



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 02:13 pm GMT

PDB ID : 3F3F  
Title : Crystal structure of the nucleoporin pair Nup85-Seh1, space group P21  
Authors : Debler, E.W.; Hseo, H.; Ma, Y.; Blobel, G.; Hoelz, A.  
Deposited on : 2008-10-30  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

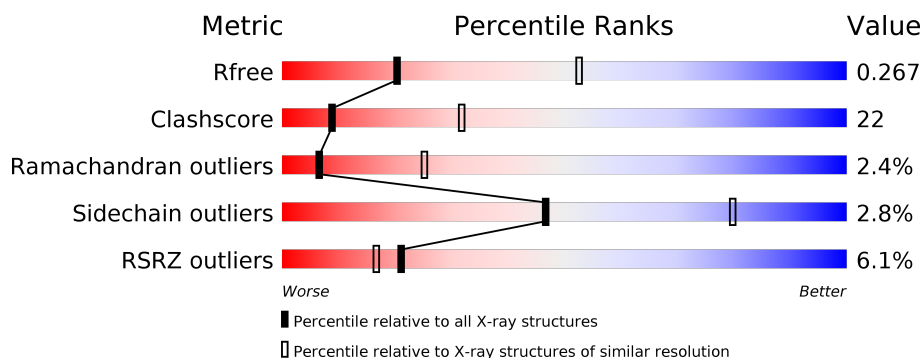
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	351	<div> <div>2%</div> <div> <div>48%</div> <div>37%</div> <div>12%</div> </div> </div>
1	B	351	<div> <div>6%</div> <div> <div>44%</div> <div>42%</div> <div>13%</div> </div> </div>
1	E	351	<div> <div>%</div> <div> <div>46%</div> <div>38%</div> <div>13%</div> </div> </div>
1	F	351	<div> <div>3%</div> <div> <div>41%</div> <div>43%</div> <div>13%</div> </div> </div>
2	C	570	<div> <div>5%</div> <div> <div>54%</div> <div>28%</div> <div>17%</div> </div> </div>
2	D	570	<div> <div>7%</div> <div> <div>54%</div> <div>31%</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	570	<div><div>5%</div><div><div></div><div>55%</div><div>26%</div><div>•</div><div>16%</div></div></div>
2	H	570	<div><div>9%</div><div><div></div><div>54%</div><div>28%</div><div>•</div><div>15%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25239 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 Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2448	1549	425	463	11			
1	B	307	Total	C	N	O	S	0	0	0
			2438	1543	423	461	11			
1	E	306	Total	C	N	O	S	0	0	0
			2432	1540	422	459	11			
1	F	306	Total	C	N	O	S	0	0	0
			2430	1538	422	459	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PRO	-	EXPRESSION TAG	UNP P53011
A	1A	HIS	-	EXPRESSION TAG	UNP P53011
B	1A	PRO	-	EXPRESSION TAG	UNP P53011
B	1B	HIS	-	EXPRESSION TAG	UNP P53011
E	1A	PRO	-	EXPRESSION TAG	UNP P53011
E	1B	HIS	-	EXPRESSION TAG	UNP P53011
F	0	PRO	-	EXPRESSION TAG	UNP P53011
F	1A	HIS	-	EXPRESSION TAG	UNP P53011

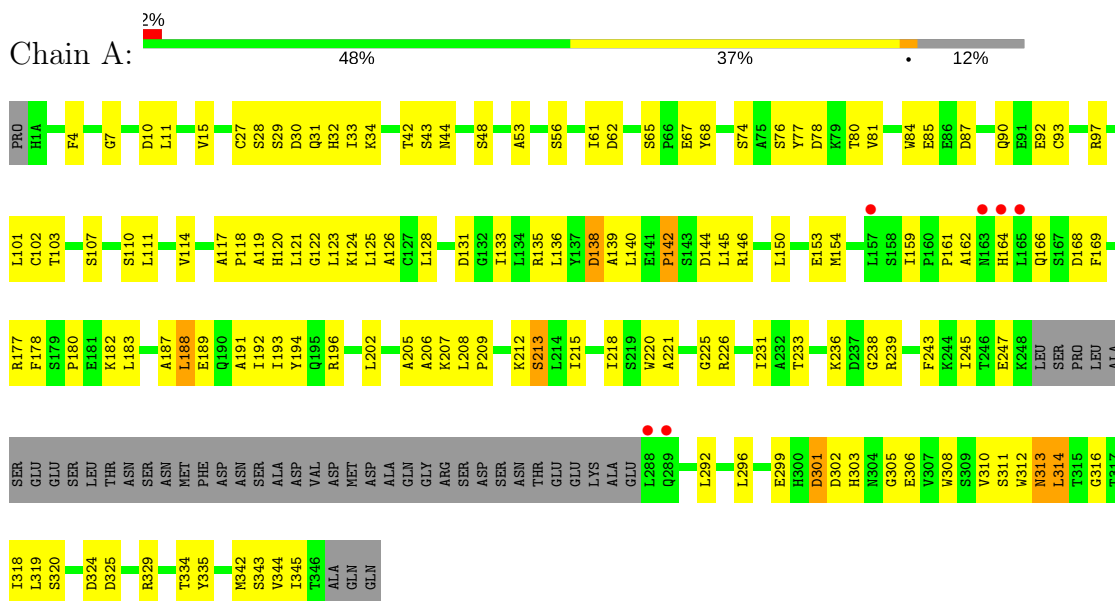
- Molecule 2 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	475	Total	C	N	O	S	0	0	0
			3812	2451	608	732	21			
2	D	495	Total	C	N	O	S	0	0	0
			3959	2533	633	770	23			
2	G	476	Total	C	N	O	S	0	0	0
			3820	2447	613	738	22			
2	H	487	Total	C	N	O	S	0	0	0
			3900	2501	624	753	22			

### 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 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: Nucleoporin SEH1



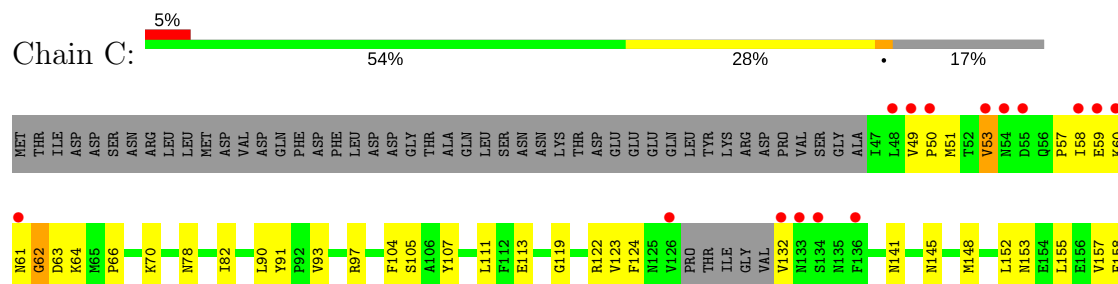
## Chain E:

