



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:11 am BST

PDB ID : 2W80  
Title : Structure of a complex between Neisseria meningitidis factor H binding protein and CCPs 6-7 of human complement factor H  
Authors : Schneider, M.C.; Prosser, B.E.; Caesar, J.J.E.; Kugelberg, E.; Li, S.; Zhang, Q.; Quoraishi, S.; Lovett, J.E.; Deane, J.E.; Sim, R.B.; Roversi, P.; Johnson, S.; Tang, C.M.; Lea, S.M.  
Deposited on : 2009-01-08  
Resolution : 2.35 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	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

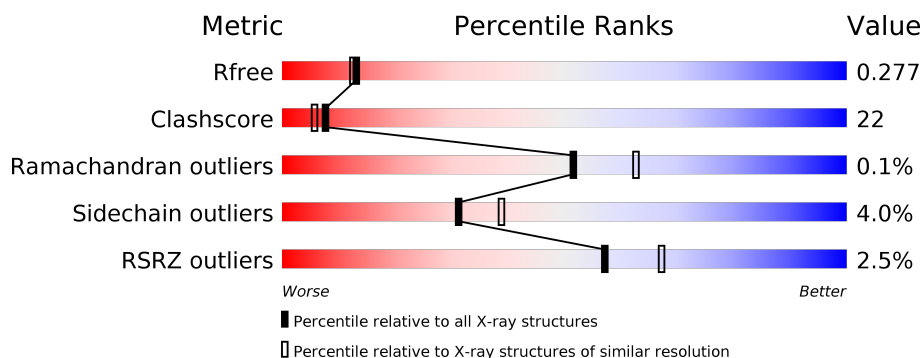
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	123	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>28%</div> <div>•</div> </div> </div>
1	B	123	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>30%</div> <div>•</div> </div> </div>
1	E	123	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>32%</div> <div>•</div> </div> </div>
1	G	123	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>33%</div> <div>•</div> </div> </div>
2	C	253	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>40%</div> <div>• •</div> </div> </div>
2	D	253	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>33%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	253	<div> <div>3%</div> <div>58%</div> <div>37%</div> <div>• •</div> </div>
2	H	253	<div> <div>4%</div> <div>57%</div> <div>36%</div> <div>• •</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11942 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 COMPLEMENT FACTOR H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	1	0
			1005	643	171	181	10			
1	B	123	Total	C	N	O	S	0	0	0
			999	639	171	179	10			
1	E	123	Total	C	N	O	S	0	0	0
			999	639	171	179	10			
1	G	123	Total	C	N	O	S	0	0	0
			999	639	171	179	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	402	HIS	TYR	variant	UNP P08603
B	402	HIS	TYR	variant	UNP P08603
E	402	HIS	TYR	variant	UNP P08603
G	402	HIS	TYR	variant	UNP P08603

- Molecule 2 is a protein called FACTOR H BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	243	Total	C	N	O	S	0	1	0
			1844	1145	331	367	1			
2	D	244	Total	C	N	O	S	0	2	0
			1861	1155	335	370	1			
2	F	244	Total	C	N	O	S	0	3	0
			1866	1158	335	372	1			
2	H	244	Total	C	N	O	S	0	2	0
			1861	1155	335	370	1			

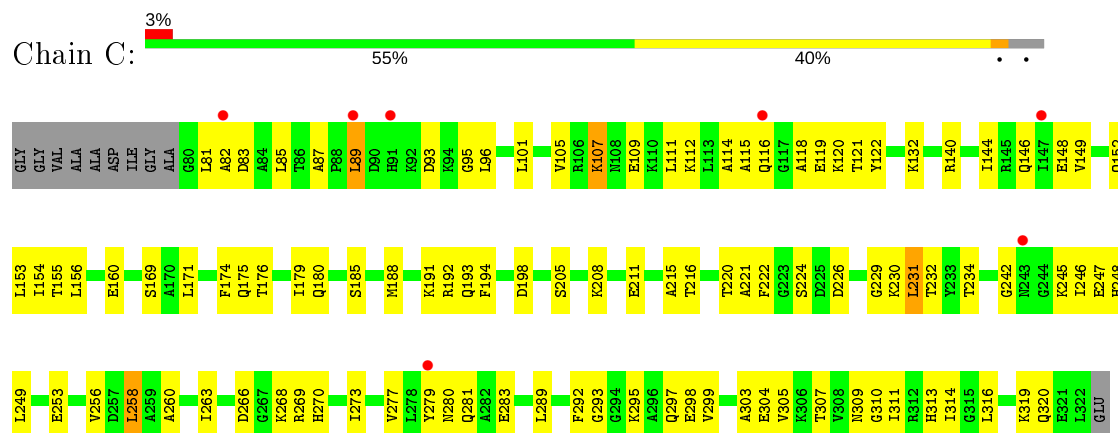
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	64	Total 64	O 64	0	0
3	B	43	Total 43	O 43	0	0
3	C	92	Total 92	O 92	0	0
3	D	104	Total 104	O 104	0	0
3	E	39	Total 39	O 39	0	0
3	F	77	Total 77	O 77	0	0
3	G	33	Total 33	O 33	0	0
3	H	56	Total 56	O 56	0	0

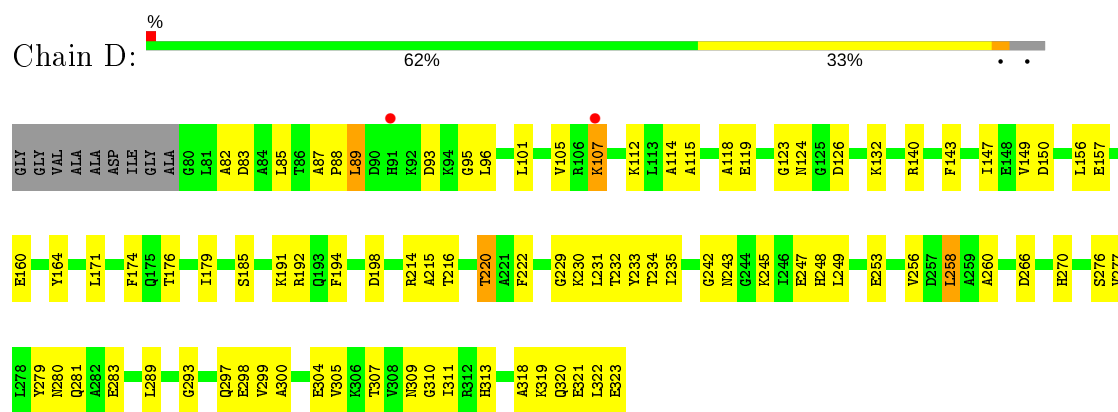




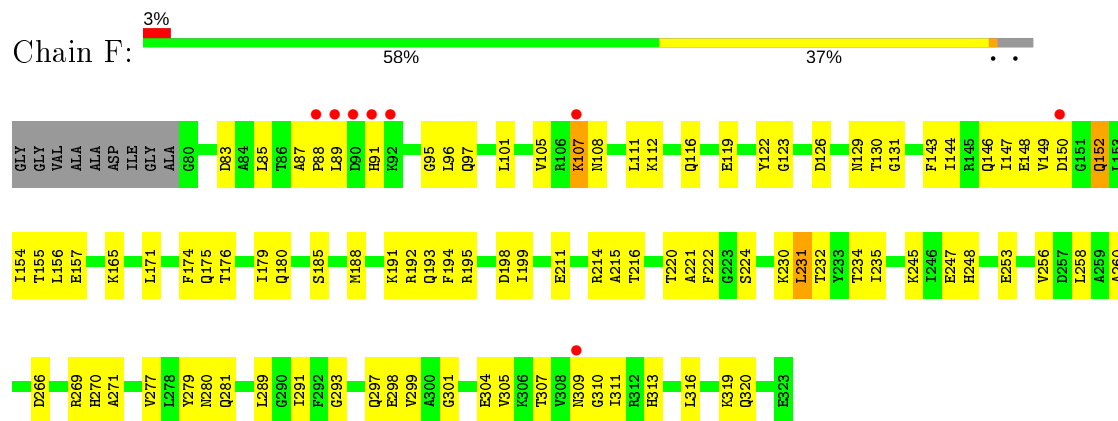
• Molecule 2: FACTOR H BINDING PROTEIN



• Molecule 2: FACTOR H BINDING PROTEIN

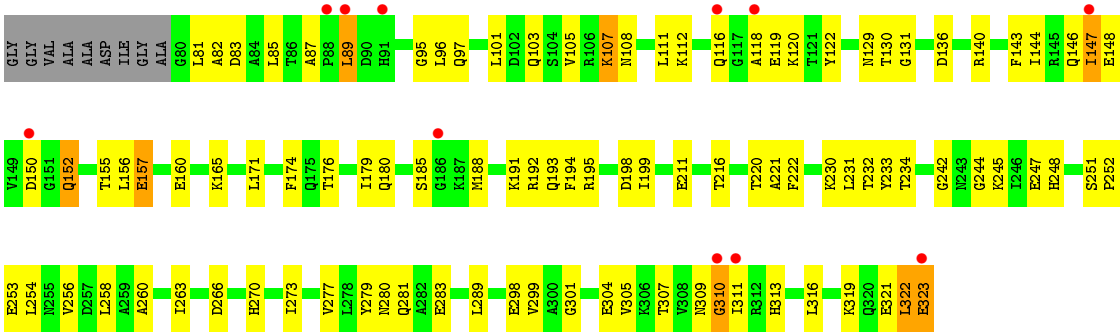


• Molecule 2: FACTOR H BINDING PROTEIN



• Molecule 2: FACTOR H BINDING PROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.70 Å 93.85 Å 99.72 Å 80.07° 80.18° 84.81°	Depositor
Resolution (Å)	95.00 – 2.35 96.99 – 2.14	Depositor EDS
% Data completeness (in resolution range)	91.8 (95.00-2.35) 82.4 (96.99-2.14)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.14 Å)	Xtriage
Refinement program		Depositor
R, $R_{free}$	0.233 , 0.263 0.237 , 0.277	Depositor DCC
$R_{free}$ test set	3938 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.6	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	0.93	EDS
Total number of atoms	11942	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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	0.47	0/1048	0.68	0/1429
