



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:08 AM GMT

PDB ID : 3O6F  
Title : Crystal structure of a human autoimmune TCR MS2-3C8 bound to MHC class II self-ligand MBP/HLA-DR4  
Authors : Yin, Y.; Li, Y.; Martin, R.; Mariuzza, R.A.  
Deposited on : 2010-07-29  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

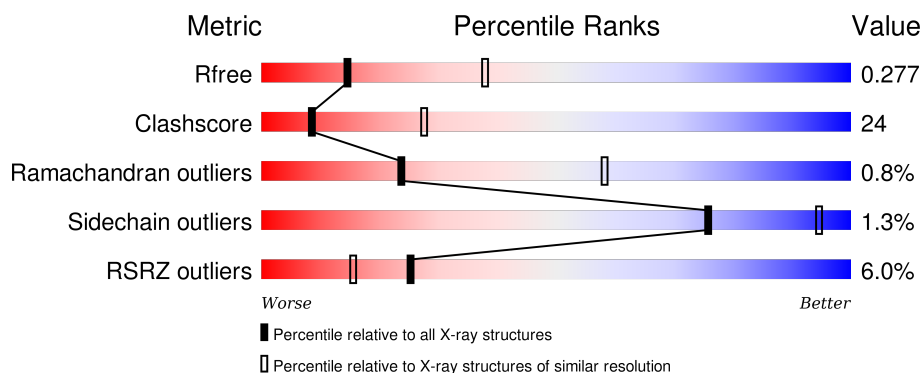
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	182	<div> <div>4%</div> <div>57%</div> <div>40%</div> <div>..</div> </div>
1	E	182	<div> <div>3%</div> <div>70%</div> <div>28%</div> <div>.</div> </div>
2	B	221	<div> <div>2%</div> <div>50%</div> <div>37%</div> <div>12%</div> </div>
2	F	221	<div> <div>2%</div> <div>62%</div> <div>29%</div> <div>5%</div> </div>
3	C	206	<div> <div>6%</div> <div>64%</div> <div>29%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	206	<div><div></div><div>13%</div><div>57%</div><div>33%</div><div>9%</div></div>
4	D	245	<div><div></div><div>%</div><div>60%</div><div>40%</div><div></div></div>
4	H	245	<div><div></div><div>13%</div><div>46%</div><div>52%</div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12887 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1446	940	232	269	5			
1	E	179	Total	C	N	O	S	0	0	0
			1456	947	237	267	5			

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-4 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	0	0
			1578	1001	271	301	5			
2	F	210	Total	C	N	O	S	0	0	0
			1671	1054	294	318	5			

- Molecule 3 is a protein called T-cell receptor alpha chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	191	Total	C	N	O	S	4	0	0
			1441	897	241	296	7			
3	G	188	Total	C	N	O	S	0	0	0
			1448	902	247	291	8			

- Molecule 4 is a protein called T-cell receptor beta-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	245	Total	C	N	O	S	0	0	0
			1919	1210	327	374	8			
4	H	243	Total	C	N	O	S	0	0	0
			1901	1201	324	369	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	189	SER	CYS	ENGINEERED MUTATION	UNP A0A5B9
H	189	SER	CYS	ENGINEERED MUTATION	UNP A0A5B9

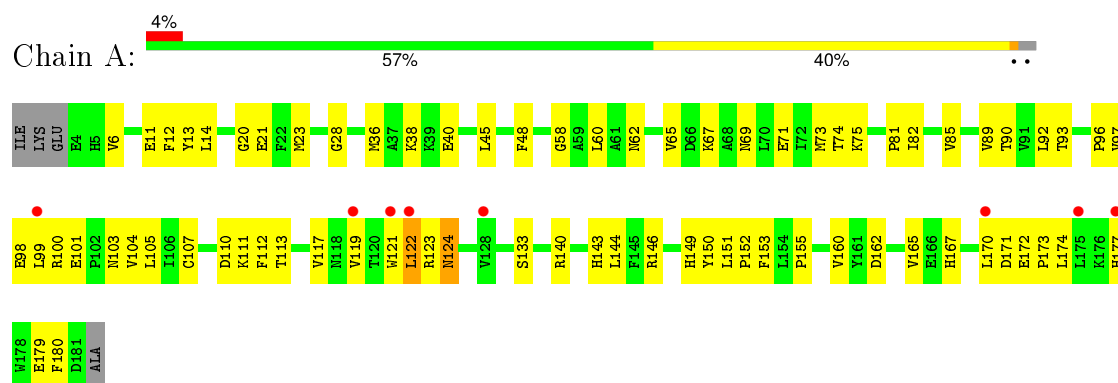
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	B	3	Total O 3 3	0	0
5	C	8	Total O 8 8	0	0
5	D	4	Total O 4 4	0	0
5	E	1	Total O 1 1	0	0
5	F	4	Total O 4 4	0	0
5	G	5	Total O 5 5	0	0

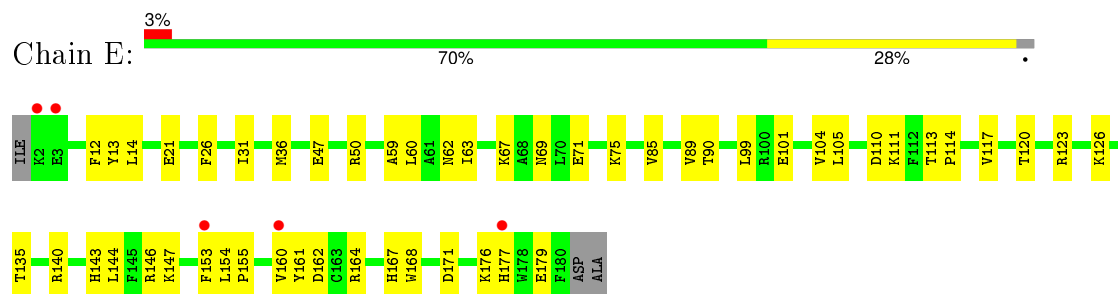
### 3 Residue-property plots [i](#)

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

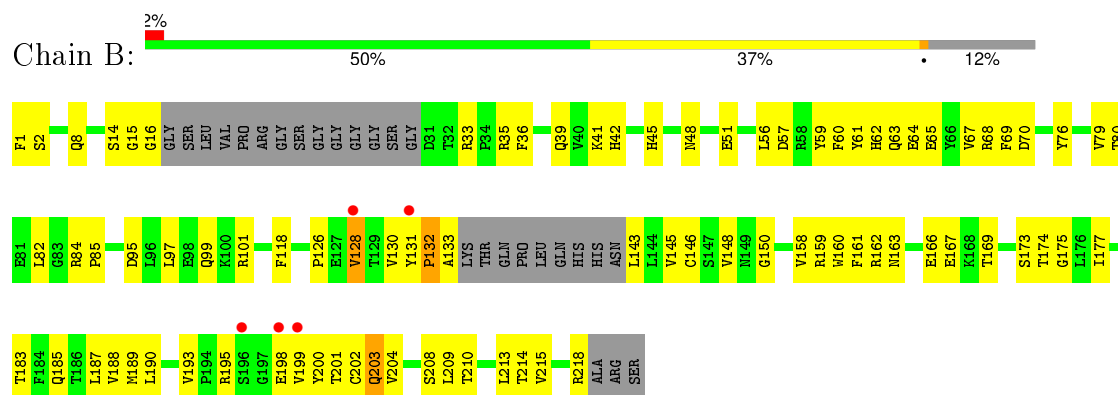
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



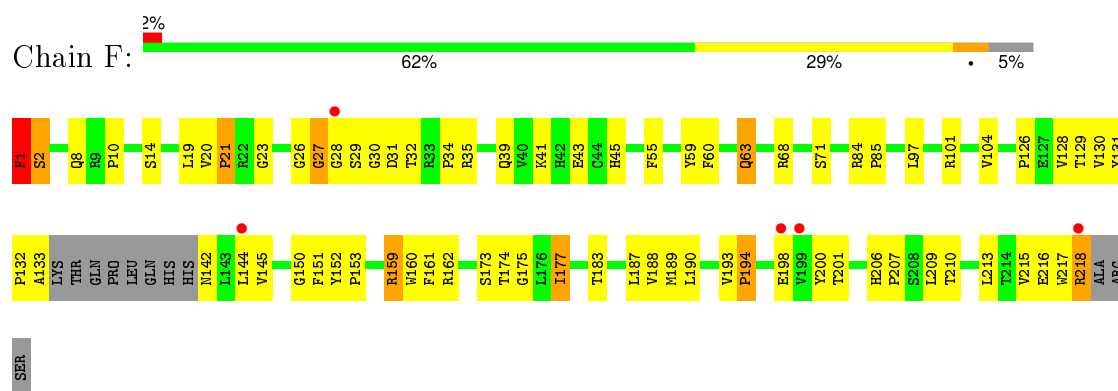
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