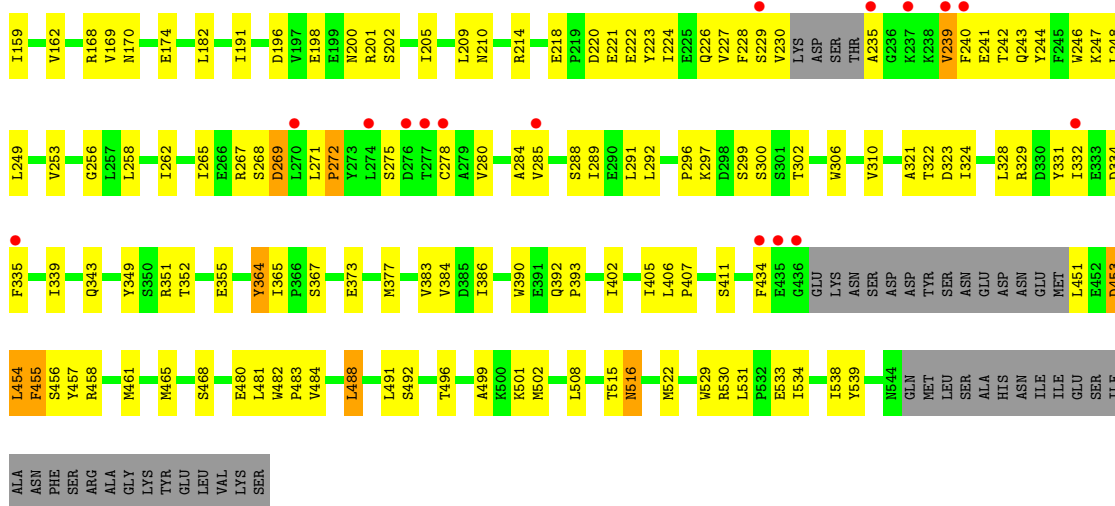


## Chain F:

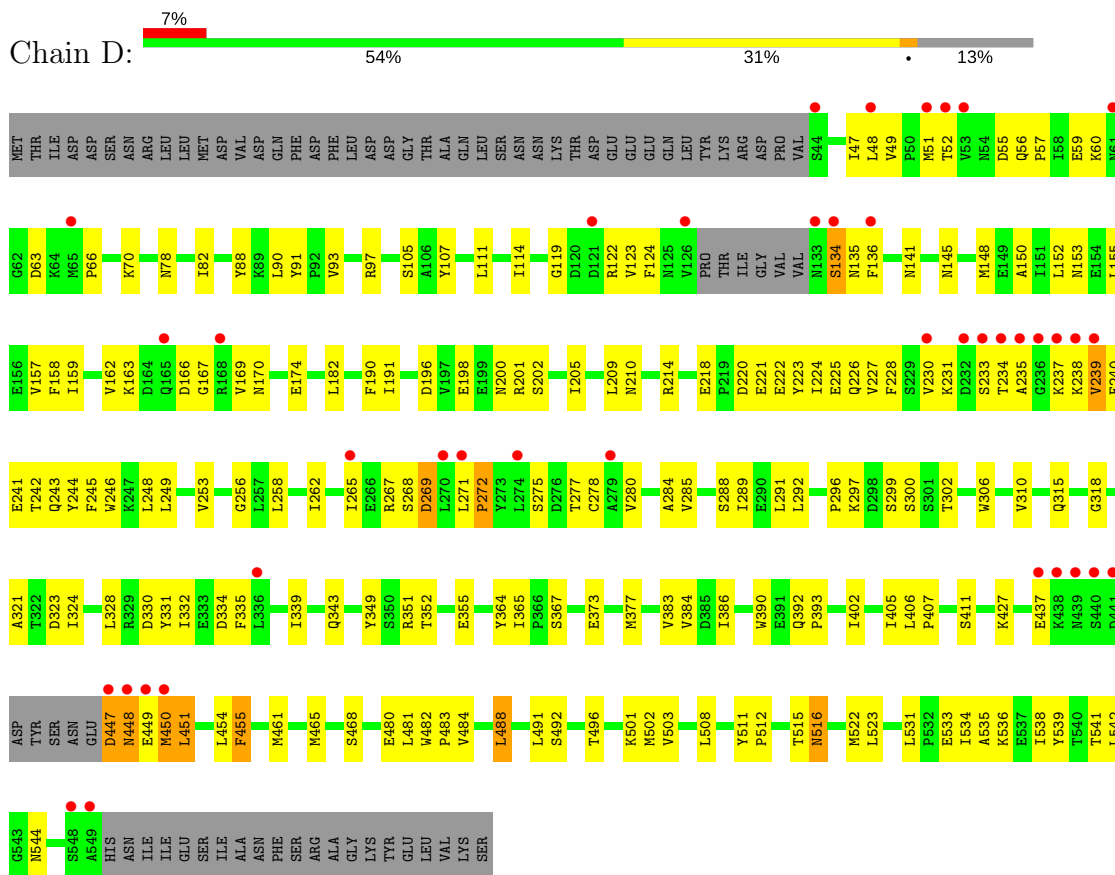


## Chain C:

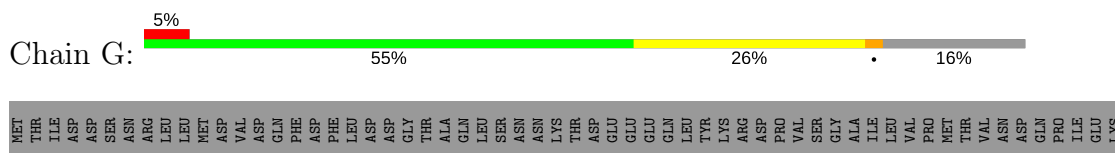


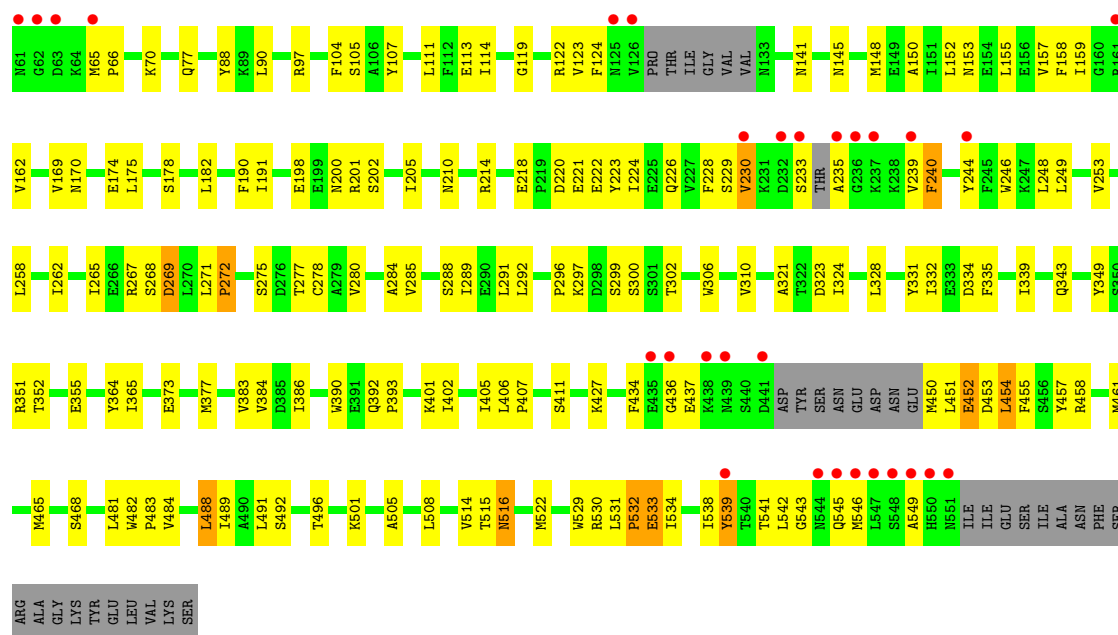


- Molecule 2: Nucleoporin NUP85

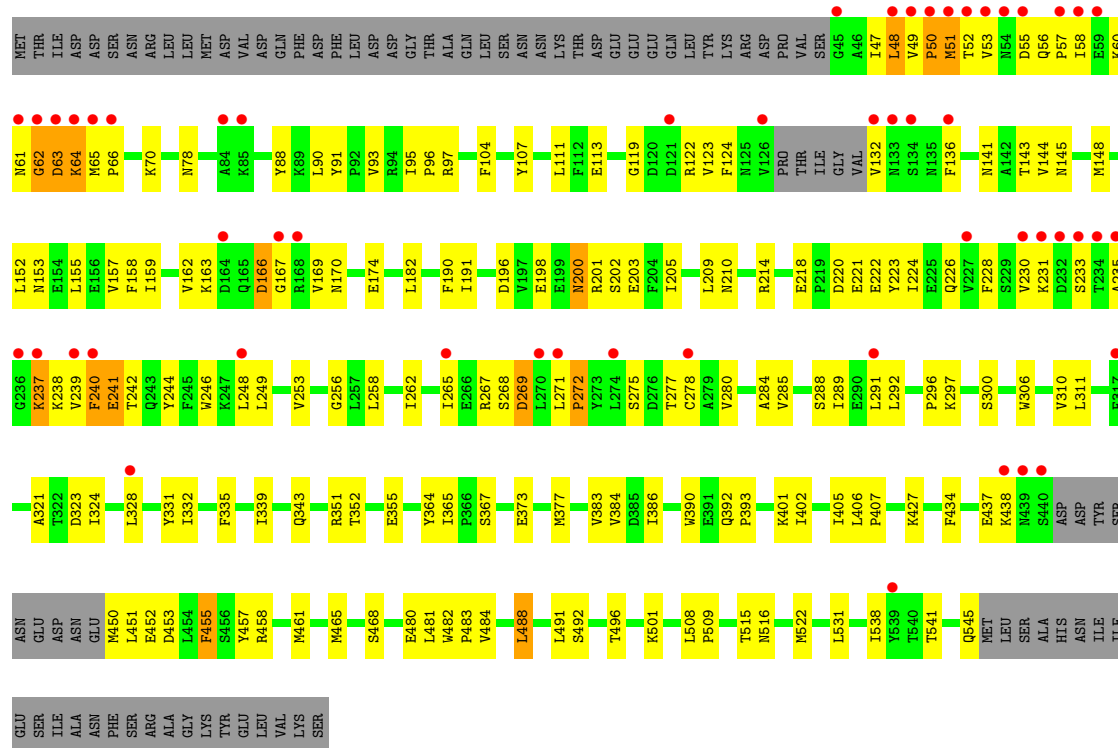


- Molecule 2: Nucleoporin NUP85





## ● Molecule 2: Nucleoporin NUP85





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.84Å 166.19Å 188.90Å 90.00° 93.02° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 48.31 – 2.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 89.0 (48.31-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.246 , 0.265 0.248 , 0.267	Depositor DCC
$R_{free}$ test set	10747 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.9	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 59.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	25239	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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](#)

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	0.45	0/2510	0.71	0/3403
1	B	0.42	0/2501	0.71	0/3391
1	E	0.45	0/2495	0.72	0/3383
1	F	0.45	0/2492	0.71	0/3379
2	C	0.44	0/3889	0.64	1/5265 (0.0%)
2	D	0.43	0/4037	0.65	0/5463
2	G	0.43	0/3896	0.63	0/5268
2	H	0.44	0/3978	0.63	0/5384
All	All	0.44	0/25798	0.67	1/34936 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	454	LEU	N-CA-C	5.65	126.26	111.00

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	2448	0	2385	110	0
1	B	2438	0	2373	138	0
1	E	2432	0	2368	120	0
1	F	2430	0	2366	147	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3812	0	3761	151	0
2	D	3959	0	3892	167	0
2	G	3820	0	3750	148	0
2	H	3900	0	3846	167	0
All	All	25239	0	24741	1082	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 22.

