



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:17 AM UTC

PDB ID : 4FC5 / pdb_00004fc5
Title : Crystal Structure of Ton_0340
Authors : Lee, S.G.; Lee, K.H.; An, Y.J.; Cha, S.S.; Oh, B.H.
Deposited on : 2012-05-24
Resolution : 2.30 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:

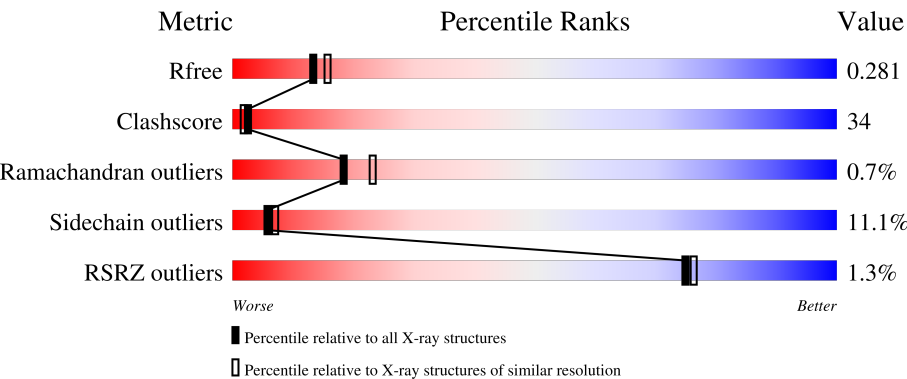
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	270	
1	B	270	
1	C	270	
1	D	270	
1	E	270	

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Mol	Chain	Length	Quality of chain
1	F	270	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: green (53%), yellow (40%), and orange (7%). The percentages are labeled below the segments.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13532 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1963	1250	334	372	7			
1	B	268	Total	C	N	O	S	0	0	0
			2022	1288	343	384	7			
1	C	269	Total	C	N	O	S	0	0	0
			2035	1297	344	386	8			
1	D	268	Total	C	N	O	S	0	0	0
			2022	1288	343	384	7			
1	E	258	Total	C	N	O	S	0	0	0
			1959	1248	333	371	7			
1	F	269	Total	C	N	O	S	0	0	0
			2035	1297	344	386	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	269	LYS	-	expression tag	UNP B6YTD8
A	270	LEU	-	expression tag	UNP B6YTD8
B	269	LYS	-	expression tag	UNP B6YTD8
B	270	LEU	-	expression tag	UNP B6YTD8
C	269	LYS	-	expression tag	UNP B6YTD8
C	270	LEU	-	expression tag	UNP B6YTD8
D	269	LYS	-	expression tag	UNP B6YTD8
D	270	LEU	-	expression tag	UNP B6YTD8
E	269	LYS	-	expression tag	UNP B6YTD8
E	270	LEU	-	expression tag	UNP B6YTD8
F	269	LYS	-	expression tag	UNP B6YTD8
F	270	LEU	-	expression tag	UNP B6YTD8

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total 8	Zn 8	0	0
2	B	11	Total 11	Zn 11	0	0
2	C	8	Total 8	Zn 8	0	0
2	D	7	Total 7	Zn 7	0	0
2	E	11	Total 11	Zn 11	0	0
2	F	8	Total 8	Zn 8	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	260	Total 260	O 260	0	0
3	B	309	Total 309	O 309	0	0
3	C	170	Total 170	O 170	0	0
3	D	191	Total 191	O 191	0	0
3	E	218	Total 218	O 218	0	0
3	F	295	Total 295	O 295	0	0

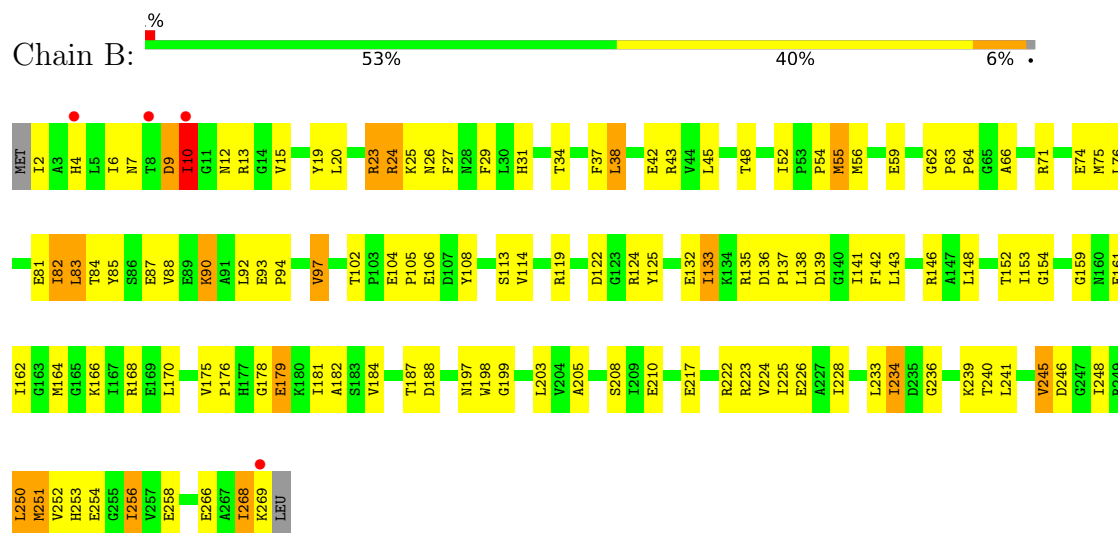
3 Residue-property plots [i](#)

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.

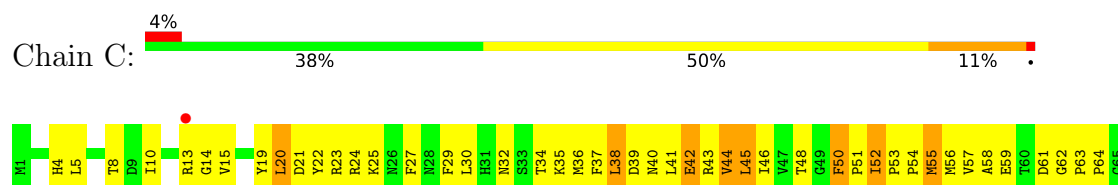
• Molecule 1: Putative uncharacterized protein

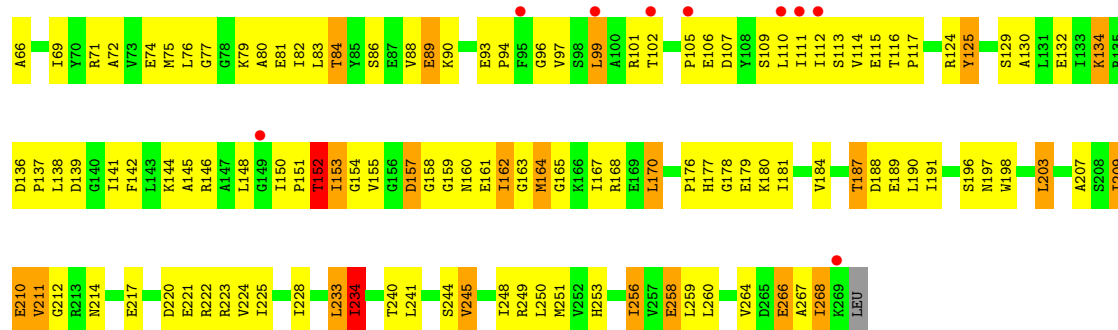


• Molecule 1: Putative uncharacterized protein

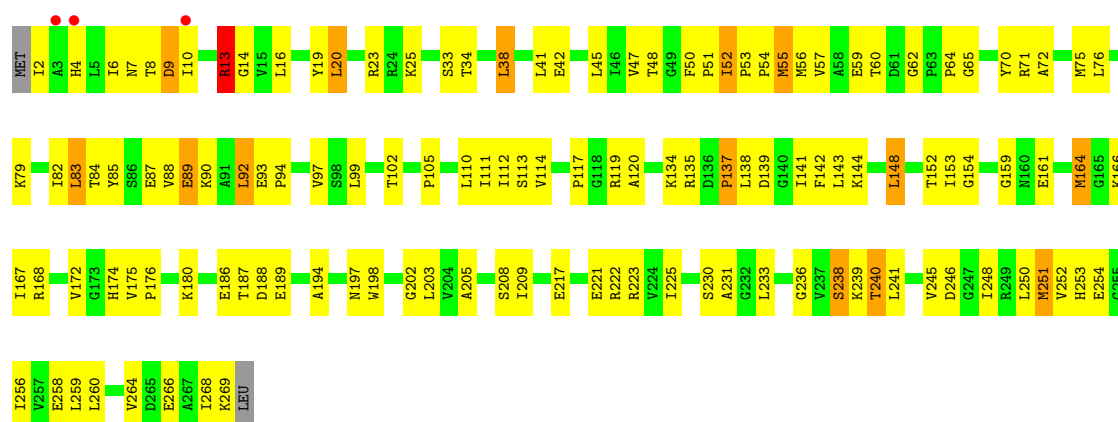


• Molecule 1: Putative uncharacterized protein

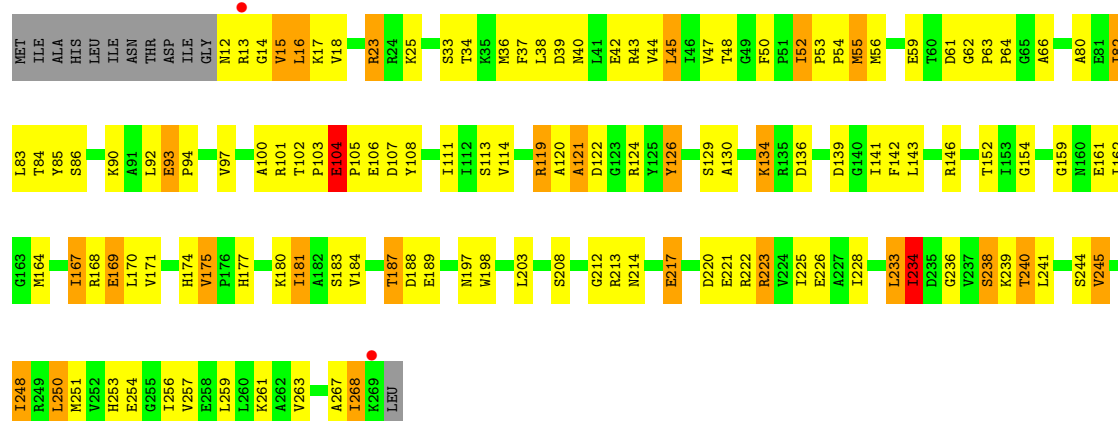




• Molecule 1: Putative uncharacterized protein

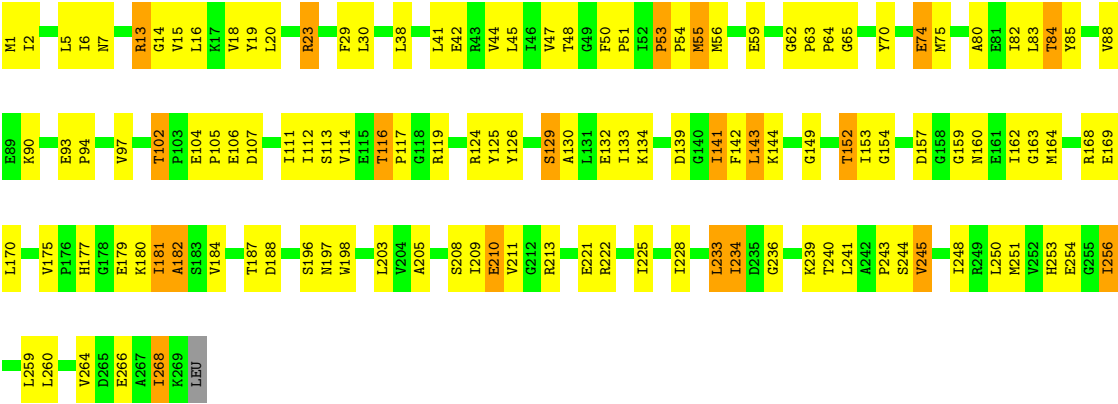


• Molecule 1: Putative uncharacterized protein



• Molecule 1: Putative uncharacterized protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.18Å 107.18Å 356.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.45 – 2.30 44.45 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.1 (44.45-2.30) 94.1 (44.45-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.22Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.281 0.223 , 0.281	Depositor DCC
R_{free} test set	9588 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13532	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.66	1/1997 (0.1%)	1.07	9/2707 (0.3%)
1	B	0.77	0/2057	1.10	7/2791 (0.3%)
1	C	0.80	2/2070 (0.1%)	1.15	15/2808 (0.5%)
1	D	0.76	0/2057	1.10	8/2791 (0.3%)
1	E	0.84	1/1993 (0.1%)	1.14	13/2702 (0.5%)
1	F	0.69	1/2070 (0.0%)	1.04	7/2808 (0.2%)
All	All	0.75	5/12244 (0.0%)	1.10	59/16607 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	ILE	CA-CB	-7.29	1.45	1.54
1	C	268	ILE	CA-CB	-5.53	1.48	1.54
1	F	53	PRO	CA-C	-5.52	1.48	1.52
1	E	15	VAL	CA-CB	-5.28	1.47	1.54
1	C	267	ALA	CA-CB	-5.17	1.47	1.54

