Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:57 am BST

PDB ID	:	4DY7
Title	:	Crystal structures of protease nexin-1 in complex with S195A thrombin
Authors	:	Huntington, J.A.; Li, W.
Deposited on	:	2012-02-28
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

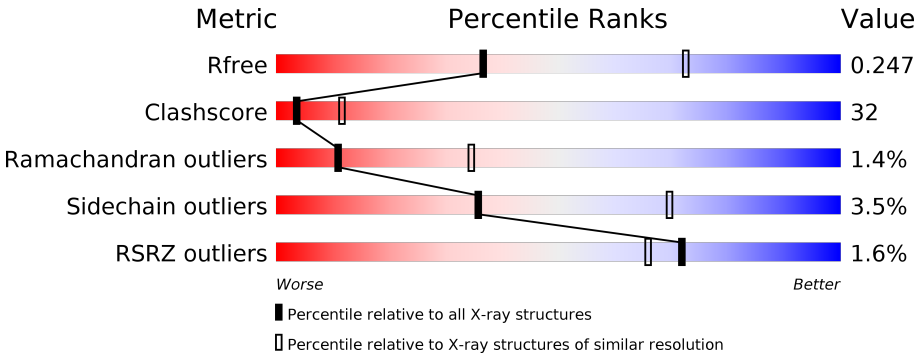
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	49	39% 47% 6% 8%
1	D	49	2% 51% 24% 20%
2	B	259	58% 38%
2	E	259	5% 58% 38%
3	C	379	% 54% 42%
3	F	379	% 61% 37%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9956 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 Thrombin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	45	Total	C	N	O	S	0	0	0
			350	222	56	71	1			
1	D	39	Total	C	N	O	S	0	0	0
			213	127	42	43	1			

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	253	Total	C	N	O	S	1	0	0
			1939	1239	334	352	14			
2	E	251	Total	C	N	O	S	0	0	0
			1727	1098	300	317	12			

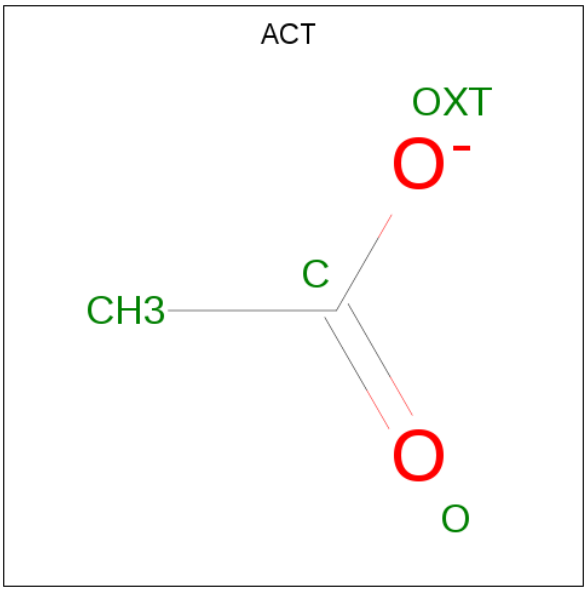
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	ALA	SER	ENGINEERED MUTATION	UNP P00734
E	195	ALA	SER	ENGINEERED MUTATION	UNP P00734

- Molecule 3 is a protein called Glia-derived nexin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	377	Total	C	N	O	S	0	0	0
			2746	1770	467	497	12			
3	F	378	Total	C	N	O	S	1	0	0
			2856	1836	485	522	13			

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	F	1	Total Ca 1 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Na 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total O 2 2	0	0

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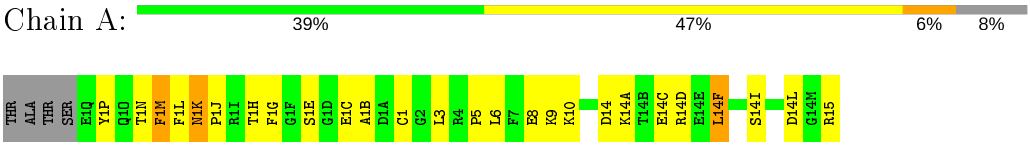
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	25	Total O 25 25	0	0
7	C	26	Total O 26 26	0	0
7	D	3	Total O 3 3	0	0
7	E	8	Total O 8 8	0	0
7	F	46	Total O 46 46	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

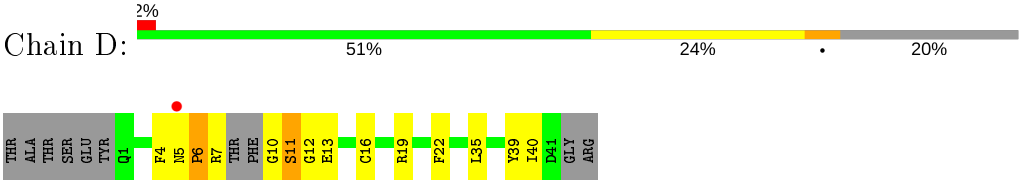
• Molecule 1: Thrombin light chain

Chain A:



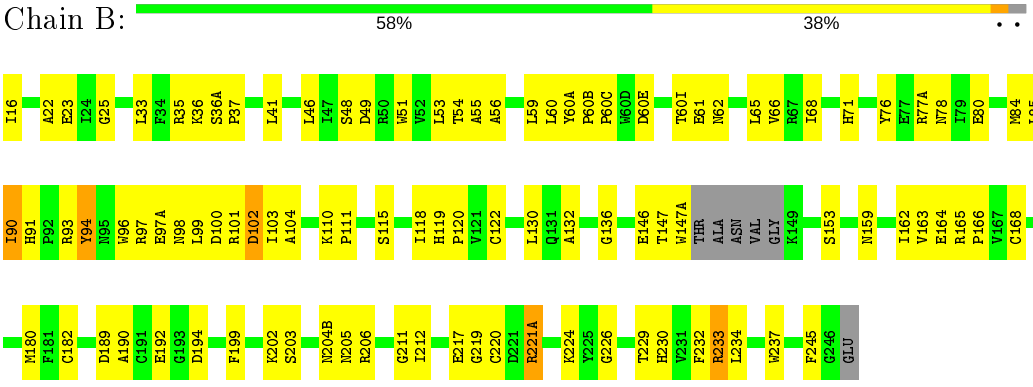
• Molecule 1: Thrombin light chain

Chain D:



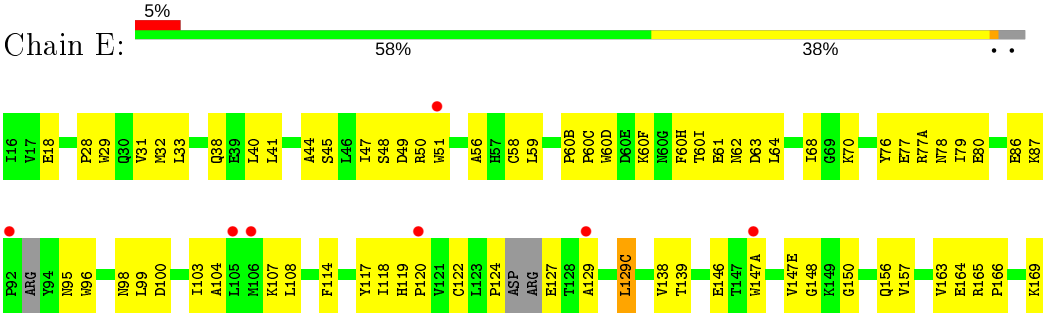
• Molecule 2: Thrombin heavy chain

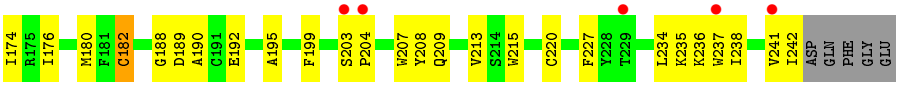
Chain B:



