



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:05 PM UTC

PDB ID : 2W81 / pdb_00002w81
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

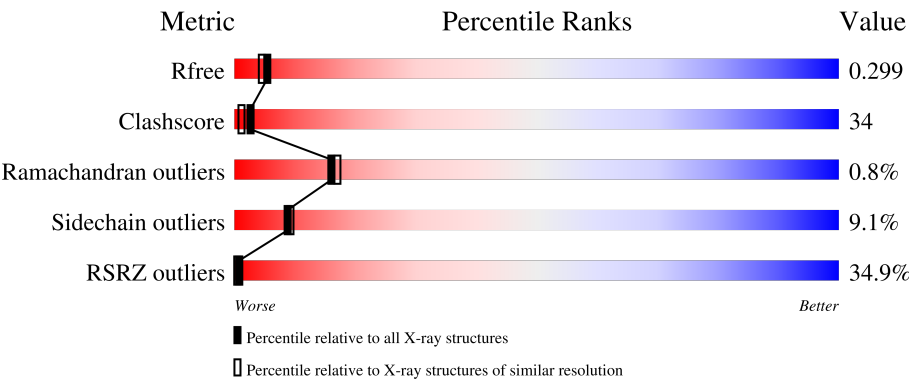
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	42% 37%48%7%7%
1	B	123	37% 54%39%5%
1	E	123	46% 48%43%7%
2	C	253	18% 57%33%5%
2	D	253	25% 47%41%8%

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Mol	Chain	Length	Quality of chain
2	F	253	45% 46% 41% 7% 5%

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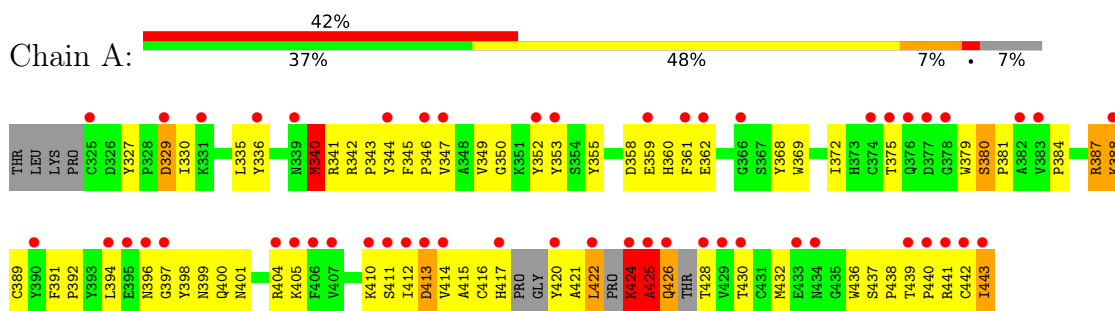
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	98	Total 98	O 98	0	0
3	D	99	Total 99	O 99	0	0
3	E	46	Total 46	O 46	0	0
3	F	90	Total 90	O 90	0	0

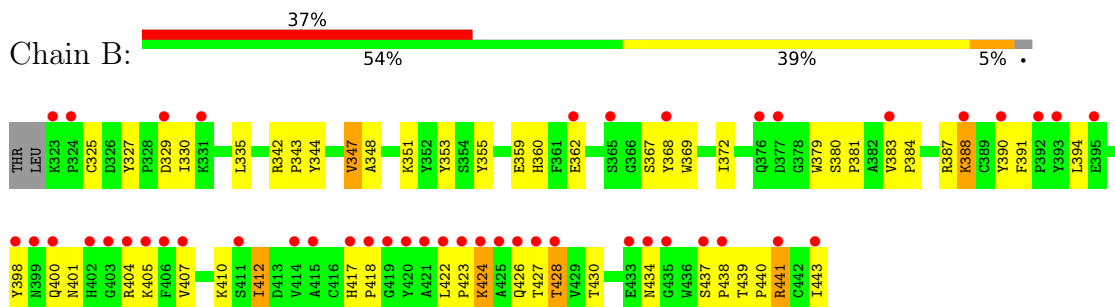
3 Residue-property plots [i](#)

