$ test set	12357 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 33.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.488 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	22146	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.33	0/2679	0.57	0/3620
1	B	0.34	0/2667	0.60	0/3605
1	C	0.31	0/2679	0.58	0/3620
1	D	0.28	0/2679	0.55	0/3620
1	E	0.31	0/2679	0.58	0/3620
1	F	0.28	0/2679	0.55	0/3620
1	G	0.33	0/2679	0.57	0/3620
1	H	0.34	0/2667	0.60	0/3605
All	All	0.32	0/21408	0.57	0/28930

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2649	0	2733	56	0
1	B	2638	0	2726	41	0
1	C	2649	0	2733	55	0
1	D	2649	0	2733	83	0
1	E	2649	0	2733	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2649	0	2733	73	0
1	G	2649	0	2733	66	0
1	H	2638	0	2726	42	0
2	A	11	0	12	1	0
2	B	11	0	12	0	0
2	C	11	0	12	1	0
2	D	11	0	12	2	0
2	E	11	0	12	2	0
2	F	11	0	12	1	0
2	G	11	0	12	1	0
2	H	11	0	12	0	0
3	A	13	0	9	0	0
3	B	13	0	9	0	0
3	C	13	0	9	0	0
3	D	13	0	9	1	0
3	E	13	0	9	0	0
3	F	13	0	9	1	0
3	G	13	0	9	0	0
3	H	13	0	9	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	110	0	0	0	0
5	B	138	0	0	3	0
5	C	80	0	0	0	0
5	D	63	0	0	2	0
5	E	86	0	0	2	0
5	F	71	0	0	2	0
5	G	104	0	0	3	0
5	H	124	0	0	2	0
All	All	22146	0	22018	449	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (449) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:MET:HE1	1:G:38:THR:HG21	1.41	1.01
1:E:328:ALA:HB2	1:E:336:LEU:HD11	1.51	0.91
1:E:18:THR:HG22	1:E:27:GLU:HG2	1.54	0.89
1:A:328:ALA:HB2	1:A:336:LEU:HD11	1.55	0.86
1:G:276:LYS:HG2	1:H:279:GLN:HG3	1.57	0.84
1:G:330:VAL:HG22	1:G:353:SER:O	1.78	0.84
1:B:1:MET:CE	1:B:42:LEU:HD12	2.09	0.83
1:E:275:LEU:O	1:E:279:GLN:HG2	1.78	0.82
1:F:18:THR:HG22	1:F:27:GLU:HG2	1.61	0.82
1:A:330:VAL:HG22	1:A:353:SER:O	1.79	0.82
1:G:139:GLU:HB2	1:G:142:VAL:HG23	1.62	0.82
1:C:328:ALA:HB2	1:C:336:LEU:HD11	1.60	0.80
1:A:167:GLU:HG2	1:A:168:ALA:H	1.48	0.79
1:A:253:VAL:HG12	1:A:286:ILE:HD12	1.64	0.79
1:A:139:GLU:HB2	1:A:142:VAL:HG23	1.65	0.79
1:C:18:THR:HG22	1:C:27:GLU:HG2	1.65	0.78
1:G:1:MET:CE	1:G:38:THR:HG21	2.14	0.78
1:B:1:MET:HE1	1:B:42:LEU:HD12	1.66	0.78
1:D:133:ILE:HD13	1:D:150:LYS:HD2	1.65	0.77
1:H:1:MET:CE	1:H:42:LEU:HD12	2.15	0.76
1:F:1:MET:HG3	1:F:40:GLU:OE1	1.85	0.76
1:C:279:GLN:OE1	1:D:279:GLN:HG3	1.87	0.74
1:H:15:LEU:HD11	1:H:26:ILE:HD12	1.66	0.74
1:D:18:THR:HG22	1:D:27:GLU:HG2	1.69	0.74
1:F:133:ILE:HD13	1:F:150:LYS:HD2	1.69	0.74
1:F:275:LEU:O	1:F:279:GLN:HG2	1.88	0.73
1:G:276:LYS:HG2	1:H:279:GLN:CG	2.18	0.73
1:F:264:LYS:HD2	1:F:267:LYS:HD3	1.69	0.73
1:A:275:LEU:O	1:A:279:GLN:HG2	1.89	0.73
1:D:264:LYS:HD2	1:D:267:LYS:HD3	1.72	0.70
1:B:247:GLN:HG3	5:B:411:HOH:O	1.90	0.70
1:C:330:VAL:HG11	1:C:352:ILE:HG23	1.73	0.70
1:G:221:ARG:HB3	1:G:221:ARG:HH21	1.57	0.70
1:H:26:ILE:HD11	1:H:28:SER:O	1.92	0.70
1:B:15:LEU:HD11	1:B:26:ILE:HD12	1.72	0.69
1:G:13:ILE:HD11	1:G:329:PRO:HB3	1.74	0.69
1:D:328:ALA:HB2	1:D:336:LEU:HD11	1.73	0.69
1:C:38:THR:OG1	1:C:40:GLU:HG2	1.93	0.68
1:H:160:ILE:HD11	1:H:186:LEU:HD22	1.74	0.68
1:B:26:ILE:HD11	1:B:28:SER:O	1.94	0.68
1:B:250:LEU:HG	1:B:254:LYS:HE3	1.76	0.67
1:D:146:LYS:O	1:D:150:LYS:HG2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:ILE:HG22	1:E:174:LYS:HE2	1.76	0.67
1:D:1:MET:HG3	1:D:40:GLU:OE1	1.94	0.67
1:D:275:LEU:O	1:D:279:GLN:HG2	1.95	0.66
1:A:239:ALA:HB2	1:A:258:VAL:HG11	1.78	0.66
1:D:149:GLU:O	1:D:153:LEU:HD13	1.96	0.66