• Molecule 2: Thrombin heavy chain

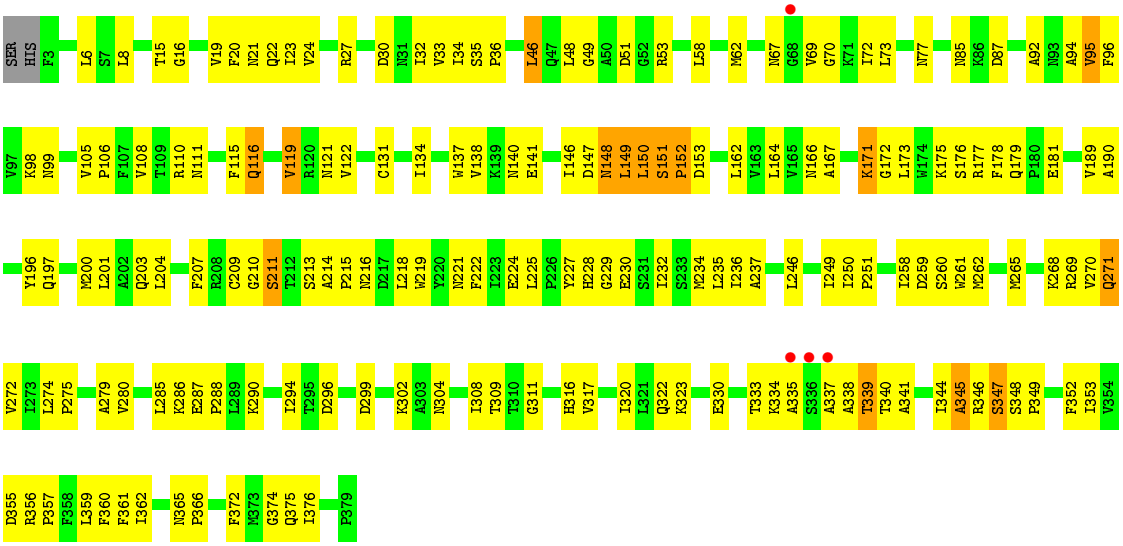
Chain E:





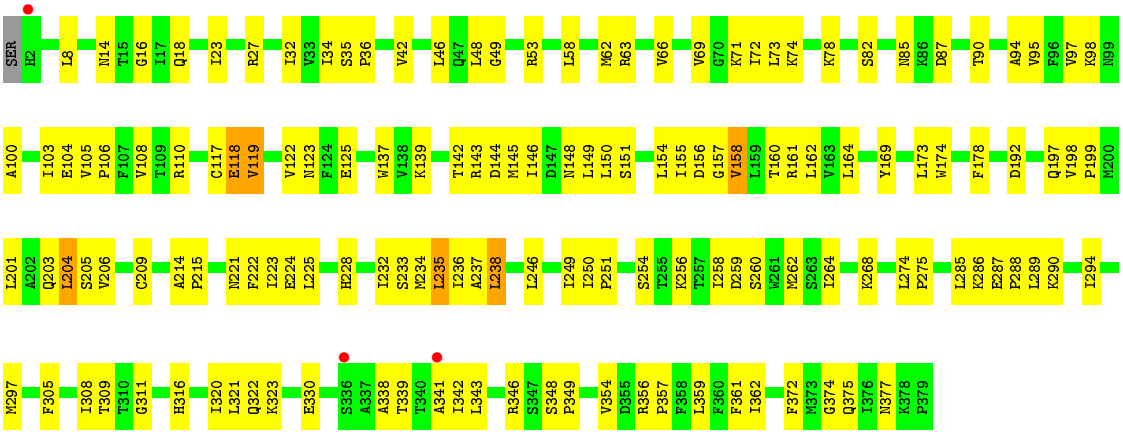
- Molecule 3: Glia-derived nexin

Chain C:



- Molecule 3: Glia-derived nexin

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	191.96Å 86.67Å 101.89Å 90.00° 94.44° 90.00°	Depositor
Resolution (Å)	47.04 – 2.80 47.04 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (47.04-2.80) 95.1 (47.04-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0098	Depositor
R, R_{free}	0.223 , 0.268 0.241 , 0.247	Depositor DCC
R_{free} test set	1987 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	61.9	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9956	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, ACT

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	0.23	0/357	0.38	0/479
1	D	0.23	0/213	0.38	0/292
2	B	0.30	0/1988	0.39	0/2703
2	E	0.20	0/1770	0.37	0/2430
3	C	0.21	0/2806	0.39	0/3840
3	F	0.35	1/2916 (0.0%)	0.41	0/3972
All	All	0.28	1/10050 (0.0%)	0.39	0/13716