1	B	0.40	0/1039	0.58	0/1417
1	E	0.37	0/1039	0.59	0/1417
1	G	0.39	0/1039	0.63	0/1417
2	C	0.39	0/1872	0.68	1/2511 (0.0%)
2	D	0.42	0/1892	0.68	0/2537
2	F	0.42	0/1900	0.68	0/2548
2	H	0.41	0/1892	0.66	0/2537
All	All	0.41	0/11721	0.65	1/15813 (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	153	LEU	CB-CG-CD1	-5.01	102.49	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	1005	0	921	40	0
1	B	999	0	915	34	0
1	E	999	0	915	33	0
1	G	999	0	915	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1844	0	1833	92	0
2	D	1861	0	1852	74	0
2	F	1866	0	1856	87	0
2	H	1861	0	1852	97	0
3	A	64	0	0	2	0
3	B	43	0	0	1	0
3	C	92	0	0	1	0
3	D	104	0	0	4	0
3	E	39	0	0	3	0
3	F	77	0	0	3	0
3	G	33	0	0	3	0
3	H	56	0	0	3	0
All	All	11942	0	11059	492	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 (492) 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:C:89:LEU:H	2:C:89:LEU:HD13	1.10	1.12
2:C:149:VAL:O	2:C:152:GLN:HG2	1.47	1.12
2:H:147:ILE:HG12	2:H:156:LEU:HD11	1.29	1.09
2:H:89:LEU:HD13	2:H:89:LEU:H	1.13	1.02
2:H:322:LEU:C	2:H:323:GLU:HG2	1.79	1.00
2:D:105:VAL:O	2:D:124:ASN:ND2	1.96	0.99
1:A:420:TYR:CD1	1:A:443:ILE:HG12	1.99	0.98
2:C:231:LEU:HD12	2:C:232:THR:N	1.82	0.95
2:D:89:LEU:HD13	2:D:89:LEU:H	1.31	0.94
2:H:147:ILE:HG12	2:H:156:LEU:CD1	1.99	0.92
2:H:171:LEU:HD11	2:H:222:PHE:HZ	1.33	0.92
2:C:231:LEU:HD22	2:C:316:LEU:HD22	1.52	0.91
1:B:407:VAL:HG12	1:B:410:LYS:HE3	1.52	0.91
2:H:231:LEU:HD12	2:H:232:THR:N	1.86	0.90
2:C:171:LEU:HD11	2:C:222:PHE:HZ	1.37	0.90
2:F:231:LEU:HD22	2:F:316:LEU:HD22	1.51	0.90
2:H:152:GLN:HA	2:H:152:GLN:NE2	1.84	0.90
2:C:230:LYS:HD3	2:C:248:HIS:ND1	1.87	0.90
2:F:171:LEU:HD11	2:F:222:PHE:CZ	2.06	0.90
1:A:442:CYS:O	1:A:443:ILE:HG13	1.72	0.90
2:C:289:LEU:HD13	2:C:299:VAL:HG11	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:171:LEU:HD11	2:F:222:PHE:HZ	1.36	0.88
1:B:407:VAL:HG12	1:B:410:LYS:CE	2.03	0.87
2:H:171:LEU:HD11	2:H:222:PHE:CZ	2.09	0.87
2:F:231:LEU:HD12	2:F:232:THR:N	1.89	0.86
2:F:215:ALA:HB1	2:F:320:GLN:OE1	1.75	0.86
2:C:89:LEU:N	2:C:89:LEU:HD13	1.90	0.86
1:A:420:TYR:HD1	1:A:443:ILE:HG12	1.43	0.83
2:H:322:LEU:O	2:H:323:GLU:HG2	1.77	0.83
2:D:230:LYS:HD3	2:D:248:HIS:ND1	1.93	0.83
2:C:171:LEU:HD11	2:C:222:PHE:CZ	2.14	0.82
2:H:89:LEU:CD1	2:H:89:LEU:H	1.93	0.82
1:B:407:VAL:H	1:B:410:LYS:HD2	1.44	0.81
2:F:289:LEU:HD13	2:F:299:VAL:HG11	1.63	0.81
2:C:89:LEU:H	2:C:89:LEU:CD1	1.89	0.81
2:H:231:LEU:HD22	2:H:316:LEU:HD22	1.63	0.81
2:H:253:GLU:OE1	2:H:307:THR:HB	1.81	0.80
1:A:410:LYS:HD2	1:A:411:SER:H	1.47	0.80
2:D:89:LEU:CD1	2:D:89:LEU:H	1.96	0.79
2:F:253:GLU:OE1	2:F:307:THR:HB	1.83	0.79
2:D:231:LEU:HD13	2:D:232:THR:N	1.98	0.78
2:D:89:LEU:HD13	2:D:89:LEU:N	1.98	0.77
2:H:131:GLY:HA2	2:H:165:LYS:NZ	1.99	0.77
2:D:253:GLU:OE1	2:D:307:THR:HB	1.85	0.77
2:C:149:VAL:O	2:C:152:GLN:CG	2.28	0.77
2:C:215:ALA:HB1	2:C:320:GLN:OE1	1.86	0.76
2:H:230:LYS:HD3	2:H:248:HIS:ND1	1.98	0.76
1:A:410:LYS:HD2	1:A:411:SER:N	2.01	0.76
2:H:231:LEU:HD12	2:H:232:THR:H	1.50	0.76
1:B:407:VAL:N	1:B:410:LYS:HD2	2.00	0.75
2:H:309:ASN:H	2:H:310:GLY:HA2	1.49	0.75
2:H:309:ASN:N	2:H:310:GLY:HA2	2.02	0.75
1:G:423:PRO:HA	1:G:443:ILE:HD11	1.68	0.75
1:G:372:ILE:HG13	1:G:379:TRP:CE3	2.21	0.75
2:C:107:LYS:O	2:C:107:LYS:HD3	1.88	0.74
2:H:116:GLN:HA	3:H:2008:HOH:O	1.86	0.74
2:F:230:LYS:HD3	2:F:248:HIS:ND1	2.02	0.74
2:F:309:ASN:N	2:F:310:GLY:HA2	2.02	0.73
2:C:309:ASN:N	2:C:310:GLY:HA2	2.04	0.73
2:H:289:LEU:HD22	2:H:299:VAL:HG12	1.70	0.73
2:D:289:LEU:HD13	2:D:299:VAL:HG11	1.69	0.72
2:F:107:LYS:HD3	2:F:107:LYS:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:TYR:CE2	2:D:220:THR:HG21	2.25	0.72