1:C:133:ILE:HD13	1:C:150:LYS:HG3	1.78	0.65
1:F:330:VAL:HG22	1:F:353:SER:O	1.96	0.65
1:G:133:ILE:HG21	1:G:150:LYS:HG2	1.78	0.65
1:A:1:MET:HE3	1:A:42:LEU:HD12	1.78	0.65
1:A:1:MET:CE	1:A:42:LEU:HD12	2.27	0.65
1:G:166:ILE:O	1:G:170:ILE:HG13	1.97	0.65
1:C:330:VAL:CG1	1:C:352:ILE:HG23	2.27	0.64
1:B:19:PHE:HB3	1:B:26:ILE:HG22	1.80	0.64
1:C:247:GLN:HB3	1:G:221:ARG:HH22	1.60	0.64
1:H:1:MET:HE3	1:H:42:LEU:HD12	1.78	0.64
1:F:143:MET:SD	1:F:172:ARG:HD3	2.38	0.64
1:F:250:LEU:O	1:F:253:VAL:HG22	1.98	0.64
1:F:273:GLU:HG2	5:F:366:HOH:O	1.96	0.64
1:F:250:LEU:HG	1:F:254:LYS:HE3	1.80	0.64
1:G:21:ILE:HG13	1:G:23:LEU:H	1.63	0.63
1:E:253:VAL:HG12	1:E:286:ILE:HD12	1.79	0.63
1:D:250:LEU:HG	1:D:254:LYS:HE3	1.80	0.63
1:F:174:LYS:O	1:F:178:GLU:HG3	1.97	0.63
1:F:45:TYR:CE2	1:F:353:SER:HA	2.34	0.62
1:G:239:ALA:HB2	1:G:258:VAL:HG11	1.81	0.62
1:F:146:LYS:O	1:F:150:LYS:HG2	1.98	0.62
1:C:253:VAL:HG12	1:C:286:ILE:HD12	1.81	0.62
1:D:330:VAL:HG22	1:D:353:SER:O	1.99	0.62
1:F:149:GLU:O	1:F:153:LEU:HD13	1.99	0.62
1:D:1:MET:HE2	1:D:38:THR:HG21	1.80	0.61
1:D:129:VAL:HG13	1:D:342:LEU:HB2	1.82	0.61
1:F:174:LYS:HE2	1:F:209:TYR:CE2	2.36	0.61
1:H:170:ILE:HG23	1:H:206:LEU:HD11	1.82	0.61
1:F:202:ALA:O	1:F:206:LEU:HD13	2.00	0.61
1:H:26:ILE:HD13	1:H:27:GLU:N	2.15	0.61
1:B:26:ILE:HD13	1:B:27:GLU:N	2.16	0.60
1:E:200:VAL:O	1:E:204:GLN:HG3	2.02	0.60
1:A:279:GLN:HG3	1:B:279:GLN:OE1	2.01	0.60
1:G:150:LYS:H	1:G:150:LYS:HD2	1.67	0.60
1:C:200:VAL:O	1:C:204:GLN:HG3	2.02	0.60
1:G:174:LYS:HE2	1:G:209:TYR:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:THR:HG1	2:C:355:ARG:N	1.99	0.60
1:A:254:LYS:HE3	1:B:254:LYS:HA	1.84	0.60
1:E:133:ILE:HD13	1:E:150:LYS:HD2	1.83	0.60
1:E:202:ALA:O	1:E:206:LEU:HD13	2.02	0.59
1:D:143:MET:SD	1:D:172:ARG:HD3	2.42	0.59
1:H:220:ARG:HG3	1:H:241:GLU:O	2.02	0.59
1:F:328:ALA:HB2	1:F:336:LEU:HD11	1.84	0.59
1:G:146:LYS:O	1:G:149:GLU:HB2	2.03	0.59
1:F:5:GLN:HG2	1:F:7:HIS:CE1	2.37	0.59
1:A:251:GLU:OE1	1:A:255:LYS:HE2	2.03	0.59
1:C:180:VAL:HB	1:C:184:ILE:HG13	1.86	0.58
1:E:170:ILE:HG12	1:E:206:LEU:HD11	1.86	0.58
1:F:243:CYS:O	1:F:267:LYS:HE3	2.04	0.58
1:D:273:GLU:HG2	5:D:378:HOH:O	2.03	0.58
1:D:117:PRO:HG2	1:D:120:GLN:HG2	1.87	0.57
1:G:139:GLU:HB2	1:G:142:VAL:CG2	2.34	0.57
1:A:173:VAL:HG11	1:A:206:LEU:HD23	1.86	0.57
1:D:170:ILE:HG12	1:D:206:LEU:HD11	1.87	0.57
1:E:26:ILE:HD12	1:E:27:GLU:H	1.70	0.57
1:D:45:TYR:CE2	1:D:353:SER:HA	2.40	0.57
1:F:83:LYS:O	1:F:87:VAL:HG23	2.05	0.57
1:C:330:VAL:HG11	1:C:352:ILE:CG2	2.34	0.57
1:D:202:ALA:O	1:D:206:LEU:HD13	2.04	0.57
1:C:185:LYS:HE2	1:C:212:GLU:CD	2.25	0.56
1:F:301:ILE:CG2	1:F:334:VAL:HG11	2.35	0.56
1:C:16:LYS:HE3	1:C:325:LEU:O	2.04	0.56
1:A:325:LEU:HB2	1:A:336:LEU:HD23	1.87	0.56
1:A:166:ILE:O	1:A:170:ILE:HG13	2.05	0.56
1:A:168:ALA:O	1:A:172:ARG:HG3	2.06	0.56
1:C:275:LEU:O	1:C:279:GLN:HG3	2.05	0.56
1:D:134:THR:HG1	2:D:355:ARG:N	2.04	0.56
1:A:174:LYS:HG3	1:A:175:ALA:N	2.20	0.55
1:D:1:MET:CE	1:D:42:LEU:HD12	2.36	0.55
1:D:306:HIS:ND1	1:D:344:LEU:HD13	2.20	0.55
1:F:21:ILE:HD11	1:F:53:PHE:HE2	1.71	0.55
1:E:1:MET:HE2	1:E:38:THR:HG21	1.88	0.55
1:C:247:GLN:CB	1:G:221:ARG:HH22	2.19	0.55
1:E:147:ALA:O	1:E:151:VAL:HG23	2.07	0.55
1:F:206:LEU:HA	1:F:209:TYR:HD2	1.72	0.55
1:B:298:THR:HG23	1:B:334:VAL:O	2.07	0.54
1:C:250:LEU:O	1:C:253:VAL:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:GLU:HG2	5:G:387:HOH:O	2.08	0.54