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	158	VAL	CB-CG1	-15.07	1.21	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	350	0	307	42	0
1	D	213	0	123	20	0
2	B	1939	0	1806	122	0
2	E	1727	0	1421	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2746	0	2610	197	0
3	F	2856	0	2827	141	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
5	A	1	0	0	0	0
5	F	1	0	0	0	0
6	B	1	0	0	0	0
7	A	2	0	0	0	0
7	B	25	0	0	3	0
7	C	26	0	0	5	0
7	D	3	0	0	1	0
7	E	8	0	0	1	0
7	F	46	0	0	0	0
All	All	9956	0	9103	597	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (597) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:116:GLN:HE21	3:C:116:GLN:N	1.17	1.40
1:D:19:ARG:NH2	2:E:207:TRP:NE1	1.68	1.38
1:D:19:ARG:NH2	2:E:207:TRP:HE1	1.16	1.34
1:A:1(M):PHE:HD2	1:A:1(L):PHE:N	1.23	1.32
3:C:179:GLN:HG3	3:C:181:GLU:OE2	1.33	1.25
1:D:19:ARG:NH2	2:E:207:TRP:CE2	2.11	1.18
1:A:1(M):PHE:O	1:A:1(C):GLU:OE2	1.60	1.16
3:C:131:CYS:SG	3:C:151:SER:O	2.02	1.15
1:A:1(M):PHE:CD2	1:A:1(L):PHE:N	2.16	1.14
3:C:179:GLN:CG	3:C:181:GLU:OE2	1.98	1.11
2:B:168:CYS:O	2:B:171:SER:OG	1.65	1.10
3:C:116:GLN:NE2	3:C:116:GLN:N	1.99	1.10
1:D:11:SER:CB	2:E:49:ASP:CB	2.28	1.10
2:B:97:ARG:O	3:C:339:THR:OG1	1.71	1.07
3:F:48:LEU:HD11	3:F:110:ARG:HH11	1.21	1.04
1:A:1(N):THR:H	1:A:1(M):PHE:HB2	1.18	1.03
1:D:19:ARG:NH2	2:E:207:TRP:CZ2	2.26	1.02
2:B:146:GLU:OE2	2:B:221(A):ARG:NH1	1.91	1.02
3:C:23:ILE:HD12	3:C:34:ILE:HD11	1.36	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:169:LYS:HA	2:E:176:ILE:HD11	1.41	1.02
2:B:60(I):THR:HG22	2:B:61:GLU:OE2	1.60	1.00
3:F:48:LEU:HD11	3:F:110:ARG:NH1	1.76	1.00
2:E:169:LYS:HA	2:E:176:ILE:CD1	1.94	0.96
2:B:99:LEU:HG	3:C:340:THR:HG21	1.47	0.94
1:D:11:SER:O	1:D:13:GLU:N	2.00	0.93
2:B:60:LEU:HD23	2:B:90:ILE:CD1	1.98	0.93
3:C:204:LEU:CD2	3:C:271:GLN:HG2	2.00	0.92
1:A:1(M):PHE:HD2	1:A:1(L):PHE:H	1.00	0.92
2:B:91:HIS:CD2	2:B:237:TRP:CG	2.59	0.91
1:A:1(N):THR:N	1:A:1(M):PHE:HB2	1.84	0.91
3:F:95:VAL:HG22	3:F:164:LEU:HD13	1.51	0.91
3:C:116:GLN:H	3:C:116:GLN:HE21	0.92	0.91
3:F:8:LEU:HD21	3:F:73:LEU:CD1	2.00	0.90
3:F:95:VAL:HG22	3:F:164:LEU:CD1	2.01	0.90
1:A:1(M):PHE:O	1:A:1(L):PHE:HB2	1.70	0.90
3:C:204:LEU:HD21	3:C:271:GLN:HG2	1.55	0.87
1:D:19:ARG:CZ	2:E:207:TRP:HE1	1.86	0.87
2:B:146:GLU:HB2	2:B:220:CYS:HB2	1.54	0.86
1:A:1(N):THR:CB	1:A:1(M):PHE:HA	2.05	0.86
3:F:150:LEU:HD13	3:F:155:ILE:HD11	1.57	0.86
3:F:23:ILE:HD12	3:F:34:ILE:HD11	1.57	0.85
3:C:173:LEU:HB2	3:C:228:HIS:ND1	1.91	0.85
3:F:48:LEU:HD21	3:F:110:ARG:HB3	1.56	0.85
1:D:19:ARG:CZ	2:E:207:TRP:NE1	2.39	0.85
2:E:50:ARG:O	2:E:108:LEU:HD13	1.77	0.84
3:C:335:ALA:HA	3:C:338:ALA:HB3	1.58	0.84
3:C:246:LEU:HD12	3:C:249:ILE:HD11	1.60	0.84
3:C:359:LEU:HD13	3:C:361:PHE:HE1	1.43	0.83
3:C:346:ARG:O	3:C:347:SER:HB3	1.75	0.83
3:F:359:LEU:HD23	3:F:359:LEU:H	1.42	0.83
3:F:94:ALA:HB2	3:F:137:TRP:CH2	2.16	0.81
1:A:14(L):ASP:OD1	1:A:15:ARG:CG	2.28	0.81
3:C:359:LEU:HD13	3:C:361:PHE:CE1	2.15	0.81
3:C:8:LEU:HD21	3:C:73:LEU:CD1	2.11	0.81
1:A:14(L):ASP:OD1	1:A:15:ARG:HG3	1.81	0.80
3:C:116:GLN:H	3:C:116:GLN:NE2	1.71	0.80
3:C:149:LEU:HD12	3:C:149:LEU:N	1.96	0.80
2:B:192:GLU:HB2	3:C:346:ARG:O	1.81	0.80
2:B:119:HIS:CD2	2:B:120:PRO:HD2	2.16	0.80
2:B:60:LEU:HD23	2:B:90:ILE:HD11	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:PHE:CB	1:D:5:ASN:CB	2.60	0.80
3:F:48:LEU:CD1	3:F:110:ARG:NH1	2.46	0.79
2:B:77(A):ARG:HA	7:B:418:HOH:O	1.83	0.78
3:C:234:MET:CE	3:C:362:ILE:HD11	2.12	0.78
3:C:337:ALA:O	3:C:341:ALA:CB	2.32	0.78
3:C:309:THR:HG23	3:C:311:GLY:O	1.82	0.78
3:C:346:ARG:O	3:C:347:SER:CB	2.32	0.78
1:A:3:LEU:CD1	2:B:206:ARG:HG2	2.14	0.77
3:C:345:ALA:HB2	7:C:514:HOH:O	1.84	0.77
3:C:175:LYS:O	3:C:333:THR:CG2	2.33	0.77
3:C:359:LEU:O	3:C:359:LEU:HD12	1.83	0.76
2:B:146:GLU:CD	2:B:221(A):ARG:NH1	2.38	0.76
3:C:337:ALA:O	3:C:341:ALA:HB2	1.85	0.75
2:E:60(B):PRO:HB2	2:E:60(C):PRO:HD3	1.68	0.75
3:C:209:CYS:O	3:C:265:MET:HA	1.86	0.75
3:C:151:SER:CB	3:C:152:PRO:CD	2.66	0.74
2:E:234:LEU:O	2:E:237:TRP:HB3	1.87	0.74
2:B:130:LEU:HD12	2:B:162:ILE:HD13	1.68	0.74
1:D:19:ARG:HH22	2:E:207:TRP:HZ2	1.33	0.74
2:B:60(A):TYR:CE2	2:B:60(C):PRO:HG2	2.22	0.74
2:B:221(A):ARG:HB2	2:B:224:LYS:HB2	1.70	0.74
3:C:211:SER:HA	3:C:222:PHE:CE2	2.21	0.74
3:F:342:ILE:HG22	3:F:343:LEU:O	1.87	0.73
2:B:93:ARG:CB	2:B:101:ARG:HD3	2.18	0.73
1:D:6:PRO:O	1:D:7:ARG:CB	2.34	0.73
2:B:91:HIS:HD2	2:B:237:TRP:CG	2.04	0.73
2:E:124:PRO:HG2	2:E:208:TYR:CB	2.19	0.73
3:F:260:SER:O	3:F:264:ILE:HG13	1.89	0.73
1:A:14:ASP:OD1	1:A:14(C):GLU:HB3	1.88	0.72
3:C:359:LEU:CD1	3:C:361:PHE:HE1	2.02	0.72
2:B:99:LEU:HG	3:C:340:THR:CG2	2.18	0.72
3:F:8:LEU:HD21	3:F:73:LEU:HD13	1.70	0.72
1:A:1(M):PHE:CD2	1:A:1(M):PHE:C	2.63	0.72
2:B:219:GLY:O	3:C:346:ARG:NH1	2.23	0.72
2:B:61:GLU:CD	2:B:61:GLU:H	1.94	0.71
3:F:148:ASN:OD1	3:F:148:ASN:O	2.07	0.71
3:C:23:ILE:HD12	3:C:34:ILE:CD1	2.16	0.71
1:A:1(N):THR:CB	1:A:1(M):PHE:CA	2.69	0.71
3:F:8:LEU:CD2	3:F:73:LEU:CD1	2.68	0.70
2:E:47:ILE:O	2:E:120:PRO:HB2	1.91	0.70
2:E:170:ASP:OD2	7:E:405:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:125:GLU:HA	3:F:158:VAL:HG22	1.74	0.70
1:A:1:CYS:O	2:B:206:ARG:NH1	2.25	0.69
2:B:165:ARG:HB3	2:B:166:PRO:HD3	1.72	0.69
3:C:234:MET:HE3	3:C:362:ILE:HD11	1.74	0.69
2:B:61:GLU:HB3	2:B:85:LEU:O	1.92	0.69
1:A:1(K):ASN:HD22	1:A:1(J):PRO:HD2	1.57	0.69
2:E:31:VAL:HB	2:E:44:ALA:HB3	1.73	0.69
2:E:77:GLU:O	2:E:80:GLU:HG2	1.93	0.68