2:H:107:LYS:HD3	2:H:107:LYS:O	1.90	0.72
2:H:156:LEU:HD23	2:H:180:GLN:NE2	2.05	0.71
2:D:171:LEU:HD11	2:D:222:PHE:CZ	2.24	0.71
2:H:89:LEU:HD13	2:H:89:LEU:N	1.98	0.71
2:H:131:GLY:HA2	2:H:165:LYS:HZ1	1.55	0.71
2:C:253:GLU:OE1	2:C:307:THR:HB	1.90	0.70
2:F:123:GLY:HA3	2:F:126:ASP:OD2	1.90	0.70
2:C:146:GLN:HG2	2:C:155:THR:HA	1.73	0.69
1:E:372:ILE:HG13	1:E:379:TRP:CE3	2.28	0.69
2:F:309:ASN:H	2:F:310:GLY:HA2	1.56	0.69
2:D:231:LEU:HD13	2:D:231:LEU:C	2.13	0.69
2:H:146:GLN:HG2	2:H:155:THR:HA	1.74	0.69
2:H:289:LEU:HD13	2:H:299:VAL:HG11	1.75	0.69
2:D:215:ALA:HB1	2:D:320:GLN:OE1	1.92	0.68
1:E:332:HIS:NE2	1:E:433:GLU:OE2	2.18	0.68
2:F:256:VAL:HG21	2:F:277:VAL:HG13	1.73	0.68
2:F:171:LEU:CD1	2:F:222:PHE:HZ	2.06	0.67
2:C:289:LEU:HD22	2:C:299:VAL:HG12	1.76	0.67
1:E:321:THR:N	3:E:2001:HOH:O	2.27	0.67
2:H:174:PHE:HB3	3:H:2021:HOH:O	1.93	0.67
1:B:372:ILE:HG12	1:B:379:TRP:CE3	2.29	0.67
2:F:256:VAL:HG21	2:F:277:VAL:CG1	2.25	0.67
2:F:289:LEU:HD22	2:F:299:VAL:HG12	1.76	0.67
1:A:428:THR:HG22	3:A:2056:HOH:O	1.95	0.66
2:D:309:ASN:N	2:D:310:GLY:HA2	2.10	0.66
2:D:107:LYS:O	2:D:107:LYS:HD3	1.96	0.66
2:C:93:ASP:OD2	2:C:132:LYS:HE2	1.97	0.65
2:D:171:LEU:HD11	2:D:222:PHE:HZ	1.61	0.65
2:F:107:LYS:C	2:F:107:LYS:HD3	2.15	0.65
2:H:256:VAL:HG12	2:H:279:TYR:HB2	1.79	0.65
2:D:304:GLU:HG2	2:D:313:HIS:CD2	2.32	0.65
1:A:442:CYS:O	1:A:443:ILE:CG1	2.44	0.65
2:C:107:LYS:HA	2:C:107:LYS:HE3	1.79	0.65
1:A:372:ILE:HG12	1:A:379:TRP:CE3	2.31	0.64
2:H:107:LYS:HE3	2:H:107:LYS:HA	1.78	0.64
2:H:180:GLN:OE1	2:H:185:SER:HA	1.98	0.64
2:C:156:LEU:HD23	2:C:180:GLN:NE2	2.12	0.64
2:F:156:LEU:HD23	2:F:180:GLN:NE2	2.12	0.64
2:F:149:VAL:O	2:F:150:ASP:HB2	1.97	0.64
1:A:347:VAL:CG1	1:A:351:LYS:HB2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:342:ARG:HB3	1:G:343:PRO:HD3	1.79	0.63
1:A:359[A]:GLU:H	1:A:359[A]:GLU:CD	2.02	0.63
2:H:304:GLU:HG2	2:H:313:HIS:CD2	2.34	0.63
2:D:107:LYS:C	2:D:107:LYS:HD3	2.17	0.63
2:D:309:ASN:H	2:D:310:GLY:HA2	1.64	0.62
2:C:309:ASN:H	2:C:310:GLY:HA2	1.63	0.62
1:A:420:TYR:CE1	1:A:443:ILE:HG12	2.35	0.62
1:B:342:ARG:HB3	1:B:343:PRO:HD3	1.80	0.62
2:C:216:THR:HG22	2:C:234:THR:OG1	1.99	0.62
1:E:362:GLU:OE1	1:E:388:LYS:NZ	2.33	0.62
2:H:107:LYS:HD3	2:H:107:LYS:C	2.19	0.62
1:A:362:GLU:OE1	1:A:388:LYS:NZ	2.32	0.62
1:A:327:TYR:OH	1:A:338:GLU:HG3	1.98	0.62
2:C:144:ILE:HG22	2:C:146:GLN:HG3	1.82	0.62
2:D:93:ASP:OD2	2:D:132:LYS:HE2	1.98	0.62
2:F:179:ILE:HD13	2:F:191:LYS:HD3	1.80	0.62
2:H:83:ASP:OD1	2:H:87:ALA:HB2	1.98	0.62
2:C:107:LYS:C	2:C:107:LYS:HD3	2.19	0.62
2:C:231:LEU:HD12	2:C:232:THR:H	1.61	0.61
2:D:289:LEU:HD22	2:D:299:VAL:HG12	1.80	0.61
2:H:322:LEU:C	2:H:323:GLU:CG	2.59	0.61
1:E:355:TYR:CD2	1:E:372:ILE:HG23	2.35	0.61
2:F:131:GLY:HA2	2:F:165:LYS:HZ1	1.66	0.61
2:D:107:LYS:HA	2:D:107:LYS:HE3	1.82	0.61
2:F:107:LYS:HA	2:F:107:LYS:HE3	1.83	0.61
2:F:143:PHE:HE1	2:F:157:GLU:HG2	1.65	0.61
1:G:355:TYR:CD2	1:G:372:ILE:CG2	2.84	0.61
1:B:387:ARG:HG2	1:B:432:MET:O	2.00	0.60
2:H:256:VAL:HG21	2:H:277:VAL:HG13	1.82	0.60
2:F:256:VAL:CG2	2:F:277:VAL:HG13	2.30	0.60
1:B:332:HIS:NE2	1:B:433:GLU:OE2	2.25	0.60
2:F:180:GLN:OE1	2:F:185:SER:HA	2.02	0.59
1:A:420:TYR:HD1	1:A:443:ILE:CG1	2.12	0.59
1:B:327:TYR:OH	1:B:338:GLU:HG3	2.02	0.59
1:B:359:GLU:O	1:B:360:HIS:HB2	2.01	0.59
2:D:179:ILE:HD13	2:D:191:LYS:HD3	1.83	0.59
2:F:147:ILE:CG2	2:F:156:LEU:HD11	2.33	0.59
2:C:171:LEU:CD1	2:C:222:PHE:HZ	2.14	0.59
1:E:342:ARG:HB3	1:E:343:PRO:HD3	1.84	0.59
2:D:123:GLY:O	2:D:126:ASP:HB2	2.03	0.58
1:G:330:ILE:HG23	1:G:384:PRO:CG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:171:LEU:CD1	2:D:222:PHE:HZ	2.16	0.58
2:F:149:VAL:HB	2:F:154:ILE:HD13	1.85	0.58
