



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 06:38 PM UTC

PDB ID : 3HNP / pdb_00003hnp
Title : Crystal Structure of an Oxidoreductase from Bacillus cereus. Northeast Structural Genomics Consortium target id BcR251
Authors : Seetharaman, J.; Su, M.; Sahdev, S.; Janjua, H.; Xiao, R.; Ciccocanti, C.; Foote, E.L.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2009-05-31
Resolution : 2.60 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

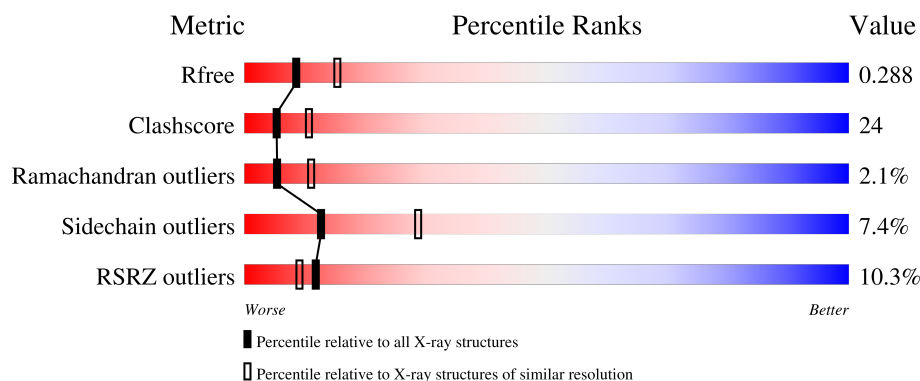
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

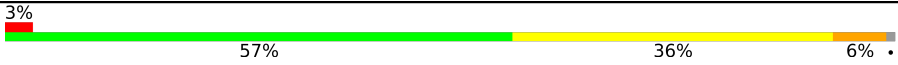
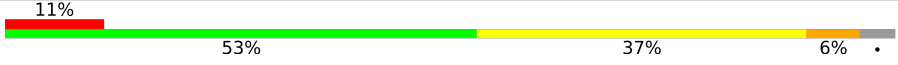
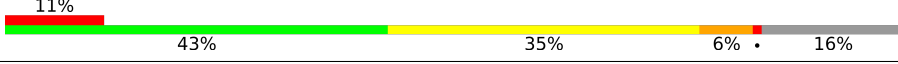
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	353	
1	B	353	
1	C	353	
1	D	353	
1	E	353	

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Mol	Chain	Length	Quality of chain
1	F	353	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 15535 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 Oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2767	1772	466	521	8			
1	B	350	Total	C	N	O	S	0	0	0
			2777	1778	468	523	8			
1	C	340	Total	C	N	O	S	0	0	0
			2667	1709	449	501	8			
1	D	344	Total	C	N	O	S	0	0	0
			2731	1749	458	516	8			
1	E	297	Total	C	N	O	S	0	0	0
			2299	1465	387	440	7			
1	F	294	Total	C	N	O	S	0	0	0
			2205	1401	376	422	6			

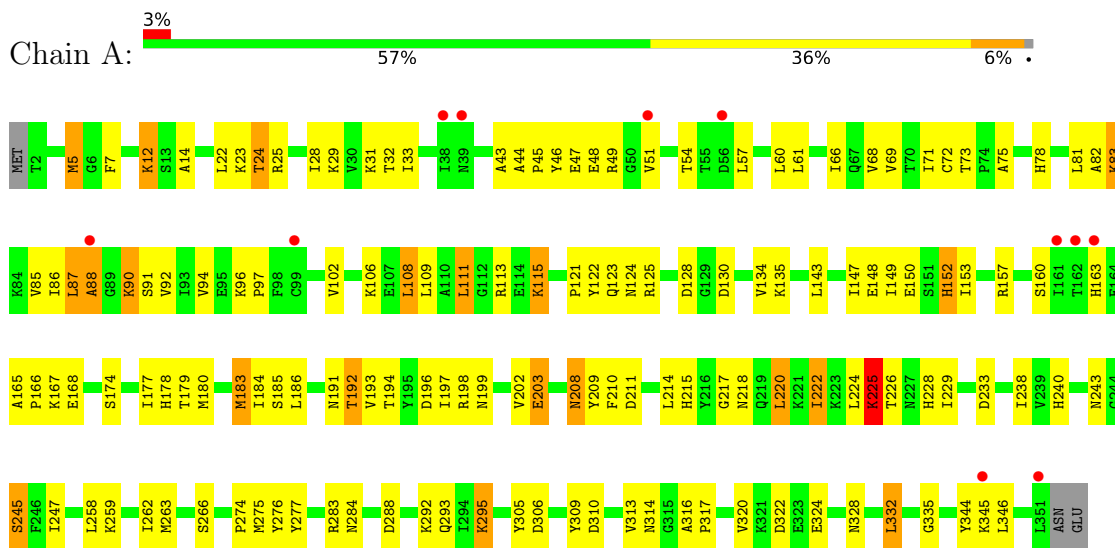
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	41	Total	O	0	0
			41	41		
2	B	12	Total	O	0	0
			12	12		
2	C	6	Total	O	0	0
			6	6		
2	D	10	Total	O	0	0
			10	10		
2	E	17	Total	O	0	0
			17	17		
2	F	3	Total	O	0	0
			3	3		