3:C:269:ARG:HH12	3:C:345:ALA:HA	1.58	0.68
2:E:50:ARG:O	2:E:108:LEU:CD1	2.41	0.68
2:E:79:ILE:HG23	2:E:117:TYR:CD2	2.27	0.68
3:F:23:ILE:HD12	3:F:34:ILE:CD1	2.22	0.68
3:C:53:ARG:HB3	3:C:296:ASP:OD2	1.94	0.68
3:F:198:VAL:HG23	3:F:199:PRO:HD2	1.76	0.68
3:F:23:ILE:CD1	3:F:34:ILE:HD11	2.23	0.67
3:F:274:LEU:HD12	3:F:275:PRO:HD2	1.75	0.67
3:C:22:GLN:HE22	3:C:288:PRO:HA	1.57	0.67
3:F:201:LEU:HD22	3:F:330:GLU:HG3	1.76	0.67
1:A:14(A):LYS:HG3	2:B:23:GLU:OE2	1.95	0.67
2:E:129(C):LEU:N	2:E:129(C):LEU:HD12	2.10	0.67
2:E:169:LYS:CA	2:E:176:ILE:CD1	2.72	0.67
2:B:60(C):PRO:HB3	3:C:337:ALA:HB1	1.76	0.67
1:A:1(M):PHE:O	1:A:1(C):GLU:CD	2.32	0.66
3:C:189:VAL:O	3:C:357:PRO:HD3	1.96	0.66
3:C:335:ALA:CA	3:C:338:ALA:HB3	2.25	0.66
2:B:60(B):PRO:N	2:B:60(C):PRO:HD2	2.10	0.66
2:B:189:ASP:OD1	2:B:190:ALA:N	2.29	0.66
3:C:22:GLN:NE2	3:C:288:PRO:HA	2.11	0.66
3:C:359:LEU:C	3:C:359:LEU:HD12	2.16	0.66
2:E:169:LYS:HA	2:E:176:ILE:HD12	1.78	0.66
3:F:97:VAL:HG22	3:F:162:LEU:CD1	2.26	0.66
3:C:23:ILE:CD1	3:C:34:ILE:HD11	2.22	0.65
3:C:246:LEU:CD1	3:C:249:ILE:HD11	2.26	0.65
3:C:108:VAL:HA	3:C:119:VAL:HG11	1.77	0.65
2:E:124:PRO:CG	2:E:208:TYR:CB	2.74	0.65
3:C:95:VAL:HG13	3:C:119:VAL:HB	1.77	0.65
3:C:105:VAL:N	3:C:106:PRO:HD2	2.12	0.65
1:A:1(K):ASN:HB3	1:A:1(H):THR:HG22	1.79	0.65
3:F:235:LEU:HD21	3:F:262:MET:HE1	1.79	0.65
2:B:146:GLU:OE1	2:B:221(A):ARG:NH1	2.30	0.64
3:C:274:LEU:HD23	3:C:274:LEU:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:161:ARG:HE	3:F:316:HIS:HD2	1.45	0.64
1:A:1(M):PHE:HD2	1:A:1(M):PHE:C	1.91	0.64
2:E:122:CYS:HB2	2:E:207:TRP:O	1.98	0.64
3:F:246:LEU:HD11	3:F:359:LEU:HD22	1.79	0.64
3:F:234:MET:CE	3:F:362:ILE:HD11	2.28	0.64
3:C:235:LEU:HB2	3:C:361:PHE:HB2	1.80	0.64
2:E:33:LEU:HD21	2:E:64:LEU:HD13	1.79	0.64
2:E:189:ASP:OD1	2:E:190:ALA:N	2.31	0.63
2:E:86:GLU:N	2:E:107:LYS:O	2.24	0.63
3:F:155:ILE:CG2	3:F:156:ASP:N	2.61	0.63
1:A:1(K):ASN:HD22	1:A:1(J):PRO:CD	2.12	0.63
3:C:360:PHE:HE1	3:C:376:ILE:HD11	1.64	0.63
2:B:60:LEU:HD23	2:B:90:ILE:HD13	1.81	0.63
3:C:58:LEU:HD23	3:C:294:ILE:HD13	1.81	0.62
2:E:172:THR:OG1	2:E:174:ILE:HG12	1.98	0.62
3:F:143:ARG:O	3:F:144:ASP:HB2	1.99	0.62
2:B:176:ILE:HG22	2:B:177:THR:N	2.15	0.62
3:F:237:ALA:O	3:F:359:LEU:HD23	2.00	0.62
2:B:60(A):TYR:CZ	2:B:60(C):PRO:HG2	2.34	0.62
3:C:261:TRP:O	3:C:265:MET:HG3	2.00	0.61
3:C:337:ALA:O	3:C:341:ALA:HB3	2.01	0.61
2:E:98:ASN:O	2:E:99:LEU:HB2	1.99	0.61
3:C:234:MET:HE2	3:C:362:ILE:HD11	1.83	0.61
2:E:138:VAL:CG2	2:E:199:PHE:HD2	2.13	0.61
2:E:79:ILE:HG23	2:E:117:TYR:CE2	2.36	0.61
2:E:61:GLU:CG	2:E:87:LYS:HA	2.31	0.61
3:F:204:LEU:HD23	3:F:205:SER:N	2.14	0.61
3:F:285:LEU:O	3:F:289:LEU:HG	2.01	0.61
3:F:155:ILE:CG2	3:F:160:THR:OG1	2.50	0.60
3:F:95:VAL:HG22	3:F:164:LEU:HD11	1.83	0.60
2:B:65:LEU:CD2	2:B:84:MET:HG2	2.31	0.60
3:C:149:LEU:CD1	3:C:149:LEU:N	2.64	0.60
2:B:176:ILE:HG22	2:B:177:THR:H	1.66	0.60
3:C:250:ILE:N	3:C:251:PRO:HD2	2.17	0.60
3:C:173:LEU:HB2	3:C:228:HIS:CE1	2.36	0.60
3:F:46:LEU:HD13	3:F:297:MET:SD	2.42	0.59
1:A:1(E):SER:O	2:B:49:ASP:HB2	2.02	0.59
2:E:47:ILE:HG13	2:E:48:SER:N	2.16	0.59
2:B:65:LEU:HD21	2:B:84:MET:HG2	1.84	0.59
2:E:60(B):PRO:HG2	2:E:96:TRP:CZ2	2.37	0.59
2:E:241:VAL:O	2:E:242:ILE:C	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:346:ARG:NH2	7:C:515:HOH:O	2.24	0.58
3:C:69:VAL:CG1	3:C:73:LEU:HD13	2.33	0.58
3:C:134:ILE:HG21	3:C:150:LEU:HD11	1.86	0.58
3:C:8:LEU:HD21	3:C:73:LEU:HD11	1.84	0.58
3:C:201:LEU:HD22	3:C:330:GLU:HG3	1.85	0.58
2:B:60:LEU:CD2	2:B:90:ILE:CD1	2.78	0.58
3:C:58:LEU:O	3:C:62:MET:HG3	2.03	0.58
2:B:60(B):PRO:O	2:B:60(E):ASP:N	2.33	0.57
3:C:69:VAL:HG12	3:C:73:LEU:HD13	1.85	0.57
3:C:268:LYS:HG3	3:C:270:VAL:HG23	1.87	0.57
3:F:155:ILE:HG23	3:F:160:THR:OG1	2.04	0.57
1:A:14(F):LEU:HD11	2:B:159:ASN:CG	2.25	0.57
3:F:151:SER:O	3:F:154:LEU:N	2.37	0.57
2:E:108:LEU:N	2:E:108:LEU:HD12	2.20	0.57
2:E:124:PRO:CD	2:E:208:TYR:CB	2.82	0.57
3:C:214:ALA:HB3	3:C:216:ASN:OD1	2.04	0.57
2:E:91:HIS:H	2:E:237:TRP:HZ2	1.52	0.57
3:F:356:ARG:HB3	3:F:357:PRO:HD2	1.87	0.57
1:A:3:LEU:HD13	2:B:206:ARG:HG2	1.86	0.56
3:C:320:ILE:O	3:C:320:ILE:HG23	2.05	0.56
2:B:77(A):ARG:O	2:B:78:ASN:HB2	2.04	0.56
3:C:227:TYR:HD2	3:C:232:ILE:O	1.88	0.56
2:B:130:LEU:CD1	2:B:162:ILE:HD13	2.36	0.56
3:C:116:GLN:CA	3:C:116:GLN:HE21	2.09	0.56
3:C:286:LYS:HG2	3:C:290:LYS:HE3	1.88	0.56
2:B:100:ASP:OD2	2:B:101:ARG:N	2.37	0.56
2:B:66:VAL:HG13	2:B:85:LEU:HD21	1.88	0.56
3:C:98:LYS:O	3:C:121:ASN:ND2	2.38	0.56
3:C:146:ILE:HD12	3:C:167:ALA:HB1	1.88	0.56
3:C:6:LEU:HD22	3:C:6:LEU:N	2.21	0.56
3:C:258:ILE:O	3:C:261:TRP:HB2	2.07	0.55
3:F:98:LYS:HD3	3:F:100:ALA:HB3	1.87	0.55
2:E:68:ILE:HG21	2:E:118:ILE:HD12	1.88	0.55
2:B:60(C):PRO:HB3	3:C:337:ALA:CB	2.36	0.55
2:E:41:LEU:HA	3:F:348:SER:HB2	1.88	0.55
2:B:119:HIS:CG	2:B:120:PRO:HD2	2.41	0.55
3:C:49:GLY:HA3	3:C:308:ILE:HG13	1.89	0.55
2:B:146:GLU:CD	2:B:221(A):ARG:HH12	1.98	0.55
2:B:97(A):GLU:HG3	2:B:98:ASN:N	2.22	0.55
2:E:95:ASN:O	2:E:99:LEU:N	2.35	0.55
3:F:35:SER:HB3	3:F:322:GLN:NE2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:ALA:CB	3:C:196:TYR:HE2	2.20	0.55
3:C:85:ASN:C	3:C:87:ASP:H	2.09	0.55
3:F:48:LEU:HD13	3:F:66:VAL:HG11	1.88	0.55
3:C:108:VAL:HA	3:C:119:VAL:CG1	2.37	0.55
3:F:94:ALA:HA	3:F:118:GLU:O	2.07	0.55
1:A:1(M):PHE:O	1:A:1(L):PHE:CB	2.49	0.55
3:F:145:MET:HG3	3:F:169:TYR:CE2	2.41	0.55
3:C:204:LEU:HD23	3:C:271:GLN:HG2	1.86	0.55