All (1082) 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)
2:D:450:MET:HG3	2:D:451:LEU:H	1.26	0.99
2:D:59:GLU:HG3	2:D:60:LYS:H	1.28	0.98
2:G:169:VAL:HG12	2:G:170:ASN:H	1.25	0.97
2:C:240:PHE:O	2:C:241:GLU:HG3	1.66	0.95
2:D:515:THR:HG22	2:D:516:ASN:H	1.32	0.92
1:B:159:ILE:C	1:B:161:PRO:HD3	1.93	0.89
1:F:221:ALA:HB2	1:F:312:TRP:CE2	2.08	0.88
1:E:221:ALA:HB2	1:E:312:TRP:CE2	2.07	0.88
2:H:50:PRO:HB2	2:H:53:VAL:HG22	1.54	0.88
2:C:515:THR:HG22	2:C:516:ASN:H	1.39	0.88
2:H:515:THR:HG22	2:H:516:ASN:H	1.36	0.87
1:A:221:ALA:HB2	1:A:312:TRP:CE2	2.10	0.86
2:G:515:THR:HG22	2:G:516:ASN:H	1.39	0.86
1:B:221:ALA:HB2	1:B:312:TRP:CE2	2.10	0.86
2:D:227:VAL:HG12	2:D:239:VAL:HG13	1.59	0.85
2:C:280:VAL:HG21	2:C:321:ALA:HB3	1.59	0.84
2:H:280:VAL:HG21	2:H:321:ALA:HB3	1.61	0.82
2:G:280:VAL:HG21	2:G:321:ALA:HB3	1.61	0.82
2:G:538:ILE:O	2:G:542:LEU:HG	1.80	0.81
2:D:280:VAL:HG21	2:D:321:ALA:HB3	1.62	0.81
1:A:329:ARG:HG2	1:A:344:VAL:HG22	1.62	0.80
1:B:329:ARG:HG2	1:B:344:VAL:HG22	1.63	0.80
2:D:163:LYS:O	2:D:167:GLY:HA2	1.82	0.79
1:B:208:LEU:HD11	1:B:231:ILE:HD11	1.62	0.79
2:G:532:PRO:HG2	2:G:533:GLU:H	1.45	0.79
1:B:3:PRO:CG	2:D:52:THR:HG21	2.13	0.79
1:F:329:ARG:HG2	1:F:344:VAL:HG22	1.66	0.78
1:B:208:LEU:HD11	1:B:231:ILE:CD1	2.13	0.78
1:A:225:GLY:O	2:C:453:ASP:HB3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:265:ILE:HG21	2:H:289:ILE:HD11	1.65	0.78
2:H:163:LYS:O	2:H:167:GLY:HA2	1.84	0.78
2:C:265:ILE:HG21	2:C:289:ILE:HD11	1.64	0.78
2:D:534:ILE:O	2:D:538:ILE:HG12	1.83	0.78
1:F:157:LEU:HD11	1:F:187:ALA:HB1	1.66	0.77
2:H:239:VAL:HB	2:H:268:SER:HB2	1.67	0.77
1:E:329:ARG:HG2	1:E:344:VAL:HG22	1.66	0.77
2:G:169:VAL:HG12	2:G:170:ASN:N	2.00	0.76
1:A:81:VAL:HG23	1:A:111:LEU:HD13	1.67	0.76
1:F:208:LEU:HD11	1:F:231:ILE:HD11	1.67	0.76
2:H:541:THR:O	2:H:545:GLN:HB2	1.85	0.76
2:D:265:ILE:HG21	2:D:289:ILE:HD11	1.65	0.76
2:G:265:ILE:HG21	2:G:289:ILE:HD11	1.66	0.76
1:E:225:GLY:HA2	2:G:452:GLU:OE2	1.85	0.75
1:E:208:LEU:HD11	1:E:231:ILE:HD11	1.69	0.74
2:C:454:LEU:O	2:C:456:SER:N	2.21	0.73
1:F:208:LEU:HD11	1:F:231:ILE:CD1	2.18	0.73
1:F:227:TRP:CZ3	2:H:452:GLU:HB2	2.24	0.73
1:A:208:LEU:HD11	1:A:231:ILE:HD11	1.70	0.73
1:E:238:GLY:HA2	1:E:305:GLY:O	1.88	0.73
2:H:132:VAL:O	2:H:136:PHE:HB2	1.89	0.73
2:H:278:CYS:SG	2:H:323:ASP:HB2	2.29	0.72
1:F:81:VAL:HG23	1:F:111:LEU:HD13	1.71	0.72
2:H:509:PRO:HA	2:H:538:ILE:HD11	1.71	0.72
2:D:148:MET:HE2	2:D:152:LEU:HG	1.72	0.71
2:H:198:GLU:HG2	2:H:300:SER:CB	2.19	0.71
1:F:220:TRP:HA	1:F:231:ILE:HG22	1.72	0.71
1:A:208:LEU:HD11	1:A:231:ILE:CD1	2.20	0.71
2:C:278:CYS:SG	2:C:323:ASP:HB2	2.31	0.70
2:G:148:MET:HE2	2:G:152:LEU:HG	1.71	0.70
1:A:68:TYR:OH	1:A:122:GLY:HA2	1.91	0.70
2:H:148:MET:HE2	2:H:152:LEU:HG	1.72	0.70
2:G:240:PHE:CD1	2:G:240:PHE:C	2.65	0.69
1:E:236:LYS:HG3	1:E:306:GLU:OE1	1.92	0.69
1:B:68:TYR:OH	1:B:122:GLY:HA2	1.93	0.69
1:A:220:TRP:HA	1:A:231:ILE:HG22	1.75	0.68
1:B:81:VAL:HG23	1:B:111:LEU:HD13	1.74	0.68
2:G:152:LEU:HD21	2:G:182:LEU:HB3	1.75	0.68
2:H:246:TRP:CD1	2:H:331:TYR:CD2	2.81	0.68
2:G:278:CYS:SG	2:G:323:ASP:HB2	2.33	0.68
2:G:246:TRP:CD1	2:G:331:TYR:CD2	2.82	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:240:PHE:CD1	2:C:268:SER:HB3	2.29	0.68
2:D:258:LEU:HD22	2:D:292:LEU:HD22	1.75	0.68
1:E:208:LEU:HD11	1:E:231:ILE:CD1	2.23	0.68
2:D:97:ARG:NH2	2:D:411:SER:O	2.28	0.67
1:E:68:TYR:OH	1:E:122:GLY:HA2	1.94	0.67
2:H:242:THR:HG22	2:H:244:TYR:H	1.59	0.67
2:C:60:LYS:C	2:C:62:GLY:H	1.94	0.67
2:G:169:VAL:CG1	2:G:170:ASN:H	2.05	0.67
2:H:50:PRO:CB	2:H:53:VAL:HG22	2.24	0.67
2:D:515:THR:HG22	2:D:516:ASN:N	2.06	0.67
2:H:258:LEU:HD22	2:H:292:LEU:HD22	1.76	0.67
1:B:196:ARG:HH11	1:B:202:LEU:HD21	1.60	0.67
2:D:169:VAL:HG12	2:D:170:ASN:H	1.60	0.67
1:E:81:VAL:HG23	1:E:111:LEU:HD13	1.77	0.67
2:G:119:GLY:O	2:G:122:ARG:HG2	1.95	0.67
2:H:231:LYS:HE2	2:H:233:SER:OG	1.94	0.67
2:C:228:PHE:HE1	2:C:267:ARG:HB3	1.58	0.67
2:D:246:TRP:CD1	2:D:331:TYR:CD2	2.82	0.67
2:C:148:MET:HE2	2:C:152:LEU:HG	1.76	0.66
2:C:58:ILE:HG22	2:C:59:GLU:N	2.10	0.66
2:D:202:SER:HA	2:D:297:LYS:O	1.95	0.66
1:F:238:GLY:HA2	1:F:305:GLY:O	1.96	0.66
2:H:373:GLU:O	2:H:377:MET:HG3	1.94	0.66
2:C:280:VAL:HG21	2:C:321:ALA:CB	2.26	0.66
2:D:119:GLY:O	2:D:122:ARG:HG2	1.96	0.66
2:D:373:GLU:O	2:D:377:MET:HG3	1.96	0.66
2:G:258:LEU:HD22	2:G:292:LEU:HD22	1.77	0.66
2:D:450:MET:CG	2:D:451:LEU:H	2.05	0.66
2:H:515:THR:HG22	2:H:516:ASN:N	2.08	0.66
2:C:244:TYR:O	2:C:248:LEU:HG	1.96	0.65
1:A:238:GLY:HA2	1:A:305:GLY:O	1.97	0.65
2:H:280:VAL:HG21	2:H:321:ALA:CB	2.27	0.65
1:B:31:GLN:HG2	1:B:56:SER:O	1.96	0.65
2:C:246:TRP:CD1	2:C:331:TYR:CD2	2.84	0.65
2:D:306:TRP:O	2:D:310:VAL:HG23	1.97	0.65
2:G:198:GLU:HG2	2:G:300:SER:CB	2.27	0.65
2:H:50:PRO:HB2	2:H:53:VAL:CG2	2.24	0.65
1:A:85:GLU:HB2	1:A:101:LEU:HD11	1.78	0.65
2:C:155:LEU:O	2:C:159:ILE:HG13	1.97	0.65
2:C:258:LEU:HD22	2:C:292:LEU:HD22	1.78	0.65
1:B:345:ILE:HG22	2:D:51:MET:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:198:GLU:HG2	2:C:300:SER:CB	2.27	0.65
2:D:278:CYS:SG	2:D:323:ASP:HB2	2.37	0.65
2:H:119:GLY:O	2:H:122:ARG:HG2	1.96	0.65
2:H:450:MET:HG3	2:H:451:LEU:H	1.62	0.65
2:H:383:VAL:HG12	2:H:384:VAL:N	2.12	0.65
2:C:373:GLU:O	2:C:377:MET:HG3	1.97	0.64
2:D:60:LYS:HB2	2:D:63:ASP:OD2	1.96	0.64
1:E:220:TRP:HA	1:E:231:ILE:HG22	1.78	0.64
2:H:166:ASP:OD2	2:H:169:VAL:HG11	1.97	0.64
1:E:31:GLN:HG2	1:E:56:SER:O	1.97	0.64
1:A:196:ARG:HH11	1:A:202:LEU:HD21	1.62	0.64
1:B:238:GLY:HA2	1:B:305:GLY:O	1.98	0.64
2:D:155:LEU:O	2:D:159:ILE:HG13	1.98	0.64
2:H:306:TRP:O	2:H:310:VAL:HG23	1.98	0.64
1:B:85:GLU:HB2	1:B:101:LEU:HD11	1.79	0.64
2:C:241:GLU:HG2	2:C:328:LEU:HD13	1.80	0.64
2:C:454:LEU:HG	2:C:455:PHE:N	2.13	0.64
1:B:313:ASN:HB2	1:B:318:ILE:H	1.63	0.64
2:H:155:LEU:O	2:H:159:ILE:HG13	1.98	0.64
2:G:244:TYR:O	2:G:248:LEU:HG	1.98	0.63
1:F:314:LEU:HD12	1:F:314:LEU:O	1.97	0.63
1:A:159:ILE:O	1:A:161:PRO:HD3	1.98	0.63
2:C:170:ASN:O	2:C:174:GLU:HG3	1.99	0.63
2:D:198:GLU:HG2	2:D:300:SER:CB	2.29	0.63
2:C:242:THR:HG22	2:C:243:GLN:N	2.14	0.63
2:D:59:GLU:HG3	2:D:60:LYS:N	2.07	0.63
2:H:240:PHE:HD2	2:H:241:GLU:N	1.96	0.63
2:G:373:GLU:O	2:G:377:MET:HG3	1.97	0.63
2:G:383:VAL:HG12	2:G:384:VAL:N	2.14	0.63
2:C:515:THR:HG22	2:C:516:ASN:N	2.10	0.63
1:F:151:THR:HG21	1:F:196:ARG:HH22	1.63	0.63
2:G:545:GLN:O	2:G:549:ALA:HB3	1.98	0.63
2:D:390:TRP:O	2:D:393:PRO:HD2	1.99	0.62
2:G:280:VAL:HG21	2:G:321:ALA:CB	2.28	0.62
2:C:227:VAL:C	2:C:229:SER:H	2.02	0.62
2:C:434:PHE:CD1	2:C:458:ARG:HA	2.34	0.62
1:F:42:THR:O	1:F:44:ASN:N	2.31	0.62
2:D:383:VAL:HG12	2:D:384:VAL:N	2.15	0.62
2:G:240:PHE:CD1	2:G:269:ASP:OD2	2.53	0.62
1:B:53:ALA:HB1	1:B:84:TRP:CZ2	2.35	0.62
1:E:196:ARG:HH11	1:E:202:LEU:HD21	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:O	2:C:70:LYS:HD2	2.00	0.62
1:E:313:ASN:HB2	1:E:318:ILE:H	1.65	0.62
2:H:239:VAL:CG1	2:H:268:SER:HB3	2.30	0.62
2:C:406:LEU:HB2	2:C:407:PRO:HD3	1.82	0.61
1:B:10:ASP:HB3	1:B:29:SER:HB2	1.83	0.61
1:F:68:TYR:OH	1:F:122:GLY:HA2	2.00	0.61
2:C:241:GLU:HG2	2:C:328:LEU:CD1	2.30	0.61
1:E:53:ALA:HB1	1:E:84:TRP:CZ2	2.35	0.61
2:G:515:THR:HG22	2:G:516:ASN:N	2.11	0.61
2:H:244:TYR:O	2:H:248:LEU:HG	2.00	0.61
2:H:202:SER:HA	2:H:297:LYS:O	2.00	0.61
2:D:163:LYS:HA	2:D:167:GLY:O	2.00	0.61
1:E:306:GLU:N	1:E:324:ASP:OD2	2.32	0.61
1:F:313:ASN:HB2	1:F:318:ILE:H	1.63	0.61
1:F:196:ARG:HH11	1:F:202:LEU:HD21	1.66	0.61
2:C:306:TRP:O	2:C:310:VAL:HG23	2.00	0.61
1:F:10:ASP:HB3	1:F:29:SER:HB2	1.82	0.61
2:C:119:GLY:O	2:C:122:ARG:HG2	1.99	0.61
1:F:85:GLU:HB2	1:F:101:LEU:HD11	1.82	0.61
2:D:280:VAL:HG21	2:D:321:ALA:CB	2.30	0.61
1:E:42:THR:O	1:E:44:ASN:N	2.30	0.60
2:H:406:LEU:HB2	2:H:407:PRO:HD3	1.83	0.60
2:D:240:PHE:HA	2:D:245:PHE:CB	2.31	0.60
1:F:344:VAL:O	2:H:48:LEU:HA	2.01	0.60
2:D:244:TYR:O	2:D:248:LEU:HG	2.01	0.60
2:H:240:PHE:O	2:H:242:THR:N	2.34	0.60
1:A:31:GLN:HG2	1:A:56:SER:O	2.01	0.60
2:D:169:VAL:HG12	2:D:170:ASN:N	2.16	0.60
1:A:313:ASN:HB2	1:A:318:ILE:H	1.65	0.60
2:C:158:PHE:O	2:C:162:VAL:HG23	2.02	0.60
2:C:383:VAL:HG12	2:C:384:VAL:N	2.16	0.60
2:C:201:ARG:CZ	2:C:205:ILE:HD11	2.32	0.60
1:A:53:ALA:HB1	1:A:84:TRP:CZ2	2.37	0.59
1:B:306:GLU:N	1:B:324:ASP:OD2	2.34	0.59
2:D:227:VAL:HG12	2:D:239:VAL:CG1	2.29	0.59
2:D:268:SER:O	2:D:272:PRO:HG2	2.01	0.59
2:H:166:ASP:OD2	2:H:169:VAL:CG1	2.51	0.59
2:H:291:LEU:HD13	2:H:310:VAL:HG22	1.83	0.59
2:G:268:SER:O	2:G:272:PRO:HG2	2.03	0.59
2:G:534:ILE:O	2:G:538:ILE:HG12	2.02	0.59
2:H:230:VAL:O	2:H:230:VAL:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LYS:O	1:A:209:PRO:HD3	2.02	0.59
1:B:42:THR:O	1:B:44:ASN:N	2.32	0.59
1:F:347:ALA:HB3	2:H:58:ILE:HB	1.84	0.59
2:G:401:LYS:HE2	2:H:401:LYS:HE2	1.84	0.59
2:D:170:ASN:O	2:D:174:GLU:HG3	2.02	0.59
1:E:218:ILE:HG22	1:E:233:THR:HG22	1.84	0.59
2:G:306:TRP:O	2:G:310:VAL:HG23	2.03	0.59
2:H:240:PHE:C	2:H:242:THR:H	2.06	0.59
2:C:226:GLN:O	2:C:230:VAL:HG23	2.02	0.59
1:E:10:ASP:HB3	1:E:29:SER:HB2	1.85	0.59
2:G:170:ASN:O	2:G:174:GLU:HG3	2.02	0.59
2:H:390:TRP:O	2:H:393:PRO:HD2	2.02	0.59
1:A:10:ASP:HB3	1:A:29:SER:HB2	1.85	0.59
2:G:406:LEU:HB2	2:G:407:PRO:HD3	1.83	0.59
2:C:268:SER:O	2:C:272:PRO:HG2	2.01	0.59
1:F:306:GLU:N	1:F:324:ASP:OD2	2.35	0.59
1:F:53:ALA:HB1	1:F:84:TRP:CZ2	2.37	0.59
2:G:198:GLU:OE1	2:H:437:GLU:HA	2.03	0.59
2:D:291:LEU:HD13	2:D:310:VAL:HG22	1.83	0.59
1:F:123:LEU:HB2	1:F:139:ALA:HB3	1.85	0.59
2:G:450:MET:O	2:G:451:LEU:HD23	2.03	0.59
2:G:542:LEU:O	2:G:546:MET:N	2.35	0.59
2:H:239:VAL:HG11	2:H:268:SER:HB3	1.85	0.59
1:A:81:VAL:HG23	1:A:111:LEU:CD1	2.32	0.59
1:A:314:LEU:O	1:A:314:LEU:HD12	2.03	0.59
1:F:207:LYS:O	1:F:209:PRO:HD3	2.03	0.59
2:H:240:PHE:HD2	2:H:241:GLU:H	1.49	0.59
2:C:242:THR:CG2	2:C:243:GLN:N	2.65	0.59
1:F:157:LEU:CD1	1:F:187:ALA:HB1	2.33	0.59
1:F:77:TYR:HD2	1:F:110:SER:HB3	1.67	0.59
2:H:240:PHE:CD2	2:H:241:GLU:N	2.70	0.59
1:B:311:SER:O	1:B:319:LEU:HD12	2.02	0.58
2:C:132:VAL:HG12	2:C:132:VAL:O	2.03	0.58
2:D:231:LYS:C	2:D:233:SER:H	2.05	0.58
1:F:31:GLN:HG2	1:F:56:SER:O	2.03	0.58
2:H:49:VAL:HG21	2:H:96:PRO:HB3	1.83	0.58
1:B:220:TRP:HA	1:B:231:ILE:HG22	1.84	0.58
1:F:191:ALA:HB2	1:F:215:ILE:CD1	2.33	0.58
1:A:101:LEU:O	1:A:102:CYS:HB2	2.03	0.58
2:D:201:ARG:CZ	2:D:205:ILE:HD11	2.33	0.58
2:H:434:PHE:CD1	2:H:458:ARG:O	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:PHE:CE1	2:H:90:LEU:HD12	2.39	0.58
1:E:166:GLN:O	1:E:166:GLN:HG2	2.04	0.58
1:F:101:LEU:O	1:F:102:CYS:HB2	2.04	0.58
2:C:291:LEU:HD13	2:C:310:VAL:HG22	1.84	0.58
2:C:53:VAL:O	2:C:53:VAL:HG13	2.03	0.58
2:D:406:LEU:HB2	2:D:407:PRO:HD3	1.85	0.58
2:D:450:MET:HG3	2:D:451:LEU:N	2.09	0.58
1:F:81:VAL:HG23	1:F:111:LEU:CD1	2.34	0.58
2:G:268:SER:HB2	2:G:269:ASP:OD1	2.04	0.58
2:C:522:MET:HE1	2:C:538:ILE:HD12	1.84	0.58
2:H:285:VAL:O	2:H:289:ILE:HG13	2.04	0.58
1:A:191:ALA:HB2	1:A:215:ILE:CD1	2.34	0.58
1:A:4:PHE:CE1	2:C:90:LEU:HD12	2.39	0.58
2:H:386:ILE:O	2:H:386:ILE:HG22	2.04	0.58
1:F:118:PRO:HD2	1:F:121:LEU:HD12	1.86	0.57
2:G:201:ARG:CZ	2:G:205:ILE:HD11	2.32	0.57
1:E:314:LEU:O	1:E:314:LEU:HD12	2.03	0.57
1:F:218:ILE:HG22	1:F:233:THR:HG22	1.85	0.57
2:G:539:TYR:HA	2:G:542:LEU:HD12	1.87	0.57
1:B:191:ALA:HB2	1:B:215:ILE:CD1	2.34	0.57
1:E:125:LEU:HD12	1:E:125:LEU:C	2.25	0.57
1:B:96:ARG:HG2	1:E:96:ARG:HG3	1.86	0.57
2:H:170:ASN:O	2:H:174:GLU:HG3	2.05	0.57
2:H:246:TRP:CD1	2:H:331:TYR:HD2	2.21	0.57
2:C:522:MET:CE	2:C:538:ILE:HD12	2.34	0.57
2:H:268:SER:O	2:H:272:PRO:HG2	2.04	0.57
2:H:201:ARG:CZ	2:H:205:ILE:HD11	2.35	0.57
1:F:77:TYR:HA	1:F:110:SER:HB3	1.84	0.57
2:G:453:ASP:O	2:G:455:PHE:N	2.38	0.57
2:D:158:PHE:O	2:D:162:VAL:HG23	2.05	0.57
1:F:158:SER:C	1:F:160:PRO:HD3	2.24	0.57
1:E:128:LEU:HD23	1:E:169:PHE:HB3	1.87	0.57
1:A:213:SER:OG	1:A:236:LYS:HD3	2.04	0.57
1:A:218:ILE:HG22	1:A:233:THR:HG22	1.87	0.57
1:B:207:LYS:O	1:B:209:PRO:HD3	2.05	0.57
2:D:265:ILE:C	2:D:267:ARG:H	2.07	0.57