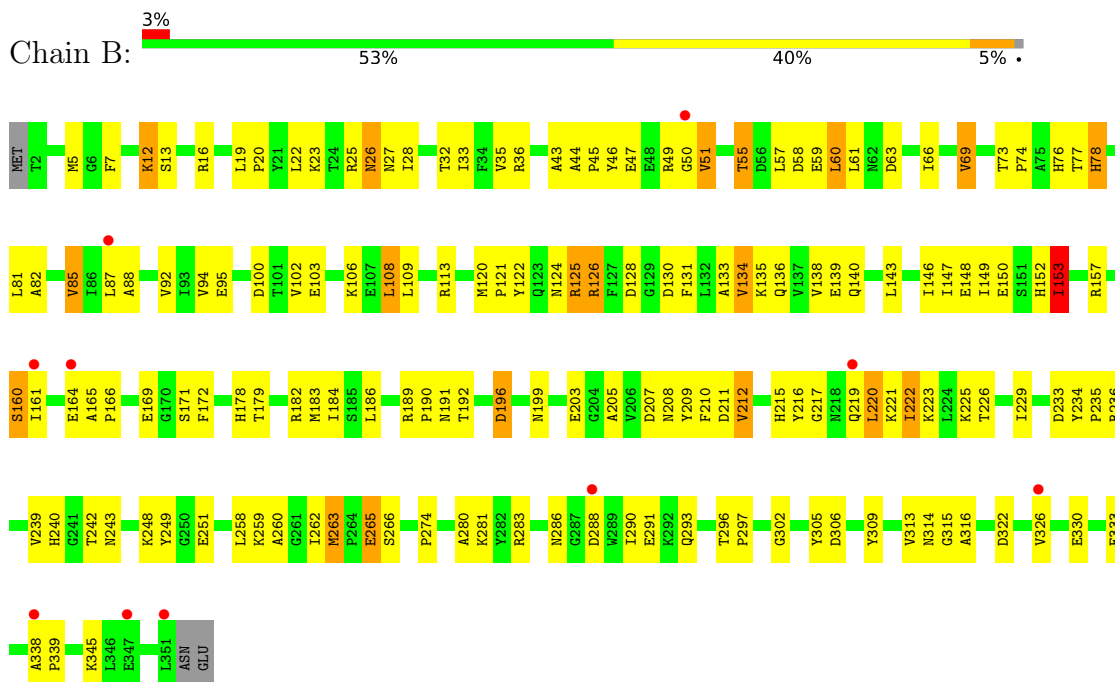
3 Residue-property plots

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.