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	250	LEU	N-CA-C	9.89	123.30	111.33
1	A	13	ARG	N-CA-C	8.54	120.58	111.28
1	A	175	VAL	N-CA-C	8.34	116.98	107.89
1	D	13	ARG	N-CA-C	7.95	127.73	110.80
1	C	52	ILE	N-CA-C	7.91	115.38	107.55
1	F	13	ARG	N-CA-C	7.71	119.69	111.28
1	E	82	ILE	N-CA-C	7.24	118.25	108.11
1	A	268	ILE	CB-CA-C	-7.23	102.38	112.14
1	D	52	ILE	N-CA-C	7.20	114.11	107.56
1	E	175	VAL	N-CA-C	7.09	115.62	107.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2	ILE	N-CA-C	-6.94	103.76	110.42
1	E	104	GLU	N-CA-C	-6.73	99.98	110.14
1	B	250	LEU	N-CA-C	6.61	119.33	111.33
1	C	44	VAL	N-CA-C	6.58	118.30	108.23
1	C	152	THR	N-CA-C	6.47	118.96	108.41
1	C	136	ASP	CA-C-N	6.44	126.81	119.92
1	C	136	ASP	C-N-CA	6.44	126.81	119.92
1	E	136	ASP	CA-C-N	6.27	126.19	119.85
1	E	136	ASP	C-N-CA	6.27	126.19	119.85
1	A	181	ILE	N-CA-C	6.10	116.89	110.72
1	C	234	ILE	N-CA-C	6.10	117.93	109.45
1	B	10	ILE	N-CA-C	6.06	121.94	109.34
1	E	234	ILE	N-CA-C	6.03	118.46	109.17
1	D	231	ALA	CA-C-N	-6.02	116.34	123.08
1	D	231	ALA	C-N-CA	-6.02	116.34	123.08
1	E	126	TYR	N-CA-C	5.97	118.94	109.50
1	C	153	ILE	CB-CA-C	-5.97	102.30	110.77
1	E	47	VAL	N-CA-C	5.92	116.40	107.75
1	A	35	LYS	CB-CG-CD	-5.84	97.86	111.30
1	E	18	VAL	N-CA-C	-5.80	104.70	110.62
1	C	153	ILE	N-CA-C	5.78	116.19	107.75
1	D	76	LEU	N-CA-C	-5.75	105.92	113.17
1	C	116	THR	CA-C-N	5.72	126.01	119.83
1	C	116	THR	C-N-CA	5.72	126.01	119.83
1	D	137	PRO	N-CA-C	5.69	121.16	111.03
1	C	249	ARG	N-CA-C	5.56	118.74	110.52
1	B	15	VAL	N-CA-C	5.51	116.24	110.62
1	F	175	VAL	N-CA-C	5.49	114.52	108.05
1	B	104	GLU	CA-C-N	5.46	124.92	119.24
1	B	104	GLU	C-N-CA	5.46	124.92	119.24
1	A	136	ASP	CA-C-N	5.45	125.43	120.03
1	A	136	ASP	C-N-CA	5.45	125.43	120.03
1	F	41	LEU	N-CA-C	5.43	119.89	113.16
1	E	52	ILE	N-CA-C	5.39	113.88	107.73
1	F	102	THR	CA-C-N	5.36	125.28	119.76
1	F	102	THR	C-N-CA	5.36	125.28	119.76
1	F	181	ILE	N-CA-C	5.36	116.84	111.00
1	E	52	ILE	CA-C-N	5.32	123.49	119.66
1	E	52	ILE	C-N-CA	5.32	123.49	119.66
1	A	28	ASN	N-CA-C	5.30	119.06	112.59
1	B	82	ILE	N-CA-C	5.30	116.11	108.48
1	B	76	LEU	N-CA-C	-5.30	106.77	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	238	SER	N-CA-C	-5.29	105.60	111.36
1	C	89	GLU	N-CA-C	-5.24	105.57	111.28
1	D	174	HIS	N-CA-C	5.21	119.63	113.12
1	C	50	PHE	CA-C-N	5.14	125.29	119.90
1	C	50	PHE	C-N-CA	5.14	125.29	119.90
1	C	42	GLU	N-CA-C	5.13	117.86	111.24
1	A	36	MET	N-CA-C	-5.12	105.78	111.36

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	1963	0	1996	122	0
1	B	2022	0	2043	154	0
1	C	2035	0	2070	198	0
1	D	2022	0	2044	141	0
1	E	1959	0	1993	132	0
1	F	2035	0	2070	134	0
2	A	8	0	0	0	0
2	B	11	0	0	0	0
2	C	8	0	0	0	0
2	D	7	0	0	0	0
2	E	11	0	0	0	0
2	F	8	0	0	0	0
3	A	260	0	0	17	0
3	B	309	0	0	19	0
3	C	170	0	0	15	0
3	D	191	0	0	11	0
3	E	218	0	0	13	0
3	F	295	0	0	15	0
All	All	13532	0	12216	835	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 34.