2:B:97(A):GLU:HA	3:C:339:THR:HB	1.88	0.55
3:F:286:LYS:HE2	3:F:290:LYS:CE	2.37	0.55
2:B:60(A):TYR:CD2	2:B:60(C):PRO:HG2	2.42	0.54
3:C:137:TRP:CE2	3:C:141:GLU:HG3	2.42	0.54
3:C:179:GLN:HG2	3:C:181:GLU:OE2	2.00	0.54
1:D:19:ARG:NE	2:E:207:TRP:NE1	2.55	0.54
3:F:8:LEU:HD21	3:F:73:LEU:HD11	1.87	0.54
3:C:95:VAL:CG1	3:C:119:VAL:HB	2.38	0.54
2:E:91:HIS:CB	2:E:237:TRP:HE1	2.20	0.54
2:B:97:ARG:O	3:C:339:THR:CB	2.55	0.54
2:B:232:PHE:C	2:B:234:LEU:H	2.09	0.54
2:B:91:HIS:NE2	2:B:237:TRP:CG	2.75	0.54
3:F:58:LEU:HD23	3:F:294:ILE:HD13	1.90	0.54
3:F:94:ALA:HB2	3:F:137:TRP:CZ2	2.43	0.54
3:C:210:GLY:O	3:C:211:SER:HB3	2.08	0.54
3:C:224:GLU:C	3:C:225:LEU:HD12	2.28	0.54
2:E:147(A):TRP:CD1	2:E:148:GLY:O	2.61	0.54
1:A:1(K):ASN:ND2	1:A:1(J):PRO:HD2	2.21	0.53
1:D:39:TYR:N	1:D:40:ILE:HA	2.21	0.53
3:C:46:LEU:HD11	3:C:164:LEU:HD21	1.90	0.53
3:C:173:LEU:HB2	3:C:228:HIS:HD1	1.73	0.53
2:E:176:ILE:HG23	2:E:180:MET:CE	2.38	0.53
2:B:203:SER:HB3	2:B:204(B):ASN:OD1	2.08	0.53
2:B:217:GLU:O	2:B:221(A):ARG:HG3	2.09	0.53
3:C:362:ILE:HB	3:C:372:PHE:HB2	1.91	0.53
2:B:60:LEU:CD2	2:B:90:ILE:HD13	2.38	0.53
2:E:164:GLU:HB3	2:E:166:PRO:HD2	1.90	0.53
3:C:214:ALA:HB1	3:C:215:PRO:HD2	1.89	0.53
3:C:51:ASP:O	3:C:304:ASN:ND2	2.42	0.53
2:E:45:SER:CB	2:E:209:GLN:OE1	2.57	0.53
1:A:14(L):ASP:OD1	1:A:15:ARG:HG2	2.07	0.53
2:B:61:GLU:HG2	2:B:87:LYS:HA	1.90	0.53
3:C:335:ALA:HA	3:C:338:ALA:CB	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:60(I):THR:HG23	2:E:62:ASN:H	1.74	0.53
3:F:198:VAL:CG2	3:F:199:PRO:HD2	2.39	0.53
3:C:335:ALA:CB	3:C:338:ALA:HB3	2.38	0.52
3:F:155:ILE:HG22	3:F:156:ASP:N	2.23	0.52
3:F:49:GLY:O	3:F:308:ILE:HG13	2.09	0.52
1:A:6:LEU:HD12	2:B:25:GLY:HA3	1.92	0.52
2:B:177:THR:HG23	2:B:180:MET:HE3	1.92	0.52
3:C:175:LYS:C	3:C:333:THR:HG22	2.30	0.52
3:F:254:SER:O	3:F:258:ILE:HG13	2.09	0.52
3:F:104:GLU:HG3	3:F:106:PRO:HD2	1.92	0.52
2:E:165:ARG:N	2:E:166:PRO:CD	2.73	0.52
3:F:235:LEU:HD21	3:F:262:MET:CE	2.38	0.52
2:B:163:VAL:HG12	2:B:164:GLU:N	2.25	0.52
3:F:238:LEU:H	3:F:238:LEU:HD23	1.75	0.52
2:B:60(B):PRO:HB2	2:B:60(C):PRO:CD	2.40	0.52
2:E:156:GLN:HA	2:E:156:GLN:NE2	2.25	0.52
3:F:250:ILE:N	3:F:251:PRO:HD2	2.24	0.52
3:F:234:MET:HE3	3:F:362:ILE:HD11	1.91	0.51
2:B:96:TRP:O	2:B:96:TRP:HE3	1.92	0.51
3:C:105:VAL:N	3:C:106:PRO:CD	2.73	0.51
3:C:162:LEU:HB3	3:C:317:VAL:HA	1.92	0.51
3:C:204:LEU:HD21	3:C:271:GLN:CG	2.36	0.51
2:E:169:LYS:CA	2:E:176:ILE:HD12	2.39	0.51
3:C:280:VAL:O	3:C:280:VAL:HG13	2.11	0.51
3:C:8:LEU:HD21	3:C:73:LEU:HD13	1.89	0.51
3:C:309:THR:CG2	3:C:311:GLY:O	2.57	0.51
3:C:246:LEU:HD12	3:C:249:ILE:CD1	2.39	0.51
3:C:375:GLN:HG3	3:C:375:GLN:O	2.11	0.51
3:F:359:LEU:H	3:F:359:LEU:CD2	2.19	0.51
2:B:35:ARG:HB2	2:B:41:LEU:HD11	1.92	0.51
3:C:48:LEU:HD21	3:C:110:ARG:HB3	1.93	0.51
2:E:40:LEU:HD12	2:E:41:LEU:N	2.26	0.51
3:F:119:VAL:O	3:F:119:VAL:HG22	2.10	0.51
2:B:60(A):TYR:OH	3:C:341:ALA:CA	2.59	0.51
3:C:34:ILE:CG2	3:C:35:SER:N	2.74	0.51
2:E:60(B):PRO:HB2	2:E:60(C):PRO:CD	2.39	0.51
3:C:115:PHE:C	3:C:116:GLN:NE2	2.62	0.51
2:E:114:PHE:CE1	2:E:120:PRO:HD3	2.47	0.50
2:E:146:GLU:HB2	2:E:220:CYS:HB2	1.94	0.50
1:A:8:GLU:OE2	2:B:202:LYS:NZ	2.37	0.50
1:D:16:CYS:C	2:E:122:CYS:SG	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:250:ILE:HB	3:F:251:PRO:HD3	1.93	0.50
3:F:214:ALA:HB1	3:F:215:PRO:HD2	1.93	0.50
3:C:151:SER:CB	3:C:152:PRO:HD2	2.39	0.50
3:F:149:LEU:HD23	3:F:323:LYS:HD2	1.93	0.50
3:F:48:LEU:CD1	3:F:110:ARG:HH12	2.25	0.50
1:A:1(G):PHE:CE2	2:B:48:SER:HB3	2.47	0.50
3:C:229:GLY:O	3:C:230:GLU:CB	2.57	0.50
1:D:10:GLY:O	1:D:11:SER:CB	2.60	0.50
3:C:32:ILE:O	3:C:374:GLY:HA2	2.13	0.49
3:F:246:LEU:O	3:F:250:ILE:HG13	2.12	0.49
3:F:234:MET:HE2	3:F:362:ILE:HD11	1.92	0.49
2:B:101:ARG:O	2:B:103:ILE:HG22	2.13	0.49
3:C:365:ASN:HB2	3:C:366:PRO:HD3	1.94	0.49
3:C:148:ASN:H	3:C:149:LEU:HD12	1.77	0.49
3:C:138:VAL:HG21	3:C:149:LEU:CD2	2.42	0.49
2:E:28:PRO:HB2	2:E:119:HIS:H	1.77	0.49
2:E:40:LEU:HD12	2:E:41:LEU:H	1.78	0.49
1:A:1(N):THR:N	1:A:1(M):PHE:CB	2.68	0.49
1:A:5:PRO:HA	1:A:9:LYS:HB2	1.93	0.49
2:B:16:ILE:N	2:B:194:ASP:OD2	2.45	0.49
2:E:18:GLU:HB2	2:E:188:GLY:HA2	1.95	0.49
3:F:250:ILE:HB	3:F:251:PRO:CD	2.43	0.49
2:E:147(A):TRP:NE1	2:E:148:GLY:O	2.46	0.49
3:F:155:ILE:HG22	3:F:157:GLY:N	2.27	0.49
3:F:178:PHE:CE2	3:F:203:GLN:HB3	2.47	0.49
2:B:136:GLY:HA3	2:B:199:PHE:CZ	2.48	0.49
3:C:222:PHE:HA	3:C:236:ILE:O	2.13	0.49
3:C:344:ILE:C	3:C:346:ARG:H	2.16	0.49
3:C:34:ILE:HG22	3:C:35:SER:N	2.28	0.49
3:F:108:VAL:HA	3:F:119:VAL:CG1	2.41	0.49
3:F:78:LYS:O	3:F:82:SER:HB2	2.13	0.49
3:F:85:ASN:O	3:F:87:ASP:N	2.37	0.49
1:A:14(F):LEU:O	1:A:14(I):SER:HB3	2.12	0.48
3:F:285:LEU:HD11	3:F:322:GLN:HB2	1.95	0.48
2:E:176:ILE:HG23	2:E:180:MET:HE2	1.94	0.48
3:F:320:ILE:HG23	3:F:320:ILE:O	2.13	0.48
3:F:204:LEU:CD2	3:F:205:SER:N	2.76	0.48
3:F:209:CYS:HB3	3:F:223:ILE:HG13	1.94	0.48
2:B:94:TYR:CZ	2:B:96:TRP:HB3	2.48	0.48
3:F:95:VAL:HB	3:F:119:VAL:HB	1.95	0.48
2:B:232:PHE:O	2:B:234:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:207:PHE:CE2	3:C:272:VAL:HG11	2.49	0.48
3:C:73:LEU:O	3:C:77:ASN:ND2	2.45	0.48
2:E:169:LYS:CA	2:E:176:ILE:HD11	2.28	0.48
2:E:70:LYS:HD2	2:E:80:GLU:OE2	2.13	0.48
3:C:177:ARG:HE	3:C:334:LYS:HA	1.78	0.48
1:D:19:ARG:HH21	2:E:207:TRP:HE1	0.50	0.48
2:E:190:ALA:HB3	3:F:346:ARG:NH1	2.29	0.48
2:B:98:ASN:O	2:B:99:LEU:HB2	2.14	0.48
3:C:190:ALA:HB2	3:C:196:TYR:HE2	1.79	0.48