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

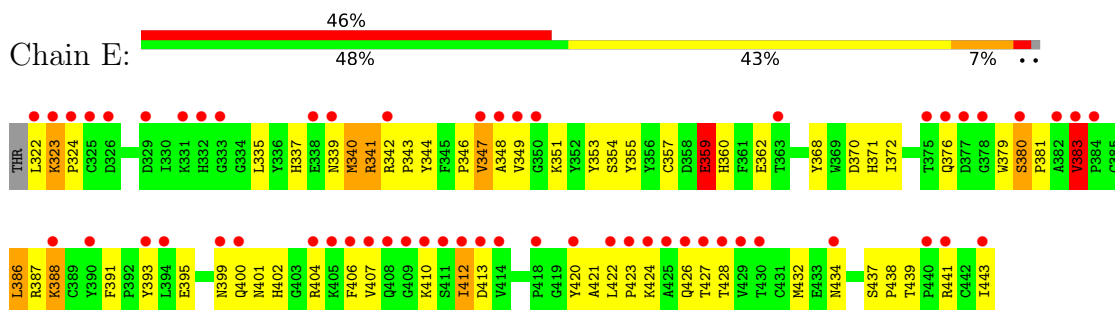
• Molecule 1: COMPLEMENT FACTOR H



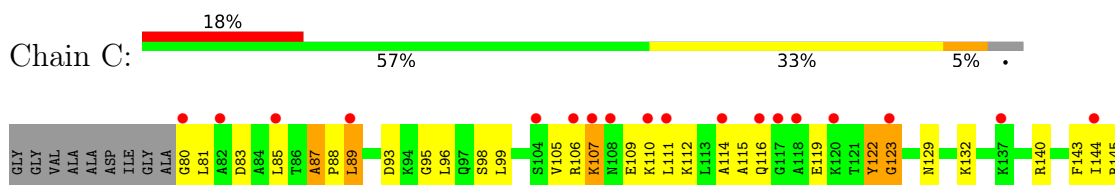
• Molecule 1: COMPLEMENT FACTOR H

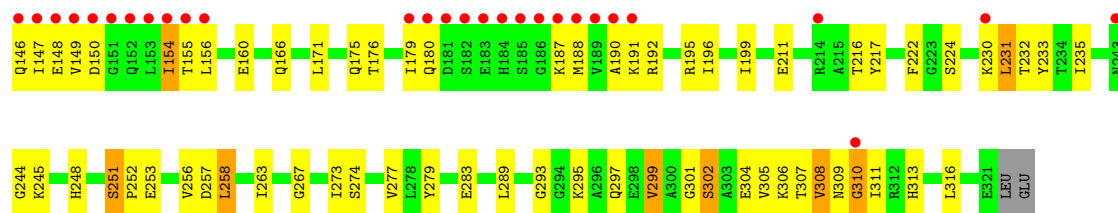


• Molecule 1: COMPLEMENT FACTOR H

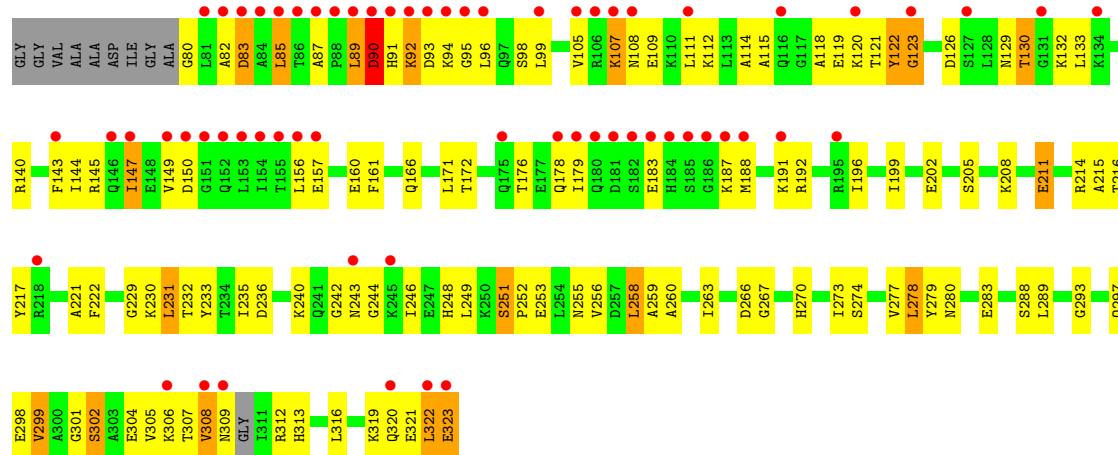


• Molecule 2: FACTOR H BINDING PROTEIN

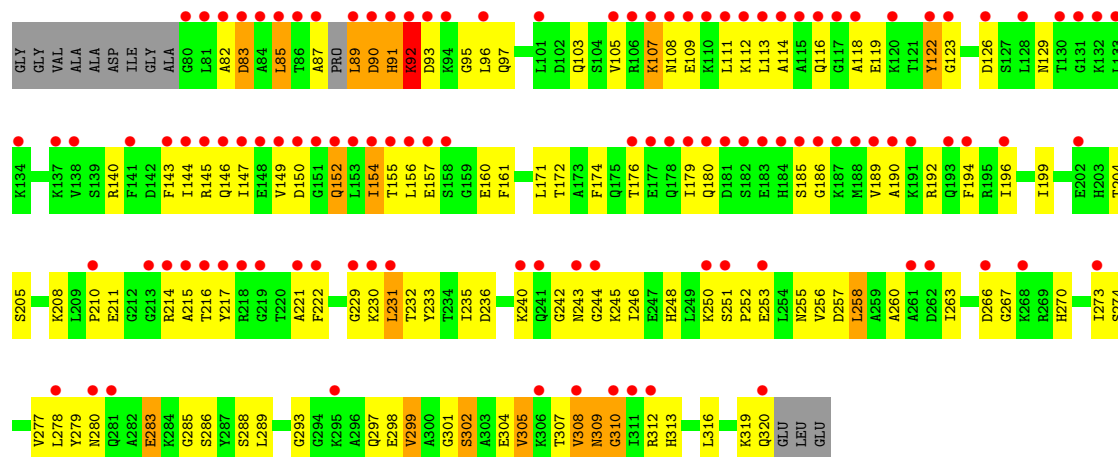




• Molecule 2: FACTOR H BINDING PROTEIN



• 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 38.81 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.8 (38.81-2.35) 94.0 (38.81-2.35)	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		Depositor
R, R_{free}	0.274 , 0.283 0.289 , 0.299	Depositor DCC
R_{free} test set	2187 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.74	1/977 (0.1%)	1.14	11/1325 (0.8%)
1	B	0.44	0/1024	0.87	5/1396 (0.4%)
1	E	0.56	1/1032 (0.1%)	0.99	6/1407 (0.4%)
2	C	0.41	0/1857	0.91	6/2491 (0.2%)
2	D	0.43	0/1869	0.95	10/2506 (0.4%)
2	F	0.40	0/1839	0.85	7/2464 (0.3%)
All	All	0.48	2/8598 (0.0%)	0.94	45/11589 (0.4%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	MET	SD-CE	-9.86	1.54	1.79
1	E	340	MET	SD-CE	-8.19	1.59	1.79

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	90	ASP	N-CA-C	-15.22	86.52	109.81
2	C	87	ALA	CA-C-N	11.15	131.07	120.03
2	C	87	ALA	C-N-CA	11.15	131.07	120.03
2	D	92	LYS	N-CA-C	-10.03	100.45	112.89
2	C	87	ALA	N-CA-C	9.21	121.34	109.64
1	E	383	VAL	CA-C-N	9.12	129.17	119.05
1	E	383	VAL	C-N-CA	9.12	129.17	119.05
2	C	251	SER	CA-C-N	8.99	129.57	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	251	SER	C-N-CA	8.99	129.57	119.32
2	F	251	SER	CA-C-N	7.39	127.74	119.32
2	F	251	SER	C-N-CA	7.39	127.74	119.32
1	A	329	ASP	N-CA-C	-7.24	97.44	109.46
1	A	425	ALA	N-CA-C	6.82	125.33	110.80
1	E	341	ARG	N-CA-C	6.58	119.42	111.40
2	D	91	HIS	N-CA-CB	-6.47	100.75	111.49
2	D	83	ASP	CB-CA-C	-6.45	98.97	111.03
1	E	368	TYR	N-CA-C	-6.24	105.31	113.17
2	D	322	LEU	N-CA-C	6.22	120.03	110.20
2	F	90	ASP	N-CA-C	6.17	118.79	109.23
2	D	251	SER	CA-C-N	6.15	126.33	119.32
2	D	251	SER	C-N-CA	6.15	126.33	119.32
1	E	357	CYS	N-CA-C	-6.11	100.96	110.42
1	A	424	LYS	CA-C-N	6.09	133.16	121.54
1	A	424	LYS	C-N-CA	6.09	133.16	121.54
2	F	267	GLY	N-CA-C	-6.09	106.79	114.16
2	D	321	GLU	N-CA-C	5.82	118.92	110.42
2	F	92	LYS	N-CA-C	5.73	119.47	111.56
1	A	350	GLY	N-CA-C	-5.68	107.21	114.37
1	A	425	ALA	CA-C-N	5.67	131.91	121.70
1	A	425	ALA	C-N-CA	5.67	131.91	121.70
2	D	211	GLU	N-CA-C	5.64	120.31	113.38
2	D	267	GLY	N-CA-C	-5.57	107.42	114.16
1	B	325	CYS	N-CA-C	5.57	117.37	108.41
1	B	383	VAL	CA-C-N	5.56	125.22	119.05
1	B	383	VAL	C-N-CA	5.56	125.22	119.05
1	E	359	GLU	N-CA-C	5.53	118.83	111.75
1	A	327	TYR	CA-C-N	5.42	125.68	119.83
1	A	327	TYR	C-N-CA	5.42	125.68	119.83
2	F	309	ASN	N-CA-C	5.39	121.71	113.19
1	A	388	LYS	CB-CA-C	-5.29	99.85	109.38
1	A	422	LEU	CA-CB-CG	-5.25	97.92	116.30
2	C	267	GLY	N-CA-C	-5.15	107.92	114.16
2	F	305	VAL	N-CA-C	5.06	115.26	108.17
1	B	327	TYR	CA-C-N	-5.05	113.53	119.84
1	B	327	TYR	C-N-CA	-5.05	113.53	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