1:F:15:VAL:O	2:H:70:LYS:HD2	2.04	0.57
2:G:365:ILE:HG21	2:H:457:TYR:OH	2.05	0.57
1:A:27:CYS:HB3	1:A:61:ILE:HD12	1.87	0.56
1:F:30:ASP:OD1	1:F:32:HIS:HB2	2.04	0.56
1:A:161:PRO:HB2	1:A:164:HIS:CD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:285:VAL:O	2:C:289:ILE:HG13	2.05	0.56
2:G:97:ARG:NH1	2:G:97:ARG:HB3	2.20	0.56
1:E:101:LEU:O	1:E:102:CYS:HB2	2.04	0.56
1:E:164:HIS:O	1:E:166:GLN:N	2.38	0.56
2:G:240:PHE:CE2	2:G:269:ASP:HB2	2.40	0.56
1:B:101:LEU:O	1:B:102:CYS:HB2	2.06	0.56
1:B:314:LEU:O	1:B:314:LEU:HD12	2.04	0.56
2:C:60:LYS:C	2:C:62:GLY:N	2.58	0.56
2:D:209:LEU:CD2	2:D:256:GLY:HA3	2.36	0.56
2:D:230:VAL:O	2:D:230:VAL:HG12	2.06	0.56
1:A:311:SER:O	1:A:319:LEU:HD12	2.06	0.56
1:B:118:PRO:HD2	1:B:121:LEU:HD12	1.87	0.56
1:E:123:LEU:HB2	1:E:139:ALA:HB3	1.88	0.56
1:A:123:LEU:HB2	1:A:139:ALA:HB3	1.86	0.56
1:A:42:THR:O	1:A:44:ASN:N	2.33	0.56
2:C:152:LEU:HD21	2:C:182:LEU:HB3	1.87	0.56
2:C:268:SER:HB2	2:C:269:ASP:OD1	2.06	0.56
2:C:386:ILE:O	2:C:386:ILE:HG22	2.06	0.56
2:H:268:SER:HB2	2:H:269:ASP:OD1	2.06	0.56
1:A:324:ASP:HB3	2:C:64:LYS:HB3	1.88	0.56
2:D:246:TRP:CD1	2:D:331:TYR:HD2	2.22	0.56
2:D:97:ARG:NH1	2:D:97:ARG:HB3	2.20	0.56
1:E:207:LYS:O	1:E:209:PRO:HD3	2.04	0.56
1:B:27:CYS:HB3	1:B:61:ILE:HD12	1.88	0.56
1:F:27:CYS:HB3	1:F:61:ILE:HD12	1.88	0.56
2:G:246:TRP:CD1	2:G:331:TYR:HD2	2.22	0.56
2:G:386:ILE:O	2:G:386:ILE:HG22	2.06	0.56
1:B:153:GLU:O	1:B:154:MET:HE3	2.06	0.55
1:F:77:TYR:CD2	1:F:110:SER:HB3	2.42	0.55
2:G:265:ILE:C	2:G:267:ARG:H	2.09	0.55
2:H:390:TRP:C	2:H:393:PRO:HD2	2.27	0.55
2:D:166:ASP:OD2	2:D:169:VAL:CG2	2.54	0.55
2:D:285:VAL:O	2:D:289:ILE:HG13	2.06	0.55
2:D:386:ILE:HG22	2:D:386:ILE:O	2.05	0.55
1:F:324:ASP:HB3	2:H:64:LYS:HB3	1.88	0.55
2:G:505:ALA:HB1	2:G:534:ILE:HD11	1.87	0.55
2:H:265:ILE:C	2:H:267:ARG:H	2.08	0.55
2:H:49:VAL:HG21	2:H:96:PRO:HG3	1.88	0.55
1:A:125:LEU:HD12	1:A:125:LEU:C	2.27	0.55
1:E:191:ALA:HB2	1:E:215:ILE:CD1	2.37	0.55
2:G:228:PHE:HE1	2:G:267:ARG:HG3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:C	1:B:125:LEU:HD12	2.27	0.55
1:B:218:ILE:O	1:B:218:ILE:HG13	2.06	0.55
1:E:15:VAL:O	2:G:70:LYS:HD2	2.06	0.55
1:A:218:ILE:HG13	1:A:218:ILE:O	2.06	0.55
2:D:461:MET:O	2:D:465:MET:HG3	2.06	0.55
1:A:306:GLU:N	1:A:324:ASP:OD2	2.36	0.55
2:D:249:LEU:O	2:D:253:VAL:HG23	2.06	0.55
2:H:57:PRO:HG3	2:H:91:TYR:CZ	2.41	0.55
2:C:271:LEU:N	2:C:272:PRO:CD	2.70	0.55
1:F:335:TYR:HB3	2:G:373:GLU:HG3	1.88	0.55
2:C:246:TRP:CD1	2:C:331:TYR:HD2	2.24	0.55
2:G:230:VAL:O	2:G:230:VAL:HG12	2.07	0.55
2:G:271:LEU:N	2:G:272:PRO:CD	2.69	0.55
2:G:291:LEU:HD13	2:G:310:VAL:HG22	1.88	0.55
2:G:202:SER:HA	2:G:297:LYS:O	2.07	0.55
2:H:158:PHE:O	2:H:162:VAL:HG23	2.06	0.55
1:E:311:SER:O	1:E:319:LEU:HD12	2.06	0.55
2:G:390:TRP:O	2:G:393:PRO:HD2	2.07	0.55
1:B:128:LEU:HD23	1:B:169:PHE:HB3	1.89	0.55
1:E:85:GLU:HB2	1:E:101:LEU:HD11	1.88	0.55
2:G:240:PHE:CE1	2:G:269:ASP:OD2	2.60	0.55
2:H:240:PHE:CZ	2:H:269:ASP:OD2	2.60	0.55
2:D:271:LEU:N	2:D:272:PRO:CD	2.70	0.54
2:C:265:ILE:C	2:C:267:ARG:H	2.09	0.54
2:C:249:LEU:O	2:C:253:VAL:HG23	2.06	0.54
1:E:247:GLU:HB3	1:E:292:LEU:HD23	1.90	0.54
1:F:346:THR:OG1	1:F:347:ALA:N	2.39	0.54
2:H:152:LEU:HD21	2:H:182:LEU:HB3	1.88	0.54
2:H:49:VAL:HG21	2:H:96:PRO:CG	2.37	0.54
1:A:30:ASP:OD1	1:A:32:HIS:HB2	2.07	0.54
2:D:152:LEU:HD21	2:D:182:LEU:HB3	1.89	0.54
2:D:271:LEU:O	2:D:275:SER:HB3	2.08	0.54
1:E:140:LEU:O	1:E:142:PRO:HD3	2.08	0.54
1:F:126:ALA:HB2	1:F:136:LEU:CD2	2.38	0.54
2:G:240:PHE:CZ	2:G:328:LEU:HD11	2.43	0.54
2:H:352:THR:OG1	2:H:355:GLU:HG3	2.07	0.54
2:C:202:SER:HA	2:C:297:LYS:O	2.08	0.54
2:C:63:ASP:O	2:C:64:LYS:C	2.43	0.54
2:D:335:PHE:CZ	2:D:339:ILE:HD11	2.42	0.54
2:G:97:ARG:HH11	2:G:97:ARG:HB3	1.73	0.54
2:G:436:GLY:O	2:H:198:GLU:OE2	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:383:VAL:HG12	2:H:384:VAL:H	1.72	0.54
2:G:343:GLN:NE2	2:G:364:TYR:CZ	2.72	0.54
2:C:58:ILE:HG22	2:C:59:GLU:H	1.72	0.54
1:B:221:ALA:HB2	1:B:312:TRP:CD2	2.42	0.53
1:F:125:LEU:C	1:F:125:LEU:HD12	2.28	0.53
2:D:97:ARG:HH11	2:D:97:ARG:HB3	1.73	0.53
1:E:218:ILE:O	1:E:218:ILE:HG13	2.08	0.53
1:F:347:ALA:CB	2:H:58:ILE:HB	2.38	0.53
2:G:539:TYR:HA	2:G:542:LEU:HB2	1.90	0.53
2:H:228:PHE:HE2	2:H:267:ARG:HB3	1.73	0.53
1:E:335:TYR:HB3	2:H:373:GLU:HG3	1.90	0.53
2:C:271:LEU:O	2:C:275:SER:HB3	2.09	0.53
2:C:534:ILE:O	2:C:538:ILE:HG12	2.08	0.53
1:A:308:TRP:CD1	2:C:66:PRO:HA	2.43	0.53
2:D:390:TRP:C	2:D:393:PRO:HD2	2.28	0.53
2:H:97:ARG:NH1	2:H:97:ARG:HB3	2.23	0.53
2:D:268:SER:HB2	2:D:269:ASP:OD1	2.07	0.53
1:A:209:PRO:HB2	2:D:318:GLY:HA3	1.91	0.53
1:F:221:ALA:HB2	1:F:312:TRP:CD2	2.42	0.53
2:H:249:LEU:O	2:H:253:VAL:HG23	2.09	0.53
2:H:239:VAL:HB	2:H:268:SER:CB	2.35	0.53
2:H:271:LEU:N	2:H:272:PRO:CD	2.71	0.53
1:A:92:GLU:O	1:A:93:CYS:HB2	2.08	0.53
1:B:236:LYS:HG3	1:B:306:GLU:OE1	2.08	0.53
2:C:97:ARG:NH1	2:C:97:ARG:HB3	2.24	0.53
1:F:74:SER:O	1:F:81:VAL:HA	2.09	0.53
1:A:85:GLU:OE2	1:A:145:LEU:HD12	2.08	0.53
1:B:159:ILE:C	1:B:161:PRO:CD	2.74	0.53
1:B:92:GLU:O	1:B:93:CYS:HB2	2.09	0.53
1:F:205:ALA:O	1:F:206:ALA:HB2	2.07	0.53
2:H:335:PHE:O	2:H:339:ILE:HG13	2.09	0.53
1:B:192:ILE:HD11	1:B:194:TYR:CE1	2.44	0.53
1:B:1(A):PRO:O	1:B:1(B):HIS:HB3	2.08	0.53
2:D:352:THR:OG1	2:D:355:GLU:HG3	2.09	0.53
2:D:343:GLN:NE2	2:D:364:TYR:CZ	2.71	0.53
1:E:205:ALA:O	1:E:206:ALA:HB2	2.09	0.53
2:H:271:LEU:O	2:H:275:SER:HB3	2.09	0.53
1:B:123:LEU:HB2	1:B:139:ALA:HB3	1.90	0.53
1:B:303:HIS:HA	1:B:325:ASP:OD2	2.08	0.53
1:B:30:ASP:OD1	1:B:32:HIS:HB2	2.09	0.53
1:B:345:ILE:CG2	2:D:51:MET:HA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:THR:CG2	1:F:196:ARG:HH22	2.21	0.53
1:F:218:ILE:HG13	1:F:218:ILE:O	2.08	0.53
1:B:85:GLU:OE2	1:B:145:LEU:HD12	2.09	0.52
1:F:311:SER:O	1:F:319:LEU:HD12	2.09	0.52
2:G:271:LEU:O	2:G:275:SER:HB3	2.09	0.52
2:H:335:PHE:CZ	2:H:339:ILE:HD11	2.44	0.52
2:H:364:TYR:CD2	2:H:365:ILE:HG13	2.44	0.52
2:D:240:PHE:CE2	2:D:269:ASP:OD2	2.62	0.52
2:G:269:ASP:N	2:G:269:ASP:OD1	2.41	0.52
2:G:285:VAL:O	2:G:289:ILE:HG13	2.09	0.52
2:G:155:LEU:O	2:G:159:ILE:HG13	2.09	0.52
2:G:158:PHE:O	2:G:162:VAL:HG23	2.09	0.52
2:G:352:THR:OG1	2:G:355:GLU:HG3	2.08	0.52
2:H:292:LEU:HD11	2:H:335:PHE:HZ	1.74	0.52
1:A:183:LEU:C	1:A:183:LEU:HD12	2.29	0.52
1:B:247:GLU:HB3	1:B:292:LEU:HD23	1.91	0.52
2:C:451:LEU:HD22	2:C:458:ARG:NE	2.24	0.52
2:C:461:MET:O	2:C:465:MET:HG3	2.09	0.52
2:C:169:VAL:HG12	2:C:169:VAL:O	2.10	0.52
1:E:68:TYR:CD1	1:E:123:LEU:HD11	2.45	0.52
2:G:383:VAL:HG12	2:G:384:VAL:H	1.74	0.52
1:B:126:ALA:HB2	1:B:136:LEU:CD2	2.39	0.52
2:C:364:TYR:CD2	2:C:365:ILE:HG13	2.45	0.52
1:F:291:ASN:HD22	1:F:291:ASN:N	2.08	0.52
1:A:212:LYS:NZ	2:D:330:ASP:OD1	2.38	0.52
2:C:335:PHE:CZ	2:C:339:ILE:HD11	2.45	0.52
1:E:303:HIS:HA	1:E:325:ASP:OD2	2.09	0.52
1:F:162:ALA:O	1:F:164:HIS:N	2.43	0.52
1:A:140:LEU:O	1:A:142:PRO:HD3	2.09	0.52
2:C:390:TRP:O	2:C:393:PRO:HD2	2.09	0.52
2:D:383:VAL:HG12	2:D:384:VAL:H	1.74	0.52
1:E:126:ALA:HB2	1:E:136:LEU:CD2	2.40	0.52
1:E:157:LEU:HD13	1:E:161:PRO:HD2	1.92	0.52
1:F:303:HIS:HA	1:F:325:ASP:OD2	2.10	0.52
1:A:335:TYR:HB3	2:D:373:GLU:HG3	1.92	0.51
2:G:364:TYR:CD2	2:G:365:ILE:HG13	2.45	0.51
1:A:131:ASP:OD1	1:A:135:ARG:NH2	2.43	0.51
1:B:140:LEU:O	1:B:142:PRO:HD3	2.10	0.51
2:G:153:ASN:O	2:G:157:VAL:HG23	2.10	0.51
2:G:190:PHE:CE2	2:G:427:LYS:HG3	2.45	0.51
2:C:352:THR:OG1	2:C:355:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:PRO:N	1:F:161:PRO:CD	2.73	0.51
2:G:249:LEU:O	2:G:253:VAL:HG23	2.09	0.51
2:C:141:ASN:O	2:C:145:ASN:ND2	2.43	0.51
2:C:292:LEU:HD11	2:C:335:PHE:HZ	1.75	0.51
2:G:539:TYR:O	2:G:543:GLY:N	2.44	0.51
2:H:269:ASP:N	2:H:269:ASP:OD1	2.42	0.51
2:D:269:ASP:N	2:D:269:ASP:OD1	2.43	0.51
1:F:153:GLU:O	1:F:154:MET:HE3	2.11	0.51
2:G:532:PRO:CG	2:G:533:GLU:H	2.21	0.51
2:H:223:TYR:O	2:H:226:GLN:HB2	2.11	0.51
1:B:81:VAL:HG23	1:B:111:LEU:CD1	2.40	0.51
1:B:239:ARG:HH11	1:B:239:ARG:HG3	1.75	0.51
1:F:167:SER:HA	1:F:188:LEU:HD21	1.91	0.51
1:F:140:LEU:O	1:F:142:PRO:HD3	2.10	0.51
1:B:159:ILE:O	1:B:161:PRO:HD3	2.09	0.51
2:D:262:ILE:HG12	2:D:289:ILE:HG23	1.93	0.51
1:B:3:PRO:CD	2:D:52:THR:HG21	2.41	0.51
1:E:77:TYR:HD2	1:E:110:SER:HB3	1.76	0.51
2:G:453:ASP:O	2:G:454:LEU:C	2.47	0.51
1:A:192:ILE:HD11	1:A:194:TYR:CE1	2.46	0.51
1:B:151:THR:HG21	1:B:196:ARG:HH22	1.76	0.51
2:H:49:VAL:HG21	2:H:96:PRO:CB	2.40	0.51
2:C:390:TRP:C	2:C:393:PRO:HD2	2.31	0.51
2:D:364:TYR:CD2	2:D:365:ILE:HG13	2.46	0.51
1:E:124:LYS:HG3	1:E:138:ASP:OD1	2.11	0.51
1:E:30:ASP:OD1	1:E:32:HIS:HB2	2.10	0.51
1:F:159:ILE:O	1:F:159:ILE:HG22	2.11	0.51
1:F:3:PRO:HG3	2:H:52:THR:HG21	1.92	0.51
2:D:515:THR:CG2	2:D:516:ASN:H	2.13	0.50
1:F:92:GLU:O	1:F:93:CYS:HB2	2.11	0.50
1:A:239:ARG:HG3	1:A:239:ARG:HH11	1.76	0.50
1:A:178:PHE:CD1	2:C:502:MET:HE2	2.46	0.50
2:G:522:MET:HE2	2:G:538:ILE:HG13	1.94	0.50
1:A:68:TYR:CD1	1:A:123:LEU:HD11	2.46	0.50
1:A:225:GLY:O	2:C:453:ASP:CB	2.56	0.50
2:D:523:LEU:CD2	2:D:535:ALA:HB1	2.41	0.50
1:E:136:LEU:HD11	1:E:202:LEU:HD11	1.93	0.50
2:H:163:LYS:HA	2:H:167:GLY:O	2.10	0.50
1:A:102:CYS:SG	1:A:103:THR:N	2.85	0.50
1:E:27:CYS:HB3	1:E:61:ILE:HD12	1.92	0.50
1:F:247:GLU:HB3	1:F:292:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:PRO:HA	1:F:97:ARG:HH12	1.76	0.50
1:A:303:HIS:HA	1:A:325:ASP:OD2	2.11	0.50
1:B:74:SER:O	1:B:81:VAL:HA	2.11	0.50
2:C:262:ILE:HG12	2:C:289:ILE:HG23	1.93	0.50
2:C:269:ASP:N	2:C:269:ASP:OD1	2.44	0.50
2:C:343:GLN:NE2	2:C:364:TYR:CZ	2.68	0.50
1:A:324:ASP:HB3	2:C:64:LYS:HD3	1.93	0.50
1:F:131:ASP:OD1	1:F:135:ARG:NH2	2.44	0.50
2:G:390:TRP:C	2:G:393:PRO:HD2	2.32	0.50
1:A:183:LEU:O	1:A:183:LEU:HD12	2.11	0.50
2:D:240:PHE:HA	2:D:245:PHE:CG	2.47	0.50
1:E:131:ASP:OD1	1:E:135:ARG:NH2	2.44	0.50
1:A:77:TYR:HA	1:A:110:SER:HB3	1.92	0.50
1:E:92:GLU:O	1:E:93:CYS:HB2	2.11	0.50
1:F:236:LYS:HG3	1:F:306:GLU:OE1	2.12	0.50
1:E:154:MET:HA	1:E:154:MET:HE2	1.94	0.50
1:F:131:ASP:O	1:F:159:ILE:HD11	2.11	0.50
1:A:126:ALA:HB2	1:A:136:LEU:CD2	2.41	0.50
1:B:102:CYS:SG	1:B:103:THR:N	2.85	0.50
1:E:308:TRP:CD1	2:G:66:PRO:HA	2.47	0.50
2:H:509:PRO:HA	2:H:538:ILE:CD1	2.42	0.49
1:B:213:SER:OG	1:B:236:LYS:HD3	2.12	0.49
2:C:218:GLU:HA	2:C:220:ASP:N	2.27	0.49
2:C:240:PHE:CD1	2:C:268:SER:CB	2.95	0.49
2:D:292:LEU:HD11	2:D:335:PHE:HZ	1.76	0.49
1:E:221:ALA:HB2	1:E:312:TRP:CD2	2.47	0.49
1:E:239:ARG:HH11	1:E:239:ARG:HG3	1.77	0.49
1:F:114:VAL:HA	1:F:126:ALA:O	2.11	0.49
1:F:239:ARG:HG3	1:F:239:ARG:HH11	1.76	0.49
1:B:65:SER:HB2	1:B:119:ALA:HB2	1.94	0.49
2:C:105:SER:HB2	2:C:481:LEU:HD21	1.95	0.49
1:E:81:VAL:HG23	1:E:111:LEU:CD1	2.40	0.49
1:F:97:ARG:HH11	1:F:97:ARG:HG3	1.77	0.49
2:H:343:GLN:NE2	2:H:364:TYR:CZ	2.68	0.49
1:B:76:SER:HB3	1:B:78:ASP:OD1	2.12	0.49
1:E:220:TRP:CG	1:E:231:ILE:HG22	2.48	0.49
2:G:218:GLU:HA	2:G:220:ASP:N	2.28	0.49
1:B:61:ILE:O	1:B:62:ASP:HB2	2.12	0.49
1:E:151:THR:HG21	1:E:196:ARG:HH22	1.78	0.49
1:F:189:GLU:HA	1:F:213:SER:O	2.13	0.49
1:F:314:LEU:C	1:F:314:LEU:HD12	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:231:LYS:O	2:H:237:LYS:HD3	2.13	0.49
1:A:221:ALA:HB2	1:A:312:TRP:CD2	2.47	0.49
1:B:189:GLU:HA	1:B:213:SER:O	2.12	0.49
2:D:153:ASN:O	2:D:157:VAL:HG23	2.12	0.49
2:D:218:GLU:HA	2:D:220:ASP:N	2.28	0.49
2:D:221:GLU:HA	2:D:224:ILE:HG13	1.94	0.49
1:A:74:SER:O	1:A:81:VAL:HA	2.12	0.49
2:D:225:GLU:HA	2:D:228:PHE:HB2	1.94	0.49
1:B:4:PHE:CE1	2:D:90:LEU:HD12	2.47	0.49
1:F:161:PRO:HB2	1:F:165:LEU:HB2	1.94	0.49
1:E:293:GLN:OE1	2:H:311:LEU:HD12	2.13	0.49
2:H:451:LEU:O	2:H:458:ARG:NH1	2.45	0.49
1:A:205:ALA:O	1:A:206:ALA:HB2	2.13	0.49
2:C:58:ILE:CG2	2:C:59:GLU:N	2.75	0.49
2:D:240:PHE:CD2	2:D:269:ASP:OD2	2.66	0.49
1:E:118:PRO:HD2	1:E:121:LEU:HD12	1.95	0.49
1:E:183:LEU:HD12	1:E:183:LEU:C	2.32	0.49
1:F:311:SER:HB3	1:F:320:SER:OG	2.13	0.49
2:G:292:LEU:HD11	2:G:335:PHE:HZ	1.77	0.49
2:G:530:ARG:O	2:G:532:PRO:HD3	2.13	0.49
1:B:205:ALA:O	1:B:206:ALA:HB2	2.12	0.49
2:C:434:PHE:CD2	2:C:457:TYR:HE1	2.30	0.49
