



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:12 AM GMT

PDB ID : 2W81
Title : STRUCTURE OF A COMPLEX BETWEEN NEISSERIA MENINGITIDIS
FACTOR H BINDING PROTEIN AND CCPS 6-7 OF HUMAN COMPLE-
MENT 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

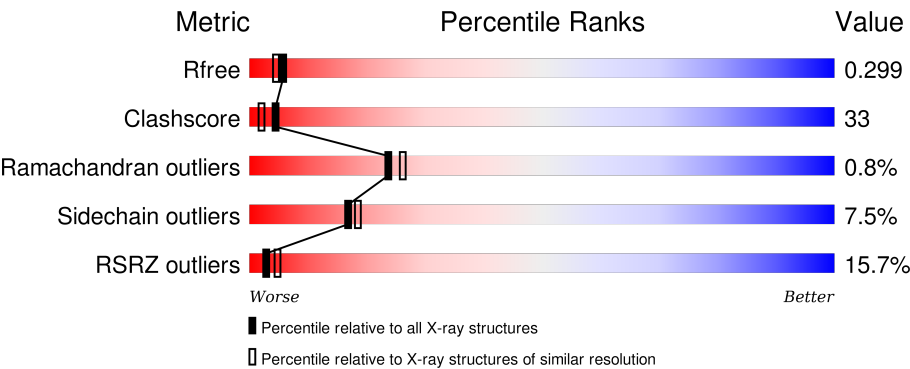
1 Overall quality at a glance i

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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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 ≥ 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	123	<div><div>20%</div><div>38%47%7%7%</div></div>
1	B	123	<div><div>22%</div><div>57%39%..</div></div>
1	E	123	<div><div>17%</div><div>50%44%6%.</div></div>
2	C	253	<div><div>11%</div><div>58%34%. .</div></div>
2	D	253	<div><div>9%</div><div>49%43%. .</div></div>

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Mol	Chain	Length	Quality of chain
2	F	253	<div><div></div><div></div><div></div><div></div><div></div></div> <div>19%49%40%6%5%</div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8836 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	115	Total	C	N	O	S	0	0	0
			943	602	162	169	10			
1	B	121	Total	C	N	O	S	0	0	0
			984	629	169	176	10			
1	E	122	Total	C	N	O	S	0	0	0
			992	635	170	177	10			

There are 3 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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	242	Total	C	N	O	S	0	0	0
			1832	1137	329	365	1			
2	D	243	Total	C	N	O	S	0	0	0
			1845	1146	330	368	1			
2	F	240	Total	C	N	O	S	0	0	0
			1816	1127	327	361	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	55	Total	O	0	0
			55	55		

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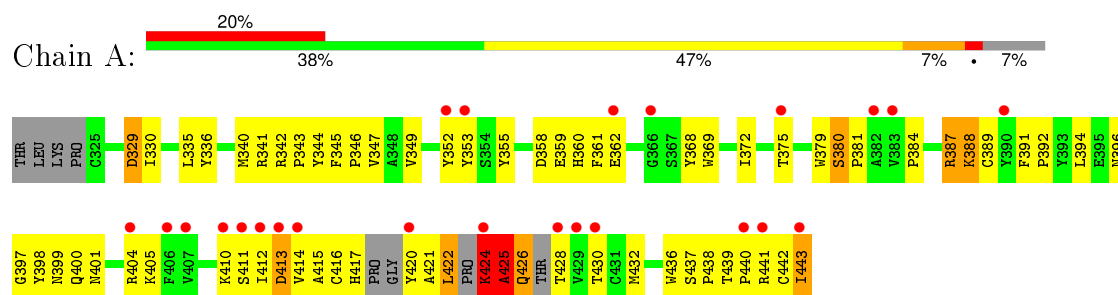
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	98	Total 98	O 98	0	0
3	D	99	Total 99	O 99	0	0
3	E	46	Total 46	O 46	0	0
3	F	90	Total 90	O 90	0	0