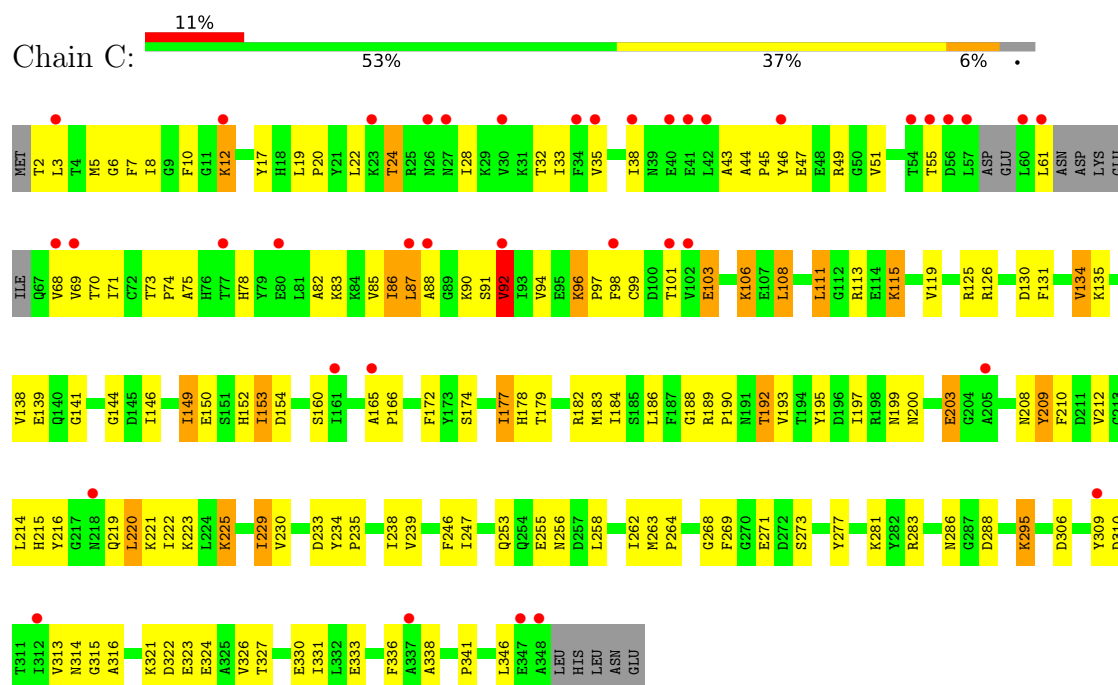
• Molecule 1: Oxidoreductase



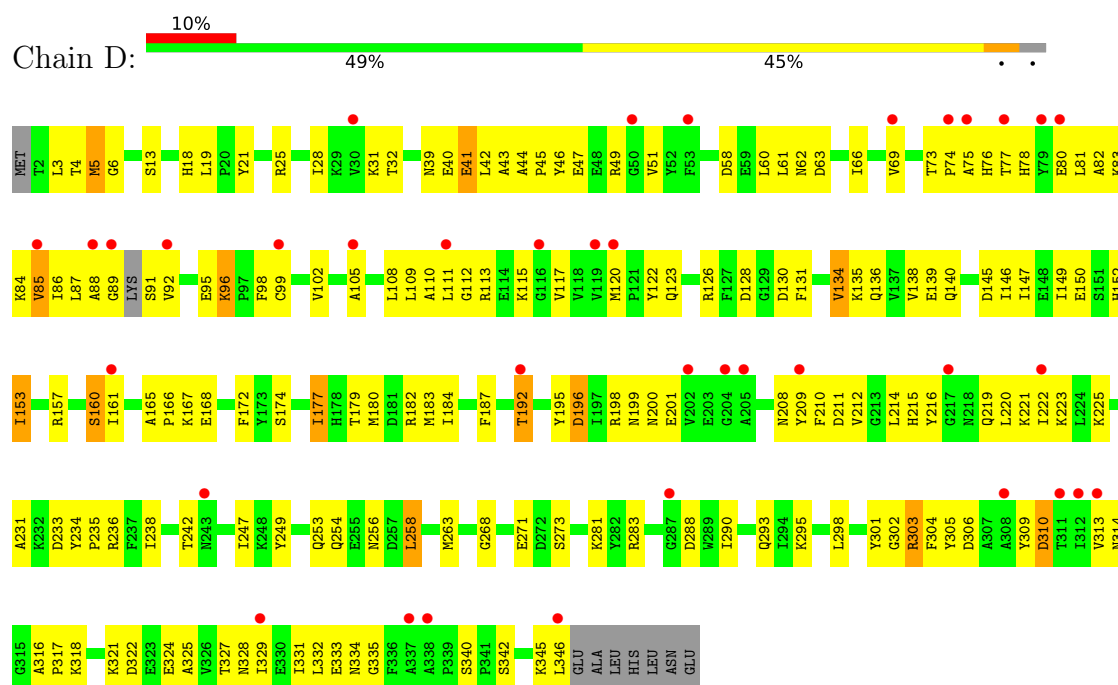
• Molecule 1: Oxidoreductase



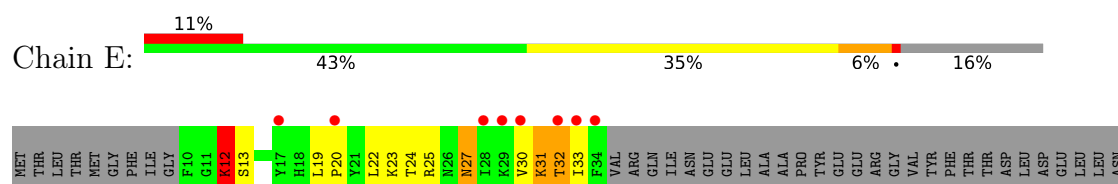
• Molecule 1: Oxidoreductase

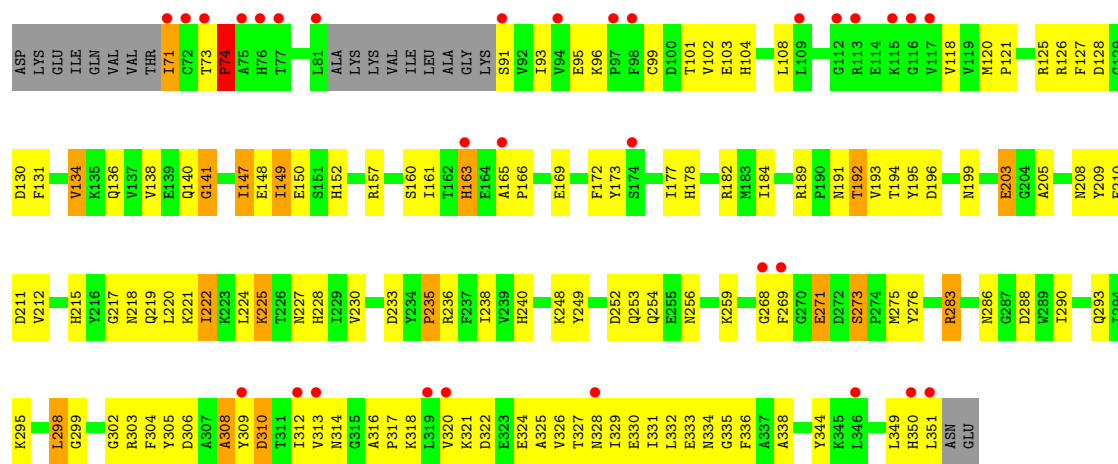


• Molecule 1: Oxidoreductase

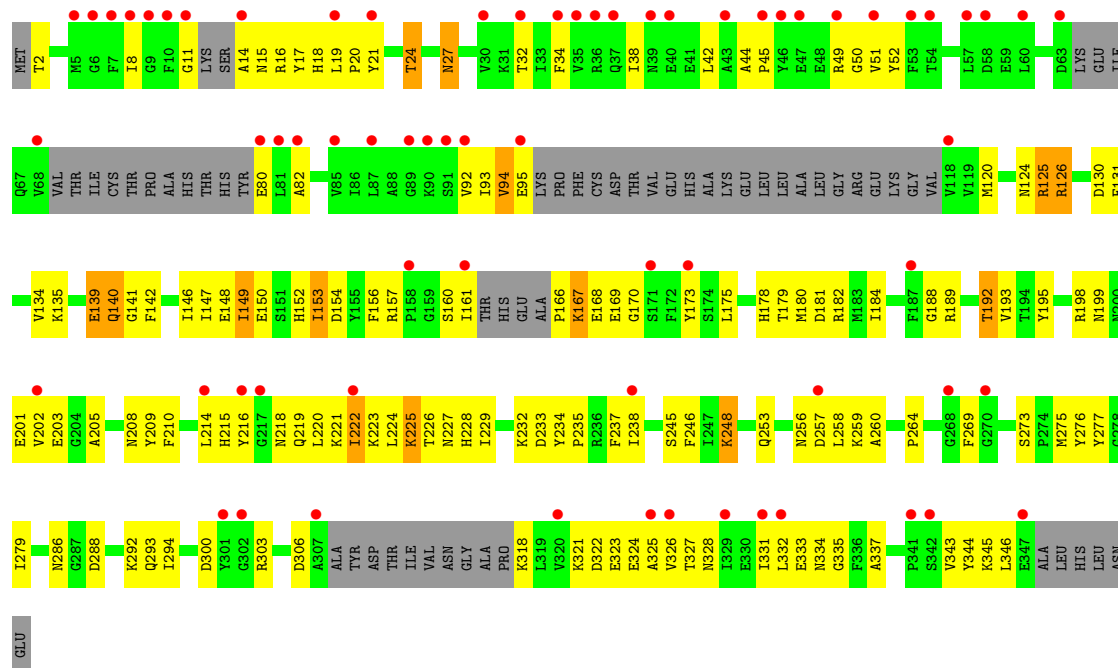


• Molecule 1: Oxidoreductase





● Molecule 1: Oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.66Å 149.51Å 95.77Å 90.00° 92.13° 90.00°	Depositor
Resolution (Å)	43.79 – 2.60 43.79 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (43.79-2.60) 94.6 (43.79-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.59 (at 2.58Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.239 , 0.282 0.245 , 0.288	Depositor DCC
R_{free} test set	5637 reflections (3.58%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.016 for h,-k,-l 0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15535	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.57	2/2831 (0.1%)	0.98	13/3833 (0.3%)
1	B	0.47	0/2841	0.94	14/3846 (0.4%)
1	C	0.46	0/2728	0.92	8/3694 (0.2%)
1	D	0.46	0/2793	0.92	8/3780 (0.2%)
1	E	0.50	0/2352	0.96	10/3187 (0.3%)
1	F	0.42	0/2247	0.86	5/3038 (0.2%)
All	All	0.48	2/15792 (0.0%)	0.93	58/21378 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	MET	SD-CE	-6.75	1.62	1.79
1	A	5	MET	SD-CE	-5.18	1.66	1.79

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	ARG	N-CA-C	-9.09	102.11	113.02
1	B	126	ARG	N-CA-C	-8.24	102.94	113.16
1	E	126	ARG	N-CA-C	-8.08	103.53	113.15
1	A	233	ASP	N-CA-C	7.90	121.10	110.35
1	D	234	TYR	N-CA-C	-7.75	98.76	110.07
1	B	220	LEU	N-CA-C	7.69	122.36	110.20
1	B	233	ASP	N-CA-C	7.59	120.94	110.24
1	E	233	ASP	N-CA-C	7.20	120.14	110.35
1	F	126	ARG	N-CA-C	-6.84	104.68	113.16
1	D	233	ASP	N-CA-C	6.76	119.02	110.24
1	C	234	TYR	N-CA-C	-6.69	100.30	110.07
1	F	170	GLY	N-CA-C	6.53	119.00	111.36
1	E	74	PRO	N-CA-CB	6.46	110.03	103.25
1	C	233	ASP	N-CA-C	6.37	119.01	110.35
1	A	78	HIS	N-CA-C	6.36	118.74	111.11