2:D:190:PHE:CE2	2:D:427:LYS:HG3	2.48	0.49
1:F:128:LEU:HD23	1:F:169:PHE:HB3	1.95	0.49
1:A:76:SER:HB3	1:A:78:ASP:OD1	2.13	0.48
1:B:218:ILE:HG22	1:B:233:THR:HG22	1.95	0.48
2:C:392:GLN:HB3	2:C:393:PRO:HD3	1.95	0.48
1:E:48:SER:O	1:E:92:GLU:HB3	2.13	0.48
2:G:262:ILE:HG12	2:G:289:ILE:HG23	1.95	0.48
2:G:454:LEU:HD21	2:G:489:ILE:HG23	1.94	0.48
1:A:153:GLU:O	1:A:154:MET:HE3	2.13	0.48
1:B:15:VAL:O	2:D:70:LYS:HD2	2.12	0.48
1:B:48:SER:O	1:B:92:GLU:HB3	2.12	0.48
2:C:220:ASP:OD2	2:C:222:GLU:HB3	2.13	0.48
1:F:119:ALA:C	1:F:121:LEU:H	2.17	0.48
2:G:461:MET:O	2:G:465:MET:HG3	2.14	0.48
2:H:218:GLU:HA	2:H:220:ASP:N	2.28	0.48
2:H:220:ASP:OD2	2:H:222:GLU:HB3	2.13	0.48
1:A:131:ASP:O	1:A:133:ILE:HG13	2.13	0.48
2:D:234:THR:O	2:D:234:THR:HG22	2.13	0.48
2:H:107:TYR:CZ	2:H:111:LEU:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:TYR:CD1	1:B:123:LEU:HD11	2.48	0.48
2:C:141:ASN:HD22	2:C:141:ASN:N	2.11	0.48
2:C:515:THR:CG2	2:C:516:ASN:H	2.20	0.48
2:D:220:ASP:OD2	2:D:222:GLU:HB3	2.12	0.48
2:D:335:PHE:O	2:D:339:ILE:HG13	2.14	0.48
1:B:227:TRP:CD1	2:D:450:MET:HB2	2.49	0.48
1:F:101:LEU:HB3	1:F:145:LEU:O	2.13	0.48
1:B:159:ILE:O	1:B:161:PRO:CD	2.61	0.48
2:C:153:ASN:O	2:C:157:VAL:HG23	2.13	0.48
2:C:383:VAL:HG12	2:C:384:VAL:H	1.75	0.48
1:E:187:ALA:O	1:E:188:LEU:HB2	2.13	0.48
1:E:74:SER:O	1:E:81:VAL:HA	2.13	0.48
2:H:97:ARG:HH11	2:H:97:ARG:HB3	1.78	0.48
1:A:196:ARG:NH1	1:A:202:LEU:HD21	2.29	0.48
1:B:157:LEU:O	1:B:158:SER:C	2.51	0.48
1:B:77:TYR:HA	1:B:110:SER:HB3	1.96	0.48
2:H:221:GLU:HA	2:H:224:ILE:HG13	1.95	0.48
1:A:314:LEU:C	1:A:314:LEU:HD12	2.34	0.48
1:F:192:ILE:HD11	1:F:194:TYR:CE1	2.48	0.48
1:F:247:GLU:HB3	1:F:292:LEU:CD2	2.44	0.48
2:G:220:ASP:OD2	2:G:222:GLU:HB3	2.13	0.48
1:B:114:VAL:HA	1:B:126:ALA:O	2.14	0.48
2:D:223:TYR:O	2:D:226:GLN:HB2	2.14	0.48
2:D:231:LYS:C	2:D:233:SER:N	2.67	0.48
1:F:131:ASP:O	1:F:133:ILE:HG13	2.14	0.48
1:F:312:TRP:CZ3	1:F:319:LEU:HB2	2.49	0.48
2:H:141:ASN:HD22	2:H:141:ASN:N	2.12	0.48
2:H:484:VAL:O	2:H:488:LEU:HB2	2.13	0.48
1:F:346:THR:HG22	2:H:49:VAL:O	2.13	0.48
2:H:57:PRO:CG	2:H:91:TYR:CZ	2.97	0.48
1:B:183:LEU:C	1:B:183:LEU:HD12	2.34	0.48
2:C:223:TYR:HA	2:C:226:GLN:HB2	1.95	0.48
1:F:213:SER:OG	1:F:236:LYS:HD3	2.14	0.48
2:G:508:LEU:HG	2:G:522:MET:HE3	1.96	0.48
2:G:532:PRO:HG2	2:G:533:GLU:N	2.23	0.48
2:H:190:PHE:CE2	2:H:427:LYS:HG3	2.48	0.48
1:A:189:GLU:HA	1:A:213:SER:O	2.14	0.48
2:G:436:GLY:O	2:G:437:GLU:HG3	2.13	0.48
2:H:461:MET:O	2:H:465:MET:HG3	2.14	0.48
1:A:118:PRO:HD2	1:A:121:LEU:HD12	1.96	0.47
1:B:131:ASP:OD1	1:B:135:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ILE:CD1	1:B:245:ILE:HD13	2.44	0.47
1:B:296:LEU:HD21	1:B:299:GLU:HG3	1.96	0.47
2:C:453:ASP:OD1	2:C:499:ALA:HB1	2.13	0.47
2:C:97:ARG:HB3	2:C:97:ARG:HH11	1.77	0.47
1:E:189:GLU:HA	1:E:213:SER:O	2.14	0.47
1:E:29:SER:C	1:E:31:GLN:H	2.18	0.47
1:E:1:MET:O	1:E:3:PRO:HD3	2.14	0.47
2:G:335:PHE:CZ	2:G:339:ILE:HD11	2.49	0.47
1:E:101:LEU:HB3	1:E:145:LEU:O	2.13	0.47
1:E:20:TYR:OH	2:G:541:THR:HG21	2.14	0.47
2:G:198:GLU:HG2	2:G:300:SER:HB2	1.95	0.47
2:H:198:GLU:HG2	2:H:300:SER:HB2	1.92	0.47
1:A:187:ALA:O	1:A:188:LEU:HB2	2.13	0.47
1:E:192:ILE:HD11	1:E:194:TYR:CE1	2.49	0.47
1:F:166:GLN:HB3	1:F:214:LEU:HD11	1.96	0.47
1:B:131:ASP:O	1:B:133:ILE:HG13	2.14	0.47
1:E:247:GLU:HB3	1:E:292:LEU:CD2	2.44	0.47
2:H:153:ASN:O	2:H:157:VAL:HG23	2.14	0.47
1:A:48:SER:O	1:A:92:GLU:HB3	2.15	0.47
2:D:196:ASP:OD1	2:D:367:SER:HA	2.14	0.47
1:F:86:GLU:HB2	1:F:98:TRP:CZ2	2.49	0.47
2:G:223:TYR:HA	2:G:226:GLN:HB2	1.96	0.47
2:H:480:GLU:O	2:H:483:PRO:HD2	2.15	0.47
2:C:508:LEU:HG	2:C:522:MET:HE3	1.96	0.47
2:H:240:PHE:CE2	2:H:269:ASP:OD2	2.68	0.47
2:H:455:PHE:HE1	2:H:468:SER:OG	1.96	0.47
2:C:454:LEU:CG	2:C:455:PHE:N	2.78	0.47
2:G:392:GLN:HB3	2:G:393:PRO:HD3	1.96	0.47
2:G:505:ALA:HA	2:G:534:ILE:HD12	1.96	0.47
2:H:262:ILE:HG12	2:H:289:ILE:HG23	1.96	0.47
1:B:196:ARG:HD2	1:B:202:LEU:HD23	1.97	0.47
2:C:223:TYR:O	2:C:226:GLN:HB2	2.15	0.47
1:F:48:SER:O	1:F:92:GLU:HB3	2.14	0.47
1:F:20:TYR:OH	2:H:541:THR:HG21	2.15	0.47
1:A:123:LEU:HD12	1:A:123:LEU:H	1.80	0.47
1:A:296:LEU:HD21	1:A:299:GLU:HG3	1.96	0.47
1:B:187:ALA:O	1:B:188:LEU:HB2	2.14	0.47
2:G:223:TYR:O	2:G:226:GLN:HB2	2.15	0.47
2:C:221:GLU:HA	2:C:224:ILE:HG13	1.96	0.47
2:D:402:ILE:O	2:D:405:ILE:HG12	2.14	0.47
2:D:455:PHE:CD2	2:D:455:PHE:O	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:484:VAL:O	2:D:488:LEU:HB2	2.14	0.47
2:D:533:GLU:H	2:D:533:GLU:CD	2.16	0.47
1:E:183:LEU:HD12	1:E:183:LEU:O	2.15	0.47
1:E:314:LEU:C	1:E:314:LEU:HD12	2.35	0.47
1:B:301:ASP:OD1	1:B:301:ASP:N	2.47	0.47
1:B:9:ASP:O	2:D:88:TYR:CZ	2.68	0.47
2:G:457:TYR:OH	2:H:365:ILE:HG21	2.15	0.47
2:H:223:TYR:HA	2:H:226:GLN:HB2	1.95	0.47
2:H:196:ASP:OD1	2:H:367:SER:HA	2.15	0.47
2:H:515:THR:CG2	2:H:516:ASN:H	2.17	0.47
1:A:119:ALA:C	1:A:121:LEU:H	2.19	0.46
1:B:119:ALA:C	1:B:121:LEU:H	2.18	0.46
2:C:335:PHE:O	2:C:339:ILE:HG13	2.15	0.46
2:C:484:VAL:O	2:C:488:LEU:HB2	2.15	0.46
2:D:123:VAL:HG12	2:D:124:PHE:N	2.30	0.46
2:D:482:TRP:N	2:D:483:PRO:CD	2.78	0.46
1:E:4:PHE:CE1	2:G:90:LEU:HD12	2.50	0.46
2:G:105:SER:HB2	2:G:481:LEU:HD21	1.96	0.46
1:A:124:LYS:HG3	1:A:138:ASP:OD1	2.16	0.46
2:C:57:PRO:HB2	2:C:82:ILE:HD11	1.97	0.46
2:D:105:SER:HB2	2:D:481:LEU:HD21	1.96	0.46
1:A:114:VAL:HA	1:A:126:ALA:O	2.16	0.46
1:B:107:SER:HA	1:B:135:ARG:HH21	1.80	0.46
2:D:59:GLU:CG	2:D:60:LYS:H	2.10	0.46
1:E:296:LEU:HD21	1:E:299:GLU:HG3	1.97	0.46
2:H:209:LEU:HD21	2:H:256:GLY:HA3	1.97	0.46
1:B:196:ARG:NH1	1:B:202:LEU:HD21	2.27	0.46
1:B:29:SER:C	1:B:31:GLN:H	2.19	0.46
2:C:198:GLU:HG2	2:C:300:SER:HB2	1.97	0.46
2:D:480:GLU:O	2:D:483:PRO:HD2	2.15	0.46
1:E:157:LEU:HD13	1:E:161:PRO:CD	2.46	0.46
1:F:113:SER:O	1:F:127:CYS:HA	2.15	0.46
1:F:11:LEU:O	1:F:28:SER:HB2	2.14	0.46
1:F:167:SER:HA	1:F:188:LEU:CD2	2.46	0.46
1:F:296:LEU:HD21	1:F:299:GLU:HG3	1.97	0.46
2:G:107:TYR:CZ	2:G:111:LEU:HD11	2.51	0.46
1:B:1(B):HIS:ND1	1:B:1(B):HIS:O	2.45	0.46
2:C:123:VAL:HG12	2:C:124:PHE:N	2.31	0.46
2:C:57:PRO:HB2	2:C:82:ILE:CD1	2.45	0.46
2:C:61:ASN:O	2:C:63:ASP:N	2.49	0.46
2:D:107:TYR:CZ	2:D:111:LEU:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:TYR:HA	2:D:226:GLN:HB2	1.97	0.46
2:D:235:ALA:C	2:D:237:LYS:H	2.18	0.46
1:E:97:ARG:HH11	1:E:97:ARG:HG3	1.81	0.46
1:F:134:LEU:HD11	1:F:183:LEU:HD11	1.97	0.46
1:F:183:LEU:HD12	1:F:183:LEU:C	2.36	0.46
1:F:7:GLY:C	1:F:34:LYS:HE3	2.36	0.46
2:G:484:VAL:O	2:G:488:LEU:HB2	2.15	0.46
1:A:301:ASP:O	1:A:303:HIS:N	2.49	0.46
2:C:243:GLN:O	2:C:247:LYS:HG3	2.16	0.46
2:C:58:ILE:CG2	2:C:59:GLU:H	2.28	0.46
2:D:210:ASN:OD1	2:D:214:ARG:HD2	2.16	0.46
1:F:68:TYR:CD1	1:F:123:LEU:HD11	2.51	0.46
1:F:29:SER:C	1:F:31:GLN:H	2.19	0.46
1:E:77:TYR:CD2	1:E:110:SER:HB3	2.50	0.46
2:H:209:LEU:CD2	2:H:256:GLY:HA3	2.46	0.46
2:H:242:THR:CG2	2:H:244:TYR:HB2	2.46	0.46
1:A:117:ALA:HB3	1:A:124:LYS:HB3	1.98	0.46
1:B:124:LYS:HG3	1:B:138:ASP:OD1	2.16	0.46
1:B:87:ASP:OD2	1:B:90:GLN:HG2	2.15	0.46
2:D:209:LEU:HD21	2:D:256:GLY:HA3	1.97	0.46
2:G:335:PHE:O	2:G:339:ILE:HG13	2.16	0.46
2:H:392:GLN:HB3	2:H:393:PRO:HD3	1.98	0.46
1:F:225:GLY:O	2:H:453:ASP:HA	2.16	0.46
1:F:308:TRP:CD1	2:H:66:PRO:HA	2.51	0.46
1:B:83:LEU:HD13	1:B:148:TRP:CE2	2.51	0.46
1:B:314:LEU:C	1:B:314:LEU:HD12	2.36	0.46
1:E:76:SER:HB3	1:E:78:ASP:OD1	2.16	0.46
2:G:278:CYS:HB2	2:G:323:ASP:O	2.16	0.46
2:C:455:PHE:CD2	2:C:455:PHE:O	2.69	0.45
2:D:141:ASN:O	2:D:145:ASN:ND2	2.49	0.45
1:F:159:ILE:N	1:F:160:PRO:CD	2.79	0.45
1:F:220:TRP:CG	1:F:231:ILE:HG22	2.51	0.45
1:B:178:PHE:CD1	2:D:502:MET:HE2	2.51	0.45
1:E:45:TRP:HZ2	2:G:77:GLN:HG2	1.81	0.45
2:G:296:PRO:HD3	2:G:306:TRP:CD1	2.50	0.45
2:G:515:THR:CG2	2:G:516:ASN:H	2.20	0.45
2:H:278:CYS:HB2	2:H:323:ASP:O	2.16	0.45
1:B:154:MET:HE2	1:B:154:MET:HA	1.99	0.45
2:C:296:PRO:HD3	2:C:306:TRP:CD1	2.51	0.45
2:C:533:GLU:HG2	2:C:533:GLU:H	1.29	0.45
2:D:508:LEU:HG	2:D:522:MET:HE3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:CYS:SG	1:E:103:THR:N	2.89	0.45
1:E:301:ASP:O	1:E:303:HIS:N	2.49	0.45
1:F:154:MET:HE2	1:F:154:MET:HA	1.98	0.45
2:G:221:GLU:HA	2:G:224:ILE:HG13	1.97	0.45
2:G:453:ASP:C	2:G:455:PHE:N	2.69	0.45
1:B:1:MET:HA	1:B:1:MET:CE	2.46	0.45
1:B:301:ASP:O	1:B:303:HIS:N	2.50	0.45
2:C:434:PHE:CE2	2:C:457:TYR:CE1	3.04	0.45
2:C:482:TRP:N	2:C:483:PRO:CD	2.78	0.45
2:G:141:ASN:N	2:G:141:ASN:HD22	2.14	0.45
2:H:481:LEU:O	2:H:484:VAL:HB	2.17	0.45
1:B:97:ARG:HG3	1:B:97:ARG:HH11	1.81	0.45
2:C:434:PHE:CE2	2:C:457:TYR:HE1	2.34	0.45
1:A:209:PRO:HG3	2:D:315:GLN:HA	1.99	0.45
1:F:161:PRO:HA	1:F:165:LEU:HD12	1.99	0.45
1:F:128:LEU:HD22	1:F:185:VAL:HG13	1.97	0.45
2:H:296:PRO:HD3	2:H:306:TRP:CD1	2.51	0.45
1:A:114:VAL:HG13	1:A:114:VAL:O	2.16	0.45
1:B:114:VAL:O	1:B:114:VAL:HG13	2.17	0.45
1:B:247:GLU:HB3	1:B:292:LEU:CD2	2.46	0.45
2:D:163:LYS:O	2:D:167:GLY:CA	2.60	0.45
2:D:328:LEU:O	2:D:332:ILE:HG13	2.16	0.45
1:E:7:GLY:C	1:E:34:LYS:HE3	2.37	0.45
1:F:87:ASP:OD2	1:F:90:GLN:HG2	2.16	0.45
2:G:152:LEU:CD2	2:G:182:LEU:HB3	2.43	0.45
2:H:210:ASN:OD1	2:H:214:ARG:HD2	2.16	0.45
2:H:78:ASN:HB2	2:H:93:VAL:O	2.17	0.45
1:A:29:SER:C	1:A:31:GLN:H	2.19	0.45
1:B:123:LEU:H	1:B:123:LEU:HD12	1.82	0.45
2:C:278:CYS:HB2	2:C:323:ASP:O	2.17	0.45
2:D:501:LYS:HG2	2:D:531:LEU:HD21	1.98	0.45
1:B:3:PRO:HG2	2:D:52:THR:HG21	1.95	0.45
1:E:196:ARG:NH1	1:E:202:LEU:HD21	2.32	0.45
2:G:97:ARG:NH2	2:G:411:SER:O	2.50	0.45
2:D:447:ASP:O	2:D:448:ASN:HB2	2.17	0.45
1:E:114:VAL:HA	1:E:126:ALA:O	2.16	0.45
1:A:154:MET:HE2	1:A:154:MET:HA	1.99	0.45
1:A:87:ASP:OD2	1:A:90:GLN:HG2	2.16	0.45
1:B:150:LEU:C	1:B:150:LEU:HD23	2.37	0.45
2:C:209:LEU:HD21	2:C:256:GLY:HA3	1.99	0.45
2:C:49:VAL:CG1	2:C:50:PRO:HD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:278:CYS:HB2	2:D:323:ASP:O	2.16	0.45
1:E:107:SER:HA	1:E:135:ARG:HH21	1.82	0.45
1:E:77:TYR:HA	1:E:110:SER:HB3	1.98	0.45
2:G:159:ILE:HG12	2:G:175:LEU:HB3	1.99	0.45
2:G:481:LEU:O	2:G:484:VAL:HB	2.17	0.45
2:H:123:VAL:HG12	2:H:124:PHE:N	2.32	0.45
2:H:402:ILE:O	2:H:405:ILE:HG12	2.17	0.45
2:C:49:VAL:HG13	2:C:50:PRO:HD2	1.99	0.45
2:D:454:LEU:HD13	2:D:503:VAL:HG21	1.98	0.45
1:F:162:ALA:C	1:F:164:HIS:N	2.70	0.45
1:F:76:SER:HB3	1:F:78:ASP:OD1	2.16	0.45
1:B:308:TRP:CD1	2:D:66:PRO:HA	2.52	0.44
2:C:269:ASP:HA	2:C:272:PRO:HB2	1.99	0.44
2:D:209:LEU:HD22	2:D:256:GLY:HA3	1.99	0.44
2:D:491:LEU:O	2:D:492:SER:C	2.54	0.44
1:E:153:GLU:O	1:E:154:MET:HE3	2.17	0.44
2:G:402:ILE:O	2:G:405:ILE:HG12	2.17	0.44
1:B:117:ALA:HB3	1:B:124:LYS:HB3	2.00	0.44
2:D:240:PHE:CZ	2:D:269:ASP:OD2	2.70	0.44
1:E:123:LEU:H	1:E:123:LEU:HD12	1.82	0.44
1:E:196:ARG:HD2	1:E:202:LEU:HD23	1.99	0.44
2:H:482:TRP:N	2:H:483:PRO:CD	2.80	0.44
1:A:97:ARG:HH11	1:A:97:ARG:HG3	1.82	0.44
1:B:313:ASN:HA	1:B:313:ASN:HD22	1.62	0.44
2:C:230:VAL:O	2:C:235:ALA:HB2	2.18	0.44
2:D:166:ASP:OD2	2:D:169:VAL:HG21	2.17	0.44
2:D:450:MET:CG	2:D:451:LEU:N	2.76	0.44
1:E:131:ASP:O	1:E:133:ILE:HG13	2.17	0.44
1:F:117:ALA:HB3	1:F:124:LYS:HB3	1.99	0.44
2:H:60:LYS:C	2:H:62:GLY:H	2.20	0.44
2:C:501:LYS:HG2	2:C:531:LEU:HD21	1.99	0.44
2:D:392:GLN:HB3	2:D:393:PRO:HD3	2.00	0.44
1:E:85:GLU:OE2	1:E:145:LEU:HD12	2.17	0.44
1:F:124:LYS:HG3	1:F:138:ASP:OD1	2.17	0.44
1:F:196:ARG:NH1	1:F:202:LEU:HD21	2.32	0.44
2:G:228:PHE:CD2	2:G:228:PHE:N	2.85	0.44
1:B:80:THR:HG22	1:B:104:LEU:O	2.18	0.44
2:D:141:ASN:HD22	2:D:141:ASN:N	2.16	0.44
1:F:102:CYS:SG	1:F:103:THR:N	2.90	0.44
2:G:505:ALA:HB1	2:G:534:ILE:CD1	2.48	0.44
1:A:236:LYS:HG3	1:A:306:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:SER:HB3	1:B:320:SER:OG	2.18	0.44
2:C:402:ILE:O	2:C:405:ILE:HG12	2.18	0.44
2:D:78:ASN:HB2	2:D:93:VAL:O	2.17	0.44
1:E:126:ALA:HB2	1:E:136:LEU:HD22	2.00	0.44
1:F:291:ASN:ND2	1:F:291:ASN:N	2.66	0.44
2:G:437:GLU:OE1	2:G:458:ARG:NH2	2.47	0.44
2:H:241:GLU:HG2	2:H:241:GLU:O	2.18	0.44
2:H:328:LEU:O	2:H:332:ILE:HG13	2.17	0.44
2:H:491:LEU:O	2:H:492:SER:C	2.56	0.44