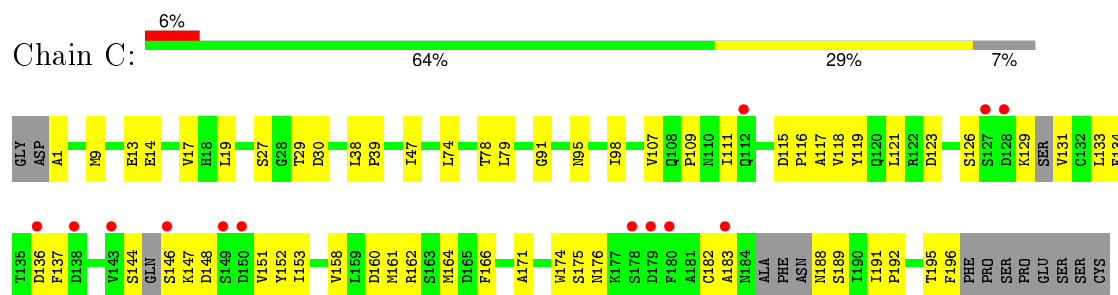
- Molecule 2: HLA class II histocompatibility antigen, DRB1-4 beta chain



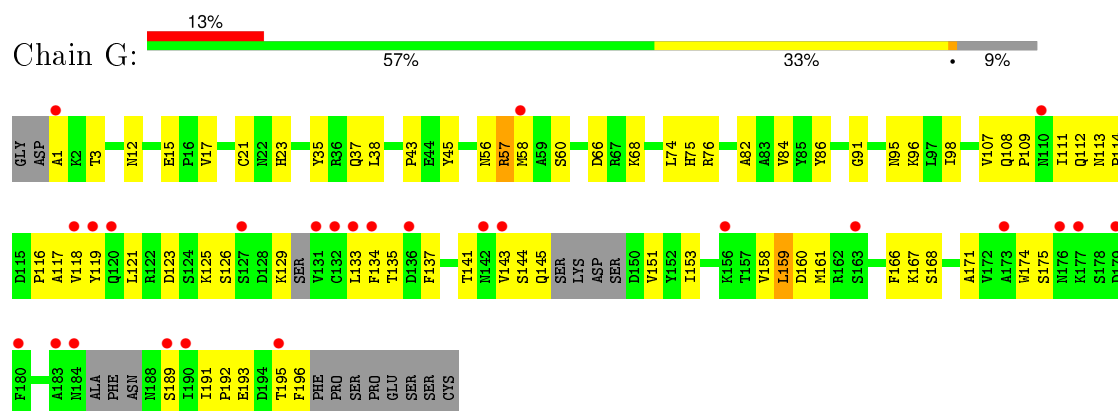
- Molecule 2: HLA class II histocompatibility antigen, DRB1-4 beta chain



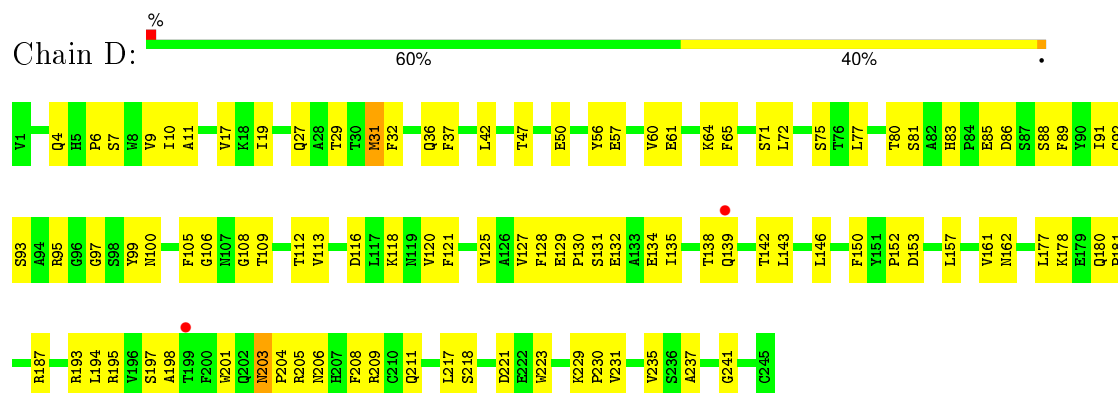
- Molecule 3: T-cell receptor alpha chain C region



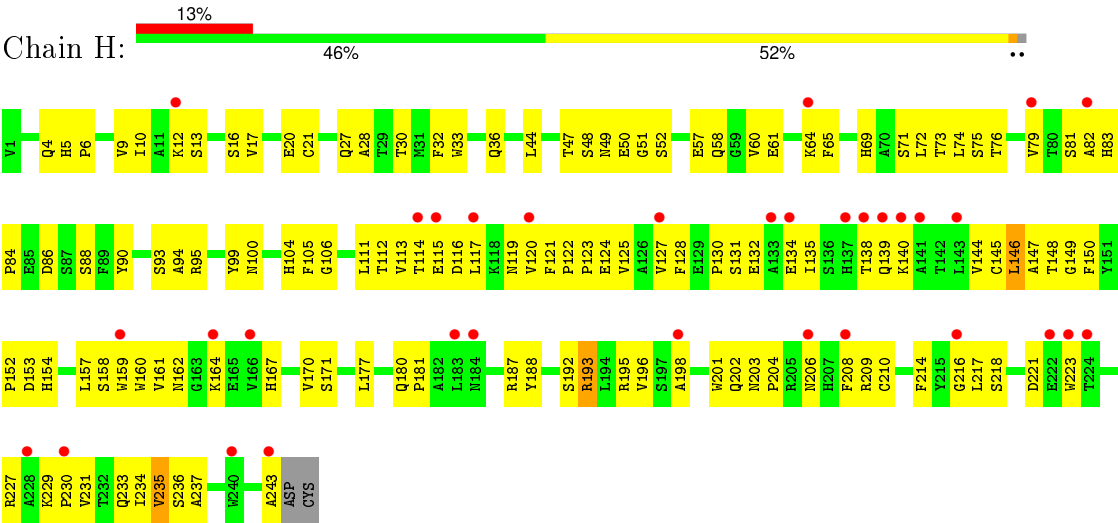
- Molecule 3: T-cell receptor alpha chain C region



- Molecule 4: T-cell receptor beta-1 chain C region



- Molecule 4: T-cell receptor beta-1 chain C region





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.48 Å   218.40 Å   98.41 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.20 – 2.80 49.21 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.20-2.80) 99.8 (49.21-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.51 (at 2.81 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.2_432)	Depositor
R, $R_{free}$	0.239 , 0.279 0.236 , 0.277	Depositor DCC
$R_{free}$ test set	2782 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.4	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 47.2	EDS
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 55112 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.48	0/1491	0.64	0/2036
1	E	0.47	0/1501	0.64	0/2048
2	B	0.51	0/1622	0.69	0/2204
2	F	0.62	1/1717 (0.1%)	0.72	3/2330 (0.1%)
3	C	0.50	0/1469	0.68	0/2005
3	G	0.45	0/1476	0.62	0/2008
4	D	0.48	0/1972	0.65	0/2690
4	H	0.45	0/1954	0.66	0/2666
All	All	0.50	1/13202 (0.0%)	0.66	3/17987 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	PHE	CD2-CE2	5.22	1.49	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	218	ARG	NE-CZ-NH2	6.10	123.35	120.30
2	F	159	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	F	194	PRO	N-CA-C	5.01	125.13	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	68	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	1446	0	1370	83	0
1	E	1456	0	1393	50	0
2	B	1578	0	1451	83	0
2	F	1671	0	1552	70	0
3	C	1441	0	1333	67	0
3	G	1448	0	1377	71	0
4	D	1919	0	1809	114	0
4	H	1901	0	1794	138	0
5	A	2	0	0	0	0
5	B	3	0	0	0	0
5	C	8	0	0	0	0
5	D	4	0	0	0	0
5	E	1	0	0	0	0
5	F	4	0	0	3	0
5	G	5	0	0	1	0
All	All	12887	0	12079	597	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 24.