1:C:1:MET:HE1	1:C:38:THR:HG21	1.90	0.54
1:E:330:VAL:HG22	1:E:353:SER:O	2.07	0.54
1:F:334:VAL:HG23	1:F:342:LEU:HD22	1.89	0.54
1:G:174:LYS:HG2	1:G:209:TYR:CZ	2.43	0.54
1:D:250:LEU:O	1:D:253:VAL:HG22	2.08	0.54
1:D:301:ILE:HD11	1:D:321:ALA:HB3	1.90	0.54
1:H:1:MET:HE1	1:H:42:LEU:HD12	1.88	0.54
1:C:239:ALA:HB2	1:C:258:VAL:HG11	1.90	0.53
1:C:202:ALA:O	1:C:206:LEU:HD13	2.09	0.53
1:D:5:GLN:HG2	1:D:7:HIS:CE1	2.42	0.53
1:H:250:LEU:HG	1:H:254:LYS:HD2	1.90	0.53
1:B:250:LEU:O	1:B:254:LYS:HG3	2.08	0.53
1:C:330:VAL:CG1	1:C:331:THR:N	2.71	0.53
1:C:330:VAL:HG13	1:C:331:THR:N	2.24	0.53
1:G:147:ALA:HB1	1:G:180:VAL:HG11	1.91	0.53
1:B:19:PHE:HB3	1:B:26:ILE:CG2	2.37	0.53
1:F:147:ALA:O	1:F:151:VAL:HG23	2.09	0.53
1:G:51:GLY:HA2	1:G:295:GLU:OE2	2.08	0.53
1:E:143:MET:SD	1:E:172:ARG:HD3	2.49	0.53
1:B:210:GLN:O	1:B:210:GLN:HG2	2.09	0.53
1:A:159:LYS:HA	1:A:187:ARG:HG3	1.91	0.52
1:B:170:ILE:HG23	1:B:206:LEU:HD11	1.91	0.52
1:B:192:GLN:HB3	1:B:219:LYS:HA	1.91	0.52
1:H:210:GLN:O	1:H:210:GLN:HG2	2.10	0.52
1:D:299:ILE:HD12	1:D:299:ILE:H	1.74	0.52
1:A:192:GLN:HB3	1:A:219:LYS:HA	1.91	0.52
1:E:210:GLN:HG2	1:E:210:GLN:O	2.10	0.52
1:C:174:LYS:O	1:C:178:GLU:HG3	2.09	0.52
1:F:306:HIS:ND1	1:F:344:LEU:HD13	2.23	0.52
1:H:146:LYS:O	1:H:150:LYS:HG2	2.09	0.52
1:A:139:GLU:HB2	1:A:142:VAL:CG2	2.37	0.52
1:D:334:VAL:HG23	1:D:342:LEU:HD22	1.91	0.52
1:E:134:THR:HG1	2:E:355:ARG:N	2.07	0.52
1:E:18:THR:HG22	1:E:27:GLU:CG	2.35	0.52
1:E:224:GLU:HG3	5:E:518:HOH:O	2.09	0.52
1:B:143:MET:SD	1:B:172:ARG:HD3	2.50	0.52
1:F:167:GLU:H	1:F:167:GLU:CD	2.13	0.52
1:A:167:GLU:HG2	1:A:168:ALA:N	2.20	0.51
1:C:147:ALA:O	1:C:151:VAL:HG23	2.10	0.51
1:D:26:ILE:HD11	1:D:295:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:VAL:HG13	1:E:287:GLU:O	2.10	0.51
1:F:174:LYS:HE2	1:F:209:TYR:HE2	1.75	0.51
1:D:167:GLU:CD	1:D:167:GLU:H	2.13	0.51
1:D:1:MET:HE3	1:D:42:LEU:HD12	1.92	0.51
1:A:206:LEU:N	1:A:206:LEU:HD12	2.25	0.51
1:F:339:LYS:NZ	1:F:342:LEU:HD23	2.25	0.51
1:D:210:GLN:O	1:D:210:GLN:HG2	2.08	0.51
1:B:220:ARG:HG3	1:B:241:GLU:O	2.11	0.51
1:F:1:MET:CE	1:F:42:LEU:HD12	2.41	0.51
1:F:210:GLN:HG2	1:F:210:GLN:O	2.11	0.51
1:C:143:MET:SD	1:C:172:ARG:HD3	2.51	0.50
1:D:170:ILE:HG23	1:D:206:LEU:HD11	1.93	0.50
1:G:279:GLN:OE1	1:H:279:GLN:NE2	2.44	0.50
1:G:322:THR:HB	1:G:336:LEU:HD12	1.93	0.50
1:E:251:GLU:OE2	1:E:255:LYS:HE2	2.10	0.50
1:G:195:THR:HG23	5:G:402:HOH:O	2.12	0.50
1:A:197:LYS:HD3	1:F:234:ASN:O	2.12	0.50
1:G:177:ARG:C	1:G:179:ALA:H	2.14	0.50
1:A:330:VAL:HG21	1:A:352:ILE:CG2	2.42	0.50
1:B:275:LEU:O	1:B:279:GLN:HG3	2.11	0.50
1:C:1:MET:HA	1:C:40:GLU:OE2	2.11	0.50
1:D:206:LEU:HA	1:D:209:TYR:HD2	1.76	0.50
1:F:6:VAL:HG21	1:F:70:GLY:HA2	1.94	0.50
1:A:250:LEU:O	1:A:254:LYS:HB2	2.12	0.50
1:D:253:VAL:HG12	1:D:286:ILE:HD12	1.94	0.50
1:D:1:MET:CE	1:D:38:THR:HG21	2.42	0.50
1:G:192:GLN:HB3	1:G:219:LYS:HA	1.93	0.50
1:G:1:MET:HG2	1:G:40:GLU:OE1	2.12	0.50
1:D:301:ILE:CG2	1:D:334:VAL:HG11	2.41	0.50
1:G:146:LYS:HD3	1:G:149:GLU:OE2	2.12	0.50
1:D:176:ILE:O	1:D:180:VAL:HG22	2.11	0.49
1:A:133:ILE:HD13	1:A:150:LYS:HD2	1.94	0.49
1:A:330:VAL:HG22	1:A:331:THR:H	1.75	0.49
1:D:174:LYS:HE2	1:D:209:TYR:HE2	1.76	0.49
1:D:240:ASP:HB3	1:D:241:GLU:OE1	2.11	0.49
1:D:200:VAL:O	1:D:204:GLN:HG3	2.12	0.49
1:C:1:MET:CE	1:C:38:THR:HG21	2.42	0.49
1:C:260:VAL:HG13	1:C:287:GLU:O	2.12	0.49
1:D:26:ILE:CD1	1:D:295:GLU:HG3	2.41	0.49
1:G:134:THR:HG22	1:G:135:LEU:N	2.28	0.49