1	E	235	PRO	N-CA-C	-6.35	101.89	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	VAL	N-CA-C	6.33	116.97	108.11
1	C	220	LEU	N-CA-C	6.27	120.11	110.20
1	A	335	GLY	N-CA-C	-6.21	106.64	114.16
1	F	45	PRO	N-CA-CB	6.11	109.66	103.25
1	C	24	THR	N-CA-C	-6.04	107.73	114.62
1	E	141	GLY	N-CA-C	6.03	123.59	114.61
1	D	263	MET	CA-C-N	5.94	127.27	119.84
1	D	263	MET	C-N-CA	5.94	127.27	119.84
1	A	263	MET	CA-C-N	5.87	127.18	119.84
1	A	263	MET	C-N-CA	5.87	127.18	119.84
1	A	225	LYS	N-CA-C	5.83	118.61	108.76
1	C	141	GLY	N-CA-C	5.81	123.26	114.61
1	B	78	HIS	N-CA-C	5.80	117.46	111.03
1	B	88	ALA	N-CA-C	-5.79	103.02	110.19
1	E	335	GLY	N-CA-C	-5.78	108.31	114.67
1	A	88	ALA	N-CA-C	-5.66	101.31	110.32
1	E	220	LEU	N-CA-C	5.55	118.53	109.59
1	C	86	ILE	N-CA-C	-5.52	105.15	110.72
1	B	51	VAL	N-CA-C	5.50	116.17	109.30
1	E	195	TYR	N-CA-C	5.44	118.26	109.40
1	E	308	ALA	N-CA-C	-5.43	105.28	111.14
1	A	94	VAL	N-CA-C	5.43	115.77	108.17
1	C	225	LYS	N-CA-C	5.42	117.33	108.55
1	B	94	VAL	N-CA-C	5.41	115.75	108.17
1	B	196	ASP	N-CA-C	-5.41	98.44	107.80
1	B	263	MET	CA-C-N	5.40	125.47	119.32
1	B	263	MET	C-N-CA	5.40	125.47	119.32
1	B	207	ASP	N-CA-C	5.34	118.10	110.24
1	D	5	MET	N-CA-C	5.31	117.48	109.41
1	A	220	LEU	N-CA-C	5.30	118.12	109.59
1	D	234	TYR	CA-C-N	-5.29	114.80	120.03
1	D	234	TYR	C-N-CA	-5.29	114.80	120.03
1	E	219	GLN	N-CA-C	5.26	118.16	111.69
1	F	142	PHE	N-CA-C	-5.26	106.82	113.18
1	B	234	TYR	N-CA-C	-5.22	101.42	109.41
1	B	60	LEU	N-CA-C	-5.20	106.27	113.18
1	B	212	VAL	N-CA-C	5.12	115.23	107.80
1	F	233	ASP	N-CA-C	5.10	116.87	110.24
1	A	128	ASP	N-CA-C	-5.08	102.17	110.20
1	A	208	ASN	N-CA-C	-5.06	105.42	112.30
1	A	111	LEU	N-CA-C	-5.04	105.91	111.71
1	A	152	HIS	N-CA-C	5.03	117.94	109.95

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	2767	0	2702	117	0
1	B	2777	0	2721	132	0
1	C	2667	0	2578	122	0
1	D	2731	0	2674	158	0
1	E	2299	0	2150	116	0
1	F	2205	0	1996	129	0
2	A	41	0	0	2	0
2	B	12	0	0	0	0
2	C	6	0	0	0	0
2	D	10	0	0	0	0
2	E	17	0	0	1	0
2	F	3	0	0	0	0
All	All	15535	0	14821	731	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 24.