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	84	1
1	B	984	0	897	64	0
1	E	992	0	908	92	0
2	C	1832	0	1820	94	0
2	D	1845	0	1833	115	0
2	F	1816	0	1806	134	1
3	A	36	0	0	9	0
3	B	55	0	0	18	0
3	C	98	0	0	15	0
3	D	99	0	0	18	0
3	E	46	0	0	19	0
3	F	90	0	0	25	0
All	All	8836	0	8114	557	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 34.

All (557) 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
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
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
1:A:422:LEU:HD12	1:A:426:GLN:C	1.99	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:171:LEU:HD11	2:C:222:PHE:HZ	1.45	0.81
1:E:407:VAL:HG12	1:E:410:LYS:HE3	1.62	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
1:E:362:GLU:HG3	1:E:388:LYS:HZ2	1.45	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
1:A:442:CYS:C	1:A:443:ILE:HG13	2.07	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:362:GLU:CD	1:A:388:LYS:NZ	2.45	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: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
2:F:152:GLN:HB2	3:F:2088:HOH:O	1.93	0.69
1:E:337:HIS:HB3	1:E:340:MET:HE3	1.73	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:E:362:GLU:HG3	1:E:388:LYS:NZ	2.08	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:A:359:GLU:H	1:A:359:GLU:CD	2.02	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:D:89:LEU:HD23	2:D:89:LEU:H	1.58	0.67
2:F:277:VAL:HG11	2:F:305:VAL:HG22	1.77	0.67
1:E:407:VAL:CG1	1:E:410:LYS:HE3	2.25	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
1:E:406:PHE:HA	1:E:410:LYS:HZ2	1.59	0.66
1:B:410:LYS:HG3	3:B:2043:HOH:O	1.94	0.66
2:F:253:GLU:OE1	2:F:307:THR:HB	1.96	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
2:F:156:LEU:HD23	2:F:180:GLN:NE2	2.11	0.65
1:A:410:LYS:O	1:A:430:THR:HG23	1.97	0.65
2:C:289:LEU:HD13	2:C:299:VAL:CG1	2.25	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:F:231:LEU:HD22	2:F:316:LEU:HD22	1.78	0.65
1:A:362:GLU:CD	1:A:388:LYS:HZ2	2.05	0.65
2:D:89:LEU:H	2:D:89:LEU:CD2	2.01	0.65
1:B:359:GLU:HG2	3:B:2014:HOH:O	1.97	0.65
2:F:289:LEU:HD13	2:F:299:VAL:CG1	2.24	0.65
2:F:107:LYS:HD3	2:F:107:LYS:C	2.21	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
2:C:310:GLY:HA3	1:E:393:TYR:CD2	2.32	0.64
1:E:322:LEU:HD12	1:E:323:LYS:N	2.13	0.64
2:D:95:GLY:HA2	2:D:96:LEU:C	2.22	0.64
2:D:188:MET:HB3	3:D:2033:HOH:O	1.97	0.64
1:E:406:PHE:HA	1:E:410:LYS:NZ	2.13	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
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:107:LYS:HD3	2:D:107:LYS:C	2.23	0.62
2:D:188:MET:H	2:F:190:ALA:HB3	1.63	0.62
1:E:362:GLU:CD	1:E:388:LYS:HZ1	2.06	0.62
2:F:112:LYS:HE2	2:F:119:GLU:OE2	1.97	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:C:107:LYS:HD3	2:C:107:LYS:C	2.23	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
2:C:93:ASP:OD2	2:C:132:LYS:HE2	1.98	0.62
1:E:407:VAL:H	1:E:410:LYS:CE	2.12	0.62
2:C:309:ASN:ND2	2:F:150:ASP:HB3	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:231:LEU:HD12	2:D:232:THR:H	1.65	0.61
1:E:322:LEU:CD1	1:E:324:PRO:HD3	2.29	0.61
2:C:95:GLY:HA2	2:C:96:LEU:C	2.25	0.61
1:E:323:LYS:HD2	1:E:346:PRO:O	2.01	0.61
1:B:438:PRO:HA	3:B:2054:HOH:O	1.99	0.61
2:D:93:ASP:OD2	2:D:132:LYS:HE2	2.01	0.61
2:D:108:ASN:HB2	3:D:2012:HOH:O	2.00	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:F:147:ILE:HG23	2:F:156:LEU:HD12	1.83	0.61
2:C:112:LYS:HE2	2:C:119:GLU:OE2	2.00	0.61
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
1:B:417:HIS:CE1	3:B:2033:HOH:O	2.56	0.59
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
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
1:A:347:VAL:HG11	1:A:353:TYR:OH	2.03	0.59
2:C:166:GLN:HA	3:C:2026:HOH:O	2.02	0.59
2:D:82:ALA:C	3:D:2002:HOH:O	2.46	0.59
2:D:82:ALA:CB	2:D:118:ALA:HB2	2.33	0.58
2:D:147:ILE:CG2	2:D:156:LEU:HD11	2.33	0.58
2:D:277:VAL:HG11	2:D:305:VAL:HG22	1.85	0.58
2:F:250:LYS:HG2	3:F:2064:HOH:O	2.03	0.58
2:F:109:GLU:OE2	2:F:145:ARG:NH1	2.36	0.58
2:F:308:VAL:O	2:F:309:ASN:ND2	2.37	0.58
1:B:407:VAL:HG12	1:B:410:LYS:CE	2.33	0.58
2:D:112:LYS:HE2	2:D:119:GLU:OE2	2.03	0.58
1:E:359:GLU:OE1	1:E:360:HIS:NE2	2.36	0.58
2:C:176:THR:O	2:C:192:ARG:HA	2.04	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
1:B:387:ARG:HH11	1:B:434:ASN:C	2.12	0.58
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:422:LEU:C	3:E:2041:HOH:O	2.46	0.57
2:D:90:ASP:OD1	2:D:92:LYS:HG3	2.05	0.57
1:E:434:ASN:HB2	3:E:2044:HOH:O	2.05	0.57
2:D:187:LYS:HG3	2:F:189:VAL:CG1	2.33	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
2:F:143:PHE:N	3:F:2033:HOH:O	2.38	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
1:A:372:ILE:HD11	1:A:379:TRP:HB3	1.88	0.56
1:A:420:TYR:CD1	1:A:443:ILE:CG2	2.88	0.56
1:A:422:LEU:CD1	1:A:426:GLN:C	2.78	0.56
1:E:340:MET:HE2	3:E:2009:HOH:O	2.05	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:F:113:LEU:C	3:F:2013:HOH:O	2.48	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: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:F:289:LEU:HD22	2:F:299:VAL:CG1	2.37	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:D:115:ALA:HB1	3:D:2022:HOH:O	2.07	0.55
2:F:304:GLU:HG2	2:F:313:HIS:CD2	2.42	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:LYS:N	1:E:324:PRO:HD3	2.22	0.54
1:A:380:SER:HA	1:A:381:PRO:C	2.32	0.54
1:B:388:LYS:HZ2	1:B:405:LYS:NZ	2.06	0.54
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: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
1:E:421:ALA:O	1:E:443:ILE:HG13	2.08	0.54
2:F:82:ALA:HA	2:F:118:ALA:CB	2.37	0.54
2:C:89:LEU:N	2:C:89:LEU:HD12	2.23	0.54
1:A:422:LEU:HB2	1:A:426:GLN:C	2.31	0.54
2:C:148:GLU:HB2	3:C:2034:HOH:O	2.06	0.54
1:E:421:ALA:N	1:E:443:ILE:O	2.41	0.54
1:A:424:LYS:N	1:A:425:ALA:HB2	2.23	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:CB	2.72	0.54
2:F:97:GLN:HG3	3:F:2006:HOH:O	2.06	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