1:H:16:LYS:O	1:H:17:GLU:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:GLY:HA3	1:E:109:LEU:HG	1.95	0.49
1:G:20:THR:HG23	1:G:25:THR:HG22	1.94	0.49
1:G:168:ALA:O	1:G:172:ARG:HG3	2.13	0.49
1:A:213:LEU:C	1:A:213:LEU:HD12	2.33	0.49
1:F:142:VAL:O	1:F:145:GLN:HB2	2.12	0.49
1:F:166:ILE:O	1:F:170:ILE:HG13	2.13	0.49
1:D:174:LYS:HG2	1:D:209:TYR:CE2	2.48	0.48
1:D:320:ASP:OD1	2:D:355:ARG:HG3	2.12	0.48
1:F:15:LEU:HG	1:F:27:GLU:O	2.13	0.48
1:A:336:LEU:HD12	1:A:336:LEU:N	2.28	0.48
1:E:84:ILE:HD13	1:E:106:CYS:SG	2.52	0.48
1:D:6:VAL:HG21	1:D:70:GLY:HA2	1.95	0.48
1:B:202:ALA:O	1:B:206:LEU:HD13	2.13	0.48
1:C:84:ILE:HD13	1:C:106:CYS:SG	2.53	0.48
1:E:146:LYS:O	1:E:150:LYS:HG2	2.13	0.48
1:C:213:LEU:HD12	1:C:213:LEU:C	2.34	0.48
1:D:339:LYS:NZ	1:D:342:LEU:HD23	2.29	0.48
1:G:276:LYS:HA	1:H:279:GLN:HG2	1.96	0.48
1:D:166:ILE:O	1:D:170:ILE:HG13	2.14	0.48
1:H:19:PHE:HB3	1:H:26:ILE:HG22	1.96	0.48
1:D:83:LYS:O	1:D:87:VAL:HG23	2.14	0.48
1:A:177:ARG:C	1:A:179:ALA:H	2.17	0.48
1:C:174:LYS:HE2	1:C:209:TYR:CE2	2.49	0.48
1:C:210:GLN:O	1:C:210:GLN:HG2	2.14	0.48
1:D:147:ALA:O	1:D:151:VAL:HG23	2.14	0.48
1:F:112:GLN:HA	1:F:348:ALA:HB1	1.96	0.47
1:F:240:ASP:HB3	1:F:241:GLU:OE1	2.13	0.47
1:H:143:MET:SD	1:H:172:ARG:HD3	2.54	0.47
1:A:225:GLY:O	1:A:228:TYR:HB3	2.14	0.47
1:B:160:ILE:HD11	1:B:186:LEU:HD22	1.95	0.47
1:E:174:LYS:HB3	1:E:174:LYS:NZ	2.29	0.47
1:F:299:ILE:HD12	1:F:299:ILE:H	1.79	0.47
1:G:249:ALA:O	1:G:253:VAL:HG13	2.14	0.47
1:F:146:LYS:HA	1:F:149:GLU:HB3	1.96	0.47
1:F:206:LEU:O	1:F:209:TYR:HB2	2.14	0.47
1:G:170:ILE:HG23	1:G:206:LEU:HD11	1.96	0.47
1:G:213:LEU:HD12	1:G:213:LEU:C	2.34	0.47
1:E:250:LEU:O	1:E:253:VAL:HG22	2.15	0.47
1:F:16:LYS:HE3	1:F:325:LEU:O	2.14	0.47
1:G:134:THR:HG1	2:G:355:ARG:N	2.13	0.47
1:B:146:LYS:O	1:B:150:LYS:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:LYS:HG2	1:F:254:LYS:HG2	1.95	0.47
1:E:35:GLU:HG2	1:E:45:TYR:CE1	2.50	0.47
1:C:234:ASN:O	1:F:197:LYS:HD3	2.14	0.47
1:A:202:ALA:O	1:A:206:LEU:HD13	2.15	0.47
1:D:264:LYS:HB2	1:D:267:LYS:HD3	1.96	0.47
1:F:213:LEU:HD12	1:F:213:LEU:C	2.35	0.47
1:H:247:GLN:HG3	5:H:404:HOH:O	2.14	0.47
1:D:21:ILE:HD13	3:D:356:TYR:CD1	2.50	0.47
1:F:143:MET:HE1	1:F:160:ILE:HG23	1.96	0.47
1:F:73:ILE:HA	1:F:76:LEU:HD12	1.97	0.47
1:F:20:THR:HG23	1:F:25:THR:HG22	1.97	0.47
1:G:322:THR:HA	1:G:325:LEU:HG	1.95	0.47
1:H:298:THR:HG23	1:H:334:VAL:O	2.14	0.47
1:A:26:ILE:CD1	1:A:295:GLU:HG3	2.45	0.47
1:G:330:VAL:HG22	1:G:331:THR:H	1.80	0.47
1:H:192:GLN:HB3	1:H:219:LYS:HA	1.97	0.47
1:E:83:LYS:O	1:E:87:VAL:HG23	2.15	0.46
1:B:20:THR:OG1	1:B:25:THR:HG22	2.15	0.46
1:C:37:GLU:HA	1:C:42:LEU:O	2.15	0.46
1:G:225:GLY:O	1:G:228:TYR:HB3	2.16	0.46
1:C:264:LYS:HB2	1:C:267:LYS:HE2	1.96	0.46
1:D:15:LEU:HG	1:D:27:GLU:O	2.15	0.46
1:H:220:ARG:HG2	1:H:220:ARG:HH11	1.80	0.46
1:H:250:LEU:O	1:H:253:VAL:HG22	2.15	0.46
1:E:167:GLU:CD	1:E:167:GLU:H	2.18	0.46
1:D:234:ASN:O	1:G:197:LYS:HD3	2.16	0.46
1:G:44:GLY:HA3	1:G:109:LEU:HG	1.96	0.46
1:B:133:ILE:HD13	1:B:150:LYS:HD2	1.97	0.46
1:D:213:LEU:HD12	1:D:213:LEU:C	2.35	0.46
1:F:228:TYR:O	1:F:232:GLN:HG2	2.16	0.46
1:A:79:PHE:CZ	1:B:116:LEU:HD11	2.51	0.46
1:D:146:LYS:O	1:D:149:GLU:HB3	2.15	0.46
1:E:330:VAL:HG22	1:E:331:THR:H	1.81	0.46
1:F:33:ILE:CD1	1:F:329:PRO:HB2	2.46	0.46
1:A:134:THR:HG1	2:A:355:ARG:N	2.14	0.46
1:A:51:GLY:HA2	1:A:295:GLU:OE2	2.16	0.46
1:G:167:GLU:H	1:G:167:GLU:CD	2.19	0.46