All (731) 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:F:235:PRO:HG2	1:F:238:ILE:HD11	1.45	0.97
1:C:35:VAL:O	1:C:55:THR:HG22	1.65	0.95
1:D:5:MET:HE3	1:D:28:ILE:HG21	1.46	0.95
1:B:191:ASN:HD21	1:B:217:GLY:H	1.10	0.93
1:B:26:ASN:H	1:B:26:ASN:ND2	1.67	0.91
1:D:110:ALA:HA	1:D:113:ARG:HD2	1.53	0.90
1:F:321:LYS:HB2	1:F:324:GLU:HG3	1.53	0.89
1:B:191:ASN:ND2	1:B:217:GLY:H	1.69	0.88
1:A:46:TYR:HB3	1:A:51:VAL:HG11	1.55	0.88
1:B:26:ASN:H	1:B:26:ASN:HD22	0.90	0.87
1:C:153:ILE:HD11	1:C:179:THR:HG23	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ASN:HD22	1:B:26:ASN:N	1.72	0.86
1:A:5:MET:HE3	1:A:28:ILE:HG21	1.56	0.86
1:B:46:TYR:HB3	1:B:51:VAL:HG11	1.59	0.85
1:A:23:LYS:HD3	1:A:49:ARG:NH1	1.92	0.85
1:F:120:MET:HB3	1:F:318:LYS:HD2	1.59	0.85
1:E:253:GLN:HE22	1:E:256:ASN:HD22	1.25	0.84
1:A:191:ASN:ND2	1:A:217:GLY:H	1.74	0.84
1:A:214:LEU:HB2	1:A:222:ILE:HG23	1.59	0.84
1:A:292:LYS:NZ	1:D:253:GLN:HE21	1.78	0.82
1:E:165:ALA:HB1	1:E:166:PRO:HD2	1.60	0.82
1:C:216:TYR:HB2	1:C:220:LEU:HB3	1.59	0.82
1:B:153:ILE:HD11	1:B:179:THR:HG21	1.63	0.81
1:E:192:THR:HG23	1:E:215:HIS:HB2	1.62	0.80
1:B:309:TYR:O	1:B:313:VAL:HG12	1.82	0.80
1:C:3:LEU:HD23	1:C:28:ILE:HD12	1.65	0.79
1:A:46:TYR:O	1:A:51:VAL:HG12	1.83	0.79
1:C:12:LYS:HE3	1:C:12:LYS:H	1.46	0.79
1:B:44:ALA:HB3	1:B:45:PRO:HD3	1.64	0.77
1:A:29:LYS:HE2	1:A:31:LYS:HZ2	1.50	0.77
1:B:46:TYR:O	1:B:51:VAL:HG12	1.84	0.76
1:C:149:ILE:HG22	1:C:222:ILE:HB	1.67	0.76
1:B:189:ARG:HH22	1:B:330:GLU:CD	1.94	0.75
1:D:5:MET:HE3	1:D:28:ILE:CG2	2.15	0.75
1:E:31:LYS:O	1:E:32:THR:CB	2.34	0.75
1:D:46:TYR:HB3	1:D:51:VAL:HG11	1.67	0.75
1:B:183:MET:HG3	1:B:222:ILE:HD13	1.68	0.75
1:A:211:ASP:CG	1:A:225:LYS:HD3	2.12	0.75
1:D:313:VAL:HG13	1:D:314:ASN:H	1.50	0.75
1:B:12:LYS:HG2	1:B:13:SER:H	1.52	0.74
1:A:29:LYS:HE2	1:A:31:LYS:NZ	2.01	0.74
1:F:189:ARG:NH1	1:F:327:THR:HG23	2.03	0.74
1:A:183:MET:HG3	1:A:222:ILE:HD11	1.69	0.74
1:E:12:LYS:H	1:E:12:LYS:HD3	1.53	0.74
1:D:177:ILE:HD13	1:D:177:ILE:O	1.87	0.73
1:A:191:ASN:HD22	1:A:217:GLY:H	1.33	0.73
1:B:166:PRO:HG2	1:B:169:GLU:HG3	1.70	0.73
1:E:316:ALA:HB1	1:E:317:PRO:HD2	1.68	0.73
1:B:165:ALA:HB1	1:B:166:PRO:HD2	1.68	0.73
1:C:43:ALA:O	1:C:47:GLU:HG3	1.88	0.73
1:D:69:VAL:HG12	1:D:85:VAL:HG21	1.71	0.72
1:D:310:ASP:HB3	1:D:316:ALA:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:GLN:O	1:E:140:GLN:HG3	1.89	0.72
1:B:149:ILE:HG12	1:B:239:VAL:HG13	1.72	0.72
1:F:131:PHE:CE1	1:F:182:ARG:HB2	2.25	0.71
1:A:135:LYS:HG3	1:A:186:LEU:HD11	1.72	0.71
1:F:149:ILE:HD12	1:F:150:GLU:N	2.05	0.71
1:D:147:ILE:HD11	1:D:242:THR:HG23	1.72	0.71
1:E:253:GLN:NE2	1:E:256:ASN:HD22	1.89	0.71
1:F:149:ILE:HA	1:F:238:ILE:O	1.91	0.70
1:C:46:TYR:HB3	1:C:51:VAL:HG11	1.73	0.70
1:B:81:LEU:O	1:B:85:VAL:HG12	1.91	0.70
1:B:211:ASP:CG	1:B:225:LYS:HD3	2.17	0.70
1:C:49:ARG:NE	1:C:49:ARG:HA	2.07	0.70
1:F:293:GLN:C	1:F:294:ILE:HD12	2.16	0.70
1:F:166:PRO:HD2	1:F:169:GLU:HG3	1.72	0.69
1:D:4:THR:HG23	1:D:31:LYS:HG2	1.73	0.69
1:D:46:TYR:O	1:D:51:VAL:HG12	1.92	0.69
1:F:220:LEU:HD12	1:F:221:LYS:H	1.55	0.69