All (597) 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)
4:D:135:ILE:HD11	4:D:198:ALA:CB	1.58	1.30
3:C:121:LEU:CD2	4:D:131:SER:N	2.08	1.17
4:D:128:PHE:CE2	4:D:146:LEU:HD12	1.80	1.16
4:D:135:ILE:HD11	4:D:198:ALA:HB2	1.17	1.15
3:C:121:LEU:HD21	4:D:131:SER:H	1.16	1.09
3:G:191:ILE:HG23	3:G:192:PRO:HD2	1.33	1.07
4:D:135:ILE:CD1	4:D:198:ALA:HB2	1.88	1.03
4:H:122:PRO:HD3	4:H:230:PRO:HB3	1.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:GLU:OE1	2:B:80:THR:HG21	1.61	0.99
1:A:107:CYS:HB2	1:A:121:TRP:CZ2	1.98	0.97
3:G:109:PRO:HG2	3:G:158:VAL:HG21	1.46	0.96
4:D:135:ILE:HD11	4:D:198:ALA:HB1	1.45	0.96
1:A:65:VAL:HG22	4:D:29:THR:HG21	1.48	0.96
4:D:128:PHE:HE2	4:D:146:LEU:HD12	1.18	0.93
4:D:178:LYS:HE3	4:D:181:PRO:HA	1.49	0.91
3:C:152:TYR:O	3:C:153:ILE:HG13	1.71	0.90
4:H:117:LEU:HD21	4:H:217:LEU:HD11	1.51	0.89
2:F:198:GLU:H	2:F:218:ARG:HH11	1.21	0.89
2:B:39:GLN:HB2	2:B:60:PHE:HB2	1.54	0.88
4:D:135:ILE:CD1	4:D:198:ALA:CB	2.48	0.88
2:B:128:VAL:HG22	2:B:128:VAL:O	1.73	0.87
1:E:123:ARG:HD3	1:E:161:TYR:CE1	2.10	0.86
2:F:162:ARG:HG3	2:F:200:TYR:HE1	1.39	0.86
1:A:65:VAL:CG2	4:D:29:THR:HG21	2.04	0.85
3:C:121:LEU:HD22	4:D:129:GLU:O	1.75	0.85
3:C:146:SER:N	3:C:153:ILE:HD12	1.92	0.84
4:H:138:THR:O	4:H:139:GLN:HB2	1.75	0.84
4:D:127:VAL:HG23	4:D:237:ALA:HB3	1.60	0.84
2:B:61:TYR:CD2	2:B:62:HIS:HD2	1.95	0.83
2:F:128:VAL:HG21	2:F:213:LEU:HD21	1.59	0.83
4:H:71:SER:O	4:H:72:LEU:HB3	1.75	0.83
2:B:14:SER:HA	4:D:27:GLN:NE2	1.93	0.82
3:G:57:ARG:H	3:G:57:ARG:HD2	1.43	0.82
4:H:125:VAL:HG21	4:H:235:VAL:O	1.79	0.82
3:C:17:VAL:HG12	3:C:74:LEU:HB2	1.61	0.81
3:G:37:GLN:HE22	4:H:36:GLN:HE22	1.26	0.81
4:H:201:TRP:O	4:H:202:GLN:HB2	1.81	0.80
2:F:29:SER:C	2:F:31:ASP:H	1.84	0.80
2:B:128:VAL:O	2:B:128:VAL:CG2	2.31	0.79
3:C:144:SER:OG	3:C:189:SER:HB3	1.82	0.79
3:G:191:ILE:CG2	3:G:192:PRO:HD2	2.12	0.79
1:E:168:TRP:CD1	2:F:28:GLY:HA3	2.18	0.79
4:D:132:GLU:HA	4:D:135:ILE:HG22	1.62	0.79
3:G:135:THR:HG21	4:H:195:ARG:HH22	1.48	0.79
4:H:223:TRP:CD1	4:H:229:LYS:HB2	2.19	0.78
1:E:13:TYR:CE2	1:E:67:LYS:HG3	2.17	0.78
1:A:144:LEU:HD23	2:B:63:GLN:OE1	1.84	0.78
3:G:109:PRO:CG	3:G:158:VAL:HG21	2.14	0.78
2:B:61:TYR:CD2	2:B:62:HIS:CD2	2.72	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:132:GLU:O	4:D:135:ILE:HG22	1.85	0.77
3:C:121:LEU:HD21	4:D:131:SER:N	1.81	0.77
1:A:71:GLU:OE1	2:B:16:GLY:HA2	1.86	0.76
2:F:174:THR:CG2	2:F:187:LEU:H	1.98	0.76
3:C:121:LEU:HD23	4:D:131:SER:N	2.01	0.76
2:B:61:TYR:CE2	2:B:62:HIS:CD2	2.73	0.76
1:A:85:VAL:HB	1:A:113:THR:HG22	1.67	0.76
3:G:57:ARG:O	3:G:58:MET:HG2	1.86	0.76
3:G:191:ILE:HG23	3:G:192:PRO:CD	2.15	0.75
4:H:127:VAL:HG23	4:H:237:ALA:HB3	1.68	0.75
1:A:123:ARG:O	1:A:124:ASN:HB2	1.85	0.75
1:A:143:HIS:HD2	2:B:41:LYS:NZ	1.84	0.75
2:B:162:ARG:HG3	2:B:200:TYR:HE1	1.50	0.75
3:C:148:ASP:HB2	3:C:151:VAL:HB	1.67	0.74
1:A:48:PHE:CD1	2:B:118:PHE:CD1	2.76	0.74
2:F:29:SER:O	2:F:31:ASP:N	2.19	0.74
3:G:159:LEU:HB3	4:H:171:SER:HB3	1.70	0.73
1:A:36:MET:HE3	1:A:60:LEU:HG	1.68	0.73
1:A:144:LEU:CD2	2:B:63:GLN:OE1	2.36	0.73
1:A:81:PRO:C	2:B:62:HIS:HE1	1.91	0.73
1:A:105:LEU:HB2	1:A:153:PHE:CE2	2.24	0.73
1:A:81:PRO:C	2:B:62:HIS:CE1	2.63	0.72
2:B:174:THR:HG23	2:B:175:GLY:O	1.88	0.72
4:H:159:TRP:CZ3	4:H:210:CYS:HB2	2.25	0.72
4:H:12:LYS:HE2	4:H:117:LEU:HB3	1.72	0.72
2:F:39:GLN:HB2	2:F:60:PHE:HB2	1.72	0.72
1:A:107:CYS:HB2	1:A:121:TRP:CH2	2.25	0.71
3:G:195:THR:O	3:G:196:PHE:HB3	1.90	0.71
1:E:12:PHE:CZ	1:E:21:GLU:HG3	2.24	0.71
1:A:107:CYS:HB2	1:A:121:TRP:HZ2	1.54	0.71
3:G:135:THR:HG21	4:H:195:ARG:NH2	2.05	0.71
1:A:12:PHE:CZ	1:A:21:GLU:HG3	2.25	0.71
3:C:152:TYR:C	3:C:153:ILE:HG13	2.09	0.71
2:F:162:ARG:HG3	2:F:200:TYR:CE1	2.25	0.70
4:D:132:GLU:CA	4:D:135:ILE:HG22	2.21	0.70
1:A:107:CYS:CB	1:A:121:TRP:CZ2	2.72	0.70
4:D:6:PRO:HG2	4:D:9:VAL:CG2	2.22	0.70
2:F:142:ASN:HB3	2:F:194:PRO:HG3	1.73	0.70
2:B:14:SER:HA	4:D:27:GLN:HE21	1.52	0.70
4:H:121:PHE:CE1	4:H:227:ARG:NH2	2.60	0.69
3:C:152:TYR:O	3:C:153:ILE:CG1	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:LYS:HG2	1:E:140:ARG:CZ	2.23	0.69
4:D:4:GLN:HG3	4:D:106:GLY:HA3	1.74	0.68
4:H:6:PRO:HG2	4:H:9:VAL:CG2	2.23	0.68
3:C:118:VAL:HG22	3:C:134:PHE:CD1	2.29	0.68
4:D:138:THR:C	4:D:139:GLN:HG2	2.14	0.68
1:A:107:CYS:CB	1:A:121:TRP:HZ2	2.07	0.67
3:G:160:ASP:OD2	3:G:167:LYS:HE2	1.95	0.67
4:H:117:LEU:HD11	4:H:217:LEU:HD21	1.75	0.67
4:H:117:LEU:HD11	4:H:217:LEU:CD2	2.25	0.67
3:C:146:SER:O	3:C:147:LYS:HB2	1.94	0.67
2:B:145:VAL:HG22	2:B:189:MET:HG2	1.77	0.67
3:C:109:PRO:HG3	3:C:158:VAL:HG21	1.76	0.67
4:D:138:THR:O	4:D:139:GLN:HG2	1.95	0.67
3:G:121:LEU:HD23	4:H:131:SER:HB2	1.77	0.67
4:H:160:TRP:HA	4:H:164:LYS:O	1.96	0.66
4:D:64:LYS:HE2	4:D:86:ASP:OD2	1.95	0.66
1:E:36:MET:HE2	1:E:63:ILE:HG13	1.77	0.66
2:F:144:LEU:HD11	2:F:217:TRP:CE3	2.31	0.66
1:A:143:HIS:CE1	2:B:60:PHE:CE1	2.84	0.66
3:C:151:VAL:HG22	3:C:175:SER:CB	2.26	0.66
4:H:130:PRO:HD2	4:H:201:TRP:CH2	2.30	0.66
1:E:62:ASN:ND2	2:F:8:GLN:HE22	1.94	0.66
1:A:98:GLU:O	1:A:155:PRO:HG2	1.96	0.66
2:B:61:TYR:CE2	2:B:62:HIS:NE2	2.64	0.66
1:E:36:MET:CE	1:E:63:ILE:HG13	2.27	0.65
1:A:113:THR:HG21	2:B:63:GLN:OE1	1.96	0.65
4:D:223:TRP:HB2	4:D:229:LYS:HD2	1.78	0.65
3:C:116:PRO:HB2	3:C:195:THR:HG22	1.79	0.65
2:F:101:ARG:O	5:F:225:HOH:O	2.13	0.65
3:C:95:ASN:HD21	4:D:95:ARG:HH22	1.43	0.65
4:H:223:TRP:CG	4:H:229:LYS:HB2	2.33	0.64
4:H:5:HIS:HB3	4:H:20:GLU:HB2	1.78	0.64