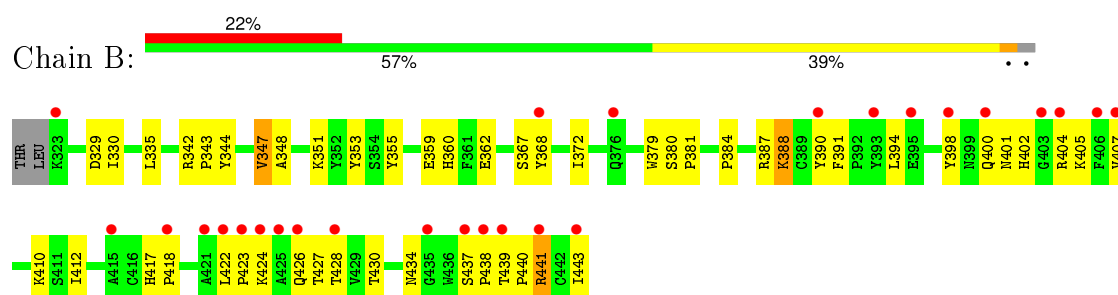
3 Residue-property plots

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

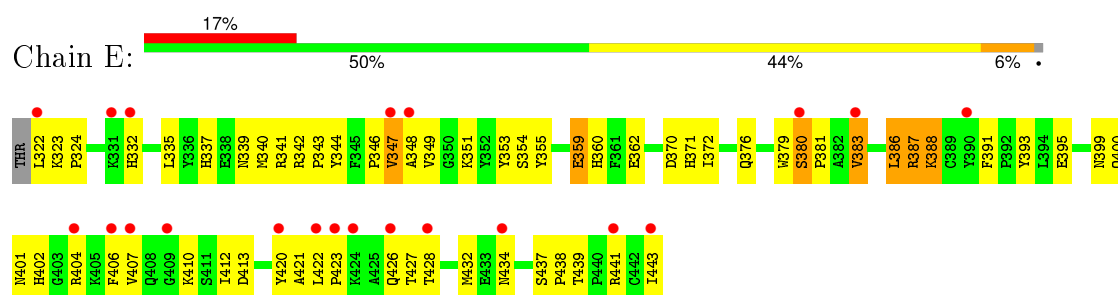
• Molecule 1: COMPLEMENT FACTOR H



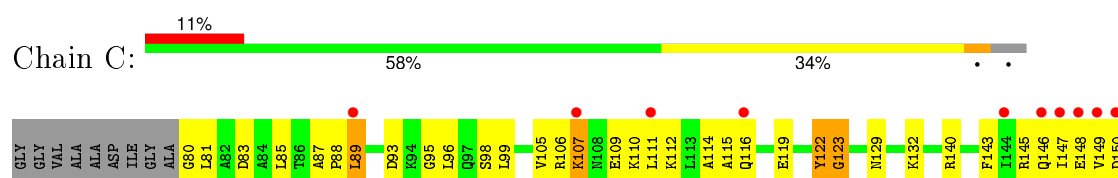
• Molecule 1: COMPLEMENT FACTOR H

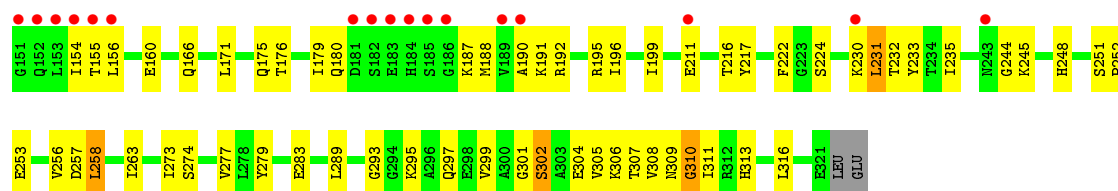


• Molecule 1: COMPLEMENT FACTOR H

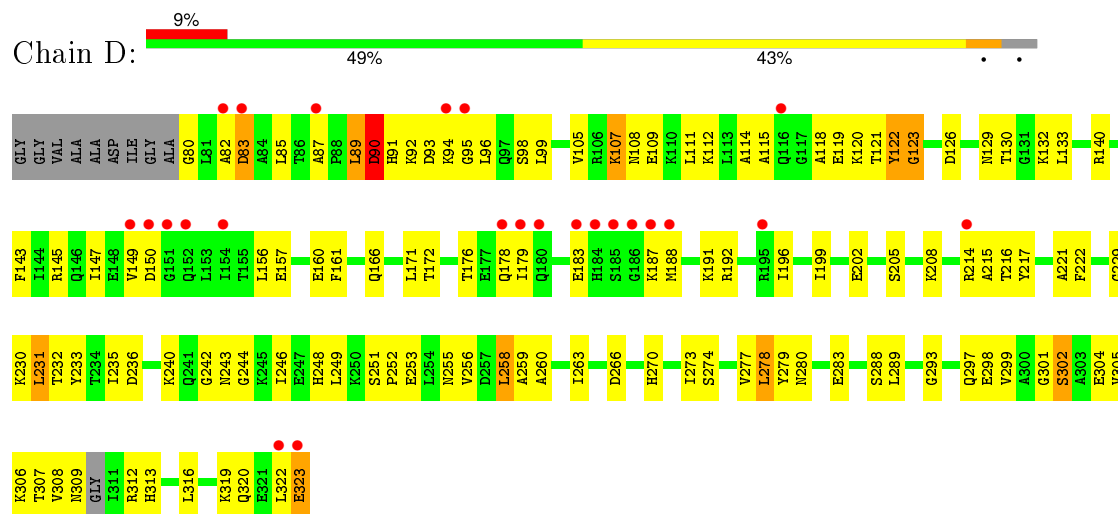


• Molecule 2: FACTOR H BINDING PROTEIN

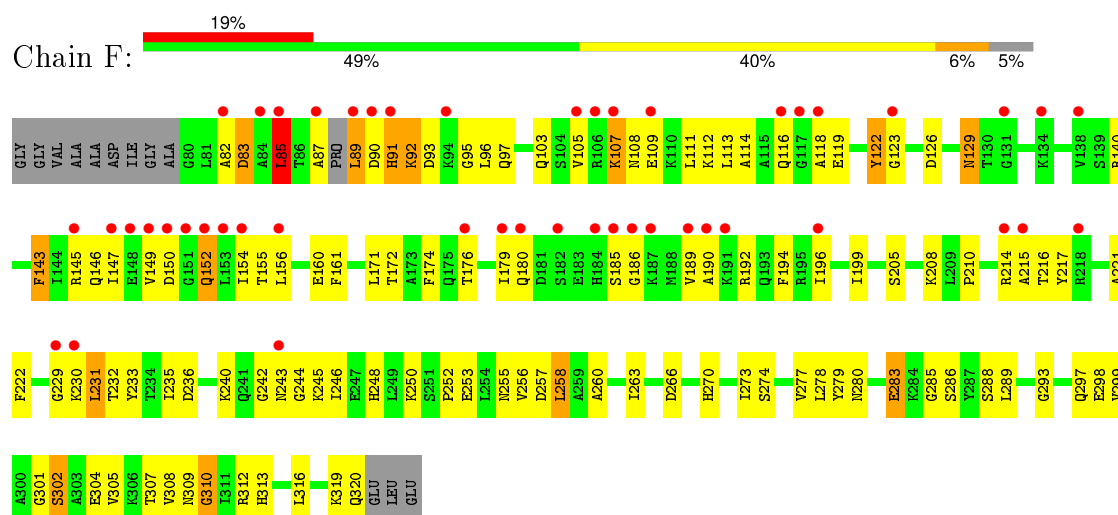




• Molecule 2: FACTOR H BINDING PROTEIN



• Molecule 2: FACTOR H BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.52Å 52.21Å 128.78Å 90.00° 118.19° 90.00°	Depositor
Resolution (Å)	38.81 – 2.35 38.82 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.8 (38.81-2.35) 94.0 (38.82-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 2.34Å)	Xtriage
Refinement program	BUSTER-TNT 2.5.1	Depositor
R, R_{free}	0.274 , 0.283 0.289 , 0.299	Depositor DCC
R_{free} test set	2187 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 43085 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8836	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.63	1/977 (0.1%)	0.87	5/1325 (0.4%)
1	B	0.39	0/1024	0.55	0/1396
1	E	0.46	0/1032	0.65	0/1407
2	C	0.35	0/1857	0.55	0/2491
2	D	0.38	0/1869	0.63	3/2506 (0.1%)
2	F	0.35	0/1839	0.54	1/2464 (0.0%)
All	All	0.41	1/8598 (0.0%)	0.62	9/11589 (0.1%)

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
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	LYS	CB-CG	-5.26	1.38	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	90	ASP	N-CA-C	-9.07	86.52	111.00
1	A	422	LEU	CA-CB-CG	-7.56	97.92	115.30
2	D	83	ASP	CB-CA-C	-5.71	98.97	110.40
2	D	91	HIS	N-CA-CB	-5.47	100.75	110.60
1	A	425	ALA	CA-C-N	-5.32	105.50	117.20
1	A	425	ALA	N-CA-C	5.31	125.33	111.00
1	A	388	LYS	CB-CA-C	-5.27	99.85	110.40
2	F	85	LEU	CB-CG-CD2	-5.27	102.05	111.00
1	A	329	ASP	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	424	LYS	Mainchain,Peptide

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	943	0	850	81	1
1	B	984	0	897	58	0
1	E	992	0	908	92	0
2	C	1832	0	1820	93	0
2	D	1845	0	1833	112	0
2	F	1816	0	1806	129	1
3	A	36	0	0	9	0
3	B	55	0	0	17	0
3	C	98	0	0	15	0
3	D	99	0	0	17	0
3	E	46	0	0	20	0
3	F	90	0	0	25	0
All	All	8836	0	8114	539	1

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 33.