1:F:2:THR:HG22	1:F:27:ASN:ND2	2.07	0.69
1:E:193:VAL:HG21	1:E:331:ILE:HD12	1.73	0.69
1:C:82:ALA:O	1:C:86:ILE:HG13	1.92	0.69
1:A:165:ALA:HB1	1:A:166:PRO:HD2	1.72	0.69
1:B:199:ASN:HA	1:B:208:ASN:OD1	1.93	0.69
1:E:120:MET:HB3	1:E:318:LYS:HD2	1.74	0.69
1:E:322:ASP:O	1:E:326:VAL:HG12	1.93	0.69
1:F:220:LEU:HD12	1:F:221:LYS:N	2.08	0.69
1:B:192:THR:HG23	1:B:215:HIS:HB2	1.75	0.68
1:E:150:GLU:OE2	1:E:152:HIS:HE1	1.76	0.68
1:A:66:ILE:HB	1:A:90:LYS:NZ	2.07	0.68
1:D:309:TYR:O	1:D:313:VAL:HG12	1.94	0.68
1:F:189:ARG:HH11	1:F:327:THR:HG23	1.57	0.67
1:D:221:LYS:HD2	1:F:198:ARG:HH21	1.57	0.67
1:C:309:TYR:O	1:C:313:VAL:HG12	1.94	0.67
1:A:57:LEU:HG	1:A:61:LEU:HD23	1.77	0.67
1:B:5:MET:HE1	1:B:305:TYR:CE1	2.30	0.67
1:C:149:ILE:HG12	1:C:239:VAL:HG22	1.76	0.67
1:A:69:VAL:CG1	1:A:85:VAL:HG21	2.24	0.67
1:B:25:ARG:NH2	1:B:302:GLY:HA3	2.10	0.67
1:B:109:LEU:HD22	1:B:322:ASP:OD1	1.95	0.67
1:B:69:VAL:HG13	1:B:85:VAL:HG21	1.78	0.66
1:D:120:MET:HB3	1:D:318:LYS:HD2	1.76	0.66
1:F:228:HIS:O	1:F:229:ILE:HD13	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:SER:HB3	1:B:161:ILE:HD12	1.76	0.66
1:C:262:ILE:O	1:C:263:MET:HE2	1.95	0.66
1:A:225:LYS:HD2	2:A:369:HOH:O	1.94	0.66
1:F:253:GLN:NE2	1:F:256:ASN:HD22	1.93	0.66
1:C:99:CYS:SG	1:C:108:LEU:HD22	2.36	0.66
1:C:327:THR:O	1:C:331:ILE:HG12	1.96	0.66
1:E:19:LEU:HB2	1:E:20:PRO:HD3	1.77	0.65
1:E:313:VAL:HG13	1:E:314:ASN:OD1	1.97	0.65
1:B:113:ARG:HH11	1:B:113:ARG:HB3	1.62	0.65
1:E:27:ASN:N	1:E:27:ASN:HD22	1.95	0.65
1:E:12:LYS:HG2	1:E:13:SER:H	1.62	0.64
1:E:306:ASP:O	1:E:310:ASP:HB2	1.97	0.64
1:E:12:LYS:H	1:E:12:LYS:CD	2.09	0.64
1:F:19:LEU:HB2	1:F:20:PRO:HD3	1.79	0.64
1:C:229:ILE:N	1:C:229:ILE:HD12	2.12	0.64
1:D:123:GLN:HE22	1:D:177:ILE:HD11	1.63	0.64
1:D:149:ILE:HB	1:D:222:ILE:HG22	1.78	0.64
1:F:94:VAL:HG12	1:F:95:GLU:H	1.61	0.64
1:E:199:ASN:HA	1:E:208:ASN:OD1	1.98	0.64
1:D:198:ARG:HB2	1:F:218:ASN:HD21	1.63	0.64
1:A:292:LYS:HZ1	1:D:253:GLN:HE21	1.46	0.64
1:C:150:GLU:OE2	1:C:152:HIS:HE1	1.81	0.64
1:B:12:LYS:H	1:B:12:LYS:HD2	1.64	0.64
1:C:75:ALA:HB1	1:C:97:PRO:HD2	1.80	0.64
1:A:7:PHE:HB2	1:A:33:ILE:HD13	1.80	0.63
1:C:192:THR:HG23	1:C:215:HIS:HB2	1.79	0.63
1:F:21:TYR:O	1:F:24:THR:HG22	1.98	0.63
1:A:81:LEU:O	1:A:85:VAL:HG12	1.98	0.63
1:F:149:ILE:HG13	1:F:222:ILE:HD13	1.81	0.63
1:F:166:PRO:HG2	1:F:169:GLU:HG2	1.79	0.63
1:C:17:TYR:OH	1:C:255:GLU:HG3	1.99	0.63
1:E:253:GLN:HE21	1:F:292:LYS:NZ	1.97	0.63
1:A:147:ILE:HG13	1:A:148:GLU:N	2.13	0.63
1:C:19:LEU:HB2	1:C:20:PRO:HD3	1.79	0.63
1:A:150:GLU:OE2	1:A:152:HIS:HE1	1.83	0.62
1:C:35:VAL:O	1:C:55:THR:CG2	2.42	0.62
1:D:96:LYS:NZ	1:D:96:LYS:HB3	2.14	0.62
1:E:222:ILE:HD11	1:E:224:LEU:HD21	1.81	0.62
1:C:6:GLY:C	1:C:69:VAL:HG23	2.23	0.62
1:A:44:ALA:HB3	1:A:45:PRO:HD3	1.81	0.62
1:C:69:VAL:HG12	1:C:85:VAL:HG21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:PHE:CE1	1:D:212:VAL:HG21	2.34	0.62
1:A:96:LYS:HD2	1:A:177:ILE:HG21	1.82	0.62
1:B:12:LYS:HG2	1:B:13:SER:N	2.14	0.62
1:D:109:LEU:HD11	1:D:322:ASP:HB3	1.81	0.62
1:D:166:PRO:HB2	1:D:168:GLU:OE1	1.99	0.62
1:F:210:PHE:CE2	1:F:226:THR:HB	2.35	0.62