1:A:375:THR:C	3:A:2016:HOH:O	2.52	0.53
2:D:230:LYS:HG2	3:D:2060:HOH:O	2.08	0.53
1:E:362:GLU:CG	1:E:388:LYS:NZ	2.71	0.53
2:D:147:ILE:HG21	2:D:156:LEU:HD11	1.89	0.53
2:D:256:VAL:CG2	2:D:277:VAL:HG13	2.37	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
1:B:422:LEU:HB3	1:B:426:GLN:HB2	1.90	0.53
2:D:188:MET:CB	3:D:2033:HOH:O	2.57	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:423:PRO:CG	3:B:2055:HOH:O	2.56	0.53
1:B:443:ILE:HD12	1:B:443:ILE:O	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
2:C:105:VAL:HG22	2:C:111:LEU:HB2	1.91	0.52
2:F:85:LEU:CD2	3:F:2013:HOH:O	2.56	0.52
1:A:362:GLU:HB2	1:A:388:LYS:CE	2.36	0.52
1:B:368:TYR:OH	2:C:195:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:256:VAL:CG2	2:C:277:VAL:HG13	2.38	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
1:B:443:ILE:HD12	1:B:443:ILE:C	2.35	0.52
2:D:266:ASP:CB	2:D:270:HIS:H	2.23	0.52
2:F:171:LEU:CD1	2:F:222:PHE:HZ	2.16	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:105:VAL:HG22	2:F:111:LEU:HB2	1.92	0.52
2:F:140:ARG:HB3	2:F:160:GLU:OE2	2.10	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:A:342:ARG:HB3	1:A:343:PRO:HD3	1.91	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:401:ASN:O	1:A:404:ARG:HB2	2.10	0.51
1:B:367:SER:HB3	3:B:2018:HOH:O	2.09	0.51
2:C:149:VAL:HG12	3:C:2037:HOH:O	2.09	0.51
2:F:107:LYS:HD3	2:F:107:LYS:O	2.10	0.51
2:F:90:ASP:OD1	2:F:91:HIS:N	2.41	0.51
2:F:250:LYS:HA	3:F:2064:HOH:O	2.10	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
2:C:146:GLN:HG2	2:C:155:THR:HA	1.91	0.51
1:E:349:VAL:CG2	3:E:2018:HOH:O	2.59	0.51
2:F:122:TYR:HB3	2:F:123:GLY:HA3	1.92	0.51
2:C:263:ILE:HG12	2:C:273:ILE:HG12	1.92	0.51
1:E:422:LEU:HB3	3:E:2041:HOH:O	2.11	0.51
1:A:375:THR:CB	1:B:418:PRO:HB2	2.40	0.51
1:E:407:VAL:CB	1:E:410:LYS:HE3	2.41	0.51
2:F:152:GLN:HG2	2:F:152:GLN:O	2.10	0.51
2:F:180:GLN:OE1	2:F:185:SER:HA	2.11	0.51
2:F:95:GLY:HA2	2:F:96:LEU:C	2.36	0.50
2:F:176:THR:HG21	2:F:179:ILE:CG2	2.41	0.50
2:D:240:LYS:NZ	3:D:2061:HOH:O	2.42	0.50
1:E:404:ARG:NE	3:E:2029:HOH:O	2.43	0.50
1:E:407:VAL:H	1:E:410:LYS:HE3	1.76	0.50
2:C:231:LEU:HD22	2:C:316:LEU:HD22	1.92	0.50
1:E:443:ILE:HD12	1:E:443:ILE:C	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:426:GLN:CB	3:E:2041:HOH:O	2.58	0.50
2:F:161:PHE:CZ	2:F:172:THR:HB	2.47	0.50
1:B:362:GLU:HG2	3:B:2016:HOH:O	2.12	0.50
2:C:175:GLN:NE2	2:C:224:SER:OG	2.37	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
1:A:335:LEU:HD23	1:A:355:TYR:HB3	1.94	0.50
1:B:359:GLU:O	1:B:360:HIS:HB2	2.12	0.50
1:E:407:VAL:O	1:E:410:LYS:HB2	2.12	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:E:337:HIS:CE1	2:F:103:GLN:NE2	2.78	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
2:D:308:VAL:O	2:D:308:VAL:HG23	2.11	0.49
1:E:423:PRO:O	3:E:2041:HOH:O	2.20	0.49
2:F:150:ASP:C	2:F:152:GLN:H	2.19	0.49
2:D:99:LEU:C	2:D:99:LEU:HD23	2.38	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
1:E:380:SER:HA	1:E:381:PRO:C	2.38	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
2:C:304:GLU:HG2	2:C:313:HIS:CD2	2.48	0.48
1:E:371:HIS:NE2	2:F:313:HIS:NE2	2.48	0.48
2:D:123:GLY:O	2:D:126:ASP:HB2	2.12	0.48
2:F:112:LYS:O	2:F:143:PHE:HA	2.14	0.48
2:C:149:VAL:CG2	2:C:154:ILE:HG13	2.44	0.48
1:B:330:ILE:HG23	1:B:384:PRO:HG2	1.96	0.48
1:E:322:LEU:N	3:E:2001:HOH:O	2.47	0.48
2:C:89:LEU:HB3	3:C:2007:HOH:O	2.12	0.48
2:C:99:LEU:HD23	2:C:99:LEU:C	2.38	0.48
2:D:304:GLU:HG2	2:D:313:HIS:CD2	2.48	0.48
1:B:362:GLU:CD	1:B:388:LYS:NZ	2.72	0.48
1:B:388:LYS:HZ2	1:B:405:LYS:HE3	1.79	0.48
1:A:396:ASN:O	1:A:417:HIS:HB2	2.13	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
1:E:407:VAL:HG12	1:E:410:LYS:CE	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:VAL:HG22	3:C:2035:HOH:O	2.14	0.47
2:F:230:LYS:HD2	3:F:2062:HOH:O	2.13	0.47
2:F:221:ALA:O	2:F:229:GLY:HA3	2.14	0.47
2:C:116:GLN:N	3:C:2015:HOH:O	2.46	0.47
1:A:413:ASP:N	1:A:413:ASP:OD2	2.45	0.47
1:A:437:SER:HA	1:A:438:PRO:HA	1.73	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
2:C:87:ALA:HA	2:C:88:PRO:HD3	1.63	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:F:231:LEU:HD12	2:F:232:THR:H	1.78	0.47
1:B:404:ARG:NH1	3:B:2040:HOH:O	2.48	0.47
2:D:215:ALA:CB	2:D:320:GLN:NE2	2.75	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
3:B:2030:HOH:O	2:D:306:LYS:HE2	2.15	0.47
2:D:205:SER:HB3	2:D:208:LYS:HB2	1.95	0.47
2:D:279:TYR:O	2:D:280:ASN:HB2	2.15	0.47
2:F:215:ALA:HB1	2:F:320:GLN:OE1	2.15	0.47
1:A:399:ASN:HA	3:A:2022:HOH:O	2.15	0.47
1:B:342:ARG:HB3	1:B:343:PRO:HD3	1.96	0.47
1:A:345:PHE:HA	1:A:346:PRO:C	2.40	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:388:LYS:HZ2	1:B:405:LYS:HZ1	1.63	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:C:106:ARG:HB2	2:C:109:GLU:CD	2.41	0.46
1:A:422:LEU:CB	1:A:426:GLN:C	2.88	0.46
1:B:388:LYS:HZ2	1:B:405:LYS:CE	2.28	0.46
2:C:89:LEU:CD1	2:C:89:LEU:H	2.29	0.46
2:D:259:ALA:HB2	2:D:278:LEU:CD1	2.42	0.46
1:B:344:TYR:CE1	2:C:274:SER:HB2	2.51	0.46
1:E:347:VAL:HG13	1:E:351:LYS:HB2	1.97	0.46
2:F:112:LYS:HZ3	2:F:119:GLU:HG3	1.80	0.46
1:A:359:GLU:HG2	3:D:2012:HOH:O	2.16	0.46
1:A:412:ILE:CG2	1:A:413:ASP:H	2.26	0.46
1:A:422:LEU:CD2	1:A:441:ARG:O	2.64	0.46
2:F:157:GLU:OE2	2:F:176:THR:OG1	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:ARG:H	2:C:109:GLU:CD	2.22	0.46
1:B:372:ILE:HD11	1:B:379:TRP:HB3	1.97	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
2:D:178:GLN:CD	3:D:2033:HOH:O	2.59	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:N	2:D:258:LEU:CD1	2.79	0.46
1:B:380:SER:HA	1:B:381:PRO:C	2.40	0.45
1:B:407:VAL:HG12	1:B:410:LYS:HE3	1.97	0.45
1:A:336:TYR:O	1:A:341:ARG:NH1	2.49	0.45
1:A:414:VAL:CG2	1:A:422:LEU:HD11	2.46	0.45
2:D:149:VAL:O	2:D:150:ASP:HB2	2.15	0.45
1:A:420:TYR:O	1:A:421:ALA:HB2	2.17	0.45
2:C:89:LEU:N	2:C:89:LEU:CD1	2.80	0.45
1:E:354:SER:HA	1:E:370:ASP:O	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:107:LYS:HD3	2:C:107:LYS: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