All (539) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:TYR:CD1	1:A:443:ILE:HG12	1.84	1.13
1:E:407:VAL:HG12	1:E:410:LYS:HG3	1.21	1.12
1:A:375:THR:HG21	1:B:418:PRO:HD2	1.40	1.02
1:E:322:LEU:HG	1:E:324:PRO:HD3	1.44	0.97
1:E:362:GLU:HG3	1:E:388:LYS:HZ2	1.28	0.97
2:D:171:LEU:HD11	2:D:222:PHE:HZ	1.30	0.94
1:E:376:GLN:HA	3:E:2018:HOH:O	1.70	0.89
2:F:171:LEU:HD11	2:F:222:PHE:HZ	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:289:LEU:HD13	2:D:299:VAL:HG11	1.56	0.88
2:C:309:ASN:H	2:C:310:GLY:HA2	1.37	0.87
1:A:349:VAL:HG22	3:A:2016:HOH:O	1.73	0.86
2:F:289:LEU:HD13	2:F:299:VAL:HG11	1.56	0.86
2:D:171:LEU:HD11	2:D:222:PHE:CZ	2.10	0.85
2:D:231:LEU:HD12	2:D:232:THR:N	1.92	0.85
1:A:362:GLU:OE1	1:A:388:LYS:NZ	2.09	0.84
1:E:407:VAL:CG1	1:E:410:LYS:HG3	2.06	0.84
2:F:309:ASN:H	2:F:310:GLY:HA2	1.42	0.84
2:F:256:VAL:HG21	2:F:277:VAL:HG13	1.61	0.83
1:A:396:ASN:HB3	1:A:420:TYR:CD2	2.14	0.82
2:C:289:LEU:HD13	2:C:299:VAL:HG11	1.61	0.82
2:C:230:LYS:HD3	2:C:248:HIS:ND1	1.94	0.82
2:F:93:ASP:N	2:F:97:GLN:OE1	2.12	0.82
1:A:422:LEU:HD12	1:A:426:GLN:C	1.99	0.82
2:F:171:LEU:HD11	2:F:222:PHE:CZ	2.15	0.82
2:C:306:LYS:HE2	1:E:395:GLU:HG3	1.59	0.81
1:B:441:ARG:HG3	3:B:2055:HOH:O	1.79	0.81
1:B:362:GLU:OE2	1:B:388:LYS:NZ	2.14	0.81
1:E:407:VAL:HG12	1:E:410:LYS:HE3	1.62	0.81
2:C:171:LEU:HD11	2:C:222:PHE:HZ	1.45	0.81
1:A:362:GLU:HB2	1:A:388:LYS:HE3	1.63	0.81
2:D:80:GLY:O	2:D:83:ASP:HB2	1.81	0.81
2:D:82:ALA:HB1	2:D:118:ALA:HB2	1.63	0.80
2:D:230:LYS:HD3	2:D:248:HIS:ND1	1.97	0.80
2:F:231:LEU:HD12	2:F:232:THR:N	1.97	0.79
1:E:407:VAL:HG12	1:E:410:LYS:CG	2.10	0.79
1:A:412:ILE:O	1:A:428:THR:HA	1.82	0.79
2:C:150:ASP:HB3	3:C:2036:HOH:O	1.81	0.78
1:E:322:LEU:HG	1:E:324:PRO:CD	2.12	0.78
2:F:82:ALA:HB1	2:F:118:ALA:HB2	1.66	0.78
1:E:322:LEU:CG	1:E:324:PRO:HD3	2.13	0.78
2:C:171:LEU:HD11	2:C:222:PHE:CZ	2.19	0.78
2:D:187:LYS:HG3	2:F:189:VAL:HG13	1.63	0.77
2:F:309:ASN:N	2:F:310:GLY:HA2	1.98	0.77
2:C:309:ASN:N	2:C:310:GLY:HA2	1.97	0.77
1:A:375:THR:HB	1:B:418:PRO:HB2	1.67	0.77
2:D:85:LEU:HB2	3:D:2002:HOH:O	1.86	0.76
2:C:231:LEU:HD12	2:C:232:THR:N	2.00	0.76
1:A:412:ILE:HG22	1:A:413:ASP:N	2.01	0.76
2:C:306:LYS:CE	1:E:395:GLU:HG3	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:LYS:HE2	3:B:2015:HOH:O	1.85	0.75
2:F:230:LYS:HD3	2:F:248:HIS:ND1	2.02	0.74
2:D:215:ALA:HB1	2:D:320:GLN:NE2	2.01	0.74
1:E:413:ASP:HB2	3:E:2034:HOH:O	1.87	0.74
2:F:256:VAL:HG21	2:F:277:VAL:CG1	2.17	0.74
2:C:256:VAL:HG21	2:C:277:VAL:HG13	1.69	0.74
2:D:259:ALA:HB2	2:D:278:LEU:HD11	1.68	0.74
1:E:337:HIS:CE1	2:F:103:GLN:HE22	2.06	0.74
2:C:190:ALA:HB3	2:F:186:GLY:O	1.88	0.73
2:D:187:LYS:HA	2:F:190:ALA:O	1.87	0.73
2:F:279:TYR:HA	3:F:2074:HOH:O	1.88	0.73
2:D:256:VAL:HG21	2:D:277:VAL:HG13	1.70	0.73
1:B:423:PRO:HB2	3:B:2048:HOH:O	1.87	0.73
1:A:442:CYS:C	1:A:443:ILE:HG13	2.07	0.73
1:B:394:LEU:HA	3:B:2031:HOH:O	1.89	0.72
2:F:149:VAL:HG22	3:F:2028:HOH:O	1.89	0.72
2:F:146:GLN:HG2	2:F:155:THR:HA	1.72	0.71
2:D:289:LEU:HD13	2:D:299:VAL:CG1	2.20	0.71
2:F:152:GLN:HA	3:F:2030:HOH:O	1.90	0.71
2:F:160:GLU:HA	3:F:2033:HOH:O	1.90	0.70
3:A:2028:HOH:O	2:D:183:GLU:HA	1.90	0.70
1:E:443:ILE:O	1:E:443:ILE:HD12	1.92	0.70
2:D:253:GLU:OE1	2:D:307:THR:HB	1.91	0.70
1:A:362:GLU:CD	1:A:388:LYS:NZ	2.45	0.69
2:F:152:GLN:HB2	3:F:2088:HOH:O	1.93	0.69
2:C:253:GLU:OE1	2:C:307:THR:HB	1.94	0.68
1:B:347:VAL:HG21	1:B:353:TYR:OH	1.93	0.68
1:A:422:LEU:HD12	1:A:426:GLN:O	1.93	0.68
1:E:426:GLN:HB2	3:E:2041:HOH:O	1.94	0.68
2:D:89:LEU:N	2:D:89:LEU:HD23	2.09	0.68
1:A:420:TYR:HD1	1:A:443:ILE:CG2	2.06	0.67
1:B:390:TYR:CE2	1:B:405:LYS:HG3	2.28	0.67
2:C:140:ARG:NH2	3:C:2028:HOH:O	2.27	0.67
2:F:277:VAL:HG11	2:F:305:VAL:HG22	1.77	0.67
2:D:89:LEU:HD23	2:D:89:LEU:H	1.58	0.67
1:E:407:VAL:CG1	1:E:410:LYS:HE3	2.25	0.66
1:E:362:GLU:CG	1:E:388:LYS:HZ2	2.06	0.66
1:A:420:TYR:HD1	1:A:443:ILE:HG23	1.60	0.66
2:C:187:LYS:HB2	3:D:2037:HOH:O	1.95	0.66
2:F:253:GLU:OE1	2:F:307:THR:HB	1.96	0.66
1:B:410:LYS:HG3	3:B:2043:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:176:THR:O	2:D:192:ARG:HA	1.96	0.65
1:E:362:GLU:HG3	1:E:388:LYS:NZ	2.08	0.65
2:F:156:LEU:HD23	2:F:180:GLN:NE2	2.11	0.65
1:E:406:PHE:CZ	1:E:412:ILE:HG13	2.30	0.65
2:F:149:VAL:O	2:F:152:GLN:NE2	2.27	0.65
2:C:289:LEU:HD13	2:C:299:VAL:CG1	2.25	0.65
1:A:410:LYS:O	1:A:430:THR:HG23	1.97	0.65
2:F:231:LEU:HD22	2:F:316:LEU:HD22	1.78	0.65
2:D:89:LEU:CD2	2:D:89:LEU:H	2.01	0.65
1:E:332:HIS:ND1	3:E:2008:HOH:O	2.28	0.65
2:F:289:LEU:HD13	2:F:299:VAL:CG1	2.24	0.65
1:B:359:GLU:HG2	3:B:2014:HOH:O	1.97	0.65
2:F:256:VAL:CG2	2:F:277:VAL:HG13	2.27	0.65
2:F:82:ALA:CB	2:F:118:ALA:HB2	2.27	0.64
1:E:322:LEU:HD12	1:E:323:LYS:N	2.13	0.64
2:C:310:GLY:HA3	1:E:393:TYR:CD2	2.32	0.64
1:E:406:PHE:HA	1:E:410:LYS:NZ	2.13	0.64
2:D:188:MET:HB3	3:D:2033:HOH:O	1.97	0.64
2:F:243:ASN:ND2	3:F:2060:HOH:O	2.30	0.64
2:F:242:GLY:O	2:F:260:ALA:HA	1.98	0.64
1:A:420:TYR:CE1	1:A:443:ILE:HG12	2.33	0.63
2:D:256:VAL:HG21	2:D:277:VAL:CG1	2.28	0.63
1:A:368:TYR:CE1	1:A:369:TRP:HD1	2.15	0.63
1:E:406:PHE:HA	1:E:410:LYS:HZ3	1.61	0.63
2:C:277:VAL:HG11	2:C:305:VAL:HG22	1.79	0.63
1:A:420:TYR:CD1	1:A:443:ILE:CG1	2.73	0.63
2:F:307:THR:N	2:F:310:GLY:O	2.32	0.63
2:C:289:LEU:HD22	2:C:299:VAL:CG1	2.29	0.63
2:D:188:MET:H	2:F:190:ALA:HB3	1.63	0.62
2:F:112:LYS:HE2	2:F:119:GLU:OE2	1.97	0.62
1:A:359:GLU:H	1:A:359:GLU:CD	2.02	0.62
1:E:387:ARG:NE	3:E:2043:HOH:O	2.31	0.62
2:C:307:THR:N	2:C:310:GLY:O	2.33	0.62
1:A:420:TYR:N	3:A:2032:HOH:O	2.32	0.62
2:F:231:LEU:CD2	2:F:316:LEU:HD22	2.30	0.62
1:E:322:LEU:HD12	1:E:323:LYS:H	1.65	0.62
1:E:407:VAL:H	1:E:410:LYS:CE	2.12	0.62
2:C:93:ASP:OD2	2:C:132:LYS:HE2	1.98	0.62
2:C:309:ASN:ND2	2:F:150:ASP:HB3	2.15	0.62
2:F:89:LEU:N	3:F:2003:HOH:O	2.32	0.61
1:E:347:VAL:HG21	1:E:353:TYR:OH	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:322:LEU:CD1	1:E:324:PRO:HD3	2.29	0.61
2:D:231:LEU:HD12	2:D:232:THR:H	1.65	0.61