2:H:289:LEU:HD22	2:H:299:VAL:CG1	2.33	0.58
2:D:143:PHE:CE1	2:D:157:GLU:HG2	2.38	0.58
1:A:347:VAL:HG11	1:A:351:LYS:HB2	1.85	0.58
2:F:131:GLY:HA2	2:F:165:LYS:NZ	2.18	0.58
1:G:442:CYS:HB2	3:G:2025:HOH:O	2.04	0.58
2:D:112:LYS:HE2	2:D:119:GLU:OE2	2.04	0.58
2:H:176:THR:O	2:H:192:ARG:HA	2.04	0.58
2:D:83:ASP:OD1	2:D:87:ALA:HB2	2.03	0.58
2:C:256:VAL:HG12	2:C:279:TYR:HB2	1.86	0.58
1:E:401:ASN:HA	1:E:404:ARG:HD3	1.85	0.58
1:G:359:GLU:O	1:G:360:HIS:HB2	2.04	0.57
2:D:140:ARG:HB3	2:D:160:GLU:OE2	2.04	0.57
2:H:216:THR:HG22	2:H:234:THR:OG1	2.05	0.57
2:F:112:LYS:HE2	2:F:119:GLU:OE2	2.04	0.57
1:B:372:ILE:HG12	1:B:379:TRP:HE3	1.69	0.57
1:E:347:VAL:CG1	1:E:351:LYS:HB2	2.34	0.57
1:A:330:ILE:HG23	1:A:384:PRO:HG2	1.87	0.57
1:B:347:VAL:CG1	1:B:351:LYS:HB2	2.34	0.57
1:E:327:TYR:OH	1:E:338:GLU:HG3	2.04	0.57
1:E:407:VAL:HG22	1:E:408:GLN:N	2.19	0.57
1:G:423:PRO:CA	1:G:443:ILE:HD11	2.34	0.57
1:G:327:TYR:OH	1:G:338:GLU:HG3	2.04	0.57
2:F:148:GLU:HA	2:F:152:GLN:O	2.04	0.56
2:H:140:ARG:HD3	2:H:160:GLU:OE2	2.05	0.56
1:E:355:TYR:CD2	1:E:372:ILE:CG2	2.88	0.56
1:G:355:TYR:CD2	1:G:372:ILE:HG22	2.40	0.56
2:D:95:GLY:HA2	2:D:96:LEU:C	2.25	0.56
2:F:89:LEU:HA	3:F:2013:HOH:O	2.05	0.56
2:H:179:ILE:HD13	2:H:191:LYS:HD3	1.86	0.56
1:E:359:GLU:O	1:E:360:HIS:HB2	2.05	0.56
2:H:171:LEU:CD1	2:H:222:PHE:HZ	2.13	0.56
2:H:256:VAL:HG21	2:H:277:VAL:CG1	2.36	0.56
2:D:143:PHE:HE1	2:D:157:GLU:HG2	1.70	0.56
1:G:408:GLN:NE2	1:G:433:GLU:HB2	2.21	0.56
2:H:152:GLN:CA	2:H:152:GLN:NE2	2.65	0.56
2:C:83:ASP:OD1	2:C:87:ALA:HB2	2.05	0.55
2:C:263:ILE:HG12	2:C:273:ILE:HG12	1.88	0.55
1:G:347:VAL:CG1	1:G:351:LYS:HB2	2.36	0.55
2:F:101:LEU:HA	2:F:198:ASP:OD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ILE:HG12	1:A:379:TRP:HE3	1.69	0.55
1:A:332:HIS:NE2	1:A:433:GLU:OE2	2.26	0.55
2:F:143:PHE:CE1	2:F:157:GLU:HG2	2.41	0.55
1:G:359:GLU:OE1	2:H:108:ASN:HB2	2.06	0.55
1:A:342:ARG:HB3	1:A:343:PRO:HD3	1.89	0.55
2:D:256:VAL:HG12	2:D:279:TYR:HB2	1.89	0.55
1:G:332:HIS:NE2	1:G:433:GLU:OE2	2.37	0.55
2:C:298:GLU:HG2	2:C:319:LYS:CB	2.37	0.54
2:D:147:ILE:HD12	2:D:149:VAL:HG23	1.88	0.54
1:A:420:TYR:CD1	1:A:443:ILE:CG1	2.81	0.54
2:C:149:VAL:N	2:C:152:GLN:O	2.34	0.54
1:G:331:LYS:HB3	3:G:2005:HOH:O	2.08	0.54
2:C:256:VAL:HG21	2:C:277:VAL:CG1	2.38	0.54
2:C:220:THR:HG22	2:C:221:ALA:N	2.22	0.54
2:H:280:ASN:O	2:H:281:GLN:HB2	2.07	0.54
1:A:401:ASN:HA	1:A:404:ARG:HD3	1.88	0.54
2:D:322:LEU:HD23	3:D:2097:HOH:O	2.07	0.54
2:D:280:ASN:O	2:D:281:GLN:HB2	2.07	0.54
2:D:101:LEU:HA	2:D:198:ASP:OD2	2.08	0.53
1:G:421:ALA:O	1:G:443:ILE:HG13	2.07	0.53
2:D:289:LEU:HD22	2:D:299:VAL:CG1	2.37	0.53
2:C:246:ILE:HD11	2:C:316:LEU:HD21	1.90	0.53
2:F:245:LYS:HE3	2:F:247:GLU:OE2	2.08	0.53
2:C:180:GLN:OE1	2:C:185:SER:HA	2.08	0.53
2:D:300:ALA:CA	3:D:2088:HOH:O	2.57	0.53
2:F:91:HIS:HA	3:F:2003:HOH:O	2.08	0.53
2:H:147:ILE:CG1	2:H:156:LEU:HD11	2.20	0.53
1:B:424:LYS:O	1:B:425:ALA:HB3	2.07	0.53
2:C:231:LEU:CD2	2:C:316:LEU:HD22	2.31	0.53
2:D:245:LYS:HE3	2:D:247:GLU:OE2	2.09	0.53
1:B:339:ASN:OD1	1:B:340:MET:N	2.42	0.53
2:C:112:LYS:HE2	2:C:119:GLU:OE2	2.09	0.52
2:C:289:LEU:HB3	2:C:299:VAL:HG13	1.91	0.52
1:A:330:ILE:HG23	1:A:384:PRO:CG	2.39	0.52
1:G:339:ASN:OD1	1:G:340:MET:N	2.43	0.52
2:C:140:ARG:HB3	2:C:160:GLU:OE2	2.09	0.52
1:G:338:GLU:OE2	1:G:342:ARG:NH2	2.28	0.52
1:B:330:ILE:HG23	1:B:384:PRO:HG2	1.91	0.52
2:H:155:THR:HG22	2:H:188:MET:SD	2.50	0.52
2:H:256:VAL:CG2	2:H:277:VAL:HG13	2.40	0.52
1:A:442:CYS:C	1:A:443:ILE:HG13	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:95:GLY:HA2	2:H:96:LEU:C	2.31	0.52
1:E:387:ARG:HG2	1:E:432:MET:O	2.10	0.52
2:F:266:ASP:CB	2:F:270:HIS:H	2.22	0.52