All (835) 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:B:125:TYR:HB2	1:B:133:ILE:CD1	1.65	1.25
1:D:82:ILE:HD12	1:D:97:VAL:HG11	1.20	1.17
1:A:159:GLY:HA2	1:A:164:MET:HG2	1.24	1.14
1:B:159:GLY:HA2	1:B:164:MET:HG2	1.26	1.12
1:E:159:GLY:HA2	1:E:164:MET:HG2	1.26	1.12
1:C:13:ARG:HD2	1:F:149:GLY:HA3	1.25	1.10
1:B:125:TYR:CB	1:B:133:ILE:HD11	1.82	1.09
1:E:55:MET:HE1	1:E:239:LYS:HD3	1.30	1.08
1:F:152:THR:HG23	1:F:187:THR:HG23	1.33	1.07
1:A:48:THR:HG22	1:A:114:VAL:O	1.54	1.07
1:C:84:THR:HG21	1:C:88:VAL:HG11	1.36	1.07
1:D:152:THR:HG23	1:D:188:ASP:H	1.20	1.04
1:F:48:THR:HG22	1:F:114:VAL:O	1.54	1.03
1:F:159:GLY:HA2	1:F:164:MET:HG2	1.43	1.01
1:C:109:SER:O	1:C:151:PRO:HG2	1.59	1.00
1:E:13:ARG:HD2	3:E:476:HOH:O	1.60	0.99
1:B:48:THR:O	1:B:84:THR:HG22	1.63	0.99
1:C:214:ASN:HB3	1:C:217:GLU:HG2	1.44	0.98
1:C:152:THR:HG22	1:C:188:ASP:H	1.23	0.97
1:D:10:ILE:HD12	1:D:194:ALA:HB1	1.45	0.97
1:E:82:ILE:HD12	1:E:97:VAL:HG11	1.46	0.97
1:C:130:ALA:HA	1:C:181:ILE:HD11	1.46	0.96
1:E:180:LYS:O	1:E:180:LYS:HG2	1.63	0.96
1:E:124:ARG:NH2	3:E:468:HOH:O	1.97	0.95
1:E:52:ILE:CD1	1:E:236:GLY:HA2	1.98	0.94
1:F:105:PRO:HG3	1:F:141:ILE:HD13	1.50	0.94
1:C:43:ARG:NH1	1:C:107:ASP:HB3	1.84	0.93
1:F:198:TRP:HE1	1:F:253:HIS:HD2	1.15	0.92
1:E:198:TRP:HE1	1:E:253:HIS:HD2	1.14	0.91
1:C:48:THR:HG21	1:C:66:ALA:HB2	1.53	0.90
1:B:125:TYR:HB2	1:B:133:ILE:HD11	0.92	0.89
1:B:133:ILE:HD12	1:B:133:ILE:O	1.73	0.89
1:D:52:ILE:HD11	1:D:59:GLU:HB3	1.54	0.89
1:B:240:THR:HG22	1:B:241:LEU:N	1.86	0.88
1:C:71:ARG:HD2	3:C:414:HOH:O	1.73	0.88
1:D:70:TYR:CE2	1:D:97:VAL:HG13	2.09	0.87
1:F:130:ALA:HA	1:F:181:ILE:HD11	1.56	0.87
1:F:209:ILE:HA	1:F:268:ILE:HD11	1.57	0.86
1:D:48:THR:HG22	1:D:114:VAL:O	1.76	0.86
1:A:245:VAL:HG13	1:A:253:HIS:CE1	2.11	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ILE:HG22	1:B:269:LYS:N	1.89	0.86
1:A:62:GLY:H	1:A:197:ASN:HD21	1.22	0.85
1:E:152:THR:HG23	1:E:188:ASP:H	1.40	0.85
1:C:266:GLU:CG	3:E:417:HOH:O	2.23	0.85
1:F:82:ILE:HD12	1:F:97:VAL:HG11	1.56	0.85
1:C:62:GLY:H	1:C:197:ASN:HD21	1.24	0.85
1:F:84:THR:HG21	1:F:88:VAL:HG11	1.59	0.84
1:F:102:THR:HB	3:F:580:HOH:O	1.76	0.84
1:F:152:THR:HG22	1:F:188:ASP:H	1.41	0.84
1:E:12:ASN:CG	1:E:15:VAL:HG23	2.02	0.84
1:F:105:PRO:HG3	1:F:141:ILE:CD1	2.07	0.84
1:C:150:ILE:HG22	1:C:151:PRO:HD2	1.57	0.83
1:B:159:GLY:CA	1:B:164:MET:HG2	2.06	0.83
1:C:209:ILE:HG22	1:C:210:GLU:N	1.93	0.83
1:B:105:PRO:HG3	1:B:141:ILE:HG13	1.61	0.83
1:B:223:ARG:HH21	1:F:74:GLU:HG2	1.41	0.83
1:B:159:GLY:HA2	1:B:164:MET:CG	2.08	0.82
1:D:221:GLU:OE2	1:D:225:ILE:HD11	1.79	0.82
1:A:159:GLY:CA	1:A:164:MET:HG2	2.09	0.82
1:F:222:ARG:HD2	1:F:254:GLU:OE2	1.79	0.82
1:F:48:THR:O	1:F:84:THR:HG23	1.79	0.82
1:D:93:GLU:HG3	3:D:505:HOH:O	1.79	0.82
1:C:152:THR:CG2	1:C:188:ASP:H	1.92	0.81
1:F:152:THR:HG23	1:F:187:THR:CG2	2.10	0.81
1:B:55:MET:HE1	1:B:239:LYS:HD3	1.63	0.81
1:F:209:ILE:HA	1:F:268:ILE:CD1	2.11	0.81
1:C:222:ARG:HG3	1:C:250:LEU:HD13	1.63	0.80
1:F:160:ASN:HB3	1:F:181:ILE:HG23	1.61	0.80
1:E:146:ARG:HD3	3:E:510:HOH:O	1.82	0.80
1:E:126:TYR:CB	1:E:181:ILE:CD1	2.59	0.80
1:F:159:GLY:CA	1:F:164:MET:HG2	2.12	0.80
1:C:209:ILE:C	1:C:211:VAL:H	1.89	0.79
1:D:52:ILE:CD1	1:D:59:GLU:HB3	2.12	0.79
1:D:82:ILE:HD12	1:D:97:VAL:CG1	2.09	0.79
1:E:220:ASP:CG	1:E:223:ARG:HB2	2.06	0.79
1:B:125:TYR:HB2	1:B:133:ILE:CG1	2.11	0.79
1:A:62:GLY:H	1:A:197:ASN:ND2	1.79	0.78
1:A:169:GLU:HG2	3:A:565:HOH:O	1.83	0.78
1:C:150:ILE:CG2	1:C:151:PRO:HD2	2.13	0.78
1:A:152:THR:CG2	1:A:188:ASP:H	1.95	0.78
1:E:245:VAL:HG13	1:E:253:HIS:CE1	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ASN:HB3	1:A:181:ILE:HG22	1.65	0.78
1:C:154:GLY:H	1:C:187:THR:HG21	1.50	0.77
1:C:152:THR:HG23	1:C:187:THR:HG23	1.64	0.77
1:C:268:ILE:O	1:C:268:ILE:HG22	1.84	0.77
1:B:152:THR:HG23	1:B:188:ASP:H	1.50	0.76
1:A:82:ILE:HD12	1:A:97:VAL:HG11	1.66	0.76
1:B:9:ASP:CB	1:D:2:ILE:N	2.48	0.76
1:D:110:LEU:HD12	1:D:111:ILE:H	1.51	0.76
1:C:82:ILE:HD12	1:C:97:VAL:HG11	1.67	0.76
1:C:214:ASN:HB3	1:C:217:GLU:CG	2.16	0.76
1:F:159:GLY:HA2	1:F:164:MET:CG	2.16	0.76
1:B:241:LEU:HD22	3:B:705:HOH:O	1.86	0.76
1:A:130:ALA:HA	1:A:181:ILE:HD11	1.67	0.75
1:E:159:GLY:CA	1:E:164:MET:HG2	2.12	0.75
1:B:62:GLY:H	1:B:197:ASN:HD21	1.32	0.75
1:A:52:ILE:HD13	1:A:236:GLY:HA2	1.69	0.75
1:C:63:PRO:HB2	1:C:64:PRO:HD3	1.69	0.75
1:A:152:THR:HG23	1:A:187:THR:HG23	1.68	0.75
1:A:258:GLU:HG3	3:D:433:HOH:O	1.86	0.74
1:B:240:THR:HG22	1:B:241:LEU:H	1.50	0.74
1:C:152:THR:HG22	1:C:188:ASP:N	2.00	0.74
1:C:110:LEU:HD12	1:C:151:PRO:O	1.87	0.74
1:C:245:VAL:HG13	1:C:253:HIS:NE2	2.01	0.74
1:F:116:THR:HB	1:F:162:ILE:HD13	1.70	0.74
1:B:198:TRP:HE1	1:B:253:HIS:HD2	1.36	0.74
1:B:82:ILE:HD12	1:B:97:VAL:HG11	1.68	0.74
1:F:124:ARG:HG3	1:F:124:ARG:HH11	1.53	0.74
1:B:268:ILE:CG2	1:B:269:LYS:N	2.50	0.73
1:E:55:MET:CE	1:E:239:LYS:HD3	2.13	0.73
1:F:169:GLU:HG3	3:F:483:HOH:O	1.87	0.73
1:B:48:THR:HG21	1:B:66:ALA:HB2	1.69	0.73
1:D:65:GLY:H	1:D:197:ASN:ND2	1.86	0.73
1:C:159:GLY:HA2	1:C:164:MET:HG2	1.71	0.73
1:C:43:ARG:HH12	1:C:107:ASP:HB3	1.50	0.73
1:A:36:MET:HE1	1:A:188:ASP:HB3	1.71	0.73
1:A:36:MET:HE1	1:A:188:ASP:CB	2.19	0.72
1:B:268:ILE:HG22	1:B:269:LYS:H	1.53	0.72
1:C:137:PRO:C	1:C:138:LEU:HD12	2.15	0.72
1:B:119:ARG:HG3	1:B:139:ASP:OD1	1.90	0.72
1:C:55:MET:HG2	3:C:487:HOH:O	1.89	0.72
1:E:56:MET:HE3	1:E:134:LYS:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:THR:HG22	1:F:85:TYR:H	1.54	0.72
1:D:93:GLU:HB3	1:D:94:PRO:HD3	1.72	0.71
1:C:145:ALA:N	3:C:445:HOH:O	2.23	0.71
1:E:52:ILE:HD11	1:E:59:GLU:HB3	1.72	0.71
1:E:126:TYR:HB3	1:E:181:ILE:CD1	2.21	0.71
1:B:9:ASP:HB2	1:D:2:ILE:N	2.05	0.70
1:C:62:GLY:H	1:C:197:ASN:ND2	1.88	0.70
1:E:82:ILE:HD12	1:E:97:VAL:CG1	2.19	0.70
1:C:260:LEU:O	1:C:264:VAL:HG23	1.90	0.70
1:D:119:ARG:HG3	1:D:139:ASP:OD1	1.92	0.70
1:E:48:THR:HG22	1:E:114:VAL:O	1.91	0.70
1:E:102:THR:HG22	1:E:102:THR:O	1.91	0.70
1:C:52:ILE:HG23	3:C:431:HOH:O	1.92	0.69
1:D:134:LYS:O	1:D:135:ARG:HB2	1.91	0.69
1:C:13:ARG:HD2	1:F:149:GLY:CA	2.14	0.69
1:B:9:ASP:HB3	1:D:2:ILE:N	2.06	0.69
1:A:113:SER:HB2	1:A:142:PHE:CZ	2.28	0.69
1:D:198:TRP:HE1	1:D:253:HIS:HD2	1.40	0.69
1:E:126:TYR:HB2	1:E:181:ILE:CD1	2.22	0.69
1:B:135:ARG:HG3	3:B:502:HOH:O	1.92	0.69
1:B:105:PRO:HG3	1:B:141:ILE:CG1	2.23	0.69
1:B:251:MET:HG3	3:B:454:HOH:O	1.91	0.69
1:B:93:GLU:HB3	1:B:94:PRO:HD3	1.74	0.68
1:E:52:ILE:HD13	1:E:236:GLY:HA2	1.72	0.68
1:E:154:GLY:N	1:E:187:THR:HG21	2.08	0.68
1:E:62:GLY:H	1:E:197:ASN:HD21	1.41	0.68
1:E:198:TRP:NE1	1:E:253:HIS:HD2	1.89	0.68
1:A:55:MET:HE1	1:A:239:LYS:HD3	1.74	0.68
1:A:240:THR:HG22	1:A:241:LEU:H	1.58	0.68
1:D:102:THR:HA	3:D:546:HOH:O	1.93	0.68
1:F:134:LYS:HA	3:F:462:HOH:O	1.93	0.68
1:A:159:GLY:HA2	1:A:164:MET:CG	2.14	0.68
1:E:169:GLU:HG3	1:E:170:LEU:N	2.09	0.68
1:A:52:ILE:CD1	1:A:236:GLY:HA2	2.24	0.68
1:B:133:ILE:CD1	1:B:133:ILE:O	2.42	0.68
1:C:137:PRO:O	1:C:138:LEU:HD12	1.94	0.67
1:F:62:GLY:HA2	1:F:114:VAL:HG12	1.76	0.67
1:A:54:PRO:HD2	1:A:55:MET:HE3	1.76	0.67
1:E:198:TRP:HE1	1:E:253:HIS:CD2	2.06	0.67
1:D:48:THR:CG2	1:D:114:VAL:HB	2.25	0.67
1:B:62:GLY:H	1:B:197:ASN:ND2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:SER:HB2	1:C:248:ILE:O	1.93	0.67
1:D:251:MET:HG3	3:D:413:HOH:O	1.95	0.67
1:B:228:ILE:O	1:B:233:LEU:HB2	1.94	0.66
3:C:434:HOH:O	1:E:17:LYS:HD3	1.94	0.66
1:C:43:ARG:HD3	1:C:107:ASP:O	1.95	0.66
1:E:152:THR:CG2	1:E:188:ASP:H	2.07	0.66
1:E:129:SER:O	1:E:130:ALA:HB3	1.95	0.66
1:B:25:LYS:HG2	1:B:26:ASN:ND2	2.11	0.66
1:B:42:GLU:HB2	3:B:465:HOH:O	1.95	0.66
1:C:144:LYS:HG3	3:C:505:HOH:O	1.95	0.66
1:B:54:PRO:HD2	1:B:55:MET:HE3	1.77	0.66
1:B:170:LEU:HD12	1:B:170:LEU:N	2.09	0.65
1:B:246:ASP:O	1:B:248:ILE:HD12	1.95	0.65
1:C:112:ILE:N	1:C:112:ILE:HD12	2.10	0.65
1:C:160:ASN:HB3	1:C:181:ILE:HG23	1.78	0.65
1:E:119:ARG:NH2	1:E:143:LEU:HD22	2.11	0.65
1:F:245:VAL:HG13	1:F:253:HIS:CE1	2.31	0.65
1:C:109:SER:O	1:C:151:PRO:CG	2.42	0.65
1:C:54:PRO:HD2	1:C:55:MET:HE1	1.78	0.65
1:C:154:GLY:N	1:C:187:THR:HG21	2.10	0.65
1:D:79:LYS:HD3	3:D:517:HOH:O	1.96	0.65
1:D:222:ARG:HA	1:D:250:LEU:HD22	1.79	0.65
1:C:45:LEU:HD23	1:C:81:GLU:O	1.97	0.65
1:B:2:ILE:N	1:D:9:ASP:CB	2.59	0.65
1:D:102:THR:HG22	1:D:102:THR:O	1.97	0.65
1:B:228:ILE:HB	1:B:233:LEU:HD22	1.79	0.65
1:C:152:THR:O	1:C:187:THR:HG23	1.96	0.65
1:E:52:ILE:CD1	1:E:59:GLU:HB3	2.27	0.65
1:A:48:THR:CG2	1:A:114:VAL:HB	2.26	0.65
1:D:54:PRO:HD2	1:D:55:MET:CE	2.27	0.65
1:E:187:THR:HG22	1:E:189:GLU:O	1.96	0.64
1:A:154:GLY:N	1:A:187:THR:HG21	2.12	0.64
1:C:266:GLU:HG3	3:E:417:HOH:O	1.91	0.64
1:E:171:VAL:O	1:E:175:VAL:HB	1.97	0.64
1:C:54:PRO:HD2	1:C:55:MET:CE	2.28	0.64
1:B:2:ILE:N	1:D:9:ASP:HB2	2.13	0.64
1:B:170:LEU:N	1:B:170:LEU:CD1	2.61	0.64
1:B:222:ARG:NH1	1:B:254:GLU:OE2	2.30	0.64
1:A:179:GLU:HG2	3:A:581:HOH:O	1.98	0.64
1:A:198:TRP:HE1	1:A:253:HIS:HD2	1.45	0.64
1:B:63:PRO:HB2	1:B:64:PRO:HD3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:HG21	1:A:157:ASP:O	1.97	0.64
1:F:152:THR:CG2	1:F:188:ASP:H	2.09	0.64
1:F:251:MET:HG3	3:F:447:HOH:O	1.96	0.64
1:D:240:THR:HG22	1:D:241:LEU:H	1.62	0.64
1:D:48:THR:O	1:D:84:THR:HG22	1.97	0.63
1:A:187:THR:HG22	1:A:189:GLU:O	1.99	0.63
1:C:222:ARG:CG	1:C:250:LEU:HD13	2.27	0.63