1:E:323:LYS:HD2	1:E:346:PRO:O	2.01	0.61
2:D:108:ASN:HB2	3:D:2012:HOH:O	2.00	0.61
2:D:93:ASP:OD2	2:D:132:LYS:HE2	2.01	0.61
1:B:438:PRO:HA	3:B:2054:HOH:O	1.99	0.61
2:F:147:ILE:HG23	2:F:156:LEU:HD12	1.83	0.61
1:A:404:ARG:NH2	3:A:2025:HOH:O	2.34	0.61
2:C:191:LYS:NZ	3:C:2046:HOH:O	2.29	0.61
2:C:112:LYS:HE2	2:C:119:GLU:OE2	2.00	0.61
2:F:107:LYS:C	2:F:107:LYS:HD3	2.21	0.60
1:A:424:LYS:N	3:A:2034:HOH:O	2.35	0.60
2:F:176:THR:O	2:F:192:ARG:HA	2.02	0.60
2:C:289:LEU:HD22	2:C:299:VAL:HG13	1.83	0.59
1:E:347:VAL:CG1	1:E:351:LYS:HB2	2.32	0.59
2:D:95:GLY:HA2	2:D:96:LEU:C	2.22	0.59
1:B:417:HIS:CE1	3:B:2033:HOH:O	2.56	0.59
1:E:432:MET:HB2	3:E:2044:HOH:O	2.03	0.59
2:D:242:GLY:O	2:D:260:ALA:HA	2.02	0.59
2:D:171:LEU:CD1	2:D:222:PHE:HZ	2.10	0.59
2:D:243:ASN:HB2	3:D:2062:HOH:O	2.02	0.59
2:F:214:ARG:HD2	3:F:2052:HOH:O	2.03	0.59
2:C:166:GLN:HA	3:C:2026:HOH:O	2.02	0.59
1:A:347:VAL:HG11	1:A:353:TYR:OH	2.03	0.59
2:D:82:ALA:CB	2:D:118:ALA:HB2	2.33	0.58
2:D:277:VAL:HG11	2:D:305:VAL:HG22	1.85	0.58
2:D:147:ILE:CG2	2:D:156:LEU:HD11	2.33	0.58
2:F:250:LYS:HG2	3:F:2064:HOH:O	2.03	0.58
2:F:308:VAL:O	2:F:309:ASN:ND2	2.37	0.58
2:F:109:GLU:OE2	2:F:145:ARG:NH1	2.36	0.58
1:B:407:VAL:HG12	1:B:410:LYS:CE	2.33	0.58
2:D:107:LYS:C	2:D:107:LYS:HD3	2.23	0.58
1:E:359:GLU:OE1	1:E:360:HIS:NE2	2.36	0.58
2:D:112:LYS:HE2	2:D:119:GLU:OE2	2.03	0.58
2:C:176:THR:O	2:C:192:ARG:HA	2.04	0.58
1:A:362:GLU:CD	1:A:388:LYS:HZ2	2.07	0.58
1:A:412:ILE:CG2	1:A:413:ASP:N	2.66	0.58
2:C:256:VAL:HG21	2:C:277:VAL:CG1	2.33	0.58
2:C:107:LYS:C	2:C:107:LYS:HD3	2.23	0.57
1:A:410:LYS:HD2	1:A:411:SER:H	1.69	0.57
2:D:109:GLU:OE2	2:D:145:ARG:NH1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ARG:NH1	1:B:434:ASN:O	2.37	0.57
1:B:391:PHE:HB3	1:B:401:ASN:O	2.05	0.57
2:D:322:LEU:HG	3:D:2089:HOH:O	2.02	0.57
2:D:231:LEU:HD22	2:D:316:LEU:HD22	1.85	0.57
1:E:434:ASN:HB2	3:E:2044:HOH:O	2.05	0.57
2:D:90:ASP:OD1	2:D:92:LYS:HG3	2.05	0.57
2:D:187:LYS:HG3	2:F:189:VAL:CG1	2.33	0.56
2:F:143:PHE:N	3:F:2033:HOH:O	2.38	0.56
2:D:323:GLU:HG3	3:D:2088:HOH:O	2.04	0.56
1:E:344:TYR:CD1	2:F:274:SER:HB2	2.40	0.56
1:A:412:ILE:HG22	1:A:413:ASP:O	2.04	0.56
1:B:410:LYS:O	1:B:430:THR:HG23	2.05	0.56
2:C:217:TYR:CE2	2:C:235:ILE:HD12	2.40	0.56
2:C:147:ILE:HG23	2:C:156:LEU:HD12	1.86	0.56
2:F:91:HIS:ND1	2:F:91:HIS:N	2.53	0.56
2:C:95:GLY:HA2	2:C:96:LEU:C	2.25	0.56
1:A:420:TYR:CD1	1:A:443:ILE:CG2	2.88	0.56
1:A:372:ILE:HD11	1:A:379:TRP:HB3	1.88	0.56
2:C:122:TYR:HB3	2:C:123:GLY:HA3	1.87	0.56
1:A:359:GLU:O	1:A:360:HIS:HB2	2.05	0.56
2:D:202:GLU:HB2	3:D:2043:HOH:O	2.06	0.56
2:D:147:ILE:HD12	2:D:149:VAL:CG2	2.36	0.56
2:F:82:ALA:HA	2:F:118:ALA:HB3	1.87	0.56
2:C:149:VAL:HG23	2:C:154:ILE:HG13	1.87	0.55
1:E:339:ASN:OD1	1:E:340:MET:N	2.39	0.55
2:D:122:TYR:HB3	2:D:123:GLY:HA3	1.89	0.55
2:D:166:GLN:HA	3:D:2021:HOH:O	2.07	0.55
2:F:289:LEU:HD22	2:F:299:VAL:CG1	2.37	0.55
2:D:83:ASP:O	2:D:87:ALA:N	2.40	0.55
1:E:351:LYS:HZ2	2:F:286:SER:CB	2.19	0.55
2:F:214:ARG:HA	2:F:235:ILE:O	2.06	0.55
2:C:147:ILE:HD12	3:C:2035:HOH:O	2.07	0.55
1:A:358:ASP:O	1:A:361:PHE:HB2	2.06	0.55
2:D:147:ILE:HD12	2:D:149:VAL:HG23	1.89	0.55
2:F:304:GLU:HG2	2:F:313:HIS:CD2	2.42	0.55
2:D:115:ALA:HB1	3:D:2022:HOH:O	2.07	0.55
2:D:82:ALA:C	3:D:2002:HOH:O	2.46	0.54
2:D:308:VAL:O	2:D:309:ASN:ND2	2.39	0.54
1:E:372:ILE:HD11	1:E:379:TRP:HB3	1.89	0.54
1:E:323:LYS:N	1:E:324:PRO:HD3	2.22	0.54
1:E:362:GLU:OE2	1:E:388:LYS:NZ	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:VAL:H	1:B:410:LYS:HD2	1.73	0.54
2:D:176:THR:HG21	2:D:179:ILE:CG2	2.38	0.54
2:F:85:LEU:HD21	3:F:2013:HOH:O	2.07	0.54
2:F:82:ALA:HA	2:F:118:ALA:CB	2.37	0.54
1:E:421:ALA:O	1:E:443:ILE:HG13	2.08	0.54
2:C:176:THR:HG21	2:C:179:ILE:CG2	2.37	0.54
2:D:130:THR:HG22	2:D:133:LEU:HD12	1.90	0.54
2:C:89:LEU:N	2:C:89:LEU:HD12	2.23	0.54
1:E:421:ALA:N	1:E:443:ILE:O	2.41	0.54
2:C:148:GLU:HB2	3:C:2034:HOH:O	2.06	0.54
2:F:279:TYR:O	2:F:280:ASN:HB2	2.07	0.54
1:A:424:LYS:N	1:A:425:ALA:HB2	2.23	0.54
2:F:97:GLN:HG3	3:F:2006:HOH:O	2.06	0.54
1:A:424:LYS:N	1:A:425:ALA:CB	2.72	0.54
1:A:412:ILE:HG22	1:A:413:ASP:H	1.73	0.53
1:E:341:ARG:NH1	1:E:353:TYR:HB3	2.24	0.53
1:E:349:VAL:HG22	3:E:2018:HOH:O	2.08	0.53
2:D:230:LYS:HG2	3:D:2060:HOH:O	2.08	0.53
2:D:256:VAL:CG2	2:D:277:VAL:HG13	2.37	0.53
2:D:147:ILE:HG21	2:D:156:LEU:HD11	1.89	0.53
1:B:387:ARG:HH11	1:B:434:ASN:C	2.12	0.53
2:F:114:ALA:HA	3:F:2013:HOH:O	2.08	0.53
2:C:80:GLY:N	3:C:2001:HOH:O	2.41	0.53
1:A:422:LEU:HB2	1:A:425:ALA:HB1	1.90	0.53
2:D:188:MET:CB	3:D:2033:HOH:O	2.57	0.53
1:B:422:LEU:HB3	1:B:426:GLN:HB2	1.90	0.53
1:B:423:PRO:CG	3:B:2055:HOH:O	2.56	0.53
1:B:388:LYS:NZ	1:B:405:LYS:NZ	2.56	0.53
1:B:390:TYR:CE2	1:B:405:LYS:CG	2.91	0.53
1:B:443:ILE:O	1:B:443:ILE:HD12	2.09	0.53
1:A:368:TYR:CE1	1:A:369:TRP:CD1	2.97	0.52
2:D:214:ARG:HA	2:D:235:ILE:O	2.08	0.52
1:E:422:LEU:C	3:E:2041:HOH:O	2.46	0.52
2:F:85:LEU:CD2	3:F:2013:HOH:O	2.56	0.52
2:C:105:VAL:HG22	2:C:111:LEU:HB2	1.91	0.52
1:A:362:GLU:HB2	1:A:388:LYS:CE	2.36	0.52
2:C:256:VAL:CG2	2:C:277:VAL:HG13	2.38	0.52
1:B:368:TYR:OH	2:C:195:ARG:NH2	2.43	0.52
3:B:2017:HOH:O	1:E:400:GLN:HG3	2.09	0.52
2:C:199:ILE:HD13	2:C:301:GLY:HA2	1.92	0.52
2:C:293:GLY:HA3	2:C:297:GLN:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:171:LEU:CD1	2:F:222:PHE:HZ	2.16	0.52
2:D:266:ASP:CB	2:D:270:HIS:H	2.23	0.52
2:D:82:ALA:HA	2:D:118:ALA:HB3	1.91	0.52
2:D:187:LYS:CG	2:F:189:VAL:HG13	2.37	0.52
2:F:140:ARG:HB3	2:F:160:GLU:OE2	2.10	0.52
2:F:105:VAL:HG22	2:F:111:LEU:HB2	1.92	0.52
1:A:410:LYS:HD2	3:A:2030:HOH:O	2.10	0.51
2:C:109:GLU:OE2	2:C:145:ARG:NH1	2.43	0.51
2:C:116:GLN:HG2	3:C:2014:HOH:O	2.10	0.51
1:B:362:GLU:HG3	1:B:388:LYS:CD	2.40	0.51
2:F:285:GLY:HA2	3:F:2079:HOH:O	2.10	0.51
1:A:342:ARG:HB3	1:A:343:PRO:HD3	1.91	0.51
1:E:362:GLU:CG	1:E:388:LYS:NZ	2.71	0.51
1:A:401:ASN:O	1:A:404:ARG:HB2	2.10	0.51
2:F:107:LYS:HD3	2:F:107:LYS:O	2.10	0.51