2:H:508:LEU:HG	2:H:522:MET:HE3	1.99	0.44
1:A:180:PRO:O	1:A:182:LYS:HG2	2.18	0.44
1:B:136:LEU:HD11	1:B:202:LEU:HD11	1.98	0.44
2:C:351:ARG:HB3	2:C:355:GLU:OE1	2.17	0.44
2:C:481:LEU:O	2:C:484:VAL:HB	2.18	0.44
1:B:20:TYR:OH	2:D:541:THR:HG21	2.17	0.44
1:F:183:LEU:O	1:F:183:LEU:HD12	2.17	0.44
2:H:141:ASN:O	2:H:145:ASN:ND2	2.50	0.44
1:A:144:ASP:C	1:A:146:ARG:H	2.21	0.44
2:C:107:TYR:CZ	2:C:111:LEU:HD11	2.53	0.44
2:C:228:PHE:CE1	2:C:267:ARG:HB3	2.46	0.44
2:D:536:LYS:C	2:D:538:ILE:N	2.69	0.44
2:D:57:PRO:HG3	2:D:91:TYR:CZ	2.53	0.44
1:E:119:ALA:C	1:E:121:LEU:H	2.20	0.44
2:G:141:ASN:O	2:G:145:ASN:ND2	2.50	0.44
2:G:482:TRP:N	2:G:483:PRO:CD	2.80	0.44
1:A:247:GLU:HB3	1:A:292:LEU:HD23	2.00	0.44
1:B:101:LEU:HB3	1:B:145:LEU:O	2.18	0.44
1:B:313:ASN:HB3	1:B:316:GLY:H	1.83	0.44
2:C:210:ASN:OD1	2:C:214:ARG:HD2	2.17	0.44
2:C:242:THR:CG2	2:C:243:GLN:H	2.31	0.44
2:D:228:PHE:HA	2:D:239:VAL:HG21	1.99	0.44
2:D:284:ALA:O	2:D:288:SER:HB3	2.18	0.44
1:B:3:PRO:HG3	2:D:52:THR:HG21	1.96	0.44
2:G:529:TRP:O	2:G:530:ARG:HB2	2.18	0.44
1:A:196:ARG:HD2	1:A:202:LEU:HD23	2.00	0.43
1:B:220:TRP:CG	1:B:231:ILE:HG22	2.53	0.43
2:C:78:ASN:HB2	2:C:93:VAL:O	2.18	0.43
2:D:114:ILE:HD13	2:D:150:ALA:HB1	2.00	0.43
2:D:238:LYS:HB2	2:D:240:PHE:CD2	2.53	0.43
1:F:84:TRP:CD1	1:F:84:TRP:N	2.86	0.43
2:G:328:LEU:O	2:G:332:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:501:LYS:HG2	2:G:531:LEU:HD21	2.00	0.43
1:A:301:ASP:N	1:A:301:ASP:OD1	2.51	0.43
1:B:117:ALA:HB2	1:B:173:TRP:CZ2	2.54	0.43
1:F:180:PRO:O	1:F:182:LYS:HG2	2.18	0.43
1:F:85:GLU:OE2	1:F:145:LEU:HD12	2.18	0.43
2:G:123:VAL:HG12	2:G:124:PHE:N	2.33	0.43
1:F:4:PHE:HE1	2:H:90:LEU:HD12	1.81	0.43
2:C:328:LEU:O	2:C:332:ILE:HG13	2.18	0.43
2:C:491:LEU:O	2:C:492:SER:C	2.56	0.43
1:E:313:ASN:OD1	1:E:317:THR:HB	2.18	0.43
1:A:33:ILE:HG23	1:A:61:ILE:HD11	2.01	0.43
2:D:269:ASP:HA	2:D:272:PRO:HB2	2.00	0.43
1:E:113:SER:O	1:E:127:CYS:HA	2.19	0.43
1:F:31:GLN:HB3	1:F:54:HIS:O	2.18	0.43
2:G:145:ASN:OD1	2:G:190:PHE:HA	2.18	0.43
2:G:228:PHE:N	2:G:228:PHE:HD2	2.17	0.43
2:H:60:LYS:C	2:H:62:GLY:N	2.71	0.43
2:H:47:ILE:HD13	2:H:97:ARG:HG3	2.01	0.43
1:A:101:LEU:HB3	1:A:145:LEU:O	2.18	0.43
1:B:342:MET:O	1:B:343:SER:HB3	2.18	0.43
1:B:84:TRP:CD1	1:B:84:TRP:N	2.85	0.43
2:C:299:SER:HB3	2:C:302:THR:OG1	2.18	0.43
2:C:529:TRP:O	2:C:530:ARG:HB2	2.19	0.43
1:E:87:ASP:OD2	1:E:90:GLN:HG2	2.19	0.43
2:H:383:VAL:CG1	2:H:384:VAL:N	2.80	0.43
1:B:7:GLY:C	1:B:34:LYS:HE3	2.39	0.43
2:C:531:LEU:HB3	2:C:534:ILE:CG1	2.48	0.43
2:G:455:PHE:HE1	2:G:468:SER:OG	2.02	0.43
2:G:455:PHE:CD2	2:G:455:PHE:O	2.72	0.43
2:G:491:LEU:O	2:G:492:SER:C	2.56	0.43
2:H:63:ASP:O	2:H:64:LYS:C	2.57	0.43
1:F:324:ASP:HB3	2:H:64:LYS:HD3	2.00	0.43
1:A:107:SER:HA	1:A:135:ARG:HH21	1.83	0.43
1:B:338:GLU:HB2	2:C:343:GLN:OE1	2.18	0.43
2:D:299:SER:HB3	2:D:302:THR:OG1	2.19	0.43
2:D:351:ARG:HB3	2:D:355:GLU:OE1	2.19	0.43
1:B:345:ILE:HA	2:D:49:VAL:O	2.19	0.43
1:E:164:HIS:O	1:E:165:LEU:C	2.56	0.43
1:E:238:GLY:CA	1:E:305:GLY:O	2.63	0.43
2:G:269:ASP:HA	2:G:272:PRO:HB2	2.01	0.43
2:G:284:ALA:O	2:G:288:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:242:THR:HG22	2:H:244:TYR:HB2	2.01	0.43
2:C:168:ARG:HD3	2:C:170:ASN:CB	2.49	0.43
1:B:9:ASP:O	2:D:88:TYR:CE1	2.72	0.43
1:F:134:LEU:CD1	1:F:185:VAL:HG21	2.49	0.43
1:F:301:ASP:O	1:F:303:HIS:N	2.52	0.43
2:H:501:LYS:HG2	2:H:531:LEU:HD21	2.01	0.43
1:B:11:LEU:O	1:B:28:SER:HB2	2.18	0.43
2:C:209:LEU:CD2	2:C:256:GLY:HA3	2.49	0.43
2:C:455:PHE:CG	2:C:455:PHE:O	2.71	0.43
2:D:134:SER:C	2:D:136:PHE:N	2.72	0.43
2:D:237:LYS:HB2	2:D:241:GLU:HG2	2.00	0.43
2:D:57:PRO:CB	2:D:82:ILE:HD11	2.49	0.43
1:E:180:PRO:O	1:E:182:LYS:HG2	2.18	0.43
1:F:107:SER:HA	1:F:135:ARG:HH21	1.82	0.43
1:F:187:ALA:O	1:F:188:LEU:HB2	2.17	0.43
2:G:114:ILE:HD13	2:G:150:ALA:CB	2.49	0.43
2:G:228:PHE:O	2:G:230:VAL:HG23	2.19	0.43
2:G:383:VAL:CG1	2:G:384:VAL:N	2.82	0.43
2:G:77:GLN:HE21	2:G:77:GLN:HB2	1.71	0.43
2:H:455:PHE:CD2	2:H:455:PHE:O	2.71	0.43
1:B:159:ILE:HG22	1:B:161:PRO:HD3	2.01	0.42
1:B:183:LEU:HD12	1:B:183:LEU:O	2.18	0.42
1:A:128:LEU:HD23	1:A:169:PHE:HB3	2.01	0.42
1:A:61:ILE:O	1:A:62:ASP:HB2	2.18	0.42
1:B:134:LEU:CD1	1:B:185:VAL:HG21	2.48	0.42
1:B:180:PRO:O	1:B:182:LYS:HG2	2.19	0.42
1:F:193:ILE:CD1	1:F:245:ILE:HD13	2.49	0.42
2:H:61:ASN:O	2:H:62:GLY:O	2.37	0.42
2:H:57:PRO:HG3	2:H:91:TYR:CE2	2.54	0.42
1:A:11:LEU:O	1:A:28:SER:HB2	2.18	0.42
1:A:207:LYS:O	1:A:209:PRO:CD	2.67	0.42
1:B:113:SER:O	1:B:127:CYS:HA	2.18	0.42
2:C:168:ARG:HD3	2:C:170:ASN:HB3	2.00	0.42
2:C:455:PHE:HE1	2:C:468:SER:OG	2.02	0.42
2:C:97:ARG:NH2	2:C:411:SER:O	2.52	0.42
1:E:342:MET:O	1:E:343:SER:HB3	2.19	0.42
2:G:104:PHE:O	2:G:107:TYR:HB3	2.19	0.42
1:A:67:GLU:OE1	1:A:119:ALA:HB1	2.19	0.42
1:A:77:TYR:HD2	1:A:110:SER:HB3	1.84	0.42
1:B:126:ALA:HB2	1:B:136:LEU:HD22	2.00	0.42
2:C:265:ILE:C	2:C:267:ARG:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:NH1	2:C:534:ILE:HD13	2.35	0.42
2:G:265:ILE:C	2:G:267:ARG:N	2.72	0.42
2:H:265:ILE:C	2:H:267:ARG:N	2.72	0.42
2:H:522:MET:CE	2:H:538:ILE:HG13	2.49	0.42
2:H:65:MET:HA	2:H:66:PRO:HD3	1.79	0.42
1:E:11:LEU:O	1:E:28:SER:HB2	2.18	0.42
1:E:123:LEU:N	1:E:123:LEU:HD12	2.35	0.42
1:F:80:THR:HG22	1:F:104:LEU:O	2.19	0.42
2:G:299:SER:HB3	2:G:302:THR:OG1	2.19	0.42
1:E:144:ASP:C	1:E:146:ARG:H	2.23	0.42
1:F:136:LEU:HD11	1:F:202:LEU:HD11	2.02	0.42
1:F:144:ASP:C	1:F:146:ARG:H	2.23	0.42
2:G:210:ASN:OD1	2:G:214:ARG:HD2	2.19	0.42
2:G:228:PHE:C	2:G:230:VAL:H	2.23	0.42
2:G:434:PHE:CD1	2:G:458:ARG:O	2.73	0.42
2:G:505:ALA:O	2:G:534:ILE:HD13	2.20	0.42
2:H:182:LEU:HD23	2:H:182:LEU:HA	1.89	0.42
2:H:95:ILE:HA	2:H:96:PRO:HD3	1.90	0.42
1:F:157:LEU:HD11	1:F:187:ALA:CB	2.44	0.42
1:F:61:ILE:O	1:F:62:ASP:HB2	2.19	0.42
2:H:104:PHE:O	2:H:107:TYR:HB3	2.20	0.42
2:H:51:MET:HG3	2:H:93:VAL:HG22	2.02	0.42
1:A:123:LEU:HD12	1:A:123:LEU:N	2.35	0.42
2:C:480:GLU:O	2:C:483:PRO:HD2	2.19	0.42
2:D:242:THR:O	2:D:244:TYR:N	2.53	0.42
2:D:296:PRO:HD3	2:D:306:TRP:CD1	2.54	0.42
2:D:455:PHE:CG	2:D:455:PHE:O	2.73	0.42
1:F:301:ASP:OD1	1:F:301:ASP:N	2.52	0.42
2:H:240:PHE:CE1	2:H:269:ASP:OD2	2.73	0.42
2:D:134:SER:C	2:D:136:PHE:H	2.23	0.42
1:E:133:ILE:HG21	1:E:135:ARG:HH12	1.84	0.42
1:E:313:ASN:HA	1:E:313:ASN:HD22	1.62	0.42
1:F:133:ILE:HG21	1:F:135:ARG:HH12	1.85	0.42
1:F:9:ASP:O	2:H:88:TYR:CZ	2.73	0.42
2:G:228:PHE:O	2:G:230:VAL:N	2.53	0.42
1:A:243:PHE:N	1:A:243:PHE:CD1	2.88	0.42
1:E:311:SER:HB3	1:E:320:SER:OG	2.20	0.42
1:E:324:ASP:C	1:E:326:GLY:H	2.23	0.42
1:B:192:ILE:HD11	1:B:194:TYR:CZ	2.55	0.41
1:B:33:ILE:HG23	1:B:61:ILE:HD11	2.02	0.41
2:C:284:ALA:O	2:C:288:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:ASP:OD1	1:E:301:ASP:N	2.52	0.41
1:F:136:LEU:HD12	1:F:196:ARG:HH12	1.84	0.41
1:A:81:VAL:CG2	1:A:111:LEU:HD13	2.44	0.41
1:A:150:LEU:HD23	1:A:150:LEU:C	2.40	0.41
1:B:144:ASP:C	1:B:146:ARG:H	2.23	0.41
2:C:227:VAL:C	2:C:229:SER:N	2.71	0.41
2:D:114:ILE:HD13	2:D:150:ALA:CB	2.50	0.41
2:D:56:GLN:HA	2:D:57:PRO:HD3	1.75	0.41
1:F:114:VAL:HG13	1:F:114:VAL:O	2.21	0.41
1:F:313:ASN:HB3	1:F:316:GLY:H	1.83	0.41
2:H:240:PHE:CD2	2:H:240:PHE:N	2.87	0.41
1:F:347:ALA:HB1	2:H:58:ILE:H	1.84	0.41
1:A:313:ASN:HB3	1:A:316:GLY:H	1.85	0.41
1:A:345:ILE:HD13	2:C:93:VAL:HG11	2.01	0.41
1:B:207:LYS:O	1:B:209:PRO:CD	2.68	0.41
2:C:334:ASP:HB3	2:C:349:TYR:HE1	1.85	0.41
2:D:242:THR:HG22	2:D:244:TYR:HD1	1.86	0.41
1:E:114:VAL:HG13	1:E:114:VAL:O	2.19	0.41
1:F:123:LEU:HD12	1:F:123:LEU:H	1.86	0.41
1:F:83:LEU:HD13	1:F:148:TRP:CE2	2.55	0.41
2:H:284:ALA:O	2:H:288:SER:HB3	2.20	0.41
1:A:193:ILE:CD1	1:A:245:ILE:HD13	2.51	0.41
2:C:113:GLU:HA	2:C:113:GLU:OE2	2.21	0.41
2:D:481:LEU:O	2:D:484:VAL:HB	2.21	0.41
2:D:536:LYS:O	2:D:538:ILE:N	2.54	0.41
1:F:221:ALA:HB2	1:F:312:TRP:NE1	2.33	0.41
2:G:65:MET:HA	2:G:66:PRO:HD3	1.86	0.41
2:H:269:ASP:HA	2:H:272:PRO:HB2	2.03	0.41
2:G:233:SER:C	2:G:235:ALA:N	2.74	0.41
1:B:236:LYS:C	1:B:238:GLY:H	2.23	0.41
1:B:344:VAL:O	2:D:48:LEU:HA	2.21	0.41
2:D:182:LEU:HA	2:D:182:LEU:HD23	1.93	0.41
2:D:265:ILE:C	2:D:267:ARG:N	2.71	0.41
2:D:455:PHE:HE1	2:D:468:SER:OG	2.02	0.41
1:E:313:ASN:HB3	1:E:316:GLY:H	1.85	0.41
1:E:84:TRP:N	1:E:84:TRP:CD1	2.87	0.41
1:F:196:ARG:HD2	1:F:202:LEU:HD23	2.02	0.41
1:F:313:ASN:OD1	1:F:317:THR:HB	2.20	0.41
2:G:532:PRO:C	2:G:534:ILE:H	2.24	0.41
2:H:50:PRO:O	2:H:51:MET:C	2.59	0.41
1:A:166:GLN:O	1:A:166:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:SER:HB3	1:A:320:SER:OG	2.20	0.41
1:B:31:GLN:HB3	1:B:54:HIS:O	2.20	0.41
2:C:104:PHE:O	2:C:107:TYR:HB3	2.20	0.41
2:D:449:GLU:HB3	2:D:450:MET:H	1.70	0.41
1:E:213:SER:OG	1:E:236:LYS:HD3	2.21	0.41
1:F:207:LYS:O	1:F:209:PRO:CD	2.68	0.41
2:H:56:GLN:HA	2:H:57:PRO:HD3	1.73	0.41
2:C:322:THR:HG23	2:C:329:ARG:HD3	2.03	0.41
2:C:383:VAL:CG1	2:C:384:VAL:N	2.83	0.41
2:D:198:GLU:HG2	2:D:300:SER:HB2	2.02	0.41
2:D:511:TYR:HA	2:D:512:PRO:HD3	1.84	0.41
1:B:3:PRO:HD3	2:D:52:THR:HG21	2.01	0.41
2:D:539:TYR:HA	2:D:542:LEU:HB2	2.02	0.41
1:E:150:LEU:HD23	1:E:150:LEU:C	2.41	0.41
1:E:61:ILE:O	1:E:62:ASP:HB2	2.21	0.41
1:F:342:MET:O	1:F:343:SER:HB3	2.21	0.41
2:G:182:LEU:HD23	2:G:182:LEU:HA	1.97	0.41
2:H:113:GLU:OE2	2:H:113:GLU:HA	2.20	0.41
2:H:240:PHE:C	2:H:242:THR:N	2.70	0.41
1:E:101:LEU:O	1:E:102:CYS:CB	2.69	0.41
1:E:9:ASP:O	2:G:88:TYR:CE1	2.74	0.41
2:H:351:ARG:HB3	2:H:355:GLU:OE1	2.21	0.41
1:A:342:MET:O	1:A:343:SER:HB3	2.21	0.41
1:B:324:ASP:C	1:B:326:GLY:H	2.25	0.41
2:D:169:VAL:CG1	2:D:170:ASN:N	2.84	0.41
1:B:4:PHE:HE1	2:D:90:LEU:HD12	1.86	0.41
1:F:125:LEU:O	1:F:136:LEU:HA	2.21	0.41
1:F:219:SER:HG	1:F:312:TRP:HD1	1.69	0.41
1:A:126:ALA:HB2	1:A:136:LEU:HD22	2.02	0.40
1:B:159:ILE:CB	1:B:161:PRO:HD3	2.51	0.40
2:C:196:ASP:OD1	2:C:367:SER:HA	2.21	0.40
2:D:238:LYS:HB2	2:D:240:PHE:CE2	2.56	0.40
2:D:334:ASP:HB3	2:D:349:TYR:HE1	1.86	0.40
2:D:51:MET:CE	2:D:57:PRO:HD2	2.51	0.40
1:E:125:LEU:O	1:E:136:LEU:HA	2.22	0.40
1:E:312:TRP:CZ3	1:E:319:LEU:HB2	2.57	0.40
1:E:31:GLN:HB3	1:E:54:HIS:O	2.21	0.40
1:F:33:ILE:HG23	1:F:61:ILE:HD11	2.02	0.40
1:A:220:TRP:CG	1:A:231:ILE:HG22	2.56	0.40
1:B:123:LEU:HD12	1:B:123:LEU:N	2.37	0.40
2:C:228:PHE:CD1	2:C:240:PHE:CE2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2:GLN:H	1:F:2:GLN:HG2	1.72	0.40
2:G:113:GLU:OE2	2:G:113:GLU:HA	2.20	0.40
2:H:278:CYS:CB	2:H:323:ASP:HB2	2.51	0.40
1:B:71:ILE:HD11	1:B:145:LEU:HD13	2.03	0.40
1:B:151:THR:CG2	1:B:196:ARG:HH22	2.34	0.40
1:B:193:ILE:HD11	1:B:208:LEU:HD21	2.04	0.40
2:C:278:CYS:CB	2:C:323:ASP:HB2	2.51	0.40
2:C:57:PRO:HB3	2:C:91:TYR:OH	2.22	0.40
1:E:117:ALA:HB3	1:E:124:LYS:HB3	2.03	0.40
1:E:134:LEU:CD1	1:E:185:VAL:HG21	2.50	0.40
1:F:126:ALA:HB2	1:F:136:LEU:HD22	2.03	0.40
2:G:190:PHE:CE2	2:G:427:LYS:CG	3.04	0.40
1:A:65:SER:HB2	1:A:119:ALA:HB2	2.04	0.40
1:A:7:GLY:C	1:A:34:LYS:HE3	2.41	0.40
1:B:344:VAL:O	2:D:48:LEU:HD12	2.21	0.40
2:D:235:ALA:C	2:D:237:LYS:N	2.74	0.40
2:D:227:VAL:O	2:D:239:VAL:CG2	2.69	0.40
1:F:336:SER:O	1:F:337:ASN:CB	2.68	0.40
2:G:278:CYS:HG	2:G:323:ASP:HB2	1.86	0.40
2:H:144:VAL:HG11	2:H:427:LYS:HG2	2.03	0.40
1:B:2:GLN:HA	1:B:3:PRO:HD3	1.97	0.40
1:E:117:ALA:HB2	1:E:173:TRP:CZ2	2.57	0.40
1:E:236:LYS:C	1:E:238:GLY:H	2.24	0.40
1:F:81:VAL:CG2	1:F:111:LEU:HD13	2.46	0.40
2:G:334:ASP:HB3	2:G:349:TYR:HE1	1.87	0.40
2:G:351:ARG:HB3	2:G:355:GLU:OE1	2.21	0.40
2:H:163:LYS:O	2:H:167:GLY:CA	2.63	0.40
2:H:200:ASN:ND2	2:H:203:GLU:HB2	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/351 (87%)	266 (88%)	31 (10%)	7 (2%)	7	26
1	B	303/351 (86%)	265 (88%)	33 (11%)	5 (2%)	10	34
1	E	302/351 (86%)	263 (87%)	30 (10%)	9 (3%)	5	19
1	F	302/351 (86%)	267 (88%)	26 (9%)	9 (3%)	5	19
2	C	467/570 (82%)	406 (87%)	53 (11%)	8 (2%)	10	34
2	D	489/570 (86%)	419 (86%)	58 (12%)	12 (2%)	6	23
2	G	468/570 (82%)	406 (87%)	52 (11%)	10 (2%)	8	29
2	H	481/570 (84%)	406 (84%)	60 (12%)	15 (3%)	4	18
All	All	3116/3684 (85%)	2698 (87%)	343 (11%)	75 (2%)	6	25