1:E:52:ILE:HD11	1:E:236:GLY:HA2	1.80	0.63
1:E:63:PRO:HB2	1:E:64:PRO:HD3	1.80	0.63
1:F:102:THR:HA	3:F:581:HOH:O	1.99	0.63
1:A:217:GLU:OE1	1:D:223:ARG:HD2	1.99	0.63
1:F:234:ILE:HG12	1:F:240:THR:O	1.99	0.63
1:A:105:PRO:HG3	1:A:141:ILE:HG13	1.79	0.63
1:C:214:ASN:CB	1:C:217:GLU:HG2	2.23	0.63
1:E:62:GLY:H	1:E:197:ASN:ND2	1.97	0.63
1:A:144:LYS:HE3	3:A:447:HOH:O	1.98	0.63
1:D:144:LYS:O	1:D:148:LEU:HD22	1.99	0.63
1:F:154:GLY:N	1:F:187:THR:HG21	2.13	0.63
1:E:119:ARG:HH21	1:E:143:LEU:HD13	1.64	0.62
1:D:110:LEU:HD12	1:D:111:ILE:N	2.15	0.62
1:F:55:MET:HE1	1:F:239:LYS:HD3	1.81	0.62
1:A:52:ILE:CD1	1:A:59:GLU:HB3	2.30	0.62
1:B:20:LEU:O	1:B:24:ARG:HB2	1.99	0.62
1:B:23:ARG:O	1:B:23:ARG:HD3	1.99	0.62
1:C:111:ILE:C	1:C:112:ILE:HD12	2.24	0.62
1:E:104:GLU:HG3	1:E:106:GLU:OE1	2.00	0.62
1:E:198:TRP:CZ2	1:E:256:ILE:HD12	2.35	0.62
1:A:248:ILE:HB	1:A:253:HIS:CE1	2.34	0.62
1:C:5:LEU:HD13	1:C:259:LEU:HD21	1.81	0.62
1:B:19:TYR:HE2	1:D:4:HIS:HE2	1.44	0.62
1:D:152:THR:HG23	1:D:188:ASP:N	2.05	0.62
1:D:161:GLU:O	1:D:164:MET:HB2	1.99	0.62
1:E:152:THR:O	1:E:187:THR:HG23	2.00	0.62
1:B:124:ARG:NH2	3:B:700:HOH:O	2.14	0.61
1:C:105:PRO:CB	3:C:445:HOH:O	2.47	0.61
1:C:209:ILE:CG2	1:C:210:GLU:N	2.61	0.61
1:C:258:GLU:CA	1:C:258:GLU:OE1	2.46	0.61
1:B:23:ARG:HG3	1:B:23:ARG:HH11	1.66	0.61
1:D:54:PRO:HD2	1:D:55:MET:HE3	1.82	0.61
1:A:26:ASN:HB3	3:A:446:HOH:O	2.01	0.61
1:D:152:THR:CG2	1:D:188:ASP:H	2.05	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLY:N	1:A:164:MET:HE3	2.16	0.61
1:D:222:ARG:NH1	1:D:254:GLU:OE2	2.31	0.61
1:A:252:VAL:HG21	1:F:266:GLU:HG3	1.82	0.61
1:A:90:LYS:HE2	3:A:640:HOH:O	2.01	0.60
1:A:130:ALA:CA	1:A:181:ILE:HD11	2.31	0.60
1:C:27:PHE:CE1	1:E:13:ARG:HG3	2.36	0.60
1:C:209:ILE:C	1:C:211:VAL:N	2.54	0.60
1:A:27:PHE:CE1	1:F:13:ARG:HG3	2.35	0.60
1:D:105:PRO:HG3	1:D:141:ILE:HG13	1.83	0.60
1:D:198:TRP:HE1	1:D:253:HIS:CD2	2.20	0.60
1:B:240:THR:CG2	1:B:241:LEU:N	2.57	0.60
1:C:105:PRO:HD2	1:C:106:GLU:OE1	2.02	0.60
1:B:223:ARG:NH2	1:F:74:GLU:HG2	2.16	0.59
1:F:198:TRP:HE1	1:F:253:HIS:CD2	2.07	0.59
1:C:105:PRO:HB3	3:C:445:HOH:O	2.02	0.59
1:A:126:TYR:HB3	1:A:181:ILE:HD12	1.84	0.59
1:F:48:THR:CG2	1:F:114:VAL:HB	2.32	0.59
1:B:6:ILE:HD12	1:B:199:GLY:HA2	1.84	0.59
1:C:110:LEU:CD2	1:C:112:ILE:HD11	2.33	0.59
1:C:129:SER:O	1:C:130:ALA:HB3	2.03	0.59
1:F:198:TRP:NE1	1:F:253:HIS:HD2	1.95	0.59
1:C:55:MET:HB2	1:C:57:VAL:HG23	1.85	0.59
1:A:217:GLU:OE1	1:D:223:ARG:CD	2.51	0.58
1:C:124:ARG:HG3	1:C:124:ARG:HH11	1.67	0.58
1:E:48:THR:HG22	1:E:114:VAL:HB	1.86	0.58
1:C:48:THR:CG2	1:C:66:ALA:HB2	2.28	0.58
1:D:55:MET:HE1	1:D:239:LYS:HD3	1.85	0.58
1:E:126:TYR:HB2	1:E:181:ILE:HD13	1.85	0.58
1:A:259:LEU:HD11	1:F:256:ILE:HD12	1.86	0.58
1:C:13:ARG:CZ	1:F:149:GLY:O	2.52	0.58
1:E:119:ARG:HH21	1:E:143:LEU:HD22	1.67	0.58
1:E:241:LEU:HD12	3:E:490:HOH:O	2.04	0.58
1:F:221:GLU:O	1:F:225:ILE:HG12	2.04	0.58
1:B:252:VAL:HG21	1:D:266:GLU:HG3	1.85	0.58
1:E:126:TYR:CB	1:E:181:ILE:HD13	2.34	0.58
1:C:159:GLY:CA	1:C:164:MET:HG2	2.33	0.57
1:C:266:GLU:HG2	3:E:417:HOH:O	1.95	0.57
1:A:152:THR:HG22	1:A:188:ASP:H	1.66	0.57
1:A:240:THR:HG21	3:A:523:HOH:O	2.02	0.57
1:E:220:ASP:OD1	1:E:223:ARG:HB2	2.03	0.57
1:B:217:GLU:OE1	3:B:701:HOH:O	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:ASN:ND2	1:E:15:VAL:CG2	2.67	0.57
1:A:130:ALA:HA	1:A:181:ILE:CD1	2.35	0.57
1:C:264:VAL:O	1:C:268:ILE:HG12	2.04	0.57
1:D:54:PRO:HG2	1:D:55:MET:HE3	1.85	0.57
1:A:223:ARG:HH22	1:D:75:MET:HB3	1.68	0.57
1:B:54:PRO:HD2	1:B:55:MET:CE	2.34	0.57
1:D:120:ALA:HB1	1:D:180:LYS:O	2.04	0.57
1:E:187:THR:CG2	1:E:189:GLU:O	2.52	0.57
1:B:240:THR:CG2	1:B:241:LEU:H	2.17	0.57
1:D:64:PRO:HD2	1:D:197:ASN:HD21	1.70	0.57
1:E:102:THR:N	1:E:103:PRO:HD3	2.19	0.57
1:E:119:ARG:HH21	1:E:143:LEU:CD1	2.18	0.57
1:C:110:LEU:HG	1:C:112:ILE:HD11	1.87	0.57
1:C:159:GLY:HA2	1:C:164:MET:CG	2.34	0.57
1:F:53:PRO:HG3	1:F:133:ILE:HD13	1.87	0.57
1:A:222:ARG:HB2	1:A:254:GLU:OE2	2.04	0.56
1:E:248:ILE:HB	1:E:253:HIS:CE1	2.39	0.56
1:F:260:LEU:O	1:F:264:VAL:HG23	2.05	0.56
1:C:34:THR:O	1:C:37:PHE:HB3	2.05	0.56
1:D:10:ILE:CG2	1:D:10:ILE:O	2.52	0.56
1:D:268:ILE:HG22	1:D:269:LYS:N	2.18	0.56
1:B:10:ILE:O	1:B:10:ILE:CG2	2.51	0.56
1:D:2:ILE:HD11	1:D:209:ILE:HD12	1.87	0.56
1:D:54:PRO:HA	1:D:56:MET:HE2	1.88	0.56
1:A:152:THR:HG23	1:A:188:ASP:H	1.68	0.56
1:A:54:PRO:HD2	1:A:55:MET:CE	2.36	0.56
1:A:62:GLY:N	1:A:197:ASN:HD21	1.98	0.56
1:B:71:ARG:HG2	1:B:75:MET:HE2	1.87	0.56
1:E:259:LEU:O	1:E:263:VAL:HG23	2.06	0.56
1:A:251:MET:HE2	3:A:445:HOH:O	2.05	0.56
1:E:177:HIS:HD2	3:E:419:HOH:O	1.87	0.56
1:B:55:MET:HE1	1:B:239:LYS:CD	2.33	0.56
1:B:71:ARG:CZ	1:B:75:MET:HE1	2.36	0.56
1:E:119:ARG:HH21	1:E:143:LEU:CD2	2.19	0.56
1:B:245:VAL:HG13	1:B:253:HIS:CE1	2.41	0.56
1:C:176:PRO:HA	1:F:106:GLU:HG2	1.88	0.56
1:C:258:GLU:OE1	1:C:258:GLU:N	2.39	0.56
1:D:10:ILE:CD1	1:D:194:ALA:HB1	2.29	0.55
1:D:48:THR:HG22	1:D:114:VAL:HB	1.89	0.55
1:A:252:VAL:CG2	1:F:266:GLU:HG3	2.37	0.55
1:B:106:GLU:H	1:B:106:GLU:CD	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:TYR:O	1:D:89:GLU:HG3	2.06	0.55
1:E:139:ASP:HB3	1:E:162:ILE:HD11	1.86	0.55
1:F:240:THR:HG22	1:F:241:LEU:N	2.21	0.55
1:B:10:ILE:HD11	1:B:198:TRP:CH2	2.42	0.55
1:B:222:ARG:HG3	1:B:250:LEU:HD13	1.88	0.55
1:E:238:SER:HB2	1:E:240:THR:OG1	2.06	0.55
1:B:12:ASN:ND2	3:B:514:HOH:O	2.38	0.55
1:C:21:ASP:O	1:C:24:ARG:HB3	2.05	0.55
1:C:221:GLU:O	1:C:225:ILE:HG12	2.07	0.55
1:F:14:GLY:O	1:F:18:VAL:HG23	2.05	0.55
1:C:20:LEU:HD21	1:E:23:ARG:HD2	1.89	0.55
1:D:50:PHE:CD1	1:D:117:PRO:HG3	2.41	0.55
1:E:221:GLU:O	1:E:225:ILE:HG12	2.07	0.55
1:C:198:TRP:CZ3	1:C:256:ILE:HD13	2.42	0.55
1:C:240:THR:HG22	1:C:241:LEU:N	2.22	0.55
1:F:70:TYR:CE2	1:F:97:VAL:HG13	2.42	0.55
1:C:268:ILE:O	1:C:268:ILE:CG2	2.54	0.55
1:E:48:THR:CG2	1:E:66:ALA:HB2	2.36	0.55
1:B:85:TYR:HB3	1:B:135:ARG:NH2	2.22	0.55
1:B:113:SER:HB2	1:B:142:PHE:CZ	2.42	0.55
1:C:258:GLU:HB3	3:E:458:HOH:O	2.07	0.55
1:D:52:ILE:HG12	1:D:236:GLY:HA2	1.88	0.55
1:D:251:MET:HE1	3:F:464:HOH:O	2.06	0.55
1:F:129:SER:O	1:F:130:ALA:HB3	2.07	0.55
1:C:113:SER:HB2	1:C:142:PHE:CZ	2.41	0.54
1:C:209:ILE:O	1:C:211:VAL:N	2.40	0.54
1:C:223:ARG:HD3	3:C:432:HOH:O	2.06	0.54
1:D:62:GLY:H	1:D:197:ASN:ND2	2.04	0.54
1:D:119:ARG:HH21	1:D:143:LEU:HD22	1.73	0.54
1:C:228:ILE:HG23	1:C:233:LEU:CD2	2.37	0.54
1:D:152:THR:HG22	1:D:188:ASP:OD2	2.08	0.54
1:E:130:ALA:HA	1:E:181:ILE:HD11	1.89	0.54
1:E:159:GLY:HA2	1:E:164:MET:CG	2.18	0.54
1:F:42:GLU:HB2	3:F:416:HOH:O	2.07	0.54
1:E:250:LEU:O	1:E:254:GLU:HG3	2.08	0.54
1:F:84:THR:HG21	1:F:88:VAL:CG1	2.35	0.54
1:F:141:ILE:HD13	1:F:141:ILE:O	2.08	0.54
1:F:184:VAL:HG12	1:F:184:VAL:O	2.07	0.54
1:A:139:ASP:HB3	1:A:162:ILE:HD11	1.90	0.54
1:A:52:ILE:HD11	1:A:59:GLU:HB3	1.90	0.54
1:F:113:SER:HB2	1:F:142:PHE:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ILE:HG22	1:A:113:SER:N	2.23	0.53
1:A:250:LEU:O	1:A:254:GLU:HG3	2.08	0.53
1:B:48:THR:HG22	1:B:114:VAL:HB	1.90	0.53
1:B:142:PHE:CD1	1:B:162:ILE:HD13	2.43	0.53
1:D:166:LYS:HG2	1:D:167:ILE:HG23	1.89	0.53
1:E:43:ARG:NH1	1:E:107:ASP:HB3	2.23	0.53
1:F:55:MET:HE1	1:F:239:LYS:CD	2.39	0.53
1:C:48:THR:HG21	1:C:66:ALA:CB	2.35	0.53
1:E:61:ASP:HB2	1:E:245:VAL:HG23	1.91	0.53
1:E:113:SER:HB2	1:E:142:PHE:CZ	2.43	0.53
1:A:176:PRO:O	1:A:177:HIS:HB2	2.09	0.53
1:B:125:TYR:O	1:B:133:ILE:HG13	2.09	0.53
1:C:214:ASN:ND2	1:C:264:VAL:HB	2.22	0.53
1:E:55:MET:HE1	1:E:239:LYS:CD	2.19	0.53
1:E:111:ILE:HG22	1:E:142:PHE:CZ	2.44	0.53
1:F:44:VAL:O	1:F:80:ALA:HA	2.09	0.53
1:C:145:ALA:HB1	1:C:150:ILE:HB	1.91	0.53
1:C:167:ILE:HB	1:C:170:LEU:HD22	1.91	0.53
1:C:152:THR:CG2	1:C:187:THR:HA	2.39	0.53
1:E:93:GLU:HG2	1:E:94:PRO:HD3	1.91	0.53
1:C:84:THR:HG21	1:C:88:VAL:CG1	2.24	0.53
1:C:110:LEU:HD13	1:C:151:PRO:HB2	1.91	0.53
1:E:167:ILE:HG13	1:E:167:ILE:O	2.08	0.53
1:F:7:ASN:ND2	1:F:19:TYR:CD1	2.77	0.53
1:D:209:ILE:HA	1:D:268:ILE:HD11	1.91	0.52
1:A:119:ARG:NH1	3:A:414:HOH:O	2.42	0.52
1:B:2:ILE:N	1:D:9:ASP:HB3	2.23	0.52
1:D:152:THR:C	1:D:187:THR:HG23	2.34	0.52
1:E:36:MET:HE1	1:E:188:ASP:HB3	1.91	0.52
1:A:159:GLY:H	1:A:164:MET:HE3	1.73	0.52
1:B:54:PRO:HA	1:B:56:MET:HE2	1.91	0.52
1:E:241:LEU:CD1	3:E:490:HOH:O	2.57	0.52
1:B:106:GLU:HG3	1:B:148:LEU:CD2	2.40	0.52
1:C:228:ILE:HG23	1:C:233:LEU:HB2	1.91	0.52
1:B:52:ILE:HG21	1:B:239:LYS:HG2	1.90	0.52
1:B:198:TRP:HE1	1:B:253:HIS:CD2	2.21	0.52
1:E:126:TYR:HB3	1:E:181:ILE:HD11	1.91	0.52
1:B:85:TYR:HB3	1:B:135:ARG:HH21	1.75	0.52
1:C:41:LEU:HD13	1:C:76:LEU:HB3	1.92	0.52
1:C:167:ILE:O	1:C:170:LEU:HB2	2.09	0.52
1:F:163:GLY:HA2	1:F:187:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ARG:HA	1:F:20:LEU:HD23	1.91	0.52
1:A:25:LYS:HE3	3:A:542:HOH:O	2.09	0.52
1:C:125:TYR:N	1:C:125:TYR:CD2	2.77	0.52
1:A:84:THR:OG1	1:A:85:TYR:N	2.42	0.52
1:E:129:SER:O	1:E:130:ALA:CB	2.58	0.52
1:E:152:THR:HG23	1:E:187:THR:HG23	1.92	0.52
1:F:112:ILE:HA	1:F:153:ILE:O	2.10	0.52
1:B:27:PHE:CZ	1:D:16:LEU:HD23	2.44	0.51
1:F:59:GLU:HA	1:F:234:ILE:O	2.11	0.51
1:A:245:VAL:HG13	1:A:253:HIS:NE2	2.26	0.51
1:C:110:LEU:CD1	1:C:151:PRO:HB2	2.40	0.51
1:B:84:THR:HG21	1:B:88:VAL:HG11	1.93	0.51
1:B:119:ARG:HE	1:B:143:LEU:HD21	1.76	0.51
1:C:132:GLU:HG2	1:C:134:LYS:HE3	1.92	0.51
1:E:12:ASN:CG	1:E:15:VAL:CG2	2.80	0.51