2:C:149:VAL:HG12	3:C:2037:HOH:O	2.09	0.51
1:B:367:SER:HB3	3:B:2018:HOH:O	2.09	0.51
2:F:250:LYS:HA	3:F:2064:HOH:O	2.10	0.51
2:F:90:ASP:OD1	2:F:91:HIS:N	2.41	0.51
1:B:347:VAL:CG1	1:B:351:LYS:HB2	2.41	0.51
1:E:391:PHE:HB3	1:E:401:ASN:O	2.10	0.51
1:E:349:VAL:CG2	3:E:2018:HOH:O	2.59	0.51
2:C:146:GLN:HG2	2:C:155:THR:HA	1.91	0.51
2:F:122:TYR:HB3	2:F:123:GLY:HA3	1.92	0.51
1:E:422:LEU:HB3	3:E:2041:HOH:O	2.11	0.51
2:C:263:ILE:HG12	2:C:273:ILE:HG12	1.92	0.51
1:E:407:VAL:CB	1:E:410:LYS:HE3	2.41	0.51
1:A:375:THR:CB	1:B:418:PRO:HB2	2.40	0.51
2:F:152:GLN:O	2:F:152:GLN:HG2	2.10	0.51
2:F:180:GLN:OE1	2:F:185:SER:HA	2.11	0.51
2:F:176:THR:HG21	2:F:179:ILE:CG2	2.41	0.50
1:E:407:VAL:H	1:E:410:LYS:HE3	1.76	0.50
2:F:113:LEU:C	3:F:2013:HOH:O	2.48	0.50
1:E:404:ARG:NE	3:E:2029:HOH:O	2.43	0.50
2:C:231:LEU:HD22	2:C:316:LEU:HD22	1.92	0.50
2:F:161:PHE:CZ	2:F:172:THR:HB	2.47	0.50
1:E:426:GLN:CB	3:E:2041:HOH:O	2.58	0.50
1:E:340:MET:HE1	3:E:2009:HOH:O	2.11	0.50
1:B:362:GLU:HG2	3:B:2016:HOH:O	2.12	0.50
2:F:217:TYR:CE2	2:F:235:ILE:HD12	2.47	0.50
2:F:233:TYR:HD1	2:F:244:GLY:HA3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:175:GLN:NE2	2:C:224:SER:OG	2.37	0.50
1:E:407:VAL:O	1:E:410:LYS:HB2	2.12	0.50
1:B:359:GLU:O	1:B:360:HIS:HB2	2.12	0.50
1:A:335:LEU:HD23	1:A:355:TYR:HB3	1.94	0.50
2:C:171:LEU:CD1	2:C:222:PHE:HZ	2.21	0.49
1:E:426:GLN:N	3:E:2041:HOH:O	2.18	0.49
1:A:380:SER:HA	1:A:381:PRO:C	2.32	0.49
1:E:337:HIS:CE1	2:F:103:GLN:NE2	2.78	0.49
1:A:422:LEU:HB2	1:A:426:GLN:C	2.31	0.49
2:F:196:ILE:HG13	2:F:302:SER:HB2	1.94	0.49
1:A:396:ASN:OD1	1:A:443:ILE:HD11	2.11	0.49
1:E:423:PRO:O	3:E:2041:HOH:O	2.20	0.49
2:D:308:VAL:HG23	2:D:308:VAL:O	2.11	0.49
2:D:289:LEU:HD22	2:D:299:VAL:CG1	2.42	0.49
2:F:266:ASP:CB	2:F:270:HIS:H	2.25	0.49
2:D:263:ILE:HG12	2:D:273:ILE:HG12	1.94	0.49
1:E:340:MET:CE	3:E:2009:HOH:O	2.61	0.48
1:E:371:HIS:NE2	2:F:313:HIS:NE2	2.48	0.48
2:C:304:GLU:HG2	2:C:313:HIS:CD2	2.48	0.48
1:A:375:THR:C	3:A:2016:HOH:O	2.52	0.48
2:F:112:LYS:O	2:F:143:PHE:HA	2.14	0.48
2:D:123:GLY:O	2:D:126:ASP:HB2	2.12	0.48
2:C:149:VAL:CG2	2:C:154:ILE:HG13	2.44	0.48
1:E:322:LEU:N	3:E:2001:HOH:O	2.47	0.48
1:B:330:ILE:HG23	1:B:384:PRO:HG2	1.96	0.48
2:C:89:LEU:HB3	3:C:2007:HOH:O	2.12	0.48
2:D:304:GLU:HG2	2:D:313:HIS:CD2	2.48	0.48
1:A:396:ASN:O	1:A:417:HIS:HB2	2.13	0.48
1:E:407:VAL:HG12	1:E:410:LYS:CE	2.39	0.48
1:B:344:TYR:CD1	2:C:274:SER:HB2	2.48	0.48
1:E:383:VAL:O	1:E:383:VAL:HG22	2.14	0.48
2:D:322:LEU:HD12	2:D:323:GLU:H	1.78	0.48
2:F:92:LYS:HE2	2:F:92:LYS:HB3	1.41	0.48
2:F:230:LYS:HD2	3:F:2062:HOH:O	2.13	0.47
2:C:149:VAL:HG22	3:C:2035:HOH:O	2.14	0.47
2:F:221:ALA:O	2:F:229:GLY:HA3	2.14	0.47
1:A:422:LEU:CD1	1:A:426:GLN:C	2.78	0.47
2:C:116:GLN:N	3:C:2015:HOH:O	2.46	0.47
1:A:413:ASP:OD2	1:A:413:ASP:N	2.45	0.47
2:C:147:ILE:HG23	2:C:156:LEU:CD1	2.43	0.47
2:D:309:ASN:O	2:D:312:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:SER:HA	1:A:438:PRO:HA	1.73	0.47
2:F:231:LEU:HD12	2:F:232:THR:H	1.78	0.47
2:D:149:VAL:O	2:D:150:ASP:HB2	2.15	0.47
2:D:246:ILE:HG22	2:D:255:ASN:HA	1.97	0.47
2:F:210:PRO:HD3	3:F:2048:HOH:O	2.14	0.47
2:C:87:ALA:HA	2:C:88:PRO:HD3	1.63	0.47
1:B:388:LYS:HZ2	1:B:405:LYS:NZ	2.12	0.47
2:D:215:ALA:CB	2:D:320:GLN:NE2	2.75	0.47
1:B:404:ARG:NH1	3:B:2040:HOH:O	2.48	0.47
1:A:397:GLY:HA2	1:A:417:HIS:N	2.29	0.47
1:B:424:LYS:HG3	3:B:2048:HOH:O	2.15	0.47
2:D:279:TYR:O	2:D:280:ASN:HB2	2.15	0.47
1:B:443:ILE:HD12	1:B:443:ILE:C	2.35	0.47
3:B:2030:HOH:O	2:D:306:LYS:HE2	2.15	0.47
2:F:215:ALA:HB1	2:F:320:GLN:OE1	2.15	0.47
2:D:205:SER:HB3	2:D:208:LYS:HB2	1.95	0.47
1:B:342:ARG:HB3	1:B:343:PRO:HD3	1.96	0.47
1:A:399:ASN:HA	3:A:2022:HOH:O	2.15	0.47
2:F:233:TYR:CD1	2:F:244:GLY:HA3	2.50	0.47
2:F:293:GLY:HA3	2:F:297:GLN:OE1	2.15	0.47
1:B:426:GLN:HG3	1:B:438:PRO:HG3	1.96	0.46
2:D:217:TYR:CE2	2:D:235:ILE:HD12	2.50	0.46
1:A:394:LEU:HD11	1:A:414:VAL:HG13	1.96	0.46
2:D:259:ALA:HB2	2:D:278:LEU:CD1	2.42	0.46
2:C:89:LEU:H	2:C:89:LEU:CD1	2.29	0.46
1:E:347:VAL:HG13	1:E:351:LYS:HB2	1.97	0.46
1:B:344:TYR:CE1	2:C:274:SER:HB2	2.51	0.46
1:A:359:GLU:HG2	3:D:2012:HOH:O	2.16	0.46
1:A:422:LEU:CD2	1:A:441:ARG:O	2.64	0.46
1:A:412:ILE:CG2	1:A:413:ASP:H	2.26	0.46
2:F:95:GLY:HA2	2:F:96:LEU:C	2.36	0.46
2:D:82:ALA:HA	2:D:118:ALA:CB	2.46	0.46
2:D:140:ARG:HB3	2:D:160:GLU:OE2	2.16	0.46
1:B:372:ILE:HD11	1:B:379:TRP:HB3	1.97	0.46
1:E:348:ALA:HB2	3:E:2002:HOH:O	2.14	0.46
1:B:398:TYR:HB3	1:B:400:GLN:OE1	2.16	0.46
2:D:258:LEU:CD1	2:D:258:LEU:N	2.79	0.46
1:E:443:ILE:HD12	1:E:443:ILE:C	2.36	0.45
1:B:407:VAL:HG12	1:B:410:LYS:HE3	1.97	0.45
1:A:414:VAL:CG2	1:A:422:LEU:HD11	2.46	0.45
1:A:336:TYR:O	1:A:341:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:TYR:O	1:A:421:ALA:HB2	2.17	0.45
2:F:140:ARG:HD3	2:F:160:GLU:OE2	2.17	0.45
2:F:263:ILE:HG12	2:F:273:ILE:HG12	1.97	0.45
2:C:89:LEU:CD1	2:C:89:LEU:N	2.80	0.45
1:E:354:SER:HA	1:E:370:ASP:O	2.17	0.45
2:C:231:LEU:CD2	2:C:316:LEU:HD22	2.46	0.45
1:E:351:LYS:HD2	2:F:286:SER:OG	2.16	0.45
2:C:107:LYS:O	2:C:107:LYS:HD3	2.17	0.45
1:E:439:THR:HG22	1:E:441:ARG:HD3	1.96	0.45
2:D:147:ILE:HG23	2:D:156:LEU:CD1	2.47	0.45
2:D:114:ALA:O	2:D:115:ALA:HB2	2.16	0.45
2:D:105:VAL:HG22	2:D:111:LEU:HB2	1.98	0.45
2:D:266:ASP:HB2	2:D:270:HIS:H	1.82	0.45
2:D:293:GLY:HA3	2:D:297:GLN:OE1	2.16	0.45
2:F:150:ASP:C	2:F:152:GLN:H	2.19	0.45
1:B:362:GLU:HG3	1:B:388:LYS:HD3	1.99	0.45
1:B:359:GLU:HG3	1:B:359:GLU:O	2.15	0.45
1:B:335:LEU:HD23	1:B:355:TYR:HB3	1.98	0.45
1:A:396:ASN:HB3	1:A:420:TYR:CG	2.51	0.45
2:C:176:THR:HG21	2:C:179:ILE:HG22	1.98	0.45
2:C:106:ARG:N	2:C:109:GLU:HG2	2.31	0.45
2:F:320:GLN:O	2:F:320:GLN:HG3	2.16	0.45
1:A:389:CYS:HB3	1:A:436:TRP:CE2	2.51	0.45
2:C:140:ARG:HD3	2:C:160:GLU:OE2	2.16	0.45
1:A:391:PHE:HB3	1:A:401:ASN:O	2.17	0.45
2:D:140:ARG:HD3	2:D:160:GLU:OE2	2.17	0.45
1:A:387:ARG:HG3	1:A:388:LYS:N	2.32	0.44
2:F:205:SER:HB3	2:F:208:LYS:HB2	1.98	0.44