1:B:407:VAL:HG22	1:B:408:GLN:N	2.25	0.51
2:C:268:LYS:O	2:C:269:ARG:HB2	2.10	0.51
2:C:289:LEU:HD13	2:C:299:VAL:CG1	2.35	0.51
1:E:339:ASN:OD1	1:E:340:MET:N	2.43	0.51
2:F:280:ASN:O	2:F:281:GLN:HB2	2.08	0.51
1:G:407:VAL:HG22	1:G:408:GLN:N	2.25	0.51
2:H:143:PHE:HE1	2:H:157:GLU:HG2	1.75	0.51
2:F:116:GLN:O	2:F:116:GLN:HG3	2.11	0.51
1:E:359:GLU:OE1	2:F:108:ASN:HB2	2.10	0.51
1:B:362:GLU:OE1	1:B:388:LYS:NZ	2.42	0.51
2:C:95:GLY:HA2	2:C:96:LEU:C	2.29	0.51
1:E:347:VAL:HG11	1:E:351:LYS:HB2	1.91	0.51
1:G:387:ARG:HG2	1:G:432:MET:O	2.11	0.51
2:D:140:ARG:HD3	2:D:160:GLU:OE2	2.10	0.51
2:D:83:ASP:HB2	3:D:2002:HOH:O	2.11	0.51
2:D:231:LEU:CD1	2:D:231:LEU:C	2.78	0.51
2:H:140:ARG:HB3	2:H:160:GLU:OE2	2.11	0.51
1:B:443:ILE:HD12	1:B:443:ILE:C	2.31	0.51
2:H:245:LYS:HE3	2:H:247:GLU:OE2	2.10	0.51
2:D:147:ILE:HG12	2:D:156:LEU:HD11	1.92	0.51
2:C:149:VAL:HG21	2:C:154:ILE:HD12	1.92	0.50
2:H:298:GLU:HG2	2:H:319:LYS:CB	2.41	0.50
1:G:330:ILE:HG23	1:G:384:PRO:HG2	1.92	0.50
2:C:231:LEU:C	2:C:231:LEU:HD12	2.28	0.50
2:C:280:ASN:O	2:C:281:GLN:HB2	2.11	0.50
1:B:322:LEU:N	1:B:322:LEU:HD12	2.27	0.50
2:F:147:ILE:HG21	2:F:156:LEU:HD11	1.94	0.50
2:H:101:LEU:HA	2:H:198:ASP:OD2	2.11	0.50
2:H:289:LEU:HB3	2:H:299:VAL:HG13	1.93	0.50
2:H:195[B]:ARG:HA	2:H:313:HIS:ND1	2.26	0.50
2:D:289:LEU:HB3	2:D:299:VAL:HG13	1.92	0.50
2:H:220:THR:CG2	2:H:221:ALA:N	2.75	0.50
1:B:347:VAL:HG11	1:B:351:LYS:HB2	1.93	0.50
2:H:195[A]:ARG:HA	2:H:313:HIS:ND1	2.26	0.50
1:A:412:ILE:O	1:A:428:THR:HB	2.12	0.49
1:G:322:LEU:HD12	1:G:322:LEU:N	2.27	0.49
2:D:149:VAL:O	2:D:150:ASP:HB2	2.12	0.49
2:D:298:GLU:HG2	2:D:319:LYS:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:410:LYS:HG3	1:G:411:SER:N	2.26	0.49
2:H:258:LEU:HD12	2:H:258:LEU:N	2.27	0.49
1:B:347:VAL:HG13	1:B:348:ALA:N	2.27	0.49
2:C:116:GLN:O	2:C:116:GLN:HG3	2.12	0.49
2:C:149:VAL:O	2:C:152:GLN:OE1	2.30	0.49
2:D:214:ARG:HA	2:D:235:ILE:O	2.12	0.49
1:G:347:VAL:HG11	1:G:351:LYS:HB2	1.94	0.49
2:F:155:THR:HG22	2:F:188:MET:SD	2.52	0.49
1:A:412:ILE:CG2	1:A:413:ASP:N	2.75	0.49
2:F:231:LEU:CD2	2:F:316:LEU:HD22	2.35	0.49
1:G:355:TYR:CE2	1:G:372:ILE:HG22	2.48	0.49
1:G:347:VAL:CG1	1:G:348:ALA:N	2.75	0.49
2:F:298:GLU:HG2	2:F:319:LYS:CB	2.42	0.49
2:F:176:THR:O	2:F:192:ARG:HA	2.13	0.49
2:F:289:LEU:HD22	2:F:299:VAL:CG1	2.42	0.49
2:D:298:GLU:HG2	2:D:319:LYS:HB3	1.93	0.49
2:F:147:ILE:O	2:F:154:ILE:N	2.40	0.49
2:H:112:LYS:HE2	2:H:119:GLU:OE2	2.13	0.49
2:H:199:ILE:HD13	2:H:301:GLY:HA2	1.95	0.49
2:H:81:LEU:HD23	2:H:81:LEU:N	2.28	0.49
2:F:260:ALA:HB1	3:F:2047:HOH:O	2.13	0.48
1:B:330:ILE:HG23	1:B:384:PRO:CG	2.42	0.48
2:C:155:THR:HG22	2:C:188:MET:SD	2.53	0.48
1:E:338:GLU:OE2	1:E:342:ARG:NH2	2.31	0.48
1:G:401:ASN:HA	1:G:404:ARG:HD2	1.94	0.48
2:C:101:LEU:HA	2:C:198:ASP:OD2	2.14	0.48
2:C:140:ARG:HD3	2:C:160:GLU:OE2	2.14	0.48
1:E:437:SER:HA	1:E:438:PRO:HA	1.64	0.48
2:F:185:SER:O	2:F:185:SER:OG	2.31	0.48
2:F:105:VAL:HG22	2:F:111:LEU:HB2	1.94	0.48
2:F:266:ASP:HB2	2:F:270:HIS:H	1.79	0.48
2:C:179:ILE:HD13	2:C:191:LYS:HD3	1.96	0.48
2:C:229:GLY:HA3	2:C:249:LEU:CD2	2.44	0.48
2:F:199:ILE:HD13	2:F:301:GLY:HA2	1.95	0.48
1:B:437:SER:HA	1:B:438:PRO:HA	1.64	0.48
1:A:407:VAL:HG22	1:A:408:GLN:N	2.29	0.47
2:C:295:LYS:HB2	2:C:297:GLN:NE2	2.29	0.47
1:E:424:LYS:O	1:E:424:LYS:HG2	2.14	0.47
1:E:369:TRP:CE2	2:F:195[B]:ARG:HD3	2.49	0.47
2:H:242:GLY:O	2:H:260:ALA:HA	2.14	0.47
2:H:258:LEU:CD1	2:H:258:LEU:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:307:THR:OG1	2:H:310:GLY:O	2.28	0.47
2:C:191:LYS:HE2	2:C:193:GLN:OE1	2.15	0.47
2:F:216:THR:HG22	2:F:234:THR:OG1	2.14	0.47
2:C:304:GLU:HG2	2:C:313:HIS:CD2	2.49	0.47