2:B:115:SER:OG	7:B:409:HOH:O	2.19	0.48
2:E:164:GLU:C	2:E:166:PRO:HD2	2.34	0.48
2:B:132:ALA:CB	2:B:164:GLU:HG3	2.44	0.47
2:B:60(A):TYR:OH	3:C:341:ALA:N	2.47	0.47
3:C:272:VAL:HG13	3:C:272:VAL:O	2.14	0.47
3:C:285:LEU:HD12	3:C:285:LEU:N	2.29	0.47
3:C:274:LEU:HD23	3:C:274:LEU:N	2.28	0.47
2:E:163:VAL:HB	2:E:182:CYS:SG	2.53	0.47
3:F:42:VAL:HG11	3:F:320:ILE:HD11	1.95	0.47
3:F:46:LEU:HD21	3:F:164:LEU:CD2	2.44	0.47
2:E:32:MET:HG3	2:E:40:LEU:HD13	1.96	0.47
1:A:1:CYS:C	2:B:122:CYS:SG	2.93	0.47
2:E:60(F):LYS:HB2	2:E:60(F):LYS:NZ	2.30	0.47
3:F:321:LEU:C	3:F:321:LEU:HD12	2.35	0.47
2:B:94:TYR:CE2	2:B:96:TRP:HB3	2.50	0.47
3:C:268:LYS:HG3	3:C:270:VAL:CG2	2.44	0.47
3:C:27:ARG:NH1	3:C:30:ASP:OD2	2.45	0.47
2:B:35:ARG:HG2	2:B:37:PRO:O	2.15	0.47
3:F:105:VAL:N	3:F:106:PRO:CD	2.77	0.47
3:F:206:VAL:HA	3:F:268:LYS:O	2.15	0.47
2:B:232:PHE:C	2:B:234:LEU:N	2.68	0.47
3:C:146:ILE:CG2	3:C:323:LYS:HD3	2.45	0.47
3:C:355:ASP:OD1	3:C:355:ASP:N	2.48	0.47
3:C:359:LEU:CD1	3:C:359:LEU:C	2.83	0.47
3:C:204:LEU:HD22	3:C:349:PRO:HG3	1.97	0.47
3:F:205:SER:OG	3:F:206:VAL:N	2.48	0.47
3:C:162:LEU:HB2	3:C:316:HIS:O	2.15	0.47
2:E:47:ILE:HD11	2:E:51:TRP:CB	2.45	0.47
2:B:202:LYS:HE3	2:B:205:ASN:O	2.15	0.47
2:B:60:LEU:CD2	2:B:90:ILE:HD11	2.41	0.47
3:F:146:ILE:CG2	3:F:323:LYS:HD3	2.45	0.47
2:B:35:ARG:HG3	2:B:36:LYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:ASN:O	3:C:87:ASP:N	2.42	0.46
2:E:60(B):PRO:CB	2:E:60(C):PRO:HD3	2.42	0.46
3:F:46:LEU:HD21	3:F:164:LEU:HD21	1.97	0.46
3:F:85:ASN:C	3:F:87:ASP:H	2.19	0.46
3:C:236:ILE:HD13	3:C:360:PHE:HB3	1.97	0.46
2:B:68:ILE:HG22	2:B:118:ILE:HG12	1.96	0.46
3:C:299:ASP:HB3	3:C:302:LYS:HB2	1.98	0.46
3:C:270:VAL:HG11	3:C:352:PHE:HB2	1.98	0.46
2:E:77(A):ARG:O	2:E:78:ASN:HB2	2.16	0.46
3:F:222:PHE:HA	3:F:236:ILE:O	2.15	0.46
3:C:96:PHE:CE1	3:C:134:ILE:HG23	2.51	0.46
3:F:361:PHE:N	3:F:361:PHE:CD1	2.83	0.46
2:B:212:ILE:HB	2:B:229:THR:HB	1.98	0.46
2:E:163:VAL:HG12	2:E:164:GLU:N	2.29	0.46
3:F:155:ILE:HG22	3:F:157:GLY:H	1.80	0.46
3:F:287:GLU:N	3:F:288:PRO:CD	2.79	0.46
2:B:176:ILE:O	2:B:177:THR:HG22	2.16	0.46
3:C:246:LEU:O	3:C:249:ILE:HG12	2.16	0.46
3:F:174:TRP:CZ3	3:F:225:LEU:HB3	2.50	0.46
1:A:1(P):TYR:CE1	1:A:1(C):GLU:HG2	2.50	0.46
2:E:79:ILE:CG2	2:E:117:TYR:CD2	2.97	0.46
2:B:60(A):TYR:OH	3:C:341:ALA:HA	2.15	0.46
3:C:108:VAL:HG13	3:C:119:VAL:HG13	1.97	0.46
2:E:235:LYS:O	2:E:236:LYS:C	2.55	0.46
2:E:59:LEU:N	2:E:59:LEU:HD12	2.30	0.46
3:F:178:PHE:HB2	3:F:330:GLU:HA	1.98	0.46
3:F:225:LEU:HD12	3:F:225:LEU:N	2.31	0.46
3:F:375:GLN:HG3	3:F:375:GLN:O	2.16	0.46
3:C:190:ALA:HB2	3:C:196:TYR:CE2	2.51	0.45
3:C:21:ASN:OD1	3:C:251:PRO:HA	2.16	0.45
2:E:180:MET:HE1	2:E:215:TRP:HZ2	1.82	0.45
3:F:48:LEU:HD21	3:F:110:ARG:CB	2.36	0.45
1:A:1(P):TYR:HE1	1:A:1(C):GLU:HG2	1.81	0.45
3:C:176:SER:O	3:C:203:GLN:NE2	2.45	0.45
2:E:47:ILE:O	2:E:120:PRO:CB	2.63	0.45
3:F:224:GLU:C	3:F:225:LEU:HD12	2.37	0.45
3:F:69:VAL:HG23	3:F:72:ILE:HD12	1.97	0.45
2:B:60(B):PRO:HB2	2:B:60(C):PRO:HD3	1.98	0.45
2:E:165:ARG:N	2:E:166:PRO:HD2	2.30	0.45
3:C:177:ARG:HG2	3:C:333:THR:O	2.16	0.45
2:B:89:TYR:CZ	2:B:245:PHE:CB	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:ASN:C	3:C:87:ASP:N	2.70	0.45
2:E:60(B):PRO:O	2:E:60(D):TRP:N	2.50	0.45
3:F:97:VAL:HG12	3:F:98:LYS:N	2.31	0.45
2:B:146:GLU:HB2	2:B:220:CYS:CB	2.37	0.45
2:B:153:SER:HB3	7:B:421:HOH:O	2.16	0.45
2:E:192:GLU:OE1	3:F:349:PRO:HG3	2.17	0.45
2:B:60(B):PRO:CD	2:B:60(C):PRO:HD2	2.47	0.45
3:C:227:TYR:HB2	3:C:232:ILE:O	2.17	0.45
3:F:362:ILE:HB	3:F:372:PHE:HB2	1.98	0.45
1:D:4:PHE:CB	1:D:5:ASN:CA	2.94	0.45
2:E:139:THR:HG22	2:E:157:VAL:HA	1.99	0.45
3:C:92:ALA:HB1	3:C:137:TRP:CH2	2.52	0.45
3:C:16:GLY:HA3	3:C:36:PRO:HA	1.99	0.45
2:B:54:THR:OG1	2:B:55:ALA:N	2.50	0.45
3:C:175:LYS:O	3:C:333:THR:HG22	2.16	0.45
2:E:47:ILE:HG13	2:E:48:SER:H	1.81	0.45
3:F:305:PHE:HB3	3:F:308:ILE:HD12	1.97	0.45
3:F:356:ARG:HB3	3:F:357:PRO:CD	2.47	0.45
2:B:61:GLU:CG	2:B:87:LYS:HA	2.47	0.44
2:B:96:TRP:O	2:B:96:TRP:CE3	2.71	0.44
3:F:103:ILE:HG23	3:F:308:ILE:O	2.17	0.44
3:F:143:ARG:O	3:F:144:ASP:CB	2.65	0.44
3:F:204:LEU:HD23	3:F:205:SER:H	1.81	0.44
3:C:138:VAL:HG11	3:C:149:LEU:HD11	1.98	0.44
2:E:235:LYS:O	2:E:238:ILE:N	2.50	0.44
2:E:138:VAL:HG23	2:E:199:PHE:HD2	1.81	0.44
3:F:173:LEU:HB2	3:F:228:HIS:ND1	2.32	0.44
3:F:256:LYS:O	3:F:259:ASP:HB2	2.17	0.44
3:F:354:VAL:O	3:F:354:VAL:HG12	2.18	0.44
1:A:14(L):ASP:CG	1:A:15:ARG:HG2	2.37	0.44
3:C:197:GLN:HA	3:C:197:GLN:OE1	2.17	0.44
3:C:360:PHE:CE1	3:C:376:ILE:HD11	2.49	0.44
3:C:95:VAL:HG13	3:C:119:VAL:CB	2.48	0.44
2:E:28:PRO:HG2	2:E:29:TRP:CE3	2.52	0.44
3:F:122:VAL:HG22	3:F:123:ASN:N	2.33	0.44
3:F:14:ASN:O	3:F:18:GLN:HG3	2.17	0.44
3:F:338:ALA:O	3:F:339:THR:C	2.56	0.44
2:B:130:LEU:HD23	2:B:230:HIS:NE2	2.32	0.44
2:E:47:ILE:HD11	2:E:51:TRP:HB3	2.00	0.44
2:B:36(A):SER:HA	2:B:37:PRO:HA	1.85	0.43
3:C:177:ARG:NH1	3:C:179:GLN:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:147(A):TRP:CE3	2:E:150:GLY:HA3	2.52	0.43
2:B:22:ALA:O	2:B:71:HIS:HE1	2.00	0.43
3:C:33:VAL:HG21	3:C:279:ALA:HB1	1.99	0.43
3:C:344:ILE:HG22	3:C:344:ILE:O	2.18	0.43
2:E:103:ILE:O	2:E:104:ALA:HB2	2.17	0.43
2:E:127:GLU:C	2:E:129:ALA:N	2.72	0.43
2:E:56:ALA:C	2:E:58:CYS:H	2.22	0.43
3:F:204:LEU:CD2	3:F:204:LEU:C	2.87	0.43
3:F:97:VAL:HG22	3:F:162:LEU:HD11	1.99	0.43
3:C:200:MET:HG2	3:C:275:PRO:HA	2.00	0.43
3:F:69:VAL:O	3:F:69:VAL:HG13	2.18	0.43