1:B:388:LYS:HZ2	1:B:405:LYS:HZ1	1.66	0.44
1:A:410:LYS:O	1:A:430:THR:HA	2.17	0.44
2:D:112:LYS:O	2:D:143:PHE:HA	2.18	0.44
2:D:266:ASP:HB2	2:D:270:HIS:O	2.17	0.44
2:D:99:LEU:HD23	2:D:99:LEU:C	2.38	0.44
2:C:114:ALA:O	2:C:115:ALA:HB2	2.17	0.44
2:C:231:LEU:HD12	2:C:232:THR:H	1.79	0.44
1:B:407:VAL:HG12	1:B:410:LYS:CD	2.47	0.44
2:F:147:ILE:HG23	2:F:156:LEU:CD1	2.48	0.44
1:E:380:SER:HA	1:E:381:PRO:C	2.38	0.44
1:E:423:PRO:HG3	1:E:443:ILE:HG12	2.00	0.44
2:F:297:GLN:HB3	3:F:2086:HOH:O	2.17	0.44
1:A:344:TYR:CE1	2:D:274:SER:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:LYS:O	2:D:107:LYS:HD3	2.17	0.44
2:F:278:LEU:HD23	2:F:283:GLU:HA	2.00	0.44
2:F:280:ASN:HB3	3:F:2075:HOH:O	2.17	0.44
1:A:398:TYR:HD2	1:A:415:ALA:HB1	1.83	0.44
1:E:347:VAL:HG11	1:E:351:LYS:HB2	2.00	0.44
2:C:89:LEU:HB2	3:C:2005:HOH:O	2.18	0.44
2:C:295:LYS:HD3	3:C:2082:HOH:O	2.16	0.44
2:C:307:THR:O	2:C:310:GLY:HA2	2.17	0.43
2:F:256:VAL:HG12	2:F:279:TYR:HB2	1.99	0.43
1:B:424:LYS:CG	3:B:2048:HOH:O	2.66	0.43
1:B:347:VAL:HG13	1:B:348:ALA:N	2.32	0.43
1:B:407:VAL:HG12	1:B:410:LYS:HD2	2.00	0.43
1:E:383:VAL:CG2	1:E:386:LEU:HD13	2.49	0.43
2:F:199:ILE:HD13	2:F:301:GLY:HA2	2.01	0.43
2:F:309:ASN:O	2:F:312:ARG:NH2	2.49	0.43
2:D:256:VAL:HG12	2:D:279:TYR:HB2	2.00	0.43
2:F:108:ASN:HB3	3:F:2010:HOH:O	2.19	0.43
2:C:99:LEU:C	2:C:99:LEU:HD23	2.38	0.43
2:F:149:VAL:HG23	2:F:154:ILE:HG13	2.00	0.43
1:B:362:GLU:CD	1:B:388:LYS:NZ	2.72	0.43
1:E:420:TYR:O	1:E:421:ALA:HB2	2.19	0.43
1:B:402:HIS:HE2	2:D:309:ASN:C	2.22	0.43
2:F:123:GLY:O	2:F:126:ASP:HB2	2.19	0.43
2:F:258:LEU:CD1	2:F:258:LEU:N	2.81	0.43
2:D:179:ILE:HD13	2:D:191:LYS:HD3	1.99	0.43
2:D:147:ILE:HG12	2:D:156:LEU:HD11	2.00	0.43
1:E:439:THR:CG2	1:E:441:ARG:HD3	2.48	0.43
1:B:439:THR:HA	1:B:440:PRO:HD3	1.84	0.43
2:D:288:SER:O	2:D:301:GLY:HA3	2.18	0.43
1:B:410:LYS:N	3:B:2043:HOH:O	2.52	0.43
1:E:404:ARG:HG2	1:E:404:ARG:NH2	2.34	0.43
1:A:381:PRO:HG2	1:A:384:PRO:HA	2.01	0.43
2:F:288:SER:O	2:F:301:GLY:HA3	2.18	0.43
2:D:196:ILE:HG13	2:D:302:SER:HB2	2.01	0.43
1:B:347:VAL:HG11	1:B:351:LYS:HB2	2.01	0.43
1:E:404:ARG:HH21	1:E:404:ARG:HG2	1.83	0.43
2:C:251:SER:HA	2:C:252:PRO:HD3	1.74	0.43
2:D:298:GLU:HG2	2:D:319:LYS:HB3	2.01	0.43
1:E:323:LYS:N	1:E:324:PRO:CD	2.82	0.43
1:A:439:THR:HA	1:A:440:PRO:HD3	1.82	0.43
2:C:112:LYS:O	2:C:143:PHE:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:250:LYS:O	2:F:252:PRO:HD3	2.19	0.43
2:F:266:ASP:HB2	2:F:270:HIS:H	1.82	0.43
2:D:233:TYR:HD1	2:D:244:GLY:HA3	1.84	0.43
2:F:174:PHE:O	2:F:194:PHE:HA	2.19	0.43
1:E:407:VAL:H	1:E:410:LYS:CD	2.30	0.42
2:F:161:PHE:N	3:F:2033:HOH:O	2.52	0.42
2:C:81:LEU:HD13	2:C:140:ARG:O	2.19	0.42
2:F:176:THR:HG21	2:F:179:ILE:HG22	2.01	0.42
2:C:196:ILE:HG13	2:C:302:SER:HB2	2.00	0.42
1:A:368:TYR:H	1:A:368:TYR:HD1	1.67	0.42
2:D:251:SER:HA	2:D:252:PRO:HD3	1.85	0.42
1:A:345:PHE:HA	1:A:346:PRO:C	2.40	0.42
1:E:322:LEU:HD21	1:E:324:PRO:HG3	2.01	0.42
1:A:422:LEU:HD23	1:A:422:LEU:HA	1.26	0.42
1:E:426:GLN:HG3	1:E:438:PRO:HG3	2.02	0.42
2:D:322:LEU:HD12	2:D:322:LEU:HA	1.51	0.42
1:A:352:TYR:HA	1:A:372:ILE:O	2.19	0.42
2:D:249:LEU:HB2	2:D:255:ASN:OD1	2.19	0.42
2:D:161:PHE:CZ	2:D:172:THR:HB	2.55	0.42
2:D:85:LEU:N	3:D:2002:HOH:O	2.07	0.42
1:A:410:LYS:HD2	1:A:411:SER:N	2.34	0.42
1:A:432:MET:HG3	1:A:437:SER:CB	2.49	0.42
2:F:307:THR:O	2:F:310:GLY:HA2	2.20	0.42
2:D:322:LEU:HG	2:D:323:GLU:N	2.35	0.42
1:E:344:TYR:OH	2:F:273:ILE:HA	2.20	0.42
2:C:156:LEU:HD23	2:C:180:GLN:NE2	2.34	0.42
2:F:83:ASP:OD1	2:F:87:ALA:HB2	2.20	0.42
1:A:439:THR:HG22	1:A:441:ARG:HD3	2.01	0.42
2:F:147:ILE:HG12	2:F:156:LEU:HD11	2.02	0.42
1:A:422:LEU:CB	1:A:426:GLN:C	2.88	0.41
2:D:83:ASP:N	3:D:2002:HOH:O	2.52	0.41
1:E:335:LEU:HD23	1:E:355:TYR:HB3	2.02	0.41
2:C:308:VAL:O	2:C:309:ASN:OD1	2.38	0.41
2:F:246:ILE:HG22	2:F:255:ASN:HA	2.01	0.41
2:C:179:ILE:HD13	2:C:191:LYS:HD3	2.02	0.41
2:C:147:ILE:HG21	2:C:156:LEU:HD11	2.03	0.41
2:C:106:ARG:HB2	2:C:109:GLU:CD	2.41	0.41
2:F:246:ILE:HD11	2:F:316:LEU:HD21	2.01	0.41
1:E:383:VAL:CG2	1:E:386:LEU:CD1	2.99	0.41
2:D:236:ASP:O	2:D:240:LYS:N	2.53	0.41
2:F:116:GLN:NE2	3:F:2014:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:PHE:HA	1:A:392:PRO:HD3	1.97	0.41
2:D:322:LEU:CD1	2:D:323:GLU:H	2.34	0.41
2:F:256:VAL:HG21	2:F:277:VAL:HG11	2.01	0.41
1:E:437:SER:HA	1:E:438:PRO:HA	1.75	0.41
1:E:383:VAL:HG13	3:E:2021:HOH:O	2.21	0.41
2:D:221:ALA:O	2:D:229:GLY:HA3	2.21	0.41
2:C:245:LYS:HG3	2:C:257:ASP:OD1	2.21	0.41
1:A:405:LYS:O	3:A:2028:HOH:O	2.22	0.41
1:B:437:SER:HA	1:B:438:PRO:HA	1.67	0.41
2:C:106:ARG:H	2:C:109:GLU:CD	2.22	0.41
1:A:398:TYR:HB3	1:A:400:GLN:OE1	2.21	0.41
2:F:245:LYS:HG3	2:F:257:ASP:OD1	2.20	0.41
2:C:311:ILE:HG13	1:E:393:TYR:OH	2.21	0.41
2:F:309:ASN:N	2:F:310:GLY:CA	2.78	0.41
2:D:178:GLN:CD	3:D:2033:HOH:O	2.59	0.41
2:C:256:VAL:HG12	2:C:279:TYR:HB2	2.02	0.41
2:F:266:ASP:HB2	2:F:270:HIS:O	2.21	0.41
1:E:407:VAL:HB	1:E:410:LYS:HE3	2.02	0.41
2:D:82:ALA:CB	2:D:118:ALA:CB	2.99	0.41
1:E:399:ASN:HB3	1:E:402:HIS:HB2	2.02	0.41
1:B:380:SER:HA	1:B:381:PRO:C	2.40	0.41
2:C:180:GLN:HA	2:C:188:MET:SD	2.61	0.41
2:C:233:TYR:HD1	2:C:244:GLY:HA3	1.86	0.41
1:E:342:ARG:HB3	1:E:343:PRO:HD3	2.02	0.41
2:C:258:LEU:N	2:C:258:LEU:CD1	2.83	0.41
2:F:236:ASP:O	2:F:240:LYS:N	2.54	0.41
2:D:199:ILE:HD13	2:D:301:GLY:HA2	2.03	0.40
1:A:397:GLY:HA2	1:A:417:HIS:H	1.85	0.40
2:F:231:LEU:HD12	2:F:231:LEU:C	2.41	0.40
2:C:147:ILE:CG2	2:C:156:LEU:CD1	2.99	0.40
2:F:91:HIS:CE1	3:F:2004:HOH:O	2.74	0.40
2:C:230:LYS:HD3	2:C:248:HIS:CE1	2.56	0.40
2:D:215:ALA:CB	2:D:320:GLN:HE22	2.33	0.40
2:F:298:GLU:HG2	2:F:319:LYS:HB3	2.02	0.40
2:F:147:ILE:CG2	2:F:156:LEU:CD1	2.99	0.40
2:F:156:LEU:CD2	2:F:180:GLN:NE2	2.80	0.40
2:D:120:LYS:HG2	2:D:121:THR:N	2.36	0.40
1:E:347:VAL:CG1	1:E:351:LYS:CB	3.00	0.40
2:C:110:LYS:NZ	3:C:2034:HOH:O	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:O	2:F:214:ARG:NH2[4_454]	2.18	0.02