1:E:347:VAL:CG1	1:E:348:ALA:N	2.78	0.47
2:C:152:GLN:CG	2:C:152:GLN:O	2.60	0.47
2:D:123:GLY:HA3	2:D:126:ASP:OD2	2.15	0.47
1:E:396:ASN:HB2	3:E:2029:HOH:O	2.14	0.47
2:D:112:LYS:HZ3	2:D:119:GLU:HG3	1.80	0.47
2:D:82:ALA:HA	2:D:118:ALA:HB3	1.97	0.47
2:H:220:THR:HG22	2:H:221:ALA:N	2.30	0.47
2:C:220:THR:CG2	2:C:221:ALA:N	2.77	0.47
2:C:226:ASP:HA	3:C:2060:HOH:O	2.14	0.47
1:E:401:ASN:HA	1:E:404:ARG:CD	2.45	0.47
1:G:377:ASP:HB2	3:G:2019:HOH:O	2.14	0.47
1:A:351:LYS:NZ	2:D:276:SER:HB3	2.30	0.46
2:C:242:GLY:O	2:C:260:ALA:HA	2.14	0.46
2:F:289:LEU:HB3	2:F:299:VAL:HG13	1.96	0.46
2:D:176:THR:O	2:D:192:ARG:HA	2.15	0.46
2:C:266:ASP:CB	2:C:270:HIS:H	2.28	0.46
2:D:107:LYS:HA	2:D:107:LYS:CE	2.39	0.46
2:F:231:LEU:HD12	2:F:231:LEU:C	2.33	0.46
1:A:387:ARG:HD3	1:A:433:GLU:O	2.15	0.46
2:H:105:VAL:HG22	2:H:111:LEU:HB2	1.98	0.46
2:D:88:PRO:O	2:D:89:LEU:C	2.54	0.46
2:F:191:LYS:HE2	2:F:193:GLN:OE1	2.16	0.46
1:A:387:ARG:HG3	1:A:388:LYS:N	2.30	0.46
1:B:432:MET:HG3	1:B:437:SER:HB2	1.97	0.46
2:C:293:GLY:HA3	2:C:297:GLN:OE1	2.16	0.46
2:D:256:VAL:HG21	2:D:277:VAL:CG1	2.45	0.46
2:H:116:GLN:HG3	2:H:116:GLN:O	2.16	0.46
1:B:385:CYS:HB2	3:B:2005:HOH:O	2.16	0.46
1:E:347:VAL:HG13	1:E:348:ALA:N	2.31	0.46
2:H:112:LYS:O	2:H:143:PHE:HA	2.16	0.46
1:A:339:ASN:OD1	1:A:340:MET:N	2.49	0.45
2:C:107:LYS:HA	2:C:107:LYS:CE	2.41	0.45
2:H:305:VAL:O	2:H:311:ILE:HA	2.17	0.45
2:D:112:LYS:HE2	3:D:2014:HOH:O	2.16	0.45
1:E:361:PHE:HA	1:E:386:LEU:O	2.16	0.45
2:F:97:GLN:O	2:F:130:THR:O	2.35	0.45
2:H:144:ILE:HG22	2:H:146:GLN:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LYS:O	1:A:332:HIS:HB2	2.16	0.45
2:C:148:GLU:HA	2:C:152:GLN:O	2.17	0.45
2:F:156:LEU:CD2	2:F:180:GLN:NE2	2.80	0.45
2:F:175:GLN:NE2	2:F:224:SER:OG	2.43	0.45
1:G:355:TYR:CD2	1:G:372:ILE:HG23	2.51	0.45
2:D:231:LEU:HD13	2:D:232:THR:CA	2.47	0.45
2:F:258:LEU:N	2:F:258:LEU:CD1	2.80	0.45
2:F:95:GLY:HA2	2:F:96:LEU:C	2.36	0.45
2:C:82:ALA:HA	2:C:118:ALA:HB3	1.99	0.45
2:C:256:VAL:HG21	2:C:277:VAL:HG11	1.98	0.45
1:E:330:ILE:HG23	1:E:384:PRO:HG2	1.98	0.45
1:E:372:ILE:HG13	1:E:379:TRP:CZ3	2.52	0.45
1:G:432:MET:HG3	1:G:437:SER:HB2	1.98	0.45
2:H:143:PHE:HE1	2:H:157:GLU:CG	2.30	0.45
1:A:437:SER:HA	1:A:438:PRO:HA	1.82	0.45
2:C:105:VAL:HG13	2:C:109:GLU:HG3	1.98	0.45
2:F:195[B]:ARG:HA	2:F:313:HIS:ND1	2.31	0.45
1:B:347:VAL:CG1	1:B:348:ALA:N	2.80	0.45
1:G:331:LYS:O	1:G:332:HIS:HB2	2.16	0.45
2:H:156:LEU:CD2	2:H:180:GLN:NE2	2.76	0.45
2:H:194:PHE:HB3	3:H:2024:HOH:O	2.15	0.45
2:H:82:ALA:HA	2:H:118:ALA:HB3	1.99	0.44
1:E:331:LYS:O	1:E:332:HIS:HB2	2.17	0.44
1:E:410:LYS:HE3	3:E:2032:HOH:O	2.16	0.44
2:F:305:VAL:O	2:F:311:ILE:HA	2.18	0.44
2:H:97:GLN:O	2:H:130:THR:O	2.35	0.44
1:B:407:VAL:HG12	1:B:410:LYS:NZ	2.33	0.44
1:E:330:ILE:HG23	1:E:384:PRO:CG	2.47	0.44
1:A:442:CYS:HB3	3:A:2037:HOH:O	2.18	0.44
2:C:307:THR:HG23	2:C:310:GLY:O	2.17	0.44
2:F:293:GLY:HA3	2:F:297:GLN:OE1	2.17	0.44
1:G:352:TYR:CE1	2:H:311:ILE:HD13	2.52	0.44
2:H:185:SER:OG	2:H:185:SER:O	2.36	0.44
2:C:303:ALA:HB3	2:C:314:ILE:HB	1.99	0.44
2:D:229:GLY:HA3	2:D:249:LEU:CD2	2.48	0.44
1:E:375:THR:OG1	1:E:378:GLY:O	2.33	0.44
2:F:256:VAL:HG12	2:F:279:TYR:HB2	1.99	0.44
2:H:266:ASP:HB2	2:H:270:HIS:H	1.83	0.44
1:A:427:THR:HG23	1:A:428:THR:HG23	1.99	0.44
2:D:293:GLY:HA3	2:D:297:GLN:OE1	2.18	0.44
2:F:195[A]:ARG:HA	2:F:313:HIS:ND1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:337:HIS:CE1	2:H:103:GLN:HE22	2.36	0.44
1:A:422:LEU:HD23	1:A:441:ARG:O	2.17	0.44
2:C:105:VAL:HG22	2:C:111:LEU:HB2	2.00	0.44
2:F:107:LYS:HA	2:F:107:LYS:CE	2.46	0.44
1:G:407:VAL:HG22	1:G:408:GLN:H	1.83	0.44
2:F:144:ILE:HG22	2:F:146:GLN:HG3	1.99	0.44
2:C:245:LYS:HE3	2:C:247:GLU:OE2	2.18	0.43