1:A:117:VAL:HG12	1:A:167:HIS:HD2	1.62	0.64
3:G:82:ALA:HB2	3:G:107:VAL:HG23	1.80	0.63
2:B:162:ARG:HG3	2:B:200:TYR:CE1	2.32	0.63
4:D:6:PRO:O	4:D:109:THR:OG1	2.15	0.63
3:G:166:PHE:CE2	3:G:168:SER:HB3	2.33	0.63
3:G:118:VAL:HG22	3:G:134:PHE:CD1	2.34	0.63
1:E:85:VAL:HB	1:E:113:THR:HG22	1.81	0.62
3:G:60:SER:OG	3:G:75:HIS:CE1	2.53	0.62
3:C:121:LEU:HD22	4:D:131:SER:N	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:201:TRP:O	4:D:241:GLY:HA2	1.98	0.62
3:C:121:LEU:HD22	4:D:130:PRO:C	2.20	0.62
2:B:167:GLU:OE1	2:B:169:THR:HG22	2.00	0.62
4:D:121:PHE:CE1	4:D:187:ARG:NH2	2.67	0.62
4:D:201:TRP:HE3	4:D:208:PHE:CE2	2.17	0.62
4:D:201:TRP:CE3	4:D:208:PHE:CE2	2.87	0.62
3:G:193:GLU:O	3:G:195:THR:HG23	1.99	0.62
2:B:174:THR:CG2	2:B:187:LEU:H	2.12	0.62
4:D:178:LYS:CE	4:D:181:PRO:HA	2.25	0.61
3:G:95:ASN:HD21	4:H:95:ARG:HH22	1.48	0.61
3:G:119:TYR:OH	4:H:138:THR:HG23	2.00	0.61
2:B:174:THR:HG21	2:B:187:LEU:H	1.65	0.61
3:G:191:ILE:CG2	3:G:192:PRO:CD	2.75	0.61
3:C:146:SER:N	3:C:153:ILE:HB	2.16	0.61
4:D:132:GLU:HG3	4:D:135:ILE:CG2	2.30	0.61
3:C:151:VAL:HG22	3:C:175:SER:HB2	1.82	0.61
3:G:60:SER:OG	3:G:75:HIS:HE1	1.83	0.61
4:H:6:PRO:HG2	4:H:9:VAL:HG22	1.81	0.61
4:D:120:VAL:HG12	4:D:230:PRO:HB2	1.81	0.61
3:C:118:VAL:HG22	3:C:134:PHE:HD1	1.64	0.61
1:E:105:LEU:HB2	1:E:153:PHE:CE2	2.36	0.61
4:D:132:GLU:HG3	4:D:135:ILE:HG21	1.82	0.61
3:C:123:ASP:HB3	3:C:126:SER:HA	1.81	0.61
3:C:95:ASN:ND2	4:D:95:ARG:HH22	1.98	0.61
2:F:29:SER:C	2:F:31:ASP:N	2.54	0.60
3:C:121:LEU:CD2	4:D:130:PRO:C	2.69	0.60
1:A:143:HIS:HD2	2:B:41:LYS:HZ1	1.47	0.60
2:F:130:VAL:HG13	2:F:130:VAL:O	2.01	0.60
4:D:57:GLU:O	4:D:60:VAL:HB	2.00	0.60
2:F:145:VAL:HG22	2:F:189:MET:HG2	1.84	0.60
1:A:58:GLY:HA3	4:D:99:TYR:OH	2.01	0.60
4:H:121:PHE:CE1	4:H:227:ARG:CZ	2.85	0.60
4:D:217:LEU:HD12	4:D:230:PRO:HD2	1.83	0.60
1:A:140:ARG:HG2	1:A:146:ARG:HD2	1.83	0.60
1:A:85:VAL:HB	1:A:113:THR:CG2	2.30	0.60
4:H:217:LEU:HD12	4:H:230:PRO:HD2	1.84	0.60
1:A:71:GLU:CD	2:B:16:GLY:HA2	2.22	0.60
3:C:151:VAL:HG22	3:C:175:SER:OG	2.01	0.59
3:C:121:LEU:HD23	4:D:131:SER:CA	2.31	0.59
1:A:121:TRP:HE1	1:A:149:HIS:HB3	1.66	0.59
2:B:61:TYR:O	2:B:62:HIS:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:LEU:C	2:B:213:LEU:HD23	2.22	0.59
3:C:115:ASP:HB3	3:C:136:ASP:HB3	1.83	0.59
4:H:71:SER:O	4:H:72:LEU:CB	2.46	0.59
3:G:57:ARG:H	3:G:57:ARG:CD	2.12	0.59
2:F:174:THR:HG21	2:F:187:LEU:H	1.66	0.59
1:A:160:VAL:HG22	1:A:179:GLU:CB	2.33	0.59
2:B:160:TRP:CD1	2:B:190:LEU:HB2	2.38	0.59
2:F:159:ARG:HG2	2:F:159:ARG:HH11	1.68	0.59
4:D:116:ASP:CG	4:D:118:LYS:HB3	2.23	0.58
1:A:36:MET:CE	1:A:60:LEU:HG	2.32	0.58
4:H:149:GLY:C	4:H:187:ARG:HD3	2.23	0.58
4:H:231:VAL:O	4:H:233:GLN:HG2	2.03	0.58
4:H:138:THR:O	4:H:139:GLN:CB	2.48	0.58
1:E:144:LEU:HD21	2:F:63:GLN:OE1	2.02	0.58
4:H:202:GLN:HG2	4:H:243:ALA:HA	1.85	0.58
4:D:130:PRO:HD2	4:D:201:TRP:CZ2	2.39	0.58
4:D:71:SER:O	4:D:72:LEU:CB	2.51	0.58
1:A:38:LYS:NZ	1:A:40:GLU:OE1	2.32	0.58
3:C:38:LEU:HB3	3:C:39:PRO:CD	2.34	0.58
4:H:12:LYS:HE2	4:H:117:LEU:CB	2.33	0.58
4:H:149:GLY:O	4:H:187:ARG:HD3	2.04	0.58
2:B:161:PHE:HB2	2:B:201:THR:HB	1.86	0.58
4:H:127:VAL:HG23	4:H:237:ALA:CB	2.34	0.58
3:G:37:GLN:NE2	4:H:36:GLN:HE22	1.99	0.57
4:D:32:PHE:CE1	4:D:47:THR:HG23	2.38	0.57
1:A:119:VAL:HG22	1:A:165:VAL:HG22	1.85	0.57
3:G:112:GLN:C	3:G:113:ASN:HD22	2.07	0.57
1:A:89:VAL:HG12	1:A:90:THR:N	2.19	0.57
4:H:117:LEU:HD21	4:H:217:LEU:CD1	2.29	0.57
1:E:111:LYS:HG2	1:E:140:ARG:NH2	2.19	0.57
4:D:127:VAL:HG23	4:D:237:ALA:CB	2.31	0.57
2:F:174:THR:HG22	2:F:187:LEU:H	1.69	0.57
4:D:116:ASP:OD2	4:D:118:LYS:HB3	2.04	0.57
3:G:151:VAL:HG22	3:G:175:SER:OG	2.04	0.57
4:H:117:LEU:CD2	4:H:217:LEU:HD11	2.30	0.56
4:H:132:GLU:HA	4:H:135:ILE:HG12	1.86	0.56
3:G:151:VAL:HG22	3:G:175:SER:CB	2.34	0.56
3:G:17:VAL:CG1	3:G:74:LEU:HB2	2.35	0.56
3:C:131:VAL:HG22	3:C:174:TRP:HB2	1.87	0.56
4:D:162:ASN:HD21	4:D:206:ASN:HB2	1.69	0.56
4:D:203:ASN:OD1	4:D:205:ARG:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:201:TRP:HE3	4:H:208:PHE:CE2	2.23	0.56
1:A:96:PRO:HB3	2:B:131:TYR:OH	2.06	0.56
4:D:71:SER:O	4:D:72:LEU:HB3	2.06	0.56
1:E:168:TRP:CH2	2:F:35:ARG:NH2	2.74	0.56
3:C:151:VAL:HG13	3:C:175:SER:HB2	1.87	0.56
2:B:193:VAL:HG23	2:B:193:VAL:O	2.06	0.56
4:H:192:SER:O	4:H:193:ARG:HD2	2.05	0.56
3:C:146:SER:N	3:C:153:ILE:CD1	2.68	0.56
3:G:133:LEU:HD12	3:G:134:PHE:H	1.70	0.56
4:D:4:GLN:HG2	4:D:92:CYS:SG	2.45	0.56
4:H:10:ILE:HD13	4:H:152:PRO:HG3	1.87	0.56
1:A:103:ASN:OD1	1:A:104:VAL:N	2.38	0.56
1:A:143:HIS:HD2	2:B:41:LYS:HZ2	1.54	0.56
3:G:161:MET:HG3	3:G:166:PHE:HD2	1.70	0.56
4:H:123:PRO:HA	4:H:150:PHE:HB3	1.87	0.56
4:H:9:VAL:HG11	4:H:17:VAL:CG1	2.37	0.55
3:C:121:LEU:HD23	4:D:131:SER:HB2	1.88	0.55
3:C:17:VAL:CG1	3:C:74:LEU:HB2	2.32	0.55
4:H:13:SER:OG	4:H:115:GLU:HG2	2.05	0.55
2:F:198:GLU:N	2:F:218:ARG:HD3	2.21	0.55
2:B:131:TYR:O	2:B:145:VAL:HB	2.07	0.55
4:D:125:VAL:HG21	4:D:235:VAL:O	2.07	0.55
4:D:95:ARG:HG2	4:D:97:GLY:O	2.07	0.55
3:G:166:PHE:HE2	3:G:168:SER:HB3	1.71	0.55
2:F:132:PRO:O	2:F:133:ALA:HB2	2.05	0.55
2:F:198:GLU:H	2:F:218:ARG:NH1	1.99	0.55
4:H:57:GLU:O	4:H:60:VAL:HB	2.06	0.55
4:H:111:LEU:HD11	4:H:113:VAL:HG23	1.88	0.55
2:F:213:LEU:HD23	2:F:213:LEU:C	2.26	0.55
4:H:234:ILE:HG22	4:H:235:VAL:N	2.22	0.55
4:H:9:VAL:HG11	4:H:17:VAL:HG11	1.88	0.55
4:H:131:SER:O	4:H:135:ILE:HG23	2.06	0.55
3:G:129:LYS:O	3:G:175:SER:O	2.24	0.55
3:C:13:GLU:OE1	3:C:79:LEU:HD21	2.07	0.54