1:A:103:PRO:HA	3:A:431:HOH:O	2.09	0.51
1:B:152:THR:OG1	1:B:187:THR:HG23	2.09	0.51
1:B:168:ARG:HG3	1:B:182:ALA:HB1	1.93	0.51
1:F:15:VAL:HG21	1:F:157:ASP:O	2.09	0.51
1:F:16:LEU:O	1:F:20:LEU:HD13	2.10	0.51
1:F:104:GLU:O	1:F:105:PRO:C	2.54	0.51
1:F:222:ARG:HH11	1:F:254:GLU:CD	2.19	0.51
1:E:54:PRO:N	1:E:55:MET:HE3	2.25	0.51
1:F:124:ARG:HH11	1:F:124:ARG:CG	2.22	0.51
1:F:144:LYS:HE3	3:F:504:HOH:O	2.11	0.51
1:F:163:GLY:CA	1:F:187:THR:OG1	2.58	0.51
1:E:93:GLU:O	1:E:93:GLU:HG3	2.03	0.51
1:A:89:GLU:OE2	1:A:99:LEU:HD13	2.10	0.51
1:E:44:VAL:O	1:E:80:ALA:HA	2.10	0.51
1:A:12:ASN:OD1	1:A:12:ASN:C	2.54	0.51
1:C:15:VAL:HG21	1:C:157:ASP:O	2.11	0.51
1:C:55:MET:HA	3:C:527:HOH:O	2.11	0.51
1:E:244:SER:HB2	1:E:248:ILE:O	2.11	0.51
1:D:166:LYS:O	1:D:166:LYS:CG	2.57	0.50
1:E:48:THR:CG2	1:E:114:VAL:HB	2.41	0.50
1:C:89:GLU:CD	1:C:99:LEU:HD13	2.36	0.50
1:C:223:ARG:HG3	1:C:223:ARG:HH11	1.76	0.50
1:D:47:VAL:HG22	1:D:83:LEU:HB3	1.93	0.50
1:F:139:ASP:HB3	1:F:162:ILE:HD11	1.93	0.50
1:F:152:THR:CG2	1:F:187:THR:HA	2.41	0.50
1:C:48:THR:HG22	1:C:114:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ILE:CG2	1:C:66:ALA:HB1	2.42	0.50
1:C:153:ILE:HG12	1:C:189:GLU:HB2	1.92	0.50
1:F:47:VAL:HG12	1:F:116:THR:HG21	1.93	0.50
1:D:54:PRO:CD	1:D:55:MET:HE3	2.41	0.50
1:D:112:ILE:HG22	1:D:113:SER:N	2.27	0.50
1:E:120:ALA:O	1:E:122:ASP:N	2.45	0.50
1:E:257:VAL:HG12	1:E:261:LYS:HE3	1.94	0.50
1:A:60:THR:HG22	1:A:228:ILE:CD1	2.41	0.50
1:D:72:ALA:HA	1:D:75:MET:HG2	1.94	0.50
1:E:168:ARG:O	1:E:169:GLU:C	2.54	0.50
1:E:177:HIS:CD2	3:E:419:HOH:O	2.64	0.50
1:F:126:TYR:HB2	1:F:181:ILE:HG13	1.94	0.50
1:C:155:VAL:HG22	1:C:191:ILE:HB	1.93	0.50
1:E:48:THR:HG21	1:E:66:ALA:HB2	1.93	0.50
1:F:29:PHE:CD1	1:F:29:PHE:C	2.89	0.50
1:F:53:PRO:CG	1:F:133:ILE:HD13	2.42	0.50
1:B:59:GLU:HA	1:B:234:ILE:O	2.11	0.49
1:C:217:GLU:HB3	3:C:471:HOH:O	2.12	0.49
1:A:160:ASN:HB3	1:A:181:ILE:CG2	2.39	0.49
1:D:113:SER:HB2	1:D:142:PHE:CZ	2.48	0.49
1:F:124:ARG:HD3	3:F:606:HOH:O	2.12	0.49
1:A:102:THR:HA	3:A:614:HOH:O	2.11	0.49
1:B:48:THR:CG2	1:B:66:ALA:HB2	2.39	0.49
1:C:180:LYS:HG2	1:C:181:ILE:HD12	1.92	0.49
1:D:222:ARG:HD2	1:D:254:GLU:OE2	2.12	0.49
1:E:222:ARG:O	1:E:226:GLU:HG3	2.13	0.49
1:F:153:ILE:HA	1:F:187:THR:HG21	1.93	0.49
1:A:52:ILE:HD12	1:A:59:GLU:HB3	1.94	0.49
1:C:256:ILE:O	1:C:260:LEU:HG	2.13	0.49
1:A:198:TRP:CH2	1:A:256:ILE:HD12	2.48	0.49
1:C:220:ASP:O	1:C:224:VAL:HG23	2.12	0.49
1:D:54:PRO:CG	1:D:55:MET:HE3	2.42	0.49
1:C:44:VAL:O	1:C:80:ALA:HA	2.13	0.49
1:C:51:PRO:HA	1:C:57:VAL:O	2.13	0.49
1:D:60:THR:HB	1:D:245:VAL:HG22	1.93	0.49
1:D:62:GLY:H	1:D:197:ASN:HD21	1.61	0.49
1:B:10:ILE:HB	3:B:628:HOH:O	2.12	0.49
1:B:87:GLU:HG2	1:B:88:VAL:N	2.28	0.49
1:A:223:ARG:HH21	1:D:71:ARG:CG	2.26	0.49
1:C:110:LEU:HG	1:C:112:ILE:CD1	2.43	0.49
1:D:269:LYS:HA	3:D:440:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:ASN:ND2	1:E:15:VAL:HG23	2.27	0.49
1:A:128:MET:HE3	3:A:416:HOH:O	2.12	0.49
1:D:168:ARG:O	1:D:172:VAL:HG23	2.13	0.49
1:B:10:ILE:O	1:B:10:ILE:HG23	2.11	0.48
1:C:184:VAL:HG12	1:C:184:VAL:O	2.13	0.48
1:D:34:THR:HG22	1:D:38:LEU:HD22	1.94	0.48
1:E:36:MET:HE1	1:E:188:ASP:CB	2.43	0.48
1:E:139:ASP:CB	1:E:162:ILE:HD11	2.43	0.48
1:F:153:ILE:HA	1:F:187:THR:CG2	2.43	0.48
1:C:167:ILE:O	1:C:168:ARG:C	2.56	0.48
1:C:228:ILE:HG23	1:C:233:LEU:HD23	1.94	0.48
1:F:124:ARG:HG3	1:F:124:ARG:NH1	2.26	0.48
1:F:153:ILE:CA	1:F:187:THR:HG21	2.43	0.48
1:B:102:THR:HG22	1:B:102:THR:O	2.11	0.48
1:D:7:ASN:ND2	1:D:19:TYR:CD1	2.82	0.48
1:E:105:PRO:HG3	1:E:141:ILE:HG13	1.95	0.48
1:A:116:THR:HB	1:A:162:ILE:HD12	1.95	0.48
1:C:46:ILE:HG21	1:C:66:ALA:HB1	1.96	0.48
1:C:115:GLU:OE1	1:C:115:GLU:HA	2.13	0.48
1:C:124:ARG:HG2	1:C:132:GLU:OE2	2.13	0.48
1:D:88:VAL:HG12	1:D:92:LEU:HD22	1.96	0.48
1:D:159:GLY:HA2	1:D:164:MET:CG	2.43	0.48
1:F:240:THR:HG22	1:F:241:LEU:H	1.78	0.48
1:A:223:ARG:NH2	1:D:71:ARG:O	2.46	0.48
1:D:54:PRO:O	1:D:56:MET:HE2	2.13	0.48
1:E:152:THR:HG23	1:E:188:ASP:N	2.21	0.48
1:F:180:LYS:HG2	1:F:181:ILE:HD12	1.96	0.48
1:A:152:THR:C	1:A:187:THR:HG23	2.39	0.48
1:A:222:ARG:HH11	1:A:254:GLU:CD	2.21	0.48
1:D:105:PRO:HG3	1:D:141:ILE:CG1	2.42	0.48
1:C:36:MET:CG	1:C:36:MET:O	2.61	0.48
1:D:55:MET:CB	1:D:57:VAL:HG23	2.44	0.48
1:F:105:PRO:HG3	1:F:141:ILE:HD11	1.94	0.48
1:A:20:LEU:HD11	1:F:23:ARG:HD2	1.95	0.48
1:C:39:ASP:C	1:C:40:ASN:OD1	2.56	0.48
1:D:230:SER:HB3	3:D:545:HOH:O	2.12	0.48
1:E:120:ALA:C	1:E:122:ASP:N	2.71	0.48
1:E:159:GLY:H	1:E:164:MET:HE3	1.78	0.48
1:C:14:GLY:N	3:C:565:HOH:O	2.46	0.47
1:D:50:PHE:CE1	1:D:117:PRO:HG3	2.49	0.47
1:F:244:SER:HB2	1:F:248:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:HG22	1:A:241:LEU:N	2.28	0.47
1:B:31:HIS:CD2	3:B:457:HOH:O	2.67	0.47
1:F:5:LEU:HD13	1:F:259:LEU:CD2	2.43	0.47
1:F:205:ALA:O	1:F:208:SER:HB2	2.14	0.47
1:A:62:GLY:HA2	1:A:114:VAL:HG12	1.95	0.47
1:B:254:GLU:HG2	1:B:258:GLU:OE1	2.14	0.47
1:A:33:SER:OG	1:A:189:GLU:HB3	2.15	0.47
1:A:36:MET:HE1	1:A:188:ASP:HB2	1.95	0.47
1:C:36:MET:O	1:C:36:MET:HG2	2.14	0.47
1:C:43:ARG:HH11	1:C:107:ASP:HB3	1.70	0.47
1:C:50:PHE:O	1:C:58:ALA:HA	2.14	0.47
1:C:176:PRO:O	1:C:177:HIS:HB2	2.15	0.47
1:B:152:THR:HG23	1:B:187:THR:HG23	1.96	0.47
1:C:167:ILE:HA	3:C:502:HOH:O	2.15	0.47
1:A:126:TYR:HB3	1:A:181:ILE:CD1	2.45	0.47
1:C:52:ILE:N	1:C:57:VAL:O	2.45	0.47
1:A:130:ALA:CB	1:A:181:ILE:HD11	2.43	0.47
1:B:82:ILE:HD12	1:B:97:VAL:CG1	2.40	0.47
1:C:38:LEU:HD11	1:C:207:ALA:HB1	1.96	0.47
1:A:165:GLY:HA2	1:A:183:SER:O	2.15	0.47
1:E:53:PRO:C	1:E:55:MET:HE3	2.40	0.47
1:B:178:GLY:O	1:B:179:GLU:C	2.58	0.47
1:C:55:MET:O	1:C:56:MET:HB2	2.15	0.47
1:B:7:ASN:ND2	1:B:19:TYR:CD1	2.83	0.46
1:B:83:LEU:HA	3:B:409:HOH:O	2.15	0.46
1:C:45:LEU:CD2	1:C:81:GLU:O	2.63	0.46
1:C:152:THR:HG21	1:C:187:THR:HA	1.97	0.46
1:E:45:LEU:HB2	1:E:108:TYR:CD1	2.50	0.46
1:E:228:ILE:HB	1:E:233:LEU:HD22	1.96	0.46
1:A:198:TRP:NE1	1:A:253:HIS:HD2	2.12	0.46
1:E:120:ALA:C	1:E:122:ASP:H	2.23	0.46
1:E:121:ALA:HA	1:E:184:VAL:HG21	1.97	0.46
1:A:222:ARG:O	1:A:226:GLU:HG3	2.15	0.46
1:D:52:ILE:N	1:D:52:ILE:HD12	2.29	0.46
1:A:248:ILE:O	1:A:253:HIS:HE1	1.98	0.46
1:B:225:ILE:HA	1:B:228:ILE:HG12	1.97	0.46
1:B:54:PRO:CD	1:B:55:MET:HE3	2.44	0.46
1:C:125:TYR:N	1:C:125:TYR:HD2	2.13	0.46
1:F:54:PRO:HA	1:F:56:MET:HE2	1.98	0.46
1:B:146:ARG:NH1	3:B:666:HOH:O	2.34	0.46
1:D:10:ILE:O	1:D:10:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:ASN:OD1	1:E:15:VAL:HG23	2.16	0.46
1:B:43:ARG:HH21	1:B:81:GLU:CD	2.23	0.46
1:B:90:LYS:HE2	3:B:517:HOH:O	2.15	0.46
1:C:152:THR:CG2	1:C:152:THR:O	2.61	0.46
1:C:152:THR:C	1:C:187:THR:HG23	2.41	0.46
1:D:79:LYS:HB3	3:D:517:HOH:O	2.15	0.46
1:D:260:LEU:O	1:D:264:VAL:HG23	2.16	0.46
1:F:5:LEU:HD13	1:F:259:LEU:HD21	1.97	0.46
1:F:125:TYR:HB2	1:F:133:ILE:HB	1.98	0.46
1:A:23:ARG:HD2	1:F:20:LEU:HD21	1.97	0.46
1:A:222:ARG:NH1	1:A:254:GLU:CD	2.74	0.46
1:B:248:ILE:O	1:B:253:HIS:HE1	1.97	0.46
1:D:225:ILE:HB	1:D:250:LEU:HD21	1.98	0.46
1:F:29:PHE:CD1	1:F:30:LEU:N	2.84	0.46
1:F:225:ILE:HB	1:F:250:LEU:HD21	1.98	0.46
1:B:241:LEU:CD2	3:B:705:HOH:O	2.56	0.46
1:B:248:ILE:HD12	1:B:248:ILE:N	2.31	0.46
1:D:51:PRO:O	1:D:53:PRO:HD3	2.16	0.46
1:E:119:ARG:O	1:E:183:SER:HA	2.15	0.46
1:D:238:SER:O	1:D:239:LYS:HB2	2.16	0.46
1:E:50:PHE:HB3	1:E:59:GLU:HG2	1.98	0.46
1:A:121:ALA:HA	1:A:184:VAL:HG21	1.98	0.45
1:B:224:VAL:O	1:B:228:ILE:HG12	2.16	0.45
1:F:168:ARG:HG3	1:F:182:ALA:HB1	1.98	0.45
1:A:27:PHE:HE1	1:F:13:ARG:HG3	1.80	0.45
1:A:153:ILE:C	1:A:187:THR:HG21	2.41	0.45
1:D:54:PRO:HD2	1:D:55:MET:HE1	1.98	0.45
1:A:54:PRO:CD	1:A:55:MET:HE3	2.46	0.45
1:B:34:THR:HG22	1:B:38:LEU:HD22	1.98	0.45
1:D:187:THR:HG22	1:D:189:GLU:O	2.16	0.45
1:A:102:THR:O	1:A:102:THR:HG22	2.17	0.45
1:A:224:VAL:O	1:A:228:ILE:HG12	2.17	0.45
1:C:145:ALA:CA	3:C:445:HOH:O	2.64	0.45
1:C:150:ILE:HG22	1:C:151:PRO:CD	2.38	0.45
1:F:177:HIS:CE1	3:F:643:HOH:O	2.69	0.45
1:B:4:HIS:HB3	1:D:8:THR:HA	1.98	0.45
1:B:19:TYR:CE2	1:D:4:HIS:NE2	2.75	0.45
1:B:34:THR:O	1:B:37:PHE:HB3	2.16	0.45
1:B:87:GLU:OE1	1:B:135:ARG:NH2	2.47	0.45
1:B:105:PRO:CG	1:B:141:ILE:HG13	2.40	0.45
1:B:245:VAL:HG13	1:B:253:HIS:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ASP:HB2	1:C:245:VAL:HG23	1.98	0.45
1:C:150:ILE:H	1:C:150:ILE:HG12	1.52	0.45
1:D:87:GLU:HG2	1:D:88:VAL:N	2.31	0.45
1:C:115:GLU:OE1	1:C:161:GLU:HG2	2.16	0.45
1:A:187:THR:CG2	1:A:189:GLU:O	2.63	0.45
1:C:152:THR:CG2	1:C:188:ASP:N	2.69	0.45
1:C:207:ALA:O	1:C:211:VAL:HB	2.17	0.45
1:E:126:TYR:HB2	1:E:181:ILE:HD12	1.97	0.45
1:E:222:ARG:HG3	1:E:250:LEU:HD13	1.98	0.45
1:C:69:ILE:O	1:C:72:ALA:HB3	2.17	0.45
1:A:223:ARG:HH21	1:D:71:ARG:HG3	1.83	0.44
1:D:89:GLU:HB3	1:D:99:LEU:HD11	1.99	0.44
1:E:33:SER:HA	1:E:189:GLU:HG3	1.99	0.44
1:F:93:GLU:N	1:F:94:PRO:CD	2.79	0.44
1:B:48:THR:C	1:B:84:THR:HG22	2.39	0.44
1:B:135:ARG:O	1:B:136:ASP:C	2.61	0.44
1:C:4:HIS:CD2	1:E:16:LEU:HD11	2.52	0.44
1:A:53:PRO:HA	1:A:54:PRO:HA	1.77	0.44
1:B:23:ARG:O	1:B:27:PHE:HA	2.17	0.44
1:C:152:THR:O	1:C:188:ASP:HB2	2.17	0.44
1:D:119:ARG:HG3	1:D:119:ARG:H	1.62	0.44
1:B:37:PHE:HD2	1:B:38:LEU:HD13	1.82	0.44
1:B:48:THR:CG2	1:B:114:VAL:HB	2.48	0.44
1:C:32:ASN:O	1:C:35:LYS:HB3	2.17	0.44
1:C:110:LEU:CG	1:C:112:ILE:HD11	2.47	0.44
1:D:166:LYS:N	1:D:186:GLU:HG2	2.33	0.44
1:C:35:LYS:C	1:C:37:PHE:H	2.26	0.44