1:D:313:VAL:HG13	1:D:314:ASN:N	2.14	0.62
1:C:101:THR:HB	1:C:103:GLU:OE2	2.00	0.61
1:E:222:ILE:C	1:E:222:ILE:HD13	2.25	0.61
1:C:73:THR:HB	1:C:74:PRO:HD2	1.81	0.61
1:C:83:LYS:HA	1:C:86:ILE:HD12	1.82	0.61
1:D:192:THR:HG23	1:D:215:HIS:HB2	1.82	0.61
1:A:12:LYS:N	1:A:12:LYS:HD2	2.15	0.61
1:B:219:GLN:HG2	1:C:200:ASN:O	2.00	0.61
1:C:126:ARG:NH2	1:C:324:GLU:OE1	2.28	0.61
1:C:209:TYR:CD1	1:C:210:PHE:N	2.69	0.61
1:B:293:GLN:HB2	1:F:273:SER:HB3	1.81	0.60
1:C:165:ALA:HB1	1:C:166:PRO:HD2	1.83	0.60
1:B:259:LYS:HZ3	1:E:286:ASN:HD21	1.46	0.60
1:E:134:VAL:O	1:E:138:VAL:HG23	2.02	0.60
1:A:23:LYS:HD3	1:A:49:ARG:CZ	2.31	0.60
1:A:210:PHE:CE2	1:A:226:THR:HB	2.36	0.60
1:D:25:ARG:HH12	1:D:302:GLY:HA3	1.66	0.60
1:C:153:ILE:CD1	1:C:179:THR:HG23	2.31	0.60
1:A:12:LYS:HZ3	1:A:12:LYS:H	1.50	0.60
1:C:125:ARG:HG3	1:C:178:HIS:CG	2.37	0.60
1:A:66:ILE:HB	1:A:90:LYS:HZ2	1.66	0.60
1:A:125:ARG:HB2	2:A:361:HOH:O	2.02	0.60
1:C:73:THR:HB	1:C:74:PRO:CD	2.31	0.60
1:D:214:LEU:HD12	1:D:222:ILE:HD11	1.82	0.60
1:B:46:TYR:O	1:B:51:VAL:CG1	2.50	0.59
1:F:199:ASN:OD1	1:F:201:GLU:HB2	2.01	0.59
1:F:146:ILE:HD12	1:F:146:ILE:H	1.66	0.59
1:B:63:ASP:HB3	1:B:66:ILE:HD13	1.85	0.59
1:E:235:PRO:HG3	1:E:249:TYR:CZ	2.37	0.59
1:F:146:ILE:HD12	1:F:146:ILE:N	2.17	0.59
1:A:262:ILE:HG22	1:A:266:SER:OG	2.03	0.59
1:C:209:TYR:CD1	1:C:209:TYR:C	2.80	0.59
1:A:344:TYR:HE2	1:A:346:LEU:HD13	1.68	0.59
1:B:26:ASN:ND2	1:B:26:ASN:N	2.38	0.59
1:E:22:LEU:HD21	1:E:305:TYR:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:MET:HE1	1:A:305:TYR:CD1	2.38	0.59
1:C:199:ASN:HA	1:C:208:ASN:OD1	2.03	0.59
1:A:75:ALA:HB1	1:A:97:PRO:HD2	1.84	0.58
1:A:214:LEU:HB2	1:A:222:ILE:CG2	2.31	0.58
1:B:131:PHE:CD1	1:B:182:ARG:HD2	2.38	0.58
1:A:96:LYS:HE3	1:A:174:SER:HA	1.85	0.58
1:C:83:LYS:O	1:C:87:LEU:HD13	2.04	0.58
1:F:248:LYS:HE3	1:F:276:TYR:O	2.04	0.58
1:E:268:GLY:HA2	1:E:271:GLU:HG3	1.86	0.58
1:F:16:ARG:NH1	1:F:259:LYS:HG2	2.19	0.58
1:A:240:HIS:CE1	1:E:230:VAL:HG13	2.38	0.58
1:B:281:LYS:HA	1:B:290:ILE:O	2.04	0.58
1:B:161:ILE:HD12	1:B:161:ILE:N	2.19	0.58
1:C:183:MET:HE2	1:C:183:MET:HA	1.87	0.57
1:D:157:ARG:O	1:D:160:SER:HB2	2.02	0.57
1:B:25:ARG:HH21	1:B:302:GLY:HA3	1.69	0.57
1:B:211:ASP:OD2	1:B:225:LYS:HD3	2.04	0.57
1:D:73:THR:OG1	1:D:74:PRO:HD2	2.05	0.57
1:A:199:ASN:HA	1:A:208:ASN:OD1	2.04	0.57
1:A:69:VAL:HG12	1:A:85:VAL:HG21	1.85	0.57
1:D:131:PHE:CE1	1:D:182:ARG:HB2	2.40	0.57
1:D:235:PRO:HG3	1:D:249:TYR:CZ	2.38	0.57
1:E:173:TYR:CD2	1:E:332:LEU:HD23	2.39	0.57
1:F:32:THR:HA	1:F:52:TYR:O	2.04	0.57
1:A:211:ASP:OD2	1:A:225:LYS:HD3	2.04	0.57
1:D:18:HIS:ND1	1:D:305:TYR:OH	2.31	0.57
1:A:7:PHE:HB2	1:A:33:ILE:CD1	2.34	0.57
1:B:150:GLU:OE2	1:B:152:HIS:HE1	1.87	0.57
1:B:191:ASN:HD21	1:B:217:GLY:N	1.91	0.56
1:D:146:ILE:HG22	1:D:220:LEU:HD13	1.86	0.56
1:E:22:LEU:C	1:E:24:THR:H	2.13	0.56
1:F:222:ILE:HD12	1:F:223:LYS:N	2.20	0.56
1:B:113:ARG:HB3	1:B:113:ARG:NH1	2.21	0.56
1:D:145:ASP:O	1:D:147:ILE:HD12	2.04	0.56
1:C:86:ILE:HG12	1:C:92:VAL:HG21	1.88	0.56
1:E:222:ILE:HD13	1:E:222:ILE:O	2.05	0.56
1:F:328:ASN:O	1:F:332:LEU:HD23	2.04	0.56