2:E:76:TYR:CD1	2:E:80:GLU:OE1	2.72	0.43
2:B:147:THR:O	2:B:147:THR:HG23	2.16	0.43
3:F:94:ALA:CB	3:F:137:TRP:CH2	2.96	0.43
2:B:119:HIS:CD2	2:B:120:PRO:CD	2.98	0.43
2:B:60(C):PRO:HD3	2:B:96:TRP:CZ3	2.54	0.43
3:C:178:PHE:CD2	3:C:201:LEU:HB3	2.53	0.43
3:C:209:CYS:O	3:C:265:MET:CA	2.61	0.43
3:C:213:SER:HB3	3:C:219:TRP:CE2	2.53	0.43
3:C:20:PHE:CE2	3:C:24:VAL:HG21	2.54	0.43
1:D:35:LEU:N	1:D:35:LEU:HD12	2.34	0.43
2:E:203:SER:HA	2:E:204:PRO:HD3	1.85	0.43
3:F:249:ILE:HG13	3:F:250:ILE:N	2.34	0.43
3:F:342:ILE:HG22	3:F:343:LEU:N	2.34	0.43
3:F:16:GLY:HA3	3:F:36:PRO:HA	1.99	0.43
3:F:90:THR:HG21	3:F:142:THR:HA	2.00	0.43
2:E:129(C):LEU:N	2:E:129(C):LEU:CD1	2.81	0.43
1:D:19:ARG:NE	2:E:207:TRP:HE1	2.13	0.43
2:E:70:LYS:HB3	2:E:70:LYS:HE3	1.92	0.43
3:F:32:ILE:O	3:F:374:GLY:HA2	2.19	0.43
3:F:309:THR:C	3:F:311:GLY:H	2.22	0.43
2:B:76:TYR:CE2	2:B:77(A):ARG:HB3	2.54	0.42
3:C:149:LEU:H	3:C:149:LEU:HD12	1.82	0.42
3:F:321:LEU:O	3:F:321:LEU:HD12	2.19	0.42
2:B:60(I):THR:O	2:B:61:GLU:C	2.57	0.42
2:E:156:GLN:HA	2:E:156:GLN:HE21	1.83	0.42
3:F:150:LEU:HD13	3:F:155:ILE:CD1	2.39	0.42
1:A:1(K):ASN:HD22	1:A:1(J):PRO:N	2.17	0.42
3:C:152:PRO:HD2	3:C:153:ASP:H	1.83	0.42
2:E:91:HIS:CB	2:E:237:TRP:CZ2	3.02	0.42
3:F:359:LEU:N	3:F:359:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:GLY:HA3	7:C:515:HOH:O	2.19	0.42
2:B:60(I):THR:CG2	2:B:61:GLU:OE2	2.50	0.42
3:C:140:ASN:ND2	7:C:518:HOH:O	2.52	0.42
3:C:270:VAL:HG12	3:C:271:GLN:N	2.34	0.42
2:E:147(A):TRP:CZ3	2:E:150:GLY:HA2	2.54	0.42
3:C:287:GLU:HB2	3:C:288:PRO:HD3	2.02	0.42
2:B:96:TRP:C	2:B:96:TRP:CE3	2.93	0.42
3:C:138:VAL:HG21	3:C:149:LEU:HD22	2.01	0.42
3:C:234:MET:HE3	3:C:362:ILE:CD1	2.46	0.42
3:C:259:ASP:O	3:C:262:MET:N	2.52	0.42
3:C:269:ARG:NH1	3:C:345:ALA:HA	2.29	0.42
3:C:69:VAL:O	3:C:72:ILE:N	2.52	0.42
1:A:1(C):GLU:O	1:A:1(B):ALA:C	2.58	0.42
3:F:150:LEU:HA	3:F:154:LEU:HD23	2.01	0.42
3:F:74:LYS:HB2	3:F:74:LYS:HE3	1.79	0.42
3:F:71:LYS:O	3:F:74:LYS:HG2	2.20	0.42
3:C:94:ALA:HB2	3:C:137:TRP:CH2	2.55	0.42
3:C:137:TRP:CZ2	3:C:141:GLU:HG3	2.54	0.42
3:C:151:SER:CB	3:C:152:PRO:HD3	2.49	0.42
3:C:236:ILE:HD13	3:C:360:PHE:CB	2.50	0.42
2:E:195:ALA:HA	2:E:213:VAL:HG12	2.02	0.42
2:E:28:PRO:HB2	2:E:119:HIS:N	2.35	0.42
2:E:58:CYS:O	2:E:60(F):LYS:HD3	2.20	0.42
2:E:60(I):THR:HG22	2:E:63:ASP:CG	2.40	0.42
3:F:62:MET:O	3:F:63:ARG:HB2	2.20	0.42
2:B:48:SER:OG	2:B:51:TRP:HB2	2.20	0.41
3:F:85:ASN:C	3:F:87:ASP:N	2.73	0.41
3:C:115:PHE:O	3:C:116:GLN:C	2.57	0.41
3:C:225:LEU:N	3:C:225:LEU:HD12	2.35	0.41
3:C:69:VAL:O	3:C:70:GLY:C	2.58	0.41
3:F:139:LYS:O	3:F:144:ASP:N	2.53	0.41
3:F:294:ILE:HG21	3:F:297:MET:HE1	2.00	0.41
2:B:147:THR:O	2:B:147(A):TRP:CB	2.67	0.41
3:C:221:ASN:O	3:C:237:ALA:HA	2.20	0.41
3:C:270:VAL:CG1	3:C:271:GLN:N	2.82	0.41
3:C:356:ARG:O	3:C:357:PRO:C	2.59	0.41
2:E:176:ILE:HG13	2:E:176:ILE:H	1.63	0.41
1:A:1(N):THR:CA	1:A:1(M):PHE:HB2	2.47	0.41
1:A:3:LEU:HD11	2:B:206:ARG:HG2	1.97	0.41
2:E:182:CYS:HB3	2:E:227:PHE:CE2	2.55	0.41
3:C:15:THR:O	3:C:19:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:227:TYR:CD2	3:C:232:ILE:O	2.71	0.41
3:C:344:ILE:O	3:C:346:ARG:N	2.47	0.41
2:E:77(A):ARG:O	2:E:79:ILE:HG13	2.20	0.41
3:F:357:PRO:HB3	3:F:377:ASN:ND2	2.35	0.41
2:B:163:VAL:CG1	2:B:164:GLU:N	2.84	0.41
2:B:61:GLU:OE2	2:B:61:GLU:N	2.49	0.41
3:C:166:ASN:O	3:C:322:GLN:HA	2.20	0.41
2:E:129(C):LEU:HD12	2:E:129(C):LEU:H	1.83	0.41
2:E:163:VAL:CG1	2:E:164:GLU:N	2.84	0.41
3:F:161:ARG:HE	3:F:316:HIS:CD2	2.32	0.41
1:A:8:GLU:C	1:A:10:LYS:H	2.23	0.41
2:B:226:GLY:CA	7:C:515:HOH:O	2.68	0.41
3:F:155:ILE:HG23	3:F:156:ASP:H	1.85	0.41
2:B:165:ARG:HB3	2:B:166:PRO:CD	2.48	0.41
3:C:171:LYS:O	3:C:171:LYS:HG2	2.20	0.41
1:D:22:PHE:CB	7:D:103:HOH:O	2.68	0.41
2:B:60(I):THR:O	2:B:62:ASN:N	2.54	0.41
3:C:108:VAL:HG22	3:C:119:VAL:HG13	2.02	0.41
3:C:259:ASP:O	3:C:260:SER:C	2.58	0.41
3:C:348:SER:HA	3:C:349:PRO:HD3	1.91	0.41
2:E:91:HIS:CB	2:E:237:TRP:HZ2	2.34	0.41
3:F:23:ILE:HG22	3:F:32:ILE:HD13	2.03	0.41
3:F:285:LEU:C	3:F:288:PRO:HD2	2.42	0.41
3:C:175:LYS:O	3:C:333:THR:HG23	2.18	0.41
2:E:60(B):PRO:CB	2:E:60(C):PRO:CD	2.99	0.41
2:E:60(F):LYS:HG3	2:E:60(H):PHE:CE2	2.55	0.41
3:F:221:ASN:O	3:F:237:ALA:HA	2.21	0.41
3:F:246:LEU:O	3:F:249:ILE:HG12	2.20	0.41
3:F:341:ALA:C	3:F:342:ILE:HG13	2.41	0.41
2:B:56:ALA:N	2:B:102:ASP:OD1	2.54	0.40
2:B:53:LEU:HD12	2:B:104:ALA:O	2.21	0.40
2:B:147:THR:O	2:B:147:THR:CG2	2.69	0.40
2:B:68:ILE:O	2:B:80:GLU:HA	2.21	0.40
3:C:67:ASN:N	3:C:67:ASN:OD1	2.54	0.40
2:B:60(B):PRO:CB	2:B:60(C):PRO:CD	2.99	0.40
3:F:232:ILE:HG22	3:F:233:SER:N	2.36	0.40
2:B:46:LEU:O	2:B:120:PRO:HA	2.22	0.40
2:B:110:LYS:HA	2:B:111:PRO:HD3	1.96	0.40
2:B:211:GLY:HA2	2:B:229:THR:O	2.21	0.40
3:C:210:GLY:O	3:C:211:SER:CB	2.70	0.40
3:C:211:SER:CA	3:C:222:PHE:CE2	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:353:ILE:O	3:C:353:ILE:HG23	2.22	0.40
3:C:46:LEU:HD11	3:C:164:LEU:CD2	2.50	0.40
2:E:127:GLU:C	2:E:129:ALA:H	2.24	0.40
3:F:359:LEU:N	3:F:359:LEU:CD2	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	43/49 (88%)	32 (74%)	11 (26%)	0	100 100
1	D	35/49 (71%)	26 (74%)	6 (17%)	3 (9%)	1 1
2	B	249/259 (96%)	218 (88%)	28 (11%)	3 (1%)	13 39
2	E	245/259 (95%)	212 (86%)	31 (13%)	2 (1%)	19 49
3	C	375/379 (99%)	335 (89%)	29 (8%)	11 (3%)	4 15
3	F	376/379 (99%)	347 (92%)	29 (8%)	0	100 100
All	All	1323/1374 (96%)	1170 (88%)	134 (10%)	19 (1%)	11 34