2:F:231:LEU:HD12	2:F:232:THR:H	1.75	0.43
2:F:304:GLU:HG2	2:F:313:HIS:CD2	2.53	0.43
2:F:147:ILE:HG23	2:F:156:LEU:CD1	2.48	0.43
1:G:442:CYS:C	1:G:443:ILE:HG23	2.39	0.43
2:H:251:SER:HB3	2:H:254:LEU:HG	2.00	0.43
2:C:112:LYS:HZ3	2:C:119:GLU:HG3	1.83	0.43
2:C:258:LEU:N	2:C:258:LEU:CD1	2.80	0.43
1:B:398:TYR:HB3	1:B:400:GLN:OE1	2.19	0.43
1:A:390:TYR:CD1	1:A:390:TYR:N	2.86	0.43
2:D:164:TYR:CE2	2:D:220:THR:CG2	2.96	0.43
2:F:149:VAL:HB	2:F:154:ILE:CD1	2.48	0.43
2:F:220:THR:HG22	2:F:221:ALA:N	2.32	0.43
2:D:258:LEU:CD1	2:D:258:LEU:N	2.80	0.43
2:D:256:VAL:HG21	2:D:277:VAL:HG13	2.01	0.43
2:D:305:VAL:O	2:D:311:ILE:HA	2.19	0.43
2:C:156:LEU:HD23	2:C:180:GLN:HE22	1.84	0.43
2:D:185:SER:O	2:D:185:SER:OG	2.33	0.43
2:F:112:LYS:HZ3	2:F:119:GLU:HG3	1.84	0.43
2:F:214:ARG:HA	2:F:235:ILE:O	2.18	0.43
2:C:307:THR:O	2:C:310:GLY:HA2	2.18	0.43
1:E:407:VAL:HG22	1:E:408:GLN:H	1.83	0.43
2:H:191:LYS:HE2	2:H:193:GLN:OE1	2.19	0.43
2:H:103:GLN:HB2	2:H:198:ASP:OD1	2.19	0.43
2:F:289:LEU:HD13	2:F:299:VAL:CG1	2.42	0.43
2:F:146:GLN:HG2	2:F:155:THR:HA	2.00	0.42
2:H:148:GLU:HG3	2:H:150:ASP:O	2.19	0.42
1:A:412:ILE:HG22	1:A:413:ASP:N	2.34	0.42
1:B:331:LYS:O	1:B:332:HIS:HB2	2.19	0.42
2:C:185:SER:O	2:C:185:SER:OG	2.37	0.42
1:G:328:PRO:HG3	1:G:372:ILE:HD11	2.01	0.42
2:H:233:TYR:HD1	2:H:244:GLY:HA3	1.83	0.42
2:D:266:ASP:HB2	2:D:270:HIS:H	1.85	0.42
1:G:413:ASP:OD1	1:G:428:THR:HG23	2.19	0.42
2:C:298:GLU:HG2	2:C:319:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:216:THR:HG22	2:D:234:THR:OG1	2.19	0.42
2:H:107:LYS:CE	2:H:107:LYS:HA	2.45	0.42
2:H:131:GLY:HA2	2:H:165:LYS:CE	2.50	0.42
1:B:432:MET:HG3	1:B:437:SER:CB	2.49	0.42
2:C:266:ASP:HB2	2:C:270:HIS:H	1.85	0.42
2:D:231:LEU:HD11	2:D:233:TYR:HB2	2.01	0.42
2:D:266:ASP:CB	2:D:270:HIS:H	2.32	0.42
2:F:271:ALA:HB1	2:F:291:ILE:HD12	2.01	0.42
2:F:112:LYS:O	2:F:143:PHE:HA	2.19	0.42
2:H:263:ILE:HG12	2:H:273:ILE:HG12	2.01	0.42
2:D:242:GLY:O	2:D:260:ALA:HA	2.20	0.42
1:G:372:ILE:HG13	1:G:379:TRP:HE3	1.76	0.42
2:H:298:GLU:HG2	2:H:319:LYS:HB3	2.00	0.42
1:A:347:VAL:CG1	1:A:348:ALA:N	2.82	0.42
1:B:401:ASN:O	1:B:404:ARG:HB2	2.20	0.42
1:B:407:VAL:H	1:B:410:LYS:NZ	2.18	0.42
2:C:175:GLN:NE2	2:C:224:SER:OG	2.48	0.42
2:F:256:VAL:HG21	2:F:277:VAL:HG11	2.01	0.42
2:H:266:ASP:CB	2:H:270:HIS:H	2.33	0.42
2:H:120:LYS:HD3	2:H:122:TYR:CZ	2.55	0.42
1:B:407:VAL:HG12	1:B:410:LYS:CD	2.49	0.41
2:H:174:PHE:O	2:H:194:PHE:HA	2.20	0.41
2:H:83:ASP:OD1	2:H:87:ALA:CB	2.66	0.41
2:C:120:LYS:HG2	2:C:121:THR:N	2.35	0.41
2:C:83:ASP:OD1	2:C:87:ALA:CB	2.69	0.41
2:C:176:THR:O	2:C:192:ARG:HA	2.21	0.41
2:C:305:VAL:O	2:C:311:ILE:HA	2.20	0.41
1:G:347:VAL:HG13	1:G:348:ALA:N	2.35	0.41
2:C:81:LEU:C	2:C:83:ASP:N	2.73	0.41
2:D:230:LYS:HD3	2:D:248:HIS:CE1	2.54	0.41
2:F:220:THR:CG2	2:F:221:ALA:N	2.84	0.41
2:C:205:SER:HB3	2:C:208:LYS:HB2	2.03	0.41
2:C:289:LEU:HD22	2:C:299:VAL:CG1	2.47	0.41
2:D:114:ALA:O	2:D:115:ALA:HB2	2.19	0.41
2:F:180:GLN:OE1	2:F:185:SER:HB2	2.21	0.41
2:F:269:ARG:NH1	2:F:269:ARG:HG2	2.36	0.41
2:D:231:LEU:HD12	2:D:318:ALA:HB2	2.02	0.41
1:G:361:PHE:HA	1:G:386:LEU:O	2.21	0.41
2:C:114:ALA:O	2:C:115:ALA:HB2	2.21	0.41
2:C:120:LYS:HD3	2:C:122:TYR:OH	2.21	0.41
2:C:289:LEU:HB3	2:C:299:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:ALA:HA	2:F:88:PRO:HD3	1.95	0.41
2:C:298:GLU:HG2	2:C:319:LYS:HB2	2.02	0.41
2:H:251:SER:HA	2:H:252:PRO:HD3	1.93	0.41
1:B:372:ILE:HD13	1:B:372:ILE:HG21	1.83	0.40
2:C:169:SER:HB3	2:C:292:PHE:CG	2.56	0.40
2:D:174:PHE:O	2:D:194:PHE:HA	2.21	0.40
1:E:322:LEU:N	1:E:322:LEU:HD12	2.36	0.40
2:F:174:PHE:O	2:F:194:PHE:HA	2.21	0.40
1:G:437:SER:HA	1:G:438:PRO:HA	1.64	0.40
2:H:231:LEU:C	2:H:231:LEU:HD12	2.36	0.40