4:H:234:ILE:CG2	4:H:235:VAL:N	2.70	0.54
2:F:126:PRO:HB3	2:F:151:PHE:HB3	1.88	0.54
3:C:175:SER:OG	3:C:176:ASN:N	2.39	0.54
1:A:92:LEU:HD12	1:A:93:THR:N	2.21	0.54
3:C:133:LEU:HD12	3:C:134:PHE:H	1.72	0.54
1:E:36:MET:HE3	1:E:60:LEU:HG	1.89	0.54
3:G:17:VAL:HG12	3:G:74:LEU:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3:THR:HG22	3:G:23:HIS:HB3	1.89	0.54
4:H:51:GLY:O	4:H:52:SER:OG	2.24	0.54
4:D:162:ASN:HD21	4:D:206:ASN:CB	2.21	0.54
3:C:1:ALA:HB2	3:C:98:ILE:HG21	1.89	0.54
4:D:61:GLU:HG2	4:D:65:PHE:HE2	1.72	0.54
4:D:89:PHE:CZ	4:D:108:GLY:HA3	2.43	0.54
1:E:71:GLU:O	1:E:75:LYS:HG3	2.08	0.54
3:G:12:ASN:O	3:G:15:GLU:HB2	2.06	0.54
2:B:143:LEU:HD12	2:B:190:LEU:O	2.08	0.53
4:D:83:HIS:ND1	4:D:85:GLU:HB2	2.22	0.53
4:H:117:LEU:O	4:H:117:LEU:HD23	2.08	0.53
1:E:144:LEU:CD2	2:F:63:GLN:OE1	2.56	0.53
4:H:117:LEU:HD21	4:H:217:LEU:HD21	1.90	0.53
1:E:123:ARG:O	1:E:126:LYS:HG2	2.09	0.53
4:D:194:LEU:HD12	4:D:195:ARG:N	2.24	0.53
4:H:201:TRP:C	4:H:203:ASN:H	2.11	0.53
3:G:151:VAL:HG22	3:G:175:SER:HB2	1.89	0.53
4:D:10:ILE:HD13	4:D:152:PRO:HG3	1.90	0.53
4:D:229:LYS:HG2	4:D:231:VAL:HG13	1.91	0.53
2:F:150:GLY:HA2	2:F:183:THR:HB	1.91	0.53
3:C:160:ASP:OD1	3:C:162:ARG:HG2	2.09	0.53
1:E:117:VAL:HG12	1:E:167:HIS:HD2	1.74	0.53
4:H:32:PHE:HB2	4:H:93:SER:OG	2.09	0.53
4:H:13:SER:OG	4:H:84:PRO:HD3	2.09	0.53
3:G:3:THR:HB	3:G:21:CYS:SG	2.48	0.53
4:D:37:PHE:CE2	4:D:88:SER:HB2	2.44	0.53
4:H:88:SER:HB3	4:H:90:TYR:CE2	2.44	0.52
4:H:201:TRP:CD1	4:H:202:GLN:N	2.77	0.52
4:H:28:ALA:CB	4:H:94:ALA:HB1	2.39	0.52
2:F:128:VAL:HG21	2:F:213:LEU:CD2	2.34	0.52
4:D:132:GLU:C	4:D:135:ILE:HG22	2.28	0.52
4:D:50:GLU:HG3	4:D:72:LEU:HD13	1.91	0.52
3:G:161:MET:HE1	4:H:196:VAL:HA	1.90	0.52
1:A:73:MET:HE3	2:B:82:LEU:HG	1.89	0.52
3:C:188:ASN:HA	3:C:191:ILE:HD11	1.90	0.52
1:A:45:LEU:HB2	1:A:48:PHE:CE2	2.45	0.52
4:H:32:PHE:CE1	4:H:47:THR:HG23	2.45	0.52
4:H:12:LYS:HA	4:H:114:THR:O	2.10	0.52
4:H:13:SER:HA	4:H:82:ALA:O	2.10	0.51
2:F:19:LEU:O	2:F:19:LEU:HD12	2.09	0.51
2:B:130:VAL:HG11	2:B:215:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:50:GLU:HG3	4:H:72:LEU:HB2	1.92	0.51
4:H:192:SER:C	4:H:193:ARG:HD2	2.30	0.51
2:F:1:PHE:O	2:F:2:SER:CB	2.57	0.51
3:G:84:VAL:HG11	3:G:86:TYR:CZ	2.45	0.51
2:F:161:PHE:HB2	2:F:201:THR:HB	1.92	0.51
4:H:234:ILE:CG2	4:H:235:VAL:H	2.24	0.51
3:G:118:VAL:HG22	3:G:134:PHE:HD1	1.75	0.51
4:H:167:HIS:O	4:H:170:VAL:HG23	2.10	0.51
4:D:223:TRP:CZ2	4:D:230:PRO:HD3	2.45	0.51
4:H:130:PRO:HD2	4:H:201:TRP:CZ2	2.46	0.51
4:H:48:SER:OG	4:H:69:HIS:ND1	2.32	0.51
2:B:150:GLY:HA2	2:B:183:THR:HB	1.92	0.51
1:A:160:VAL:HG22	1:A:179:GLU:HB2	1.91	0.51
2:B:48:ASN:ND2	2:B:51:GLU:OE2	2.44	0.51
4:H:28:ALA:HB1	4:H:94:ALA:HB1	1.93	0.51
4:H:145:CYS:O	4:H:146:LEU:HB2	2.10	0.51
3:C:115:ASP:HB3	3:C:136:ASP:CB	2.41	0.51
1:A:160:VAL:HG22	1:A:179:GLU:HB3	1.93	0.51
1:A:14:LEU:HD12	2:B:36:PHE:O	2.10	0.51
4:D:150:PHE:HE2	4:D:153:ASP:HA	1.76	0.50
1:E:99:LEU:HA	1:E:155:PRO:HB2	1.93	0.50
4:D:64:LYS:HE3	4:D:80:THR:O	2.11	0.50
3:G:133:LEU:HG	3:G:134:PHE:N	2.27	0.50
4:D:128:PHE:CE2	4:D:146:LEU:CD1	2.74	0.50
3:G:95:ASN:ND2	4:H:95:ARG:HH22	2.09	0.50
4:D:143:LEU:N	4:D:143:LEU:HD12	2.25	0.50
1:E:143:HIS:CE1	2:F:60:PHE:CE1	2.99	0.50
4:H:112:THR:OG1	4:H:154:HIS:NE2	2.35	0.50
1:A:105:LEU:HB2	1:A:153:PHE:CD2	2.46	0.50
4:H:144:VAL:HG22	4:H:193:ARG:HG3	1.92	0.50
1:A:92:LEU:O	1:A:105:LEU:HD12	2.12	0.50
3:G:56:ASN:HB2	3:G:57:ARG:HH11	1.77	0.50
2:F:200:TYR:HD2	2:F:217:TRP:CE3	2.30	0.49
3:C:148:ASP:CB	3:C:151:VAL:HB	2.38	0.49
4:H:145:CYS:HB2	4:H:159:TRP:CZ2	2.47	0.49
4:D:178:LYS:HE3	4:D:181:PRO:CA	2.32	0.49
1:A:73:MET:O	1:A:74:THR:C	2.50	0.49
3:C:9:MET:SD	3:C:19:LEU:HD23	2.52	0.49
4:H:204:PRO:C	4:H:206:ASN:H	2.15	0.49
4:H:74:LEU:HD12	4:H:75:SER:H	1.76	0.49
2:B:69:PHE:HB2	2:B:76:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:71:SER:HB2	5:F:224:HOH:O	2.12	0.49
3:G:91:GLY:HA2	4:H:100:ASN:OD1	2.12	0.49
4:H:201:TRP:CE3	4:H:208:PHE:CE2	3.00	0.49
1:A:97:VAL:HG11	1:A:180:PHE:HD1	1.77	0.49
1:A:143:HIS:CD2	2:B:41:LYS:NZ	2.73	0.49
4:H:146:LEU:CD2	4:H:148:THR:HG23	2.42	0.49
1:A:162:ASP:OD1	1:A:177:HIS:ND1	2.45	0.49
4:D:142:THR:HG1	4:D:195:ARG:HE	1.59	0.49
3:C:27:SER:OG	3:C:29:THR:HG22	2.13	0.49
3:G:144:SER:OG	3:G:189:SER:HB3	2.12	0.49
2:F:173:SER:HB2	2:F:188:VAL:HG22	1.95	0.49
3:G:191:ILE:HG22	3:G:192:PRO:N	2.27	0.49
2:B:174:THR:CG2	2:B:175:GLY:O	2.58	0.49
4:H:214:PHE:CE2	4:H:216:GLY:HA3	2.48	0.49
4:H:170:VAL:HG12	4:H:171:SER:N	2.27	0.49
1:A:11:GLU:OE1	1:A:62:ASN:HB3	2.12	0.49
2:B:65:GLU:CD	2:B:68:ARG:HH21	2.16	0.49
3:G:123:ASP:HA	4:H:128:PHE:CD1	2.48	0.49
3:C:195:THR:O	3:C:196:PHE:HB3	2.14	0.48
3:C:38:LEU:HB3	3:C:39:PRO:HD2	1.95	0.48
2:F:132:PRO:O	2:F:133:ALA:CB	2.60	0.48
2:F:160:TRP:CD1	2:F:190:LEU:HB2	2.48	0.48
4:D:65:PHE:HB3	4:D:77:LEU:HD11	1.95	0.48
2:B:95:ASP:O	2:B:99:GLN:HG3	2.13	0.48
4:H:83:HIS:C	4:H:113:VAL:HG11	2.34	0.48
2:B:214:THR:O	2:B:215:VAL:HG23	2.14	0.48
3:G:191:ILE:CG2	3:G:192:PRO:N	2.76	0.48
2:B:42:HIS:ND1	2:B:57:ASP:OD1	2.47	0.48
4:H:124:GLU:O	4:H:147:ALA:HA	2.14	0.48
2:F:128:VAL:HG11	2:F:213:LEU:HD22	1.95	0.48
4:H:21:CYS:HB2	4:H:33:TRP:CZ2	2.48	0.48
1:A:172:GLU:HG3	1:A:173:PRO:O	2.14	0.47
1:E:168:TRP:CH2	2:F:35:ARG:CZ	2.97	0.47
4:D:180:GLN:OE1	4:D:180:GLN:HA	2.13	0.47
4:D:132:GLU:O	4:D:135:ILE:CG2	2.60	0.47
4:D:9:VAL:HG11	4:D:17:VAL:HG11	1.96	0.47
2:B:159:ARG:NH1	2:B:166:GLU:OE2	2.47	0.47