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	107/123 (87%)	99 (92%)	7 (6%)	1 (1%)	21	22
1	B	119/123 (97%)	110 (92%)	9 (8%)	0	100	100
1	E	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
2	C	240/253 (95%)	219 (91%)	18 (8%)	3 (1%)	15	13
2	D	239/253 (94%)	219 (92%)	18 (8%)	2 (1%)	24	26
2	F	236/253 (93%)	217 (92%)	17 (7%)	2 (1%)	24	26
All	All	1061/1128 (94%)	977 (92%)	76 (7%)	8 (1%)	24	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	425	ALA
2	C	129	ASN
2	D	129	ASN
2	F	129	ASN
2	C	310	GLY
2	F	310	GLY
2	C	123	GLY
2	D	123	GLY

5.3.2 Protein sidechains [i](#)

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	101/108 (94%)	92 (91%)	9 (9%)	12	12
1	B	106/108 (98%)	99 (93%)	7 (7%)	21	23
1	E	107/108 (99%)	98 (92%)	9 (8%)	14	14
2	C	189/194 (97%)	177 (94%)	12 (6%)	22	25
2	D	191/194 (98%)	177 (93%)	14 (7%)	17	19
2	F	187/194 (96%)	172 (92%)	15 (8%)	15	16
All	All	881/906 (97%)	815 (92%)	66 (8%)	17	18