1:E:152:THR:C	1:E:187:THR:HG23	2.41	0.44
1:E:267:ALA:O	1:E:268:ILE:C	2.58	0.44
1:F:243:PRO:HG2	3:F:642:HOH:O	2.18	0.44
1:B:125:TYR:CB	1:B:133:ILE:CG1	2.89	0.44
1:B:153:ILE:C	1:B:187:THR:HG21	2.43	0.44
1:C:209:ILE:HG22	1:C:210:GLU:H	1.80	0.44
1:C:212:GLY:C	1:C:268:ILE:HD12	2.43	0.44
1:E:119:ARG:NH2	1:E:143:LEU:CD2	2.79	0.44
1:F:153:ILE:C	1:F:187:THR:HG21	2.41	0.44
1:B:152:THR:HG21	3:B:466:HOH:O	2.18	0.44
1:B:184:VAL:HG11	3:B:470:HOH:O	2.18	0.44
1:C:176:PRO:CA	1:F:106:GLU:HG2	2.47	0.44
1:C:241:LEU:N	1:C:241:LEU:HD12	2.33	0.44
1:D:71:ARG:HG2	1:D:75:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:GLY:HA2	1:D:164:MET:HG2	2.00	0.44
1:E:161:GLU:OE1	1:E:164:MET:HE3	2.18	0.44
1:F:7:ASN:ND2	1:F:19:TYR:CE1	2.86	0.44
1:C:129:SER:O	1:C:130:ALA:CB	2.65	0.44
1:D:175:VAL:HA	1:D:176:PRO:HD3	1.89	0.44
1:F:50:PHE:CD1	1:F:117:PRO:HG3	2.53	0.44
1:A:167:ILE:O	1:A:167:ILE:HG13	2.18	0.44
1:B:4:HIS:O	1:D:4:HIS:CE1	2.70	0.44
1:B:153:ILE:CA	1:B:187:THR:HG21	2.48	0.44
1:B:161:GLU:O	1:B:164:MET:HB2	2.18	0.44
1:C:167:ILE:O	1:C:170:LEU:N	2.46	0.44
1:E:59:GLU:HA	1:E:234:ILE:O	2.18	0.44
1:B:136:ASP:HA	1:B:137:PRO:HD3	1.79	0.43
1:C:75:MET:C	1:C:77:GLY:H	2.25	0.43
1:C:93:GLU:HB3	1:C:94:PRO:HD3	1.99	0.43
1:D:194:ALA:HA	3:D:432:HOH:O	2.17	0.43
1:E:257:VAL:O	1:E:261:LYS:HG3	2.18	0.43
1:A:136:ASP:HA	1:A:137:PRO:HD3	1.72	0.43
1:A:185:VAL:HA	3:A:492:HOH:O	2.18	0.43
1:C:163:GLY:O	1:C:165:GLY:N	2.51	0.43
1:C:233:LEU:HA	1:C:233:LEU:HD12	1.78	0.43
1:D:187:THR:CG2	1:D:189:GLU:O	2.66	0.43
1:F:104:GLU:O	1:F:107:ASP:N	2.47	0.43
1:A:154:GLY:O	1:A:190:LEU:HD12	2.18	0.43
1:B:4:HIS:CD2	1:D:16:LEU:HD11	2.54	0.43
1:B:136:ASP:HB2	3:B:460:HOH:O	2.19	0.43
1:C:258:GLU:OE1	1:C:258:GLU:HA	2.15	0.43
1:F:1:MET:O	1:F:5:LEU:HG	2.18	0.43
1:D:251:MET:HB2	3:D:570:HOH:O	2.17	0.43
1:E:126:TYR:CB	1:E:181:ILE:HD12	2.44	0.43
1:F:51:PRO:O	1:F:133:ILE:HD12	2.18	0.43
1:B:133:ILE:CD1	1:B:133:ILE:C	2.90	0.43
1:B:256:ILE:HD12	1:D:259:LEU:HD11	2.01	0.43
1:C:53:PRO:HA	1:C:54:PRO:HA	1.68	0.43
1:C:59:GLU:HA	1:C:234:ILE:O	2.17	0.43
1:F:105:PRO:HG2	1:F:144:LYS:HB2	2.00	0.43
1:B:205:ALA:O	1:B:208:SER:HB2	2.19	0.43
1:B:181:ILE:O	1:B:182:ALA:C	2.60	0.43
1:E:208:SER:O	1:E:212:GLY:N	2.52	0.43
1:B:31:HIS:HD2	3:B:457:HOH:O	2.02	0.43
1:B:122:ASP:OD2	1:B:124:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:GLY:N	3:D:416:HOH:O	2.51	0.43
1:D:137:PRO:O	1:D:138:LEU:HD12	2.19	0.43
1:F:62:GLY:H	1:F:197:ASN:ND2	2.16	0.43
1:D:166:LYS:O	1:D:166:LYS:HG3	2.18	0.43
1:F:228:ILE:HG23	1:F:233:LEU:HB2	1.99	0.43
1:B:105:PRO:HD2	1:B:106:GLU:OE1	2.19	0.43
1:B:198:TRP:NE1	1:B:253:HIS:HD2	2.10	0.43
1:C:228:ILE:O	1:C:233:LEU:HB2	2.19	0.43
1:E:100:ALA:HB1	1:E:103:PRO:HG3	2.01	0.43
1:F:124:ARG:CG	1:F:124:ARG:NH1	2.79	0.43
1:B:198:TRP:N	1:B:198:TRP:CD1	2.83	0.42
1:D:2:ILE:C	1:D:4:HIS:N	2.74	0.42
1:E:92:LEU:O	1:E:93:GLU:C	2.61	0.42
1:E:222:ARG:HB2	1:E:254:GLU:OE2	2.19	0.42
1:C:22:TYR:C	1:C:24:ARG:N	2.75	0.42
1:C:63:PRO:HB2	1:C:64:PRO:CD	2.43	0.42
1:C:178:GLY:O	1:C:179:GLU:C	2.59	0.42
1:D:33:SER:OG	1:D:189:GLU:HB3	2.20	0.42
1:C:29:PHE:CD1	1:C:30:LEU:N	2.87	0.42
1:C:44:VAL:CG1	1:C:112:ILE:HD13	2.49	0.42
1:C:154:GLY:O	1:C:190:LEU:HD12	2.19	0.42
1:D:153:ILE:C	1:D:187:THR:HG21	2.44	0.42
1:F:119:ARG:HH21	1:F:143:LEU:CD2	2.33	0.42
1:F:144:LYS:CE	3:F:504:HOH:O	2.66	0.42
1:D:6:ILE:HG21	1:D:202:GLY:HA3	2.01	0.42
1:D:154:GLY:N	1:D:187:THR:HG21	2.34	0.42
1:F:63:PRO:HB2	1:F:64:PRO:HD3	2.02	0.42
1:A:85:TYR:O	1:A:89:GLU:HG3	2.19	0.42
1:A:217:GLU:OE1	1:D:223:ARG:HD3	2.19	0.42
1:B:19:TYR:CZ	1:B:23:ARG:HG3	2.55	0.42
1:B:23:ARG:HG2	1:B:29:PHE:HE2	1.84	0.42
1:D:41:LEU:O	1:D:42:GLU:C	2.61	0.42
1:B:166:LYS:HG3	3:B:413:HOH:O	2.20	0.42
1:C:63:PRO:CB	1:C:64:PRO:HD3	2.45	0.42
1:C:101:ARG:O	1:C:102:THR:C	2.62	0.42
1:C:180:LYS:HB2	1:C:180:LYS:HE3	1.56	0.42
1:D:55:MET:HB3	1:D:57:VAL:HG23	2.01	0.42
1:F:211:VAL:CG1	1:F:213:ARG:HD3	2.49	0.42
1:A:23:ARG:HG3	1:A:23:ARG:HH11	1.85	0.42
1:A:251:MET:HG3	3:A:417:HOH:O	2.20	0.42
1:B:154:GLY:N	1:B:187:THR:HG21	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ILE:C	1:D:4:HIS:H	2.28	0.42
1:D:119:ARG:CG	1:D:139:ASP:OD1	2.63	0.42
1:D:246:ASP:O	1:D:248:ILE:HD12	2.19	0.42
1:F:159:GLY:C	1:F:164:MET:HG2	2.45	0.42
1:B:52:ILE:HG12	1:B:236:GLY:HA2	2.02	0.42
1:B:187:THR:HG22	1:B:188:ASP:N	2.34	0.42
1:C:48:THR:HG22	1:C:114:VAL:HB	2.01	0.42
1:C:42:GLU:O	1:C:79:LYS:HB2	2.20	0.42
1:E:181:ILE:HD13	1:E:181:ILE:HA	1.73	0.42
1:F:51:PRO:HD2	1:F:117:PRO:HG2	2.01	0.42
1:F:210:GLU:HG3	3:F:589:HOH:O	2.20	0.42
1:A:90:LYS:HE3	3:A:453:HOH:O	2.19	0.41
1:B:4:HIS:CE1	1:D:7:ASN:HB3	2.54	0.41
1:C:163:GLY:C	1:C:165:GLY:N	2.78	0.41
1:D:264:VAL:O	1:D:268:ILE:HD13	2.19	0.41
1:E:39:ASP:O	1:E:40:ASN:CG	2.63	0.41
1:E:152:THR:HG23	1:E:152:THR:O	2.20	0.41
1:E:187:THR:HG22	1:E:189:GLU:H	1.85	0.41
1:B:23:ARG:HD2	1:D:20:LEU:HD21	2.03	0.41
1:B:43:ARG:HG2	1:B:108:TYR:CD1	2.55	0.41
1:C:124:ARG:C	1:C:125:TYR:CD2	2.98	0.41
1:C:176:PRO:HA	1:F:106:GLU:CG	2.50	0.41
1:E:34:THR:O	1:E:37:PHE:HB3	2.20	0.41
1:F:59:GLU:OE2	1:F:236:GLY:HA3	2.20	0.41
1:A:223:ARG:NH2	1:D:75:MET:HE2	2.36	0.41
1:B:226:GLU:OE2	1:F:75:MET:HE2	2.20	0.41
1:C:44:VAL:HG13	1:C:112:ILE:HD13	2.02	0.41
1:C:146:ARG:HG3	3:C:407:HOH:O	2.19	0.41
1:D:110:LEU:HG	1:D:112:ILE:CD1	2.49	0.41
1:F:65:GLY:H	1:F:197:ASN:ND2	2.18	0.41
1:F:254:GLU:HB3	3:F:466:HOH:O	2.19	0.41
1:A:31:HIS:CE1	3:A:439:HOH:O	2.73	0.41
1:A:103:PRO:HD2	3:A:614:HOH:O	2.20	0.41
1:A:222:ARG:NH1	1:A:254:GLU:OE1	2.52	0.41
1:B:124:ARG:HB3	1:B:132:GLU:OE2	2.20	0.41
1:C:124:ARG:HH11	1:C:124:ARG:CG	2.33	0.41
1:D:161:GLU:N	1:D:161:GLU:OE1	2.53	0.41
1:F:222:ARG:HB2	1:F:254:GLU:OE2	2.20	0.41
1:A:221:GLU:O	1:A:225:ILE:HG12	2.19	0.41
1:D:111:ILE:HG22	1:D:142:PHE:CE2	2.55	0.41
1:F:130:ALA:CA	1:F:181:ILE:HD11	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:GLU:HG3	3:F:530:HOH:O	2.19	0.41
1:A:175:VAL:HA	1:A:176:PRO:HD3	1.87	0.41
1:A:259:LEU:CD1	1:F:256:ILE:HD12	2.49	0.41
1:B:175:VAL:HA	1:B:176:PRO:HD3	1.87	0.41
1:C:139:ASP:HB3	1:C:162:ILE:HD11	2.02	0.41
1:C:245:VAL:HG13	1:C:253:HIS:CE1	2.55	0.41
1:D:205:ALA:O	1:D:208:SER:HB2	2.21	0.41
1:D:252:VAL:O	1:D:256:ILE:HD13	2.20	0.41
1:E:84:THR:HG23	1:E:85:TYR:N	2.35	0.41
1:A:112:ILE:CG2	1:A:113:SER:N	2.83	0.41
1:C:196:SER:O	1:C:197:ASN:C	2.62	0.41
1:F:111:ILE:HD13	1:F:141:ILE:HD12	2.03	0.41
1:A:68:ALA:HB2	1:A:219:TRP:CZ3	2.56	0.41
1:A:196:SER:O	1:A:197:ASN:C	2.64	0.41
1:A:196:SER:O	1:A:199:GLY:N	2.53	0.41
1:B:122:ASP:OD2	1:B:122:ASP:C	2.62	0.41
1:C:37:PHE:HD2	1:C:38:LEU:HD13	1.85	0.41
1:B:19:TYR:OH	1:B:23:ARG:HG3	2.21	0.41
1:B:248:ILE:CG2	1:B:252:VAL:HB	2.51	0.41
1:C:84:THR:HB	1:C:88:VAL:HB	2.02	0.41
1:C:187:THR:CG2	1:C:189:GLU:O	2.69	0.41
1:D:222:ARG:HG2	1:F:251:MET:HE3	2.03	0.41
1:E:17:LYS:HB3	3:E:456:HOH:O	2.19	0.41
1:E:214:ASN:HB3	1:E:217:GLU:OE1	2.21	0.41
1:F:48:THR:C	1:F:84:THR:HG23	2.45	0.41
1:A:91:ALA:HA	1:A:231:ALA:CB	2.51	0.41
1:A:111:ILE:HD12	1:A:145:ALA:HB2	2.03	0.41
1:A:220:ASP:HB3	1:A:223:ARG:HB3	2.03	0.41
1:B:56:MET:O	1:B:135:ARG:NH1	2.53	0.41
1:C:48:THR:CG2	1:C:114:VAL:HB	2.51	0.41
1:E:48:THR:HG23	1:E:66:ALA:HB2	2.01	0.41
1:E:221:GLU:HB2	1:E:257:VAL:HG21	2.03	0.41
1:C:4:HIS:HA	1:C:19:TYR:OH	2.21	0.40
1:C:34:THR:CG2	1:C:207:ALA:HB2	2.50	0.40
1:C:212:GLY:HA2	1:C:268:ILE:HD12	2.04	0.40
1:C:228:ILE:HG23	1:C:233:LEU:CB	2.50	0.40
1:E:14:GLY:O	1:E:15:VAL:C	2.63	0.40
1:E:174:HIS:CE1	3:E:422:HOH:O	2.73	0.40
1:F:50:PHE:CE1	1:F:117:PRO:HG3	2.56	0.40
1:B:119:ARG:NH2	3:B:642:HOH:O	2.48	0.40
1:C:19:TYR:O	1:C:20:LEU:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:THR:HA	1:C:203:LEU:HD21	2.03	0.40
1:F:196:SER:O	1:F:197:ASN:C	2.64	0.40
1:C:22:TYR:C	1:C:24:ARG:H	2.29	0.40
1:C:112:ILE:N	1:C:112:ILE:CD1	2.80	0.40
1:F:119:ARG:NE	1:F:143:LEU:HD21	2.37	0.40
1:F:153:ILE:CA	1:F:187:THR:CG2	3.00	0.40
1:D:152:THR:OG1	1:D:187:THR:HG23	2.21	0.40
1:B:84:THR:HB	1:B:85:TYR:H	1.63	0.40
1:B:222:ARG:O	1:B:226:GLU:HG3	2.21	0.40
1:C:8:THR:O	1:C:10:ILE:HG23	2.21	0.40
1:C:35:LYS:C	1:C:37:PHE:N	2.78	0.40
1:C:35:LYS:HB2	1:C:35:LYS:HE2	1.79	0.40
1:C:50:PHE:CE1	1:C:117:PRO:HG3	2.57	0.40
1:C:187:THR:CG2	1:C:188:ASP:N	2.84	0.40
1:D:2:ILE:O	1:D:6:ILE:HG23	2.22	0.40
1:D:52:ILE:HD13	1:D:59:GLU:HB3	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	257/270 (95%)	242 (94%)	15 (6%)	0	100	100
1	B	266/270 (98%)	243 (91%)	22 (8%)	1 (0%)	30	38
1	C	267/270 (99%)	230 (86%)	32 (12%)	5 (2%)	6	5
1	D	266/270 (98%)	239 (90%)	26 (10%)	1 (0%)	30	38
1	E	256/270 (95%)	228 (89%)	25 (10%)	3 (1%)	10	12
1	F	267/270 (99%)	254 (95%)	12 (4%)	1 (0%)	30	38
All	All	1579/1620 (98%)	1436 (91%)	132 (8%)	11 (1%)	18	23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	210	GLU
1	D	13	ARG
1	E	268	ILE
1	C	164	MET
1	E	121	ALA
1	F	182	ALA
1	C	96	GLY
1	C	157	ASP
1	E	167	ILE
1	B	10	ILE
1	C	158	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/219 (95%)	192 (92%)	16 (8%)	12	16
1	B	213/219 (97%)	190 (89%)	23 (11%)	6	7
1	C	216/219 (99%)	186 (86%)	30 (14%)	3	4
1	D	213/219 (97%)	193 (91%)	20 (9%)	8	11
1	E	208/219 (95%)	179 (86%)	29 (14%)	3	4
1	F	216/219 (99%)	193 (89%)	23 (11%)	6	8
All	All	1274/1314 (97%)	1133 (89%)	141 (11%)	6	7