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	339	THR
3	C	347	SER
1	D	11	SER
1	D	12	GLY
2	E	147(E)	VAL
2	B	233	ARG
3	C	148	ASN
1	D	6	PRO

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Mol	Chain	Res	Type
2	E	100	ASP
2	B	102	ASP
2	B	94	TYR
3	C	147	ASP
3	C	171	LYS
3	C	211	SER
3	C	345	ALA
3	C	151	SER
3	C	172	GLY
3	C	122	VAL
3	C	152	PRO

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	33/43 (77%)	29 (88%)	4 (12%)	5 15
1	D	7/43 (16%)	7 (100%)	0	100 100
2	B	191/224 (85%)	185 (97%)	6 (3%)	40 74
2	E	137/224 (61%)	134 (98%)	3 (2%)	52 83
3	C	268/332 (81%)	258 (96%)	10 (4%)	34 68
3	F	301/332 (91%)	291 (97%)	10 (3%)	38 72
All	All	937/1198 (78%)	904 (96%)	33 (4%)	36 70

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1(M)	PHE
1	A	1(K)	ASN
1	A	14(D)	ARG
1	A	14(F)	LEU
2	B	33	LEU
2	B	59	LEU
2	B	90	ILE

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Mol	Chain	Res	Type
2	B	182	CYS
2	B	221(A)	ARG
2	B	233	ARG
3	C	46	LEU
3	C	95	VAL
3	C	99	ASN
3	C	111	ASN
3	C	116	GLN
3	C	119	VAL
3	C	149	LEU
3	C	150	LEU
3	C	218	LEU
3	C	271	GLN
2	E	38	GLN
2	E	129(C)	LEU
2	E	182	CYS
3	F	27	ARG
3	F	53	ARG
3	F	117	CYS
3	F	118	GLU
3	F	119	VAL
3	F	192	ASP
3	F	197	GLN
3	F	204	LEU
3	F	235	LEU
3	F	238	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1(K)	ASN
2	B	71	HIS
2	B	91	HIS
2	B	143	ASN
2	B	179	ASN
3	C	18	GLN
3	C	22	GLN
3	C	99	ASN
3	C	111	ASN
3	C	116	GLN
3	C	271	GLN
3	C	314	ASN

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Mol	Chain	Res	Type
2	E	38	GLN
2	E	143	ASN
2	E	156	GLN
2	E	205	ASN
3	F	179	GLN
3	F	197	GLN
3	F	316	HIS
3	F	377	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACT	B	301	-	1,3,3	1.35	0	0,3,3	0.00	-
4	ACT	A	101	5	1,3,3	1.29	0	0,3,3	0.00	-
4	ACT	C	401	-	1,3,3	1.36	0	0,3,3	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	45/49 (91%)	-0.32	0 100 100	15, 33, 61, 75	0
1	D	39/49 (79%)	-0.13	1 (2%) 56 46	30, 50, 69, 80	0
2	B	253/259 (97%)	-0.26	0 100 100	19, 40, 63, 80	1 (0%)
2	E	251/259 (96%)	0.02	13 (5%) 27 18	34, 63, 90, 106	0
3	C	377/379 (99%)	-0.30	4 (1%) 80 75	22, 46, 67, 97	0
3	F	378/379 (99%)	-0.37	3 (0%) 86 81	17, 36, 60, 95	1 (0%)
All	All	1343/1374 (97%)	-0.25	21 (1%) 72 66	15, 44, 78, 106	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	51	TRP	4.5
3	C	336	SER	4.0
3	F	2	HIS	3.8
2	E	237	TRP	3.7
3	F	336	SER	3.4
2	E	89	TYR	3.3
3	C	337	ALA	3.3
2	E	204	PRO	3.3
3	F	341	ALA	3.2
2	E	129	ALA	3.2
2	E	105	LEU	3.2
2	E	147(A)	TRP	2.6
2	E	120	PRO	2.6
2	E	229	THR	2.6
2	E	92	PRO	2.6
2	E	203	SER	2.5
1	D	5	ASN	2.4
2	E	106	MET	2.4
3	C	335	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	68	GLY	2.1
2	E	241	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NA	B	302	1/1	0.76	0.22	74,74,74,74	0
5	CA	F	401	1/1	0.88	0.07	106,106,106,106	0
4	ACT	C	401	4/4	0.88	0.20	74,76,77,83	0
4	ACT	B	301	4/4	0.91	0.34	59,60,64,66	0
5	CA	A	102	1/1	0.95	0.14	52,52,52,52	0
4	ACT	A	101	4/4	0.99	0.20	44,45,45,47	0

6.5 Other polymers (i)

There are no such residues in this entry.