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	ASP
1	A	340	MET
1	A	380	SER
1	A	387	ARG
1	A	413	ASP
1	A	416	CYS
1	A	424	LYS
1	A	426	GLN
1	A	443	ILE
1	B	329	ASP
1	B	347	VAL
1	B	388	LYS
1	B	412	ILE
1	B	427	THR
1	B	428	THR
1	B	441	ARG
2	C	83	ASP
2	C	85	LEU
2	C	89	LEU
2	C	98	SER
2	C	107	LYS
2	C	122	TYR
2	C	211	GLU
2	C	216	THR
2	C	231	LEU
2	C	258	LEU
2	C	283	GLU

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Mol	Chain	Res	Type
2	C	302	SER
2	D	89	LEU
2	D	90	ASP
2	D	94	LYS
2	D	98	SER
2	D	107	LYS
2	D	122	TYR
2	D	157	GLU
2	D	216	THR
2	D	231	LEU
2	D	258	LEU
2	D	278	LEU
2	D	283	GLU
2	D	302	SER
2	D	323	GLU
1	E	347	VAL
1	E	359	GLU
1	E	380	SER
1	E	383	VAL
1	E	386	LEU
1	E	387	ARG
1	E	388	LYS
1	E	427	THR
1	E	428	THR
2	F	83	ASP
2	F	85	LEU
2	F	89	LEU
2	F	91	HIS
2	F	92	LYS
2	F	107	LYS
2	F	122	TYR
2	F	129	ASN
2	F	143	PHE
2	F	152	GLN
2	F	216	THR
2	F	231	LEU
2	F	258	LEU
2	F	283	GLU
2	F	302	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	146	GLN
2	C	152	GLN
2	C	166	GLN
2	C	175	GLN
2	C	309	ASN
2	D	166	GLN
2	F	129	ASN
2	F	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, 95th 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 ²)	Q<0.9
1	A	115/123 (93%)	1.29	24 (20%) 1 2	26, 40, 68, 91	3 (2%)
1	B	121/123 (98%)	1.05	27 (22%) 1 2	20, 35, 61, 79	2 (1%)
1	E	122/123 (99%)	1.25	21 (17%) 2 3	24, 40, 65, 82	2 (1%)
2	C	242/253 (95%)	0.74	27 (11%) 7 12	14, 31, 66, 81	1 (0%)
2	D	243/253 (96%)	0.80	24 (9%) 9 16	18, 38, 70, 96	2 (0%)
2	F	240/253 (94%)	1.25	47 (19%) 1 2	27, 47, 79, 93	1 (0%)
All	All	1083/1128 (96%)	1.02	170 (15%) 3 5	14, 39, 70, 96	11 (1%)

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	151	GLY	16.7
2	C	154	ILE	8.8
2	C	147	ILE	8.5
2	C	153	LEU	7.9
2	C	149	VAL	7.7
2	C	156	LEU	7.6
2	C	184	HIS	7.0
2	F	150	ASP	6.5
2	F	149	VAL	6.5
2	D	187	LYS	5.9
2	D	323	GLU	5.8
2	D	184	HIS	5.7
2	F	152	GLN	5.7
1	E	423	PRO	5.5
2	C	183	GLU	5.3
2	F	186	GLY	5.2
1	A	424	LYS	5.1
2	D	186	GLY	5.1
2	F	151	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
2	C	186	GLY	4.7
2	C	150	ASP	4.6
2	F	87	ALA	4.5
2	C	148	GLU	4.5
1	B	424	LYS	4.5
2	C	185	SER	4.5
1	A	443	ILE	4.4
2	F	185	SER	4.4
2	D	151	GLY	4.3
2	F	89	LEU	4.2
1	B	407	VAL	4.2
2	C	155	THR	4.1
2	F	147	ILE	4.1
2	D	82	ALA	4.0
1	B	443	ILE	4.0
2	F	116	GLN	3.9
2	F	148	GLU	3.9
2	C	146	GLN	3.9
1	A	430	THR	3.9
1	A	414	VAL	3.8
2	D	195	ARG	3.8
1	E	390	TYR	3.7
2	C	182	SER	3.7
2	F	189	VAL	3.7
1	E	441	ARG	3.7
1	E	322	LEU	3.6
1	E	407	VAL	3.6
2	D	116	GLN	3.6
2	F	156	LEU	3.5
1	B	421	ALA	3.5
1	A	441	ARG	3.5
1	A	390	TYR	3.5
1	E	426	GLN	3.5
2	F	214	ARG	3.4
2	F	180	GLN	3.4
2	C	181	ASP	3.4
1	A	383	VAL	3.4
1	E	424	LYS	3.3
2	D	183	GLU	3.3
1	E	383	VAL	3.3
2	F	85	LEU	3.3
2	F	106	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	154	ILE	3.2
2	F	84	ALA	3.2
2	F	94	LYS	3.2
1	E	422	LEU	3.2
2	F	134	LYS	3.2
2	F	179	ILE	3.1
2	F	123	GLY	3.1
1	A	406	PHE	3.1
1	E	428	THR	3.1
2	D	83	ASP	3.0
2	D	149	VAL	3.0
2	F	138	VAL	2.9
1	E	443	ILE	2.9
2	F	230	LYS	2.9
2	D	154	ILE	2.9
2	C	190	ALA	2.9
2	D	214	ARG	2.9
1	B	418	PRO	2.9
1	E	434	ASN	2.9
2	D	152	GLN	2.9
2	F	184	HIS	2.8
2	F	91	HIS	2.8
1	B	439	THR	2.8
1	A	428	THR	2.8
2	D	87	ALA	2.8
2	C	152	GLN	2.7
2	F	145	ARG	2.7
2	F	117	GLY	2.7
2	F	190	ALA	2.7
2	D	178	GLN	2.7
2	F	105	VAL	2.7
2	F	218	ARG	2.6
1	B	398	TYR	2.6
2	F	90	ASP	2.6
1	A	404	ARG	2.6
1	A	412	ILE	2.6
1	A	420	TYR	2.6
1	B	422	LEU	2.6
1	A	410	LYS	2.6
2	F	191	LYS	2.6
1	E	348	ALA	2.6
2	D	322	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	413	ASP	2.5
1	B	435	GLY	2.5
1	B	393	TYR	2.5
1	E	420	TYR	2.5
1	B	438	PRO	2.5
2	F	82	ALA	2.5
1	A	411	SER	2.5
2	F	131	GLY	2.5
2	C	107	LYS	2.4
1	B	425	ALA	2.4
2	D	185	SER	2.4
2	C	89	LEU	2.4
1	E	404	ARG	2.4
2	C	111	LEU	2.4
1	A	429	VAL	2.4
2	D	150	ASP	2.4
1	B	437	SER	2.4
1	B	423	PRO	2.4
2	F	187	LYS	2.4
2	F	182	SER	2.3
1	B	441	ARG	2.3
2	F	107	LYS	2.3
2	F	118	ALA	2.3
1	E	409	GLY	2.3
1	B	323	LYS	2.3
2	D	94	LYS	2.3
2	F	153	LEU	2.3
1	B	390	TYR	2.3
1	A	362	GLU	2.3
1	B	395	GLU	2.3
1	B	400	GLN	2.3
2	F	243	ASN	2.3
2	C	189	VAL	2.3
2	F	196	ILE	2.3
2	F	176	THR	2.2
1	E	347	VAL	2.2
1	E	406	PHE	2.2
1	B	376	GLN	2.2
1	E	331	LYS	2.2
2	F	109	GLU	2.2
1	A	353	TYR	2.2
1	A	366	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	403	GLY	2.2
1	B	368	TYR	2.2
1	B	426	GLN	2.2
2	D	180	GLN	2.2
2	D	179	ILE	2.2
2	F	229	GLY	2.2
1	B	406	PHE	2.2
1	A	440	PRO	2.1
1	B	415	ALA	2.1
2	F	215	ALA	2.1
2	C	116	GLN	2.1
2	D	95	GLY	2.1
2	D	188	MET	2.1
1	A	407	VAL	2.1
1	A	352	TYR	2.1
2	C	211	GLU	2.1
1	A	375	THR	2.1
2	C	243	ASN	2.1
1	B	404	ARG	2.1
1	B	428	THR	2.1
1	E	380	SER	2.1
1	E	332	HIS	2.0
1	A	382	ALA	2.0
2	C	144	ILE	2.0
2	C	230	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.