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	16	LEU
1	A	23	ARG
1	A	25	LYS
1	A	38	LEU
1	A	45	LEU

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Mol	Chain	Res	Type
1	A	55	MET
1	A	60	THR
1	A	83	LEU
1	A	92	LEU
1	A	119	ARG
1	A	179	GLU
1	A	187	THR
1	A	203	LEU
1	A	245	VAL
1	A	256	ILE
1	B	9	ASP
1	B	13	ARG
1	B	23	ARG
1	B	24	ARG
1	B	38	LEU
1	B	45	LEU
1	B	55	MET
1	B	74	GLU
1	B	83	LEU
1	B	90	LYS
1	B	92	LEU
1	B	97	VAL
1	B	133	ILE
1	B	138	LEU
1	B	179	GLU
1	B	203	LEU
1	B	210	GLU
1	B	234	ILE
1	B	245	VAL
1	B	251	MET
1	B	256	ILE
1	B	266	GLU
1	B	268	ILE
1	C	20	LEU
1	C	23	ARG
1	C	25	LYS
1	C	38	LEU
1	C	45	LEU
1	C	55	MET
1	C	74	GLU
1	C	83	LEU
1	C	84	THR

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Mol	Chain	Res	Type
1	C	86	SER
1	C	90	LYS
1	C	99	LEU
1	C	125	TYR
1	C	134	LYS
1	C	141	ILE
1	C	148	LEU
1	C	152	THR
1	C	162	ILE
1	C	170	LEU
1	C	187	THR
1	C	203	LEU
1	C	209	ILE
1	C	211	VAL
1	C	233	LEU
1	C	234	ILE
1	C	245	VAL
1	C	251	MET
1	C	256	ILE
1	C	258	GLU
1	C	266	GLU
1	D	9	ASP
1	D	13	ARG
1	D	20	LEU
1	D	23	ARG
1	D	25	LYS
1	D	38	LEU
1	D	45	LEU
1	D	55	MET
1	D	83	LEU
1	D	89	GLU
1	D	90	LYS
1	D	92	LEU
1	D	148	LEU
1	D	164	MET
1	D	203	LEU
1	D	217	GLU
1	D	233	LEU
1	D	240	THR
1	D	251	MET
1	D	258	GLU
1	E	16	LEU