1:E:439:THR:HG22	1:E:441:ARG:HD3	1.96	0.45
2:F:231:LEU:HD12	2:F:231:LEU:C	2.41	0.45
2:D:105:VAL:HG22	2:D:111:LEU:HB2	1.98	0.45
2:D:112:LYS:HZ3	2:D:119:GLU:HG3	1.81	0.45
2:D:147:ILE:HG23	2:D:156:LEU:CD1	2.47	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
1:B:335:LEU:HD23	1:B:355:TYR:HB3	1.98	0.45
1:B:362:GLU:HG3	1:B:388:LYS:HD3	1.99	0.45
1:A:389:CYS:HB3	1:A:436:TRP:CE2	2.51	0.45
1:A:396:ASN:HB3	1:A:420:TYR:CG	2.51	0.45
2:C:106:ARG:N	2:C:109:GLU:HG2	2.31	0.45
2:C:176:THR:HG21	2:C:179:ILE:HG22	1.98	0.45
2:F:320:GLN:O	2:F:320:GLN:HG3	2.16	0.45
1:A:391:PHE:HB3	1:A:401:ASN:O	2.17	0.45
2:C:140:ARG:HD3	2:C:160:GLU:OE2	2.16	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:D:114:ALA:O	2:D:115:ALA:HB2	2.16	0.44
2:F:205:SER:HB3	2:F:208:LYS:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:LYS:O	1:A:430:THR:HA	2.17	0.44
2:C:114:ALA:O	2:C:115:ALA:HB2	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
1:A:340:MET:HE3	2:D:289:LEU:C	2.43	0.44
1:B:407:VAL:HG12	1:B:410:LYS:CD	2.47	0.44
2:C:231:LEU:HD12	2:C:232:THR:H	1.79	0.44
2:F:147:ILE:HG23	2:F:156:LEU:CD1	2.48	0.44
1:A:344:TYR:CE1	2:D:274:SER:HB2	2.52	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:422:LEU:CG	1:A:426:GLN:C	2.91	0.44
2:D:107:LYS:HD3	2:D:107:LYS:O	2.17	0.44
2:F:278:LEU:HD23	2:F:283:GLU:HA	2.00	0.44
1:A:398:TYR:HD2	1:A:415:ALA:HB1	1.83	0.44
2:F:280:ASN:HB3	3:F:2075:HOH:O	2.17	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
1:E:347:VAL:HG11	1:E:351:LYS:HB2	2.00	0.44
1:B:424:LYS:CG	3:B:2048:HOH:O	2.66	0.43
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: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: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:F:309:ASN:O	2:F:312:ARG:NH2	2.49	0.43
1:E:420:TYR:O	1:E:421:ALA:HB2	2.19	0.43
2:F:123:GLY:O	2:F:126:ASP:HB2	2.19	0.43
2:F:149:VAL:HG23	2:F:154:ILE:HG13	2.00	0.43
2:F:258:LEU:CD1	2:F:258:LEU:N	2.81	0.43
1:B:439:THR:HA	1:B:440:PRO:HD3	1.84	0.43
2:D:147:ILE:HG12	2:D:156:LEU:HD11	2.00	0.43
2:D:179:ILE:HD13	2:D:191:LYS:HD3	1.99	0.43
2:D:288:SER:O	2:D:301:GLY:HA3	2.18	0.43
1:E:439:THR:CG2	1:E:441:ARG:HD3	2.48	0.43
2:F:204:THR:OG1	2:F:293:GLY:O	2.32	0.43
1:A:381:PRO:HG2	1:A:384:PRO:HA	2.01	0.43
1:B:410:LYS:N	3:B:2043:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:ILE:HG13	2:D:302:SER:HB2	2.01	0.43
1:E:404:ARG:HG2	1:E:404:ARG:NH2	2.34	0.43
2:F:288:SER:O	2:F:301:GLY:HA3	2.18	0.43
1:B:347:VAL:HG11	1:B:351:LYS:HB2	2.01	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:404:ARG:HG2	1:E:404:ARG:HH21	1.83	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
2:D:233:TYR:HD1	2:D:244:GLY:HA3	1.84	0.43
1:E:323:LYS:N	1:E:324:PRO:CD	2.82	0.43
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:F:174:PHE:O	2:F:194:PHE:HA	2.19	0.43
2:C:81:LEU:HD13	2:C:140:ARG:O	2.19	0.42
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: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:422:LEU:HA	1:A:422:LEU:HD23	1.26	0.42
2:D:322:LEU:HD12	2:D:322:LEU:HA	1.51	0.42
1:E:322:LEU:HD21	1:E:324:PRO:HG3	2.01	0.42
1:E:426:GLN:HG3	1:E:438:PRO:HG3	2.02	0.42
2:F:150:ASP:C	2:F:152:GLN:N	2.77	0.42
1:A:352:TYR:HA	1:A:372:ILE:O	2.19	0.42
2:D:161:PHE:CZ	2:D:172:THR:HB	2.55	0.42
2:D:249:LEU:HB2	2:D:255:ASN:OD1	2.19	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
1:B:359:GLU:O	1:B:359:GLU:HG3	2.15	0.42
2:D:85:LEU:N	3:D:2002:HOH:O	2.07	0.42
2:F:307:THR:O	2:F:310:GLY:HA2	2.20	0.42
2:C:156:LEU:HD23	2:C:180:GLN:NE2	2.34	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: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:E:335:LEU:HD23	1:E:355:TYR:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:TYR:CD2	1:B:368:TYR:C	2.98	0.41
2:C:147:ILE:HG21	2:C:156:LEU:HD11	2.03	0.41
2:C:179:ILE:HD13	2:C:191:LYS:HD3	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:D:236:ASP:O	2:D:240:LYS:N	2.53	0.41
1:E:383:VAL:CG2	1:E:386:LEU:CD1	2.99	0.41
2:F:116:GLN:NE2	3:F:2014:HOH:O	2.53	0.41
2:F:246:ILE:HD11	2:F:316:LEU:HD21	2.01	0.41
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
1:E:362:GLU:CD	1:E:388:LYS:NZ	2.75	0.41
2:F:143:PHE:C	2:F:144:ILE:HG13	2.45	0.41
2:C:245:LYS:HG3	2:C:257:ASP:OD1	2.21	0.41
2:D:221:ALA:O	2:D:229:GLY:HA3	2.21	0.41
1:E:383:VAL:HG13	3:E:2021:HOH:O	2.21	0.41
1:E:437:SER:HA	1:E:438:PRO:HA	1.75	0.41
2:F:256:VAL:HG21	2:F:277:VAL:HG11	2.01	0.41
1:A:398:TYR:HB3	1:A:400:GLN:OE1	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:F:245:LYS:HG3	2:F:257:ASP:OD1	2.20	0.41
2:C:256:VAL:HG12	2:C:279:TYR:HB2	2.02	0.41
2:C:311:ILE:HG13	1:E:393:TYR:OH	2.21	0.41
2:F:266:ASP:HB2	2:F:270:HIS:O	2.21	0.41
2:F:309:ASN:N	2:F:310:GLY:CA	2.78	0.41
2:D:82:ALA:CB	2:D:118:ALA:CB	2.99	0.41
2:D:83:ASP:N	3:D:2002:HOH:O	2.52	0.41
1:E:399:ASN:HB3	1:E:402:HIS:HB2	2.02	0.41
1:E:407:VAL:HB	1:E:410:LYS:HE3	2.02	0.41
1:B:369:TRP:CD1	3:B:2018:HOH:O	2.74	0.41
2:C:143:PHE:C	2:C:144:ILE:HG13	2.46	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
2:C:258:LEU:N	2:C:258:LEU:CD1	2.83	0.41
1:E:342:ARG:HB3	1:E:343:PRO:HD3	2.02	0.41
2:F:236:ASP:O	2:F:240:LYS:N	2.54	0.41
1:B:412:ILE:C	1:B:428:THR:HG22	2.46	0.41
2:D:143:PHE:C	2:D:144:ILE:HG13	2.46	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:LYS:NZ	1:B:405:LYS:HZ1	2.18	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
1:A:442:CYS:C	1:A:443:ILE:CG1	2.87	0.40
2:D:120:LYS:HG2	2:D:121:THR:N	2.36	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
1:B:362:GLU:CD	1:B:388:LYS:HZ3	2.23	0.40
2:C:110:LYS:NZ	3:C:2034:HOH:O	2.55	0.40
1:E:347:VAL:CG1	1:E:351:LYS:CB	3.00	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%)	14	14
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%)	9	8
2	D	239/253 (94%)	219 (92%)	18 (8%)	2 (1%)	16	17
2	F	236/253 (93%)	217 (92%)	17 (7%)	2 (1%)	16	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1061/1128 (94%)	977 (92%)	76 (7%)	8 (1%)	16	17