1:E:168:TRP:CE3	2:F:27:GLY:HA2	2.49	0.47
1:A:98:GLU:CD	1:A:101:GLU:HG3	2.35	0.47
1:A:36:MET:HE1	1:A:60:LEU:HA	1.96	0.47
3:C:134:PHE:CE2	3:C:137:PHE:CE2	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:119:TYR:CZ	4:H:134:GLU:HA	2.50	0.47
4:D:50:GLU:HG3	4:D:72:LEU:CD1	2.45	0.47
2:F:43:GLU:OE1	2:F:45:HIS:HE1	1.97	0.47
1:A:98:GLU:O	1:A:155:PRO:CG	2.61	0.47
2:B:177:ILE:HB	2:B:185:GLN:O	2.15	0.47
2:B:203:GLN:HG2	2:B:203:GLN:O	2.13	0.47
3:G:137:PHE:CD1	3:G:141:THR:HB	2.50	0.47
1:A:65:VAL:HG23	4:D:29:THR:HG21	1.89	0.47
1:A:122:LEU:HD12	1:A:162:ASP:HB2	1.97	0.47
1:A:99:LEU:O	1:A:100:ARG:CB	2.63	0.47
1:A:82:ILE:N	2:B:62:HIS:CE1	2.83	0.47
1:E:135:THR:O	1:E:147:LYS:NZ	2.42	0.47
2:B:56:LEU:HD23	2:B:70:ASP:HA	1.96	0.47
3:G:117:ALA:CB	3:G:119:TYR:CZ	2.98	0.46
4:H:121:PHE:CE1	4:H:187:ARG:NH2	2.83	0.46
3:C:161:MET:HG3	3:C:166:PHE:HD2	1.80	0.46
3:C:182:CYS:O	3:C:183:ALA:HB3	2.14	0.46
3:C:121:LEU:HD23	4:D:131:SER:CB	2.45	0.46
4:D:194:LEU:HD12	4:D:195:ARG:H	1.80	0.46
1:E:89:VAL:HG12	1:E:90:THR:N	2.30	0.46
3:C:78:THR:O	3:C:107:VAL:HG11	2.14	0.46
5:G:209:HOH:O	4:H:99:TYR:HA	2.14	0.46
1:E:14:LEU:HD11	2:F:35:ARG:HG3	1.98	0.46
4:H:64:LYS:CE	4:H:86:ASP:OD2	2.63	0.46
1:A:65:VAL:HG22	4:D:29:THR:CG2	2.32	0.46
3:G:114:PRO:C	3:G:116:PRO:HD3	2.36	0.46
1:E:162:ASP:OD1	1:E:177:HIS:ND1	2.49	0.46
2:F:174:THR:HG23	2:F:175:GLY:O	2.15	0.46
4:H:201:TRP:CG	4:H:202:GLN:N	2.84	0.46
4:D:99:TYR:O	4:D:100:ASN:HB2	2.16	0.46
3:G:96:LYS:HD3	4:H:44:LEU:HD21	1.97	0.46
4:H:120:VAL:O	4:H:230:PRO:HG2	2.15	0.46
1:E:59:ALA:O	1:E:63:ILE:HG12	2.15	0.46
4:H:4:GLN:HG3	4:H:106:GLY:HA3	1.97	0.46
4:D:223:TRP:CE2	4:D:230:PRO:HD3	2.51	0.46
3:G:43:PRO:HG2	4:H:105:PHE:CD2	2.51	0.46
1:A:133:SER:OG	1:A:150:TYR:HB2	2.16	0.46
4:D:203:ASN:C	4:D:203:ASN:OD1	2.55	0.46
4:H:117:LEU:C	4:H:119:ASN:N	2.69	0.46
1:E:143:HIS:HD2	2:F:41:LYS:NZ	2.14	0.46
3:G:109:PRO:HG2	3:G:158:VAL:CG2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:6:PRO:HG2	4:D:9:VAL:HG22	1.95	0.45
4:H:81:SER:O	4:H:82:ALA:C	2.53	0.45
2:F:26:GLY:O	2:F:32:THR:HA	2.15	0.45
4:D:132:GLU:HA	4:D:135:ILE:CG2	2.41	0.45
1:A:12:PHE:CE2	1:A:21:GLU:HB2	2.51	0.45
2:F:55:PHE:HB3	2:F:71:SER:HB3	1.99	0.45
4:H:223:TRP:CZ2	4:H:230:PRO:HD3	2.51	0.45
4:H:146:LEU:HD21	4:H:148:THR:HG23	1.98	0.45
3:C:111:ILE:HD13	3:C:137:PHE:O	2.16	0.45
4:D:61:GLU:HG2	4:D:65:PHE:CE2	2.52	0.45
3:G:96:LYS:HD3	4:H:44:LEU:CD2	2.47	0.45
3:G:38:LEU:HD23	3:G:38:LEU:HA	1.75	0.45
1:A:28:GLY:O	1:A:146:ARG:NH2	2.39	0.45
2:F:206:HIS:ND1	2:F:207:PRO:HD2	2.32	0.45
4:H:154:HIS:N	4:H:154:HIS:CD2	2.83	0.45
2:F:23:GLY:HA3	2:F:34:PRO:CD	2.47	0.45
4:H:61:GLU:OE2	4:H:65:PHE:HE2	1.99	0.45
3:G:159:LEU:HD11	4:H:195:ARG:HD2	1.99	0.45
4:H:192:SER:C	4:H:193:ARG:CD	2.85	0.45
4:H:76:THR:O	4:H:76:THR:HG22	2.17	0.45
4:H:198:ALA:O	4:H:201:TRP:O	2.35	0.45
1:E:36:MET:CE	1:E:60:LEU:HG	2.47	0.44
4:H:157:LEU:HD23	4:H:158:SER:N	2.32	0.44
2:F:131:TYR:HA	2:F:132:PRO:HD2	1.79	0.44
3:C:191:ILE:HG22	3:C:192:PRO:N	2.32	0.44
4:D:177:LEU:C	4:D:177:LEU:HD12	2.37	0.44
2:B:158:VAL:HG22	2:B:204:VAL:HG22	2.00	0.44
3:G:191:ILE:HG22	3:G:192:PRO:O	2.17	0.44
4:D:7:SER:O	4:D:109:THR:HA	2.16	0.44
4:D:19:ILE:HD12	4:D:77:LEU:HD23	2.00	0.44
1:A:170:LEU:HD13	1:A:174:LEU:HB2	1.98	0.44
2:B:209:LEU:HD13	2:B:213:LEU:HB2	1.99	0.44
2:B:84:ARG:N	2:B:85:PRO:HD2	2.32	0.44
1:A:151:LEU:HD12	1:A:152:PRO:HD2	2.00	0.44
3:G:108:GLN:HA	3:G:109:PRO:HD3	1.82	0.44
1:A:65:VAL:HG12	1:A:69:ASN:ND2	2.32	0.44
1:E:168:TRP:HH2	2:F:35:ARG:NH2	2.16	0.44
1:A:89:VAL:HG12	1:A:90:THR:H	1.83	0.44
2:B:59:TYR:HB2	2:B:67:VAL:HG12	1.99	0.44
2:F:209:LEU:HD13	2:F:213:LEU:HB2	2.00	0.44
3:G:37:GLN:HE22	4:H:36:GLN:NE2	2.04	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:LYS:HG2	3:C:176:ASN:O	2.17	0.44
1:E:62:ASN:ND2	2:F:8:GLN:NE2	2.65	0.44
1:A:98:GLU:O	1:A:155:PRO:CB	2.66	0.44
3:C:79:LEU:HD21	3:C:109:PRO:HA	2.00	0.44
3:G:35:TYR:CD1	3:G:45:TYR:HA	2.53	0.44
1:E:171:ASP:N	1:E:171:ASP:OD1	2.51	0.44
4:D:203:ASN:OD1	4:D:205:ARG:CB	2.66	0.44
1:E:154:LEU:HD12	1:E:155:PRO:HD2	2.00	0.44
4:D:209:ARG:NH1	4:D:211:GLN:HB2	2.33	0.44
4:H:209:ARG:HD2	4:H:236:SER:HB3	1.99	0.44
2:B:132:PRO:O	2:B:133:ALA:HB2	2.18	0.44
1:A:143:HIS:CD2	2:B:41:LYS:HZ2	2.33	0.44
1:A:82:ILE:N	2:B:62:HIS:HE1	2.14	0.44
4:D:42:LEU:CD2	4:D:91:ILE:HD12	2.48	0.44
2:B:33:ARG:O	2:B:35:ARG:NH1	2.41	0.44
4:H:30:THR:HG23	4:H:49:ASN:ND2	2.32	0.44
2:B:145:VAL:HG22	2:B:189:MET:CG	2.48	0.43
4:H:117:LEU:O	4:H:120:VAL:HG23	2.18	0.43
2:F:206:HIS:CG	2:F:207:PRO:HD2	2.53	0.43
2:B:65:GLU:O	2:B:79:VAL:HB	2.18	0.43
2:F:43:GLU:OE1	2:F:45:HIS:CE1	2.71	0.43
2:B:126:PRO:HD3	2:B:208:SER:OG	2.18	0.43
4:H:201:TRP:O	4:H:202:GLN:CB	2.55	0.43
3:C:111:ILE:O	3:C:111:ILE:HG22	2.18	0.43
3:C:191:ILE:HG23	3:C:192:PRO:HD2	1.99	0.43
1:E:99:LEU:C	1:E:101:GLU:H	2.22	0.43
3:C:144:SER:OG	3:C:189:SER:CB	2.61	0.43
1:E:168:TRP:CD1	2:F:28:GLY:CA	2.96	0.43
2:B:213:LEU:C	2:B:213:LEU:CD2	2.87	0.43
3:G:174:TRP:CH2	4:H:177:LEU:HD21	2.53	0.43
4:D:203:ASN:HA	4:D:204:PRO:HD3	1.89	0.43
4:H:120:VAL:O	4:H:230:PRO:CG	2.66	0.43
2:F:174:THR:HG23	2:F:177:ILE:HD12	2.01	0.43
2:F:193:VAL:HA	2:F:194:PRO:HD3	1.71	0.43
1:A:117:VAL:HG12	1:A:167:HIS:CD2	2.50	0.43
4:D:31:MET:SD	4:D:75:SER:HB3	2.58	0.43
2:F:84:ARG:N	2:F:85:PRO:HD2	2.33	0.43
3:G:145:GLN:O	3:G:153:ILE:HD12	2.18	0.43
4:D:197:SER:O	4:D:198:ALA:C	2.57	0.43
4:H:5:HIS:HA	4:H:6:PRO:HA	1.80	0.43