1:B:1:MET:HE3	1:B:42:LEU:HD12	1.93	0.45
1:D:293:MET:O	1:D:296:GLU:HG2	2.15	0.45
1:G:211:ILE:N	1:G:211:ILE:HD12	2.31	0.45
1:H:26:ILE:HD13	1:H:26:ILE:C	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:26:ILE:HD13	1:H:28:SER:H	1.80	0.45
1:D:139:GLU:HB2	1:D:142:VAL:HG23	1.99	0.45
1:E:306:HIS:HA	1:E:344:LEU:HD11	1.98	0.45
1:F:200:VAL:O	1:F:204:GLN:HG3	2.16	0.45
1:A:146:LYS:O	1:A:150:LYS:HG2	2.16	0.45
1:B:260:VAL:HG12	1:B:261:ILE:N	2.30	0.45
1:A:290:ILE:HG21	1:A:308:ALA:HB2	1.99	0.45
1:D:174:LYS:HE2	1:D:209:TYR:CE2	2.52	0.45
1:D:197:LYS:HD3	1:E:234:ASN:O	2.16	0.45
1:F:132:ASP:OD1	1:F:132:ASP:C	2.55	0.45
1:D:16:LYS:HE3	1:D:325:LEU:O	2.17	0.45
1:G:336:LEU:HD13	5:G:374:HOH:O	2.16	0.45
1:A:21:ILE:HG13	1:A:23:LEU:H	1.81	0.45
1:D:250:LEU:O	1:D:254:LYS:HG3	2.17	0.45
1:B:213:LEU:C	1:B:213:LEU:HD12	2.38	0.45
1:B:239:ALA:HB2	1:B:258:VAL:HG11	1.98	0.45
1:C:132:ASP:OD1	1:C:132:ASP:C	2.56	0.44
1:C:1:MET:HG2	1:C:40:GLU:OE2	2.17	0.44
1:E:125:TYR:HA	1:F:80:ASN:OD1	2.17	0.44
1:H:19:PHE:HB3	1:H:26:ILE:CG2	2.47	0.44
1:A:279:GLN:OE1	1:A:279:GLN:HA	2.17	0.44
1:F:134:THR:HG1	2:F:355:ARG:N	2.15	0.44
1:H:26:ILE:HD13	1:H:28:SER:N	2.31	0.44
1:C:90:LYS:O	1:C:90:LYS:HD3	2.16	0.44
1:F:146:LYS:O	1:F:149:GLU:HB3	2.17	0.44
1:F:264:LYS:HB2	1:F:267:LYS:HB2	2.00	0.44
1:G:19:PHE:HB3	1:G:26:ILE:CG2	2.46	0.44
1:E:48:GLY:O	1:E:50:PRO:HD3	2.18	0.44
1:A:169:ASP:O	1:A:172:ARG:HB2	2.17	0.44
1:D:64:GLU:O	1:D:68:LEU:HG	2.18	0.44
1:F:196:PRO:O	1:F:200:VAL:HG23	2.17	0.44
1:G:13:ILE:HD12	1:G:297:THR:HG21	1.99	0.44
1:A:174:LYS:O	1:A:178:GLU:HG2	2.18	0.44
1:E:185:LYS:NZ	1:E:212:GLU:HG3	2.32	0.44
1:F:145:GLN:HA	1:F:145:GLN:OE1	2.16	0.44
1:C:281:CYS:HB3	1:C:286:ILE:O	2.18	0.44
1:E:239:ALA:HB2	1:E:258:VAL:HG11	2.00	0.44
1:H:170:ILE:CG2	1:H:174:LYS:HE2	2.47	0.44
1:C:38:THR:HG1	1:C:40:GLU:HG2	1.82	0.44
1:D:1:MET:HE3	1:D:40:GLU:OE1	2.18	0.44
1:G:132:ASP:OD1	1:G:132:ASP:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:281:CYS:HB3	1:H:286:ILE:O	2.18	0.43
1:C:192:GLN:HB3	1:C:219:LYS:HA	2.00	0.43
1:A:26:ILE:HD12	1:A:295:GLU:HG3	2.00	0.43
1:B:27:GLU:OE2	1:B:27:GLU:N	2.48	0.43
1:D:73:ILE:HA	1:D:76:LEU:HD12	2.00	0.43
1:H:132:ASP:OD1	1:H:132:ASP:C	2.57	0.43
1:B:11:SER:O	1:B:30:ASP:HA	2.19	0.43
1:D:45:TYR:HE2	1:D:353:SER:HA	1.83	0.43
1:E:336:LEU:HD12	5:E:409:HOH:O	2.17	0.43
1:H:239:ALA:HB2	1:H:258:VAL:HG11	2.01	0.43
1:B:26:ILE:HD13	1:B:26:ILE:C	2.38	0.43
1:D:170:ILE:CG2	1:D:174:LYS:HE3	2.49	0.43
1:H:260:VAL:HG12	1:H:261:ILE:N	2.33	0.43
1:D:142:VAL:O	1:D:145:GLN:HB2	2.18	0.43
1:D:33:ILE:CD1	1:D:329:PRO:HB2	2.49	0.43
1:F:206:LEU:CD1	1:F:206:LEU:N	2.81	0.43
1:F:170:ILE:HG12	1:F:206:LEU:HD11	2.00	0.43
1:A:336:LEU:HD12	1:A:336:LEU:H	1.84	0.43
1:C:35:GLU:HG2	1:C:45:TYR:CE1	2.53	0.43
1:F:51:GLY:HA2	1:F:295:GLU:OE2	2.17	0.43
1:G:170:ILE:CG2	1:G:174:LYS:HE3	2.49	0.43
1:G:159:LYS:HA	1:G:187:ARG:HG3	2.00	0.43
1:A:199:ALA:O	1:A:203:ILE:HG13	2.18	0.43
1:E:26:ILE:HD11	1:E:28:SER:O	2.19	0.43
1:B:295:GLU:HG2	5:B:479:HOH:O	2.19	0.42
1:G:133:ILE:CG2	1:G:150:LYS:HG2	2.48	0.42
1:G:162:VAL:O	1:G:190:ALA:HA	2.19	0.42
1:G:26:ILE:CD1	1:G:295:GLU:HG3	2.49	0.42
1:H:11:SER:O	1:H:30:ASP:HA	2.19	0.42
1:H:44:GLY:HA3	1:H:109:LEU:HG	2.00	0.42
1:C:250:LEU:O	1:C:253:VAL:CG2	2.66	0.42
1:E:20:THR:OG1	1:E:25:THR:HG22	2.18	0.42
1:G:20:THR:OG1	1:G:25:THR:HG22	2.19	0.42
1:H:290:ILE:HG21	1:H:308:ALA:HB2	2.01	0.42
1:C:250:LEU:HG	1:C:254:LYS:HE3	2.01	0.42