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%)	9	10
1	B	106/108 (98%)	98 (92%)	8 (8%)	12	13
1	E	107/108 (99%)	96 (90%)	11 (10%)	7	6
2	C	189/194 (97%)	174 (92%)	15 (8%)	11	12
2	D	191/194 (98%)	171 (90%)	20 (10%)	6	6
2	F	187/194 (96%)	170 (91%)	17 (9%)	9	9
All	All	881/906 (97%)	801 (91%)	80 (9%)	9	9

All (80) 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

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Mol	Chain	Res	Type
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	424	LYS
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	154	ILE
2	C	211	GLU
2	C	216	THR
2	C	231	LEU
2	C	258	LEU
2	C	283	GLU
2	C	299	VAL
2	C	302	SER
2	C	308	VAL
2	D	85	LEU
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	130	THR
2	D	147	ILE
2	D	157	GLU
2	D	211	GLU
2	D	216	THR
2	D	231	LEU
2	D	258	LEU

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Mol	Chain	Res	Type
2	D	278	LEU
2	D	283	GLU
2	D	299	VAL
2	D	302	SER
2	D	308	VAL
2	D	323	GLU
1	E	323	LYS
1	E	347	VAL
1	E	359	GLU
1	E	380	SER
1	E	383	VAL
1	E	386	LEU
1	E	388	LYS
1	E	412	ILE
1	E	424	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	152	GLN
2	F	154	ILE
2	F	211	GLU
2	F	216	THR
2	F	231	LEU
2	F	258	LEU
2	F	283	GLU
2	F	299	VAL
2	F	302	SER
2	F	308	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	417	HIS
2	C	146	GLN
2	C	152	GLN
2	C	166	GLN