1:E:110:ASP:OD1	1:E:111:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:ARG:CG	1:E:146:ARG:HD2	2.49	0.43
4:H:161:VAL:O	4:H:162:ASN:C	2.56	0.43
1:A:75:LYS:NZ	2:B:15:GLY:O	2.44	0.43
1:E:12:PHE:C	1:E:12:PHE:CD1	2.92	0.43
3:C:134:PHE:HB3	3:C:171:ALA:O	2.19	0.43
1:A:143:HIS:CE1	2:B:60:PHE:HE1	2.33	0.42
3:G:37:GLN:OE1	4:H:36:GLN:OE1	2.37	0.42
4:H:58:GLN:C	4:H:60:VAL:H	2.23	0.42
3:G:66:ASP:OD2	3:G:68:LYS:HB2	2.19	0.42
2:B:160:TRP:CH2	2:B:202:CYS:HB2	2.54	0.42
4:H:125:VAL:HG23	4:H:235:VAL:CG1	2.49	0.42
4:D:229:LYS:HA	4:D:230:PRO:HD3	1.94	0.42
1:A:89:VAL:CG1	1:A:90:THR:N	2.82	0.42
4:H:209:ARG:HD2	4:H:236:SER:CB	2.49	0.42
2:F:14:SER:HA	4:H:27:GLN:HE21	1.84	0.42
4:D:130:PRO:HD2	4:D:201:TRP:CH2	2.55	0.42
4:H:214:PHE:HE2	4:H:216:GLY:HA3	1.84	0.42
1:A:110:ASP:OD1	1:A:111:LYS:HG3	2.19	0.42
4:H:140:LYS:HD2	4:H:195:ARG:NH1	2.34	0.42
4:H:153:ASP:HB3	4:H:188:TYR:CD2	2.55	0.42
3:G:1:ALA:HB2	3:G:98:ILE:HG21	2.01	0.42
4:D:203:ASN:O	4:D:241:GLY:HA3	2.20	0.42
4:H:144:VAL:HG12	4:H:145:CYS:O	2.20	0.42
1:A:6:VAL:HG22	2:B:45:HIS:ND1	2.34	0.42
3:G:125:LYS:O	3:G:126:SER:HB3	2.20	0.42
1:A:85:VAL:O	1:A:112:PHE:HA	2.20	0.42
1:A:20:GLY:O	1:A:21:GLU:HG2	2.20	0.42
1:A:13:TYR:CD2	1:A:67:LYS:HA	2.55	0.42
4:D:11:ALA:O	4:D:113:VAL:HA	2.20	0.42
2:F:130:VAL:HG11	2:F:215:VAL:HG12	2.02	0.42
4:H:61:GLU:OE2	4:H:65:PHE:CE2	2.73	0.42
2:B:210:THR:HG22	2:B:210:THR:O	2.20	0.42
1:E:113:THR:HA	1:E:114:PRO:C	2.40	0.41
1:E:89:VAL:HG12	1:E:90:THR:H	1.86	0.41
2:B:199:VAL:HG22	2:B:218:ARG:CB	2.50	0.41
2:B:128:VAL:HB	2:B:148:VAL:HG22	2.01	0.41
1:E:113:THR:HG22	1:E:144:LEU:HD22	2.02	0.41
4:D:56:TYR:HD1	4:D:60:VAL:HG11	1.84	0.41
4:D:42:LEU:HD22	4:D:91:ILE:HD12	2.02	0.41
4:H:180:GLN:HA	4:H:181:PRO:HD2	1.88	0.41
4:H:229:LYS:HA	4:H:230:PRO:HD3	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD12	1:A:92:LEU:C	2.41	0.41
3:C:91:GLY:HA2	4:D:100:ASN:OD1	2.19	0.41
2:B:8:GLN:OE1	2:B:42:HIS:NE2	2.53	0.41
4:H:234:ILE:C	4:H:235:VAL:HG23	2.41	0.41
1:E:113:THR:CG2	1:E:144:LEU:HD22	2.50	0.41
2:F:129:THR:HG22	2:F:131:TYR:HD1	1.85	0.41
2:F:59:TYR:CD2	2:F:59:TYR:N	2.88	0.41
2:B:146:CYS:HB2	2:B:160:TRP:CZ2	2.55	0.41
4:D:10:ILE:HD12	4:D:112:THR:O	2.21	0.41
1:E:47:GLU:HG3	1:E:50:ARG:HH21	1.85	0.41
2:B:173:SER:HB2	2:B:188:VAL:HG22	2.03	0.41
2:F:20:VAL:HB	2:F:21:PRO:HD2	2.02	0.41
4:H:159:TRP:CH2	4:H:210:CYS:HB2	2.55	0.41
3:C:117:ALA:HA	3:C:196:PHE:H	1.85	0.41
4:D:218:SER:O	4:D:221:ASP:HB2	2.21	0.41
3:C:119:TYR:CZ	4:D:134:GLU:HA	2.56	0.41
2:B:163:ASN:OD1	2:B:198:GLU:HB2	2.21	0.41
2:B:163:ASN:HD21	2:B:198:GLU:HB2	1.85	0.41
1:A:171:ASP:N	1:A:171:ASP:OD1	2.46	0.41
1:E:120:THR:HB	1:E:164:ARG:HB3	2.03	0.41
1:E:176:LYS:HD2	1:E:176:LYS:HA	1.88	0.41
1:A:85:VAL:HG12	1:A:85:VAL:O	2.20	0.41
2:B:97:LEU:O	2:B:101:ARG:HG3	2.21	0.41
2:F:97:LEU:HA	2:F:97:LEU:HD23	1.84	0.41
4:H:218:SER:O	4:H:221:ASP:HB2	2.21	0.41
1:E:26:PHE:HB2	1:E:31:ILE:HD11	2.02	0.41
4:D:93:SER:HB3	4:D:105:PHE:CD1	2.56	0.41
3:C:30:ASP:HA	3:C:91:GLY:HA3	2.02	0.41
2:B:193:VAL:O	2:B:195:ARG:N	2.51	0.41
2:F:129:THR:O	2:F:129:THR:HG22	2.21	0.41
4:H:73:THR:O	4:H:73:THR:HG22	2.21	0.41
2:F:152:TYR:CG	2:F:153:PRO:HA	2.56	0.41
1:E:160:VAL:HG22	1:E:179:GLU:HB3	2.03	0.41
2:B:145:VAL:CG2	2:B:189:MET:HG2	2.49	0.40
3:G:134:PHE:HD2	3:G:171:ALA:HB3	1.85	0.40
3:C:191:ILE:CG2	3:C:192:PRO:HD2	2.51	0.40
4:D:150:PHE:CE2	4:D:153:ASP:HA	2.55	0.40
2:F:104:VAL:HG13	5:F:224:HOH:O	2.21	0.40
1:E:69:ASN:OD1	2:F:10:PRO:HA	2.21	0.40
3:C:164:MET:O	3:C:164:MET:HG3	2.21	0.40
4:H:120:VAL:HG12	4:H:230:PRO:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:TYR:CZ	2:B:62:HIS:NE2	2.89	0.40
1:E:110:ASP:OD1	1:E:111:LYS:HG3	2.20	0.40
3:C:13:GLU:O	3:C:14:GLU:HB2	2.20	0.40
4:H:93:SER:HA	4:H:104:HIS:O	2.21	0.40
4:D:143:LEU:H	4:D:143:LEU:HD12	1.85	0.40
4:D:157:LEU:C	4:D:157:LEU:HD23	2.42	0.40
1:E:104:VAL:HG12	1:E:105:LEU:N	2.36	0.40
3:G:143:VAL:HG22	3:G:144:SER:N	2.37	0.40
1:A:11:GLU:HA	1:A:21:GLU:O	2.21	0.40
2:B:143:LEU:HD12	2:B:190:LEU:C	2.42	0.40
4:D:36:GLN:HB2	4:D:42:LEU:HD23	2.04	0.40
4:H:217:LEU:H	4:H:231:VAL:HA	1.87	0.40
1:A:107:CYS:HB3	1:A:121:TRP:HZ2	1.84	0.40
2:F:216:GLU:HA	2:F:216:GLU:OE1	2.22	0.40
4:H:16:SER:HA	4:H:79:VAL:O	2.22	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	176/182 (97%)	160 (91%)	15 (8%)	1 (1%)	30	65
1	E	177/182 (97%)	164 (93%)	13 (7%)	0	100	100
2	B	189/221 (86%)	176 (93%)	11 (6%)	2 (1%)	17	50
2	F	206/221 (93%)	185 (90%)	17 (8%)	4 (2%)	10	32
3	C	183/206 (89%)	162 (88%)	20 (11%)	1 (0%)	34	69
3	G	180/206 (87%)	154 (86%)	25 (14%)	1 (1%)	30	65
4	D	243/245 (99%)	225 (93%)	18 (7%)	0	100	100
4	H	241/245 (98%)	210 (87%)	28 (12%)	3 (1%)	16	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1595/1708 (93%)	1436 (90%)	147 (9%)	12 (1%)	24 58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	2	SER
4	H	235	VAL
2	B	132	PRO
2	B	2	SER
4	H	146	LEU
1	A	124	ASN
4	H	116	ASP
3	C	47	ILE
2	F	21	PRO
2	F	27	GLY
3	G	111	ILE
2	F	30	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	159/166 (96%)	157 (99%)	2 (1%)	76 94
1	E	160/166 (96%)	160 (100%)	0	100 100
2	B	167/189 (88%)	164 (98%)	3 (2%)	66 91
2	F	176/189 (93%)	172 (98%)	4 (2%)	58 88
3	C	159/183 (87%)	159 (100%)	0	100 100
3	G	163/183 (89%)	160 (98%)	3 (2%)	66 91
4	D	212/216 (98%)	207 (98%)	5 (2%)	57 87
4	H	209/216 (97%)	208 (100%)	1 (0%)	92 98
All	All	1405/1508 (93%)	1387 (99%)	18 (1%)	76 94