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	B	43	SER
2	C	272	PRO
2	C	455	PHE
2	D	272	PRO
2	D	450	MET
2	D	451	LEU
1	E	43	SER
1	E	165	LEU
1	F	43	SER
2	G	272	PRO
2	H	62	GLY
2	H	241	GLU
2	H	272	PRO
1	A	162	ALA
1	A	302	ASP
1	B	302	ASP
2	C	62	GLY
2	C	239	VAL
2	D	448	ASN
1	E	302	ASP
1	F	163	ASN
1	F	302	ASP
2	G	239	VAL
2	H	235	ALA
2	H	238	LYS
2	H	438	LYS

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Mol	Chain	Res	Type
1	A	120	HIS
1	B	120	HIS
1	B	213	SER
2	D	243	GLN
2	D	455	PHE
1	E	120	HIS
1	E	164	HIS
1	F	120	HIS
1	F	166	GLN
1	F	213	SER
2	G	229	SER
2	G	454	LEU
1	A	213	SER
1	B	188	LEU
2	D	200	ASN
1	E	213	SER
2	H	51	MET
2	H	455	PHE
1	A	188	LEU
2	C	53	VAL
2	C	200	ASN
2	C	364	TYR
2	D	277	THR
1	E	325	ASP
1	F	161	PRO
1	F	188	LEU
2	G	200	ASN
2	G	533	GLU
2	H	64	LYS
2	H	200	ASN
2	H	237	LYS
2	D	135	ASN
2	D	239	VAL
1	E	188	LEU
2	G	277	THR
2	G	532	PRO
2	H	50	PRO
2	H	63	ASP
2	H	277	THR
2	C	191	ILE
2	D	191	ILE
1	E	142	PRO