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Mol	Chain	Res	Type
2	C	175	GLN
2	C	180	GLN
2	C	309	ASN
2	D	166	GLN
2	F	162	GLN
2	F	175	GLN
2	F	270	HIS

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 oligosaccharides 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%)	2.11	52 (45%) 0 0	26, 40, 68, 91	3 (2%)
1	B	121/123 (98%)	1.69	46 (38%) 1 0	20, 35, 61, 79	2 (1%)
1	E	122/123 (99%)	2.09	57 (46%) 0 0	24, 39, 65, 82	2 (1%)
2	C	242/253 (95%)	1.13	46 (19%) 3 3	14, 31, 66, 81	1 (0%)
2	D	243/253 (96%)	1.46	63 (25%) 1 1	18, 38, 70, 96	2 (0%)
2	F	240/253 (94%)	2.12	114 (47%) 0 0	27, 47, 79, 93	1 (0%)
All	All	1083/1128 (96%)	1.70	378 (34%) 1 0	14, 39, 70, 96	11 (1%)

All (378) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	147	ILE	7.2
2	C	151	GLY	7.0
2	F	149	VAL	6.8
2	C	156	LEU	6.4
1	A	443	ILE	6.3
2	F	185	SER	6.2
2	C	154	ILE	6.0
2	F	186	GLY	6.0
1	B	443	ILE	5.9
2	C	153	LEU	5.9
2	F	87	ALA	5.9
2	F	152	GLN	5.7
2	F	123	GLY	5.7
2	D	187	LYS	5.6
2	D	184	HIS	5.6
1	E	443	ILE	5.6
1	E	390	TYR	5.5
1	A	406	PHE	5.5
1	A	424	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
2	F	156	LEU	5.3
2	F	89	LEU	5.3
1	A	414	VAL	5.3
1	E	441	ARG	5.2
2	D	186	GLY	5.2
2	F	180	GLN	5.1
2	C	149	VAL	5.0
1	E	383	VAL	5.0
1	B	422	LEU	4.9
2	F	147	ILE	4.9
2	F	150	ASP	4.8
2	D	185	SER	4.8
2	F	189	VAL	4.7
2	D	87	ALA	4.7
2	C	184	HIS	4.6
1	E	407	VAL	4.5
1	E	322	LEU	4.4
2	D	151	GLY	4.4
2	C	182	SER	4.4
2	F	84	ALA	4.3
1	B	390	TYR	4.3
2	C	185	SER	4.3
1	B	418	PRO	4.3
1	B	395	GLU	4.3
2	F	190	ALA	4.3
1	E	347	VAL	4.2
2	F	182	SER	4.2
1	A	390	TYR	4.2
2	D	154	ILE	4.2
2	F	184	HIS	4.1
2	F	179	ILE	4.1
1	A	404	ARG	4.1
2	F	106	ARG	4.1
2	C	155	THR	4.1
2	F	191	LYS	4.1
2	D	195	ARG	4.1
2	F	154	ILE	4.1
1	B	323	LYS	4.0
2	D	89	LEU	4.0
1	A	377	ASP	4.0
2	D	94	LYS	3.9
2	F	214	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	323	GLU	3.9
2	F	187	LYS	3.9
2	C	189	VAL	3.9
2	F	153	LEU	3.9
1	E	388	LYS	3.9
1	A	441	ARG	3.9
2	F	178	GLN	3.8
1	B	421	ALA	3.8
1	A	383	VAL	3.8
1	A	422	LEU	3.8
2	C	150	ASP	3.8
1	E	411	SER	3.7
2	F	151	GLY	3.7
2	D	149	VAL	3.7
1	A	376	GLN	3.7
2	F	107	LYS	3.7
2	F	218	ARG	3.7
1	A	405	LYS	3.7
1	E	427	THR	3.7
1	E	405	LYS	3.7
1	A	428	THR	3.6
1	B	398	TYR	3.6
1	B	424	LYS	3.6
2	F	188	MET	3.6
2	F	310	GLY	3.6
1	B	441	ARG	3.6
2	F	243	ASN	3.6
2	C	146	GLN	3.6
1	E	424	LYS	3.6
2	F	105	VAL	3.6
1	E	376	GLN	3.5
1	E	422	LEU	3.5
1	B	402	HIS	3.5
2	C	123	GLY	3.5
2	F	229	GLY	3.5
2	F	148	GLU	3.5
1	B	376	GLN	3.5
1	B	383	VAL	3.5
2	C	190	ALA	3.4
1	A	426	GLN	3.4
1	E	423	PRO	3.4
2	D	179	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	406	PHE	3.4
1	E	332	HIS	3.4
1	E	410	LYS	3.4
2	D	120	LYS	3.4
1	B	428	THR	3.4
1	E	380	SER	3.3
2	F	215	ALA	3.3
2	F	146	GLN	3.3
1	A	329	ASP	3.3
2	F	85	LEU	3.3
1	A	412	ILE	3.3
2	F	145	ARG	3.3
1	A	420	TYR	3.3
1	B	407	VAL	3.3
2	F	118	ALA	3.3
2	F	96	LEU	3.3
1	A	331	LYS	3.3
1	A	407	VAL	3.3
2	D	243	ASN	3.2
1	B	400	GLN	3.2
1	E	428	THR	3.2
1	B	368	TYR	3.2
1	A	378	GLY	3.2
1	E	404	ARG	3.2
2	D	83	ASP	3.2
1	B	437	SER	3.2
1	E	393	TYR	3.2
1	B	403	GLY	3.2
1	A	434	ASN	3.2
2	C	191	LYS	3.2
2	D	156	LEU	3.2
1	E	408	GLN	3.2
2	F	253	GLU	3.2
1	E	349	VAL	3.2
2	F	120	LYS	3.1
1	A	411	SER	3.1
1	B	415	ALA	3.1
1	E	409	GLY	3.1
2	D	150	ASP	3.1
2	C	107	LYS	3.1
2	F	157	GLU	3.1
2	D	181	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	117	GLY	3.1
1	A	388	LYS	3.1
2	D	123	GLY	3.1
2	D	131	GLY	3.1
2	F	93	ASP	3.1
2	D	180	GLN	3.1
2	F	109	GLU	3.1
2	F	295	LYS	3.1
2	C	183	GLU	3.0
2	D	155	THR	3.0
2	D	182	SER	3.0
2	C	181	ASP	3.0
2	F	108	ASN	3.0
2	F	131	GLY	3.0
2	C	230	LYS	3.0
2	F	137	LYS	3.0
2	D	147	ILE	3.0
2	F	230	LYS	3.0
1	E	434	ASN	3.0
2	F	90	ASP	3.0
2	F	266	ASP	3.0
1	A	440	PRO	3.0
2	D	178	GLN	3.0
2	F	158	SER	3.0
2	F	82	ALA	2.9