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Mol	Chain	Res	Type
1	E	23	ARG
1	E	25	LYS
1	E	38	LEU
1	E	42	GLU
1	E	45	LEU
1	E	55	MET
1	E	83	LEU
1	E	86	SER
1	E	90	LYS
1	E	93	GLU
1	E	101	ARG
1	E	104	GLU
1	E	119	ARG
1	E	134	LYS
1	E	169	GLU
1	E	181	ILE
1	E	187	THR
1	E	203	LEU
1	E	213	ARG
1	E	217	GLU
1	E	223	ARG
1	E	233	LEU
1	E	234	ILE
1	E	238	SER
1	E	240	THR
1	E	245	VAL
1	E	248	ILE
1	E	251	MET
1	F	6	ILE
1	F	23	ARG
1	F	38	LEU
1	F	45	LEU
1	F	55	MET
1	F	74	GLU
1	F	83	LEU
1	F	84	THR
1	F	90	LYS
1	F	116	THR
1	F	129	SER
1	F	141	ILE
1	F	143	LEU
1	F	152	THR

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Mol	Chain	Res	Type
1	F	170	LEU
1	F	179	GLU
1	F	203	LEU
1	F	210	GLU
1	F	233	LEU
1	F	234	ILE
1	F	245	VAL
1	F	256	ILE
1	F	268	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	40	ASN
1	A	197	ASN
1	A	253	HIS
1	B	26	ASN
1	B	28	ASN
1	B	197	ASN
1	B	253	HIS
1	C	197	ASN
1	D	7	ASN
1	D	28	ASN
1	D	31	HIS
1	D	197	ASN
1	D	253	HIS
1	E	40	ASN
1	E	177	HIS
1	E	197	ASN
1	E	253	HIS
1	F	7	ASN
1	F	28	ASN
1	F	177	HIS
1	F	197	ASN
1	F	253	HIS

5.3.3 RNA ⓘ

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](#)

Of 53 ligands modelled in this entry, 53 are monoatomic - leaving 0 for Mogul analysis.

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 [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	259/270 (95%)	-0.67	1 (0%) 88 89	5, 23, 43, 65	0
1	B	268/270 (99%)	-0.42	4 (1%) 72 73	10, 29, 53, 76	0
1	C	269/270 (99%)	0.29	10 (3%) 45 48	22, 45, 69, 83	0
1	D	268/270 (99%)	-0.41	3 (1%) 78 79	14, 29, 48, 72	0
1	E	258/270 (95%)	-0.15	2 (0%) 82 83	20, 39, 59, 84	0
1	F	269/270 (99%)	-0.57	0 100 100	9, 26, 43, 52	0
All	All	1591/1620 (98%)	-0.32	20 (1%) 75 76	5, 32, 58, 84	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	HIS	4.1
1	E	13	ARG	3.3
1	B	269	LYS	3.0
1	A	11	GLY	3.0
1	E	269	LYS	2.8
1	B	4	HIS	2.8
1	D	3	ALA	2.8
1	C	269	LYS	2.8
1	C	105	PRO	2.8
1	D	10	ILE	2.7
1	C	102	THR	2.6
1	B	8	THR	2.5
1	C	111	ILE	2.5
1	C	13	ARG	2.3
1	C	95	PHE	2.3
1	B	10	ILE	2.2
1	C	149	GLY	2.2
1	C	99	LEU	2.2
1	C	110	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	112	ILE	2.1

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](#)

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, 95th 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
2	ZN	E	311	1/1	0.74	0.14	128,128,128,128	0
2	ZN	C	301	1/1	0.76	0.17	103,103,103,103	0
2	ZN	B	310	1/1	0.78	0.19	136,136,136,136	0
2	ZN	B	309	1/1	0.79	0.14	137,137,137,137	0
2	ZN	B	311	1/1	0.79	0.11	125,125,125,125	0
2	ZN	D	307	1/1	0.80	0.11	124,124,124,124	0
2	ZN	E	310	1/1	0.82	0.33	109,109,109,109	0
2	ZN	E	306	1/1	0.82	0.18	141,141,141,141	0
2	ZN	A	308	1/1	0.83	0.15	164,164,164,164	0
2	ZN	E	308	1/1	0.84	0.14	110,110,110,110	0
2	ZN	F	308	1/1	0.85	0.17	106,106,106,106	0
2	ZN	A	307	1/1	0.86	0.25	96,96,96,96	0
2	ZN	D	306	1/1	0.87	0.11	122,122,122,122	0
2	ZN	D	301	1/1	0.88	0.16	83,83,83,83	0
2	ZN	F	307	1/1	0.88	0.21	100,100,100,100	0
2	ZN	B	308	1/1	0.88	0.12	133,133,133,133	0
2	ZN	E	307	1/1	0.90	0.15	104,104,104,104	0
2	ZN	F	302	1/1	0.90	0.15	104,104,104,104	0
2	ZN	C	304	1/1	0.90	0.17	72,72,72,72	0
2	ZN	C	308	1/1	0.90	0.09	132,132,132,132	0
2	ZN	C	307	1/1	0.91	0.12	124,124,124,124	0
2	ZN	F	301	1/1	0.92	0.14	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	305	1/1	0.92	0.20	89,89,89,89	0
2	ZN	D	303	1/1	0.93	0.16	69,69,69,69	0
2	ZN	B	302	1/1	0.93	0.16	58,58,58,58	0
2	ZN	F	306	1/1	0.95	0.12	62,62,62,62	0
2	ZN	C	302	1/1	0.95	0.10	51,51,51,51	0
2	ZN	E	309	1/1	0.95	0.14	75,75,75,75	0
2	ZN	E	304	1/1	0.96	0.11	73,73,73,73	0
2	ZN	A	304	1/1	0.96	0.16	68,68,68,68	0
2	ZN	B	307	1/1	0.96	0.10	67,67,67,67	0
2	ZN	B	304	1/1	0.96	0.17	67,67,67,67	0
2	ZN	A	302	1/1	0.97	0.16	45,45,45,45	0
2	ZN	C	306	1/1	0.97	0.23	89,89,89,89	0
2	ZN	A	306	1/1	0.97	0.13	44,44,44,44	0
2	ZN	C	303	1/1	0.97	0.12	49,49,49,49	0
2	ZN	E	301	1/1	0.97	0.14	46,46,46,46	0
2	ZN	E	303	1/1	0.97	0.09	66,66,66,66	0
2	ZN	A	305	1/1	0.98	0.16	52,52,52,52	0
2	ZN	B	306	1/1	0.98	0.10	55,55,55,55	0
2	ZN	E	302	1/1	0.98	0.08	47,47,47,47	0
2	ZN	B	303	1/1	0.98	0.12	47,47,47,47	0
2	ZN	C	305	1/1	0.98	0.14	54,54,54,54	0
2	ZN	D	304	1/1	0.98	0.14	34,34,34,34	0
2	ZN	D	305	1/1	0.98	0.13	39,39,39,39	0
2	ZN	A	303	1/1	0.98	0.10	30,30,30,30	0
2	ZN	E	305	1/1	0.99	0.09	46,46,46,46	0
2	ZN	F	303	1/1	0.99	0.12	40,40,40,40	0
2	ZN	F	304	1/1	0.99	0.11	30,30,30,30	0
2	ZN	F	305	1/1	0.99	0.10	32,32,32,32	0
2	ZN	B	301	1/1	0.99	0.10	39,39,39,39	0
2	ZN	A	301	1/1	0.99	0.10	30,30,30,30	0
2	ZN	D	302	1/1	0.99	0.09	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.