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	MET
1	A	122	LEU
2	B	1	PHE
2	B	128	VAL
2	B	203	GLN
4	D	31	MET
4	D	81	SER
4	D	161	VAL
4	D	193	ARG
4	D	203	ASN
2	F	1	PHE
2	F	63	GLN
2	F	177	ILE
2	F	210	THR
3	G	57	ARG
3	G	76	ARG
3	G	159	LEU
4	H	193	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	A	149	HIS
2	B	179	ASN
2	B	185	GLN
3	C	22	ASN
3	C	37	GLN
3	C	53	ASN
3	C	75	HIS
4	D	27	GLN
4	D	49	ASN
1	E	62	ASN
1	E	84	ASN
1	E	143	HIS
2	F	45	HIS
2	F	149	ASN
3	G	22	ASN
3	G	37	GLN
3	G	53	ASN
3	G	75	HIS
3	G	95	ASN
3	G	113	ASN

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Mol	Chain	Res	Type
4	H	27	GLN
4	H	40	GLN
4	H	49	ASN

### 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 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	178/182 (97%)	0.15	8 (4%) 37 26	32, 66, 117, 124	0
1	E	179/182 (98%)	0.13	5 (2%) 56 44	27, 51, 98, 108	0
2	B	195/221 (88%)	-0.04	5 (2%) 59 47	29, 54, 93, 133	0
2	F	210/221 (95%)	0.02	5 (2%) 62 50	26, 48, 93, 116	0
3	C	191/206 (92%)	0.29	13 (6%) 20 12	24, 52, 128, 139	1 (0%)
3	G	188/206 (91%)	0.62	26 (13%) 4 2	28, 68, 137, 147	0
4	D	245/245 (100%)	0.04	2 (0%) 87 81	34, 57, 95, 125	0
4	H	243/245 (99%)	0.73	33 (13%) 4 2	30, 92, 128, 143	0
All	All	1629/1708 (95%)	0.25	97 (5%) 25 15	24, 60, 124, 147	1 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	243	ALA	7.6
3	G	190	ILE	7.2
4	H	140	LYS	5.8
3	C	143	VAL	5.4
3	G	119	TYR	5.2
3	C	128	ASP	4.8
3	G	180	PHE	4.7
3	G	118	VAL	4.2
3	G	177	LYS	4.2
3	C	127	SER	4.2
3	G	179	ASP	4.2
1	E	2	LYS	4.0
4	H	138	THR	4.0
4	H	223	TRP	3.9
4	H	208	PHE	3.9
2	F	28	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
4	H	133	ALA	3.8
1	E	177	HIS	3.6
1	A	121	TRP	3.5
2	F	144	LEU	3.4
1	E	3	GLU	3.4
3	G	120	GLN	3.4
3	C	183	ALA	3.4
3	G	131	VAL	3.3
3	G	184	ASN	3.3
1	A	177	HIS	3.3
4	H	228	ALA	3.3
4	H	184	ASN	3.2
3	G	173	ALA	3.2
2	F	218	ARG	3.2
3	G	183	ALA	3.2
3	C	180	PHE	3.2
4	H	198	ALA	3.2
3	C	149	SER	3.2
1	A	175	LEU	3.1
3	G	132	CYS	3.1
3	G	143	VAL	3.0
3	G	133	LEU	3.0
4	H	159	TRP	3.0
1	A	128	VAL	2.9
3	G	58	MET	2.9
1	A	99	LEU	2.9
4	H	216	GLY	2.9
4	H	143	LEU	2.8
1	E	153	PHE	2.8
3	G	189	SER	2.8
3	G	127	SER	2.8
3	G	176	ASN	2.8
1	A	122	LEU	2.7
4	H	139	GLN	2.7
2	F	198	GLU	2.7
3	C	136	ASP	2.6
3	G	136	ASP	2.6
4	H	183	LEU	2.6
2	B	196	SER	2.6
3	G	1	ALA	2.6
3	G	142	ASN	2.5
2	F	199	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	G	134	PHE	2.5
3	C	179	ASP	2.5
4	H	120	VAL	2.4
3	G	195	THR	2.4
4	H	64	LYS	2.4
1	E	160	VAL	2.4
2	B	128	VAL	2.4
3	C	146	SER	2.4
3	G	163	SER	2.4
4	H	134	GLU	2.3
1	A	170	LEU	2.3
4	H	117	LEU	2.3
4	D	199	THR	2.3
4	H	240	TRP	2.3
4	H	115	GLU	2.3
4	H	230	PRO	2.2
2	B	199	VAL	2.2
3	C	178	SER	2.2
4	H	114	THR	2.2
4	H	137	HIS	2.2
4	H	127	VAL	2.2
4	H	164	LYS	2.2
4	H	166	VAL	2.2
3	C	150	ASP	2.2
4	H	141	ALA	2.2
3	C	138	ASP	2.1
4	H	206	ASN	2.1
3	G	110	ASN	2.1
1	A	119	VAL	2.1
4	H	79	VAL	2.1
4	H	82	ALA	2.1
2	B	131	TYR	2.1
2	B	198	GLU	2.1
4	H	12	LYS	2.0
4	H	224	THR	2.0
3	C	112	GLN	2.0
4	H	222	GLU	2.0
3	G	156	LYS	2.0
4	D	139	GLN	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.