2	D	153	LEU	2.9
2	F	94	LYS	2.9
2	F	144	ILE	2.9
1	A	439	THR	2.9
1	B	435	GLY	2.9
1	B	404	ARG	2.9
1	E	420	TYR	2.9
1	B	423	PRO	2.9
1	B	406	PHE	2.9
2	F	306	LYS	2.9
2	C	152	GLN	2.9
1	E	429	VAL	2.9
2	F	219	GLY	2.9
2	C	187	LYS	2.9
2	D	152	GLN	2.9
1	A	362	GLU	2.9
2	F	155	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	365	SER	2.8
2	F	221	ALA	2.8
1	B	405	LYS	2.8
2	D	92	LYS	2.8
2	F	134	LYS	2.8
1	E	413	ASP	2.8
1	B	393	TYR	2.8
1	B	420	TYR	2.8
2	C	89	LEU	2.8
1	A	430	THR	2.8
2	D	309	ASN	2.8
2	F	91	HIS	2.8
1	A	359	GLU	2.8
2	D	183	GLU	2.8
1	A	425	ALA	2.8
1	A	375	THR	2.8
1	A	417	HIS	2.8
2	F	86	THR	2.8
1	B	399	ASN	2.8
2	C	243	ASN	2.8
1	B	411	SER	2.8
2	F	114	ALA	2.8
1	A	361	PHE	2.8
2	D	146	GLN	2.7
2	D	95	GLY	2.7
2	F	112	LYS	2.7
1	E	375	THR	2.7
1	B	438	PRO	2.7
1	A	395	GLU	2.7
1	A	433	GLU	2.7
1	B	388	LYS	2.7
2	D	191	LYS	2.7
2	F	268	LYS	2.7
2	D	188	MET	2.7
1	E	394	LEU	2.7
1	A	410	LYS	2.7
2	D	105	VAL	2.7
2	F	183	GLU	2.7
2	F	216	THR	2.7
1	E	426	GLN	2.6
2	C	118	ALA	2.6
2	F	116	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	414	VAL	2.6
1	A	366	GLY	2.6
2	F	278	LEU	2.6
1	A	413	ASP	2.6
2	F	138	VAL	2.6
1	E	350	GLY	2.6
2	F	244	GLY	2.6
2	C	179	ILE	2.6
2	F	196	ILE	2.6
2	F	251	SER	2.6
2	C	116	GLN	2.6
2	F	111	LEU	2.6
1	A	382	ALA	2.6
2	F	261	ALA	2.6
1	B	362	GLU	2.6
2	C	188	MET	2.6
2	D	91	HIS	2.6
1	A	396	ASN	2.5
1	B	434	ASN	2.5
1	E	324	PRO	2.5
2	C	186	GLY	2.5
1	E	338	GLU	2.5
1	E	323	LYS	2.5
2	C	80	GLY	2.5
1	E	430	THR	2.5
1	B	426	GLN	2.5
2	C	180	GLN	2.5
2	F	113	LEU	2.5
2	F	133	LEU	2.5
1	E	348	ALA	2.5
2	D	90	ASP	2.5
2	F	181	ASP	2.5
2	C	117	GLY	2.5
1	E	363	THR	2.5
2	F	320	GLN	2.5
1	A	429	VAL	2.5
2	D	157	GLU	2.5
1	A	336	TYR	2.5
1	B	377	ASP	2.5
2	D	108	ASN	2.5
1	B	425	ALA	2.5
2	D	82	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	115	ALA	2.5
2	D	116	GLN	2.5
2	F	80	GLY	2.5
2	D	86	THR	2.4
2	D	127	SER	2.4
1	E	412	ILE	2.4
1	E	331	LYS	2.4
2	C	120	LYS	2.4
1	E	339	ASN	2.4
2	F	281	GLN	2.4
1	E	378	GLY	2.4
2	C	310	GLY	2.4
2	D	218	ARG	2.4
2	F	176	THR	2.4
2	D	308	VAL	2.4
1	A	339	ASN	2.4
2	F	241	GLN	2.4
1	B	427	THR	2.4
2	D	306	LYS	2.4
2	C	214	ARG	2.4
2	D	88	PRO	2.4
1	B	414	VAL	2.4
2	F	202	GLU	2.4
1	A	353	TYR	2.3
2	F	122	TYR	2.3
2	F	210	PRO	2.3
1	A	397	GLY	2.3
2	C	82	ALA	2.3
1	A	325	CYS	2.3
1	A	442	CYS	2.3
2	F	141	PHE	2.3
2	F	81	LEU	2.3
2	D	245	LYS	2.3
2	F	240	LYS	2.3
2	C	148	GLU	2.3
2	D	99	LEU	2.3
1	B	329	ASP	2.3
2	D	106	ARG	2.3
2	F	312	ARG	2.3
2	F	308	VAL	2.3
1	B	331	LYS	2.3
2	C	85	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	111	LEU	2.3
2	C	108	ASN	2.3
1	A	346	PRO	2.3
2	C	137	LYS	2.3
1	E	326	ASP	2.2
1	E	418	PRO	2.2
1	E	440	PRO	2.2
1	E	382	ALA	2.2
2	D	84	ALA	2.2
2	D	81	LEU	2.2
2	F	231	LEU	2.2
2	D	143	PHE	2.2
2	F	194	PHE	2.2
2	C	144	ILE	2.2
1	A	347	VAL	2.2
2	F	83	ASP	2.2
1	B	417	HIS	2.2
2	F	110	LYS	2.2
2	F	250	LYS	2.2
2	C	114	ALA	2.2
1	A	344	TYR	2.2
2	F	217	TYR	2.2
1	E	342	ARG	2.2
2	D	96	LEU	2.2
2	D	322	LEU	2.2
1	E	377	ASP	2.2
1	E	425	ALA	2.2
2	C	104	SER	2.2
2	F	130	THR	2.2
2	F	128	LEU	2.1
2	F	262	ASP	2.1
2	D	134	LYS	2.1
2	F	92	LYS	2.1
2	F	143	PHE	2.1
2	D	175	GLN	2.1
1	A	394	LEU	2.1
2	F	101	LEU	2.1
1	B	433	GLU	2.1
2	D	93	ASP	2.1
2	D	320	GLN	2.1
2	F	213	GLY	2.1
1	A	374	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	106	ARG	2.1
2	D	107	LYS	2.1
2	F	132	LYS	2.1
1	A	352	TYR	2.1
2	F	311	ILE	2.1
1	E	400	GLN	2.1
1	B	392	PRO	2.1
1	B	419	GLY	2.1
1	E	325	CYS	2.1
2	C	111	LEU	2.1
2	D	85	LEU	2.1
1	B	324	PRO	2.1
2	F	177	GLU	2.0
2	F	193	GLN	2.0
1	E	329	ASP	2.0
1	E	399	ASN	2.0
2	F	280	ASN	2.0
1	E	384	PRO	2.0
1	E	333	GLY	2.0
2	F	222	PHE	2.0
2	C	110	LYS	2.0
2	F	126	ASP	2.0
2	F	273	ILE	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 oligosaccharides 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.