2:H:322:LEU:O	2:H:323:GLU:CG	2.60	0.40
2:F:258:LEU:N	2:F:258:LEU:HD12	2.36	0.40
2:H:136:ASP:OD2	2:H:319:LYS:NZ	2.46	0.40
2:H:289:LEU:HD13	2:H:299:VAL:CG1	2.48	0.40
1:A:372:ILE:HD11	1:A:379:TRP:HB3	2.03	0.40
2:C:152:GLN:HG2	2:C:152:GLN:O	2.21	0.40
2:C:174:PHE:O	2:C:194:PHE:HA	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	122/123 (99%)	115 (94%)	7 (6%)	0	100	100
1	B	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
1	E	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
1	G	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
2	C	242/253 (96%)	227 (94%)	15 (6%)	0	100	100
2	D	244/253 (96%)	231 (95%)	13 (5%)	0	100	100
2	F	245/253 (97%)	228 (93%)	16 (6%)	1 (0%)	34	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	244/253 (96%)	227 (93%)	16 (7%)	1 (0%)	34 38
All	All	1460/1504 (97%)	1371 (94%)	87 (6%)	2 (0%)	51 63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	152	GLN
2	H	310	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	109/108 (101%)	105 (96%)	4 (4%)	34 42
1	B	108/108 (100%)	105 (97%)	3 (3%)	43 53
1	E	108/108 (100%)	104 (96%)	4 (4%)	34 42
1	G	108/108 (100%)	104 (96%)	4 (4%)	34 42
2	C	191/194 (98%)	184 (96%)	7 (4%)	34 42
2	D	193/194 (100%)	185 (96%)	8 (4%)	30 37
2	F	194/194 (100%)	188 (97%)	6 (3%)	40 48
2	H	193/194 (100%)	181 (94%)	12 (6%)	18 19
All	All	1204/1208 (100%)	1156 (96%)	48 (4%)	31 39

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	413	ASP
1	A	427	THR
1	A	428	THR
1	A	443	ILE
1	B	347	VAL
1	B	411	SER

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Mol	Chain	Res	Type
1	B	427	THR
2	C	85	LEU
2	C	89	LEU
2	C	107	LYS
2	C	211	GLU
2	C	231	LEU
2	C	258	LEU
2	C	283	GLU
2	D	85	LEU
2	D	89	LEU
2	D	107	LYS
2	D	220	THR
2	D	258	LEU
2	D	283	GLU
2	D	321	GLU
2	D	323	GLU
1	E	347	VAL
1	E	387	ARG
1	E	412	ILE
1	E	427	THR
2	F	85	LEU
2	F	107	LYS
2	F	122	TYR
2	F	129	ASN
2	F	211	GLU
2	F	231	LEU
1	G	359	GLU
1	G	372	ILE
1	G	388	LYS
1	G	411	SER
2	H	85	LEU
2	H	89	LEU
2	H	107	LYS
2	H	129	ASN
2	H	147	ILE
2	H	152	GLN
2	H	157	GLU
2	H	211	GLU
2	H	283	GLU
2	H	321	GLU
2	H	322	LEU
2	H	323	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	166	GLN
2	C	175	GLN
2	D	129	ASN
2	D	166	GLN
2	F	166	GLN
2	F	175	GLN
2	H	108	ASN
2	H	152	GLN
2	H	175	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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	123/123 (100%)	0.21	3 (2%) 59 68	22, 34, 49, 66	2 (1%)
1	B	123/123 (100%)	0.19	1 (0%) 86 91	29, 40, 54, 66	2 (1%)
1	E	123/123 (100%)	0.22	2 (1%) 72 80	30, 41, 54, 68	2 (1%)
1	G	123/123 (100%)	0.26	2 (1%) 72 80	33, 44, 58, 71	1 (0%)
2	C	243/253 (96%)	0.29	7 (2%) 51 62	24, 38, 55, 68	0
2	D	244/253 (96%)	0.19	2 (0%) 86 91	19, 34, 51, 64	0
2	F	244/253 (96%)	0.29	8 (3%) 46 59	23, 39, 60, 75	0
2	H	244/253 (96%)	0.44	11 (4%) 33 46	28, 43, 62, 73	0
All	All	1467/1504 (97%)	0.28	36 (2%) 57 67	19, 39, 57, 75	7 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	89	LEU	6.0
1	A	443	ILE	5.4
2	F	90	ASP	4.9
2	H	91	HIS	4.2
2	F	91	HIS	3.5
2	H	310	GLY	3.4
2	D	91	HIS	3.3
2	F	89	LEU	3.3
2	C	116	GLN	3.0
2	H	88	PRO	2.6
2	F	150	ASP	2.6
2	H	118	ALA	2.6
1	B	404	ARG	2.6
2	D	107	LYS	2.6
2	F	88	PRO	2.5
2	H	311	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	377	ASP	2.4
2	F	309	ASN	2.4
1	A	427	THR	2.4
2	F	107	LYS	2.3
2	C	82	ALA	2.3
2	H	116	GLN	2.3
2	H	150	ASP	2.3
1	G	443	ILE	2.3
2	C	89	LEU	2.3
2	H	186	GLY	2.2
1	E	372	ILE	2.2
1	A	390	TYR	2.2
2	H	323	GLU	2.2
2	C	91	HIS	2.2
2	F	92	LYS	2.1
2	C	147	ILE	2.1
1	G	372	ILE	2.1
2	H	147	ILE	2.1
2	C	243[A]	ASN	2.0
2	C	279	TYR	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.