1:E:13:ILE:HD13	1:E:327:THR:O	2.19	0.42
1:E:281:CYS:HB3	1:E:286:ILE:O	2.19	0.42
1:E:301:ILE:HD11	1:E:321:ALA:HB3	2.02	0.42
1:F:1:MET:HE2	1:F:38:THR:HG21	2.00	0.42
1:F:336:LEU:HD12	5:F:570:HOH:O	2.20	0.42
1:F:4:LYS:HD3	1:F:37:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:LEU:HD12	5:D:385:HOH:O	2.19	0.42
1:E:260:VAL:HG12	1:E:261:ILE:N	2.34	0.42
1:E:323:PHE:CD1	1:E:338:ALA:HA	2.54	0.42
1:H:213:LEU:HD12	1:H:213:LEU:C	2.39	0.42
1:C:250:LEU:HA	1:C:253:VAL:HG22	2.01	0.42
1:B:224:GLU:HG3	5:B:406:HOH:O	2.20	0.42
1:C:166:ILE:O	1:C:170:ILE:HG13	2.19	0.42
1:D:243:CYS:O	1:D:267:LYS:HE3	2.20	0.42
1:F:21:ILE:HD13	3:F:356:TYR:CD1	2.55	0.42
1:B:264:LYS:HB2	1:B:267:LYS:HE2	2.01	0.42
1:E:145:GLN:O	1:E:149:GLU:HG3	2.20	0.42
1:F:185:LYS:HE2	1:F:212:GLU:OE2	2.19	0.42
1:D:281:CYS:HB3	1:D:286:ILE:O	2.20	0.42
1:F:199:ALA:O	1:F:203:ILE:HG13	2.20	0.42
1:G:228:TYR:O	1:G:232:GLN:HG2	2.20	0.42
1:D:132:ASP:OD1	1:D:132:ASP:C	2.57	0.42
1:D:206:LEU:N	1:D:206:LEU:CD1	2.83	0.42
1:C:197:LYS:HD3	1:H:234:ASN:O	2.20	0.42
1:G:190:ALA:O	1:G:191:ASN:C	2.58	0.42
1:C:221:ARG:HB2	1:G:247:GLN:HE22	1.84	0.42
1:A:176:ILE:O	1:A:179:ALA:HB3	2.20	0.41
1:D:11:SER:O	1:D:30:ASP:HA	2.19	0.41
1:D:177:ARG:NH1	1:D:182:PHE:HA	2.35	0.41
1:D:34:VAL:HG12	1:D:35:GLU:N	2.35	0.41
1:E:320:ASP:OD1	2:E:355:ARG:HG3	2.20	0.41
1:A:213:LEU:O	1:A:213:LEU:HD12	2.20	0.41
1:E:132:ASP:C	1:E:132:ASP:OD1	2.58	0.41
1:A:228:TYR:O	1:A:232:GLN:HG2	2.20	0.41
1:B:1:MET:HE3	1:B:113:LYS:HD3	2.02	0.41
1:B:16:LYS:HB3	1:B:16:LYS:NZ	2.36	0.41
1:D:323:PHE:N	1:D:323:PHE:CD1	2.87	0.41
1:G:169:ASP:O	1:G:172:ARG:HB2	2.19	0.41
1:C:170:ILE:HG12	1:C:206:LEU:HD11	2.02	0.41
1:F:299:ILE:N	1:F:299:ILE:HD12	2.35	0.41
1:G:199:ALA:O	1:G:203:ILE:HG13	2.20	0.41
1:G:330:VAL:HG21	1:G:352:ILE:CG2	2.50	0.41
1:E:216:GLN:HG2	1:E:241:GLU:OE1	2.20	0.41
1:H:174:LYS:HG2	1:H:209:TYR:CZ	2.56	0.41
1:A:134:THR:HG22	1:A:135:LEU:N	2.35	0.41
1:D:120:GLN:HA	1:D:120:GLN:OE1	2.21	0.41
1:D:196:PRO:O	1:D:200:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:GLY:HA2	1:D:108:ASP:OD2	2.21	0.41
1:E:261:ILE:HD12	1:E:281:CYS:SG	2.61	0.41
1:H:166:ILE:O	1:H:170:ILE:HG13	2.21	0.41
1:A:290:ILE:O	1:A:290:ILE:HG23	2.19	0.41
1:C:273:GLU:OE1	1:C:276:LYS:HD2	2.21	0.41
1:D:51:GLY:HA2	1:D:295:GLU:OE2	2.21	0.41
1:F:250:LEU:O	1:F:254:LYS:HG3	2.20	0.41
1:G:26:ILE:HD12	1:G:295:GLU:HG3	2.03	0.41
1:A:161:LYS:HD3	1:A:189:ASP:HB3	2.02	0.41
1:A:328:ALA:HB2	1:A:336:LEU:CD1	2.37	0.41
1:B:250:LEU:HA	1:B:253:VAL:HG22	2.03	0.41
1:C:168:ALA:O	1:C:172:ARG:HG3	2.21	0.41
1:F:225:GLY:O	1:F:228:TYR:HB3	2.20	0.41
1:G:206:LEU:HA	1:G:209:TYR:HD2	1.86	0.41
1:A:132:ASP:OD1	1:A:132:ASP:C	2.58	0.41
1:A:206:LEU:CD1	1:A:206:LEU:N	2.84	0.41
1:B:132:ASP:C	1:B:132:ASP:OD1	2.59	0.41
1:G:174:LYS:HE2	1:G:209:TYR:HE2	1.85	0.41
1:G:200:VAL:O	1:G:204:GLN:HG3	2.21	0.41
1:F:206:LEU:N	1:F:206:LEU:HD12	2.36	0.40
1:A:4:LYS:HG3	1:A:39:GLU:OE2	2.21	0.40
1:C:12:LYS:HG2	1:C:30:ASP:OD1	2.22	0.40
1:E:166:ILE:HG13	1:E:167:GLU:N	2.36	0.40
1:E:170:ILE:HG12	1:E:206:LEU:CD1	2.50	0.40
1:F:15:LEU:O	1:F:16:LYS:C	2.59	0.40
1:A:1:MET:HG2	1:A:78:PRO:HD2	2.04	0.40
1:H:71:GLN:HG3	5:H:385:HOH:O	2.20	0.40
1:H:84:ILE:HD13	1:H:106:CYS:SG	2.61	0.40
1:B:234:ASN:O	1:E:197:LYS:HD3	2.21	0.40
1:B:290:ILE:HG21	1:B:308:ALA:HB2	2.04	0.40
1:C:185:LYS:HE2	1:C:212:GLU:OE2	2.21	0.40
1:D:15:LEU:O	1:D:16:LYS:C	2.60	0.40