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Mol	Chain	Res	Type
2	G	191	ILE
2	H	191	ILE
1	A	142	PRO
1	F	142	PRO
2	G	230	VAL
2	D	47	ILE

### 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	270/307 (88%)	261 (97%)	9 (3%)	41	75
1	B	269/307 (88%)	260 (97%)	9 (3%)	41	75
1	E	268/307 (87%)	257 (96%)	11 (4%)	33	68
1	F	267/307 (87%)	255 (96%)	12 (4%)	30	64
2	C	424/510 (83%)	415 (98%)	9 (2%)	56	84
2	D	441/510 (86%)	431 (98%)	10 (2%)	53	83
2	G	424/510 (83%)	414 (98%)	10 (2%)	52	82
2	H	434/510 (85%)	425 (98%)	9 (2%)	56	84
All	All	2797/3268 (86%)	2718 (97%)	79 (3%)	47	80

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	THR
1	A	138	ASP
1	A	168	ASP
1	A	226	ARG
1	A	301	ASP
1	A	310	VAL
1	A	313	ASN
1	A	314	LEU
1	A	334	THR

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Mol	Chain	Res	Type
1	B	80	THR
1	B	138	ASP
1	B	168	ASP
1	B	226	ARG
1	B	301	ASP
1	B	310	VAL
1	B	313	ASN
1	B	314	LEU
1	B	334	THR
2	C	51	MET
2	C	239	VAL
2	C	269	ASP
2	C	324	ILE
2	C	453	ASP
2	C	488	LEU
2	C	496	THR
2	C	516	ASN
2	C	539	TYR
2	D	55	ASP
2	D	134	SER
2	D	269	ASP
2	D	324	ILE
2	D	437	GLU
2	D	447	ASP
2	D	488	LEU
2	D	496	THR
2	D	516	ASN
2	D	544	ASN
1	E	80	THR
1	E	138	ASP
1	E	164	HIS
1	E	168	ASP
1	E	183	LEU
1	E	226	ARG
1	E	301	ASP
1	E	310	VAL
1	E	313	ASN
1	E	314	LEU
1	E	334	THR
1	F	1(A)	HIS
1	F	80	THR
1	F	138	ASP

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Mol	Chain	Res	Type
1	F	161	PRO
1	F	168	ASP
1	F	226	ARG
1	F	291	ASN
1	F	301	ASP
1	F	310	VAL
1	F	313	ASN
1	F	314	LEU
1	F	334	THR
2	G	178	SER
2	G	240	PHE
2	G	269	ASP
2	G	324	ILE
2	G	452	GLU
2	G	488	LEU
2	G	496	THR
2	G	514	VAL
2	G	516	ASN
2	G	539	TYR
2	H	48	LEU
2	H	55	ASP
2	H	143	THR
2	H	166	ASP
2	H	240	PHE
2	H	269	ASP
2	H	324	ILE
2	H	488	LEU
2	H	496	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	308/351 (87%)	0.32	6 (1%) 66 64	77, 104, 136, 169	0
1	B	307/351 (87%)	0.39	20 (6%) 19 14	79, 107, 137, 180	0
1	E	306/351 (87%)	0.29	4 (1%) 77 76	75, 105, 134, 172	0
1	F	306/351 (87%)	0.26	9 (2%) 51 46	82, 107, 137, 180	0
2	C	475/570 (83%)	0.34	31 (6%) 19 14	74, 102, 159, 171	0
2	D	495/570 (86%)	0.40	40 (8%) 12 9	75, 106, 168, 191	0
2	G	476/570 (83%)	0.41	29 (6%) 21 17	70, 102, 159, 190	0
2	H	487/570 (85%)	0.50	53 (10%) 5 4	77, 106, 174, 192	0
All	All	3160/3684 (85%)	0.37	192 (6%) 21 17	70, 105, 160, 192	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	GLN	9.3
2	G	546	MET	8.4
2	G	545	GLN	7.2
2	D	133	ASN	6.9
2	H	45	GLY	6.6
2	D	270	LEU	6.3
2	H	58	ILE	6.2
1	B	164	HIS	6.2
2	C	436	GLY	6.1
2	H	126	VAL	5.9
2	D	440	SER	5.8
2	D	239	VAL	5.8
1	B	165	LEU	5.7
2	D	234	THR	5.5
1	A	164	HIS	5.5
2	G	539	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
2	H	438	LYS	5.4
2	G	439	ASN	5.3
2	H	234	THR	5.2
2	G	549	ALA	5.1
1	B	162	ALA	4.9
2	H	440	SER	4.8
2	G	126	VAL	4.8
2	H	132	VAL	4.7
2	H	233	SER	4.7
2	H	65	MET	4.6
2	C	435	GLU	4.6
2	H	53	VAL	4.5
2	D	51	MET	4.5
2	H	49	VAL	4.5
2	H	66	PRO	4.5
1	F	36	PHE	4.5
2	H	439	ASN	4.5
2	D	52	THR	4.5
2	H	230	VAL	4.5
2	D	448	ASN	4.4
2	G	235	ALA	4.4
2	H	235	ALA	4.4
2	C	239	VAL	4.3
2	H	48	LEU	4.3
1	A	165	LEU	4.3
2	H	168	ARG	4.3
2	C	55	ASP	4.2
2	G	548	SER	4.1
2	G	233	SER	4.1
2	D	235	ALA	4.1
2	D	441	ASP	4.1
2	H	133	ASN	4.0
2	H	134	SER	4.0
2	D	61	ASN	4.0
2	D	548	SER	4.0
2	G	438	LYS	3.9
2	D	438	LYS	3.8
2	C	49	VAL	3.8
2	D	126	VAL	3.8
2	H	54	ASN	3.8
1	B	167	SER	3.8
2	G	232	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
2	H	50	PRO	3.7
2	D	165	GLN	3.6
1	F	26	THR	3.6
2	H	239	VAL	3.6
1	A	163	ASN	3.6
2	D	232	ASP	3.6
2	D	233	SER	3.5
2	C	274	LEU	3.5
2	C	54	ASN	3.5
2	H	136	PHE	3.5
2	H	57	PRO	3.4
2	D	230	VAL	3.4
2	C	136	PHE	3.4
2	G	551	ASN	3.4
1	B	157	LEU	3.3
2	D	265	ILE	3.3
2	H	61	ASN	3.3
2	G	544	ASN	3.3
2	D	279	ALA	3.3
2	H	52	THR	3.2
2	G	62	GLY	3.2
2	G	236	GLY	3.2
2	G	61	ASN	3.2
1	E	164	HIS	3.2
2	H	55	ASP	3.2
2	G	547	LEU	3.1
2	C	59	GLU	3.1
2	H	237	LYS	3.1
2	C	276	ASP	3.1
2	G	550	HIS	3.1
2	H	164	ASP	3.1
2	D	439	ASN	3.1
1	B	163	ASN	3.0
2	G	63	ASP	3.0
1	B	158	SER	2.9
2	H	227	VAL	2.9
2	C	240	PHE	2.9
2	H	84	ALA	2.9
2	H	59	GLU	2.9
2	H	85	LYS	2.9
2	C	332	ILE	2.9
1	B	145	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	335	PHE	2.9
2	C	235	ALA	2.9
2	D	65	MET	2.9
2	H	167	GLY	2.8
2	G	237	LYS	2.8
2	D	449	GLU	2.8
2	C	285	VAL	2.8
2	H	63	ASP	2.8
2	C	60	LYS	2.8
2	D	236	GLY	2.8
2	D	447	ASP	2.8
2	H	232	ASP	2.8
1	B	194	TYR	2.8
2	D	44	SER	2.8
2	H	274	LEU	2.8
2	D	437	GLU	2.8
1	F	33	ILE	2.7
2	C	132	VAL	2.7
2	G	230	VAL	2.7
2	C	277	THR	2.7
2	G	441	ASP	2.7
1	A	288	LEU	2.7
2	C	126	VAL	2.7
2	D	48	LEU	2.7
2	D	336	LEU	2.7
2	C	53	VAL	2.6
2	C	61	ASN	2.6
1	B	1(A)	PRO	2.6
1	B	101	LEU	2.6
2	D	136	PHE	2.6
2	C	237	LYS	2.6
2	D	168	ARG	2.6
1	A	157	LEU	2.5
2	H	62	GLY	2.5
2	G	125	ASN	2.5
2	H	270	LEU	2.5
2	H	317	PHE	2.5
2	D	238	LYS	2.5
1	B	248	LYS	2.5
1	B	81	VAL	2.5
2	H	539	TYR	2.5
2	H	291	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	271	LEU	2.4
2	C	58	ILE	2.4
2	C	133	ASN	2.4
2	C	50	PRO	2.3
2	D	450	MET	2.3
2	G	161	ARG	2.3
2	G	435	GLU	2.3
2	H	236	GLY	2.3
2	D	121	ASP	2.3
2	H	271	LEU	2.3
1	F	123	LEU	2.3
1	F	68	TYR	2.3
1	A	289	GLN	2.3
2	H	121	ASP	2.2
1	E	136	LEU	2.2
2	C	270	LEU	2.2
2	D	53	VAL	2.2
1	E	158	SER	2.2
1	B	156	VAL	2.2
2	D	237	LYS	2.2
2	G	239	VAL	2.2
1	B	104	LEU	2.1
1	B	105	ASN	2.1
1	F	11	LEU	2.1
2	C	48	LEU	2.1
1	F	155	LYS	2.1
2	C	278	CYS	2.1
2	H	278	CYS	2.1
2	C	434	PHE	2.1
2	H	240	PHE	2.1
1	B	155	LYS	2.1
2	H	64	LYS	2.1
2	G	436	GLY	2.1
1	B	128	LEU	2.1
2	C	229	SER	2.1
2	D	134	SER	2.1
2	H	328	LEU	2.1
2	H	248	LEU	2.1
1	E	156	VAL	2.1
1	F	161	PRO	2.1
2	C	134	SER	2.0
2	D	549	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	G	65	MET	2.0
2	H	265	ILE	2.0
2	H	231	LYS	2.0
2	H	51	MET	2.0
2	G	244	TYR	2.0
1	B	80	THR	2.0
2	D	274	LEU	2.0
1	F	164	HIS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.