1:C:253:GLN:HE22	1:C:256:ASN:HD22	1.54	0.56
1:C:135:LYS:HG3	1:C:186:LEU:HD11	1.88	0.56
1:C:313:VAL:HG13	1:C:314:ASN:ND2	2.21	0.56
1:E:236:ARG:N	1:E:248:LYS:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:303:ARG:HA	1:F:306:ASP:OD2	2.06	0.56
1:B:135:LYS:HG3	1:B:186:LEU:HD11	1.87	0.56
1:A:46:TYR:C	1:A:51:VAL:HG12	2.30	0.56
1:E:191:ASN:HD22	1:E:217:GLY:H	1.52	0.56
1:A:60:LEU:C	1:A:60:LEU:HD23	2.31	0.55
1:B:153:ILE:CD1	1:B:179:THR:HG21	2.36	0.55
1:F:161:ILE:N	1:F:161:ILE:HD12	2.21	0.55
1:A:5:MET:HE3	1:A:28:ILE:CG2	2.32	0.55
1:C:283:ARG:HH11	1:C:283:ARG:HG3	1.71	0.55
1:D:99:CYS:SG	1:D:108:LEU:HD12	2.46	0.55
1:C:44:ALA:HB3	1:C:45:PRO:HD3	1.87	0.55
1:D:183:MET:HB3	1:D:222:ILE:HD12	1.88	0.55
1:E:321:LYS:HB2	1:E:324:GLU:HG3	1.88	0.55
1:B:82:ALA:HB3	1:B:108:LEU:HD21	1.88	0.55
1:E:30:VAL:O	1:E:31:LYS:CB	2.55	0.55
1:F:147:ILE:HG22	1:F:219:GLN:HG2	1.89	0.55
1:A:69:VAL:HG11	1:A:85:VAL:HG21	1.89	0.55
1:D:183:MET:HE2	1:D:183:MET:HA	1.89	0.55
1:B:47:GLU:C	1:B:49:ARG:H	2.14	0.54
1:C:193:VAL:HG21	1:C:331:ILE:HD12	1.89	0.54
1:B:73:THR:HB	1:B:74:PRO:CD	2.37	0.54
1:B:125:ARG:NH1	1:B:128:ASP:OD2	2.40	0.54
1:B:143:LEU:C	1:B:243:ASN:HB2	2.33	0.54
1:C:277:TYR:OH	1:C:295:LYS:HE3	2.08	0.54
1:B:280:ALA:O	1:B:291:GLU:HA	2.07	0.54
1:D:184:ILE:HD12	1:D:328:ASN:OD1	2.07	0.54
1:C:134:VAL:O	1:C:138:VAL:HG23	2.08	0.54
1:A:293:GLN:HB2	1:D:273:SER:HB2	1.90	0.54
1:B:22:LEU:HD22	1:B:28:ILE:HG21	1.90	0.54
1:E:275:MET:HB2	1:F:293:GLN:CD	2.33	0.54
1:E:298:LEU:HD23	1:E:299:GLY:H	1.73	0.54
1:F:184:ILE:HG23	1:F:188:GLY:O	2.08	0.54
1:F:345:LYS:C	1:F:346:LEU:HD22	2.33	0.54
1:F:157:ARG:HB3	1:F:160:SER:HB2	1.90	0.53
1:C:321:LYS:O	1:C:324:GLU:HB2	2.07	0.53
1:C:172:PHE:CE1	1:C:212:VAL:HG21	2.43	0.53
1:B:274:PRO:HD2	1:E:293:GLN:OE1	2.08	0.53
1:E:125:ARG:HD2	1:E:178:HIS:CG	2.43	0.53
1:F:294:ILE:HD12	1:F:294:ILE:N	2.22	0.53
1:A:111:LEU:O	1:A:115:LYS:HB2	2.09	0.53
1:A:109:LEU:HD22	1:A:322:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:ALA:HB1	1:D:166:PRO:HD2	1.89	0.53
1:C:149:ILE:CG2	1:C:222:ILE:HB	2.37	0.53
1:D:60:LEU:O	1:D:63:ASP:HB2	2.09	0.53
1:F:201:GLU:HG2	1:F:208:ASN:HD21	1.74	0.53
1:B:161:ILE:HD12	1:B:161:ILE:H	1.74	0.53
1:C:144:GLY:O	1:C:146:ILE:HD12	2.09	0.53
1:D:4:THR:HG23	1:D:31:LYS:CG	2.39	0.53
1:F:131:PHE:HA	1:F:134:VAL:HG22	1.91	0.52
1:F:202:VAL:HG23	1:F:205:ALA:CB	2.39	0.52
1:F:343:VAL:HG12	1:F:344:TYR:N	2.24	0.52
1:C:46:TYR:HB3	1:C:51:VAL:CG1	2.39	0.52
1:A:57:LEU:HG	1:A:61:LEU:CD2	2.39	0.52
1:D:150:GLU:OE2	1:D:152:HIS:HE1	1.91	0.52
1:D:321:LYS:HB2	1:D:324:GLU:HG3	1.91	0.52
1:F:175:LEU:O	1:F:178:HIS:HB2	2.09	0.52
1:F:209:TYR:O	1:F:210:PHE:HB3	2.08	0.52
1:B:138:VAL:HG22	1:B:146:ILE:CD1	2.39	0.52
1:C:326:VAL:HG13	1:C:327:THR:N	2.24	0.52
1:C:35:VAL:CG1	1:C:38:ILE:HG12	2.39	0.52
1:E:125:ARG:C	1:E:127:PHE:H	2.17	0.52
1:F:92:VAL:HG12	1:F:93:ILE:N	2.24	0.52
1:A:135:LYS:HG3	1:A:186:LEU:CD1	2.40	0.52
1:A:283:ARG:HA	1:A:288:ASP:O	2.09	0.52
1:A:121:PRO:HG2	1:A:320:VAL:HG11	1.91	0.52
1:E:131:PHE:CE1	1:E:182:ARG:HB2	2.44	0.52
1:A:29:LYS:HB3	1:A:