1:D:4:LYS:HD3	1:D:37:GLU:OE2	2.22	0.40
1:F:170:ILE:HG23	1:F:206:LEU:HD11	2.03	0.40
1:G:290:ILE:O	1:G:290:ILE:HG23	2.20	0.40
1:C:199:ALA:O	1:C:203:ILE:HG13	2.21	0.40
1:D:192:GLN:HB3	1:D:219:LYS:HA	2.03	0.40
1:G:213:LEU:O	1:G:213:LEU:HD12	2.21	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	352/354 (99%)	331 (94%)	20 (6%)	1 (0%)	41	31
1	B	351/354 (99%)	337 (96%)	14 (4%)	0	100	100
1	C	352/354 (99%)	339 (96%)	13 (4%)	0	100	100
1	D	352/354 (99%)	330 (94%)	20 (6%)	2 (1%)	25	15
1	E	352/354 (99%)	338 (96%)	14 (4%)	0	100	100
1	F	352/354 (99%)	332 (94%)	19 (5%)	1 (0%)	41	31
1	G	352/354 (99%)	332 (94%)	19 (5%)	1 (0%)	41	31
1	H	351/354 (99%)	339 (97%)	12 (3%)	0	100	100
All	All	2814/2832 (99%)	2678 (95%)	131 (5%)	5 (0%)	47	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	208	ASP
1	D	207	ALA
1	F	208	ASP
1	G	178	GLU
1	A	178	GLU

### 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	278/278 (100%)	276 (99%)	2 (1%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	277/278 (100%)	274 (99%)	3 (1%)	73	73
1	C	278/278 (100%)	274 (99%)	4 (1%)	67	65
1	D	278/278 (100%)	276 (99%)	2 (1%)	84	84
1	E	278/278 (100%)	275 (99%)	3 (1%)	73	73
1	F	278/278 (100%)	276 (99%)	2 (1%)	84	84
1	G	278/278 (100%)	275 (99%)	3 (1%)	73	73
1	H	277/278 (100%)	270 (98%)	7 (2%)	47	41
All	All	2222/2224 (100%)	2196 (99%)	26 (1%)	71	70

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	LYS
1	A	223	LEU
1	B	26	ILE
1	B	53	PHE
1	B	167	GLU
1	C	53	PHE
1	C	141	ASN
1	C	150	LYS
1	C	330	VAL
1	D	17	GLU
1	D	224	GLU
1	E	53	PHE
1	E	174	LYS
1	E	223	LEU
1	F	17	GLU
1	F	167	GLU
1	G	141	ASN
1	G	150	LYS
1	G	221	ARG
1	H	26	ILE
1	H	27	GLU
1	H	53	PHE
1	H	103	ASP
1	H	167	GLU
1	H	183	ASP
1	H	279	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	D	247	GLN
1	E	247	GLN
1	F	112	GLN
1	G	247	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	ARG	F	355	3	9,10,11	0.41	0	5,11,13	0.58	0
2	ARG	A	355	3	9,10,11	0.46	0	5,11,13	0.43	0
3	TYR	H	356	2,4	10,13,13	0.50	0	12,17,17	0.23	0
2	ARG	C	355	3	9,10,11	0.39	0	5,11,13	0.47	0
2	ARG	B	355	3	9,10,11	0.47	0	5,11,13	0.30	0
3	TYR	G	356	2,4	10,13,13	0.46	0	12,17,17	0.33	0
3	TYR	E	356	2,4	10,13,13	0.36	0	12,17,17	0.41	0
3	TYR	C	356	2,4	10,13,13	0.38	0	12,17,17	0.37	0
2	ARG	E	355	3	9,10,11	0.41	0	5,11,13	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TYR	A	356	2,4	10,13,13	0.42	0	12,17,17	0.36	0
3	TYR	F	356	2,4	10,13,13	0.39	0	12,17,17	0.28	0
3	TYR	D	356	2,4	10,13,13	0.46	0	12,17,17	0.39	0
3	TYR	B	356	2,4	10,13,13	0.54	0	12,17,17	0.20	0
2	ARG	H	355	3	9,10,11	0.52	0	5,11,13	0.60	0
2	ARG	D	355	3	9,10,11	0.40	0	5,11,13	0.34	0
2	ARG	G	355	3	9,10,11	0.46	0	5,11,13	0.46	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	ARG	F	355	3	-	3/8/9/11	-
2	ARG	A	355	3	-	0/8/9/11	-
3	TYR	H	356	2,4	-	2/4/8/8	0/1/1/1
2	ARG	C	355	3	-	2/8/9/11	-
2	ARG	B	355	3	-	2/8/9/11	-
3	TYR	G	356	2,4	-	2/4/8/8	0/1/1/1
3	TYR	E	356	2,4	-	2/4/8/8	0/1/1/1
3	TYR	C	356	2,4	-	2/4/8/8	0/1/1/1
2	ARG	E	355	3	-	0/8/9/11	-
3	TYR	A	356	2,4	-	2/4/8/8	0/1/1/1
3	TYR	F	356	2,4	-	2/4/8/8	0/1/1/1
3	TYR	D	356	2,4	-	2/4/8/8	0/1/1/1
3	TYR	B	356	2,4	-	2/4/8/8	0/1/1/1
2	ARG	H	355	3	-	2/8/9/11	-
2	ARG	D	355	3	-	0/8/9/11	-
2	ARG	G	355	3	-	2/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	355	ARG	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	G	355	ARG	N-CA-CB-CG
2	G	355	ARG	C-CA-CB-CG
2	F	355	ARG	O-C-CA-CB
3	F	356	TYR	CA-CB-CG-CD1
2	H	355	ARG	C-CA-CB-CG
3	F	356	TYR	CA-CB-CG-CD2
3	H	356	TYR	CA-CB-CG-CD2
3	C	356	TYR	CA-CB-CG-CD2
3	B	356	TYR	CA-CB-CG-CD1
3	H	356	TYR	CA-CB-CG-CD1
3	C	356	TYR	CA-CB-CG-CD1
3	B	356	TYR	CA-CB-CG-CD2
3	D	356	TYR	CA-CB-CG-CD1
3	D	356	TYR	CA-CB-CG-CD2
3	G	356	TYR	CA-CB-CG-CD2
3	E	356	TYR	CA-CB-CG-CD1
3	G	356	TYR	CA-CB-CG-CD1
3	E	356	TYR	CA-CB-CG-CD2
3	A	356	TYR	CA-CB-CG-CD2
3	A	356	TYR	CA-CB-CG-CD1
2	B	355	ARG	N-CA-CB-CG
2	H	355	ARG	N-CA-CB-CG
2	F	355	ARG	N-CA-CB-CG
2	F	355	ARG	C-CA-CB-CG
2	C	355	ARG	CG-CD-NE-CZ
2	C	355	ARG	N-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	355	ARG	1	0
2	A	355	ARG	1	0
2	C	355	ARG	1	0
2	E	355	ARG	2	0
3	F	356	TYR	1	0
3	D	356	TYR	1	0
2	D	355	ARG	2	0
2	G	355	ARG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	354/354 (100%)	0.09	10 (2%) 53 56	25, 37, 62, 71	0
1	B	353/354 (99%)	-0.09	1 (0%) 94 94	22, 33, 49, 58	0
1	C	354/354 (100%)	-0.08	0 100 100	28, 39, 53, 61	0
1	D	354/354 (100%)	0.45	16 (4%) 33 36	32, 48, 66, 74	0
1	E	354/354 (100%)	-0.08	0 100 100	28, 39, 51, 62	0
1	F	354/354 (100%)	0.42	15 (4%) 36 39	33, 48, 66, 75	0
1	G	354/354 (100%)	0.08	8 (2%) 60 63	25, 36, 62, 70	0
1	H	353/354 (99%)	-0.08	0 100 100	22, 33, 48, 58	0
All	All	2830/2832 (99%)	0.09	50 (1%) 68 71	22, 39, 61, 75	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	ILE	4.0
1	G	180	VAL	3.6
1	A	170	ILE	3.4
1	A	173	VAL	3.3
1	A	209	TYR	3.1
1	D	45	TYR	3.0
1	D	27	GLU	3.0
1	D	46	GLY	2.9
1	G	209	TYR	2.8
1	F	46	GLY	2.7
1	A	180	VAL	2.7
1	G	170	ILE	2.7
1	F	16	LYS	2.7
1	A	208	ASP	2.6
1	A	178	GLU	2.5
1	G	208	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	166	ILE	2.5
1	A	174	LYS	2.4
1	D	152	LYS	2.4
1	F	45	TYR	2.4
1	F	336	LEU	2.3
1	D	16	LYS	2.3
1	F	10	ALA	2.3
1	F	147	ALA	2.3
1	F	152	LYS	2.3
1	F	13	ILE	2.3
1	F	53	PHE	2.3
1	G	145	GLN	2.3
1	D	135	LEU	2.3
1	A	160	ILE	2.2
1	G	173	VAL	2.2
1	D	342	LEU	2.2
1	F	129	VAL	2.2
1	D	140	PRO	2.1
1	F	179	ALA	2.1
1	F	27	GLU	2.1
1	G	178	GLU	2.1
1	D	145	GLN	2.1
1	F	37	GLU	2.1
1	A	148	VAL	2.1
1	D	141	ASN	2.1
1	D	166	ILE	2.1
1	D	133	ILE	2.1
1	D	184	ILE	2.1
1	D	179	ALA	2.1
1	F	341	LEU	2.0
1	D	53	PHE	2.0
1	F	39	GLU	2.0
1	B	166	ILE	2.0
1	D	336	LEU	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 monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ARG	B	355	11/12	0.86	0.14	36,40,46,48	0
2	ARG	A	355	11/12	0.86	0.12	45,48,56,59	0
2	ARG	H	355	11/12	0.87	0.13	35,40,46,47	0
2	ARG	G	355	11/12	0.87	0.13	46,48,57,58	0
3	TYR	D	356	13/13	0.88	0.15	43,49,53,54	0
2	ARG	D	355	11/12	0.88	0.15	46,48,55,56	0
3	TYR	A	356	13/13	0.90	0.17	41,43,45,45	0
3	TYR	B	356	13/13	0.91	0.14	37,41,45,45	0
3	TYR	F	356	13/13	0.91	0.14	43,50,53,54	0
2	ARG	C	355	11/12	0.92	0.10	38,42,50,51	0
4	MG	A	357	1/1	0.93	0.04	36,36,36,36	0
3	TYR	H	356	13/13	0.93	0.15	34,43,48,49	0
3	TYR	G	356	13/13	0.93	0.19	40,45,46,46	0
2	ARG	F	355	11/12	0.93	0.17	47,50,56,58	0
3	TYR	E	356	13/13	0.94	0.10	36,40,44,47	0
3	TYR	C	356	13/13	0.94	0.12	39,41,42,43	0
4	MG	G	357	1/1	0.95	0.06	35,35,35,35	0
2	ARG	E	355	11/12	0.95	0.08	34,39,45,47	0
4	MG	F	357	1/1	0.96	0.08	41,41,41,41	0
4	MG	E	357	1/1	0.96	0.05	35,35,35,35	0
4	MG	D	357	1/1	0.96	0.07	37,37,37,37	0
4	MG	C	357	1/1	0.97	0.09	36,36,36,36	0
4	MG	B	357	1/1	0.98	0.05	34,34,34,34	0
4	MG	H	357	1/1	0.98	0.06	35,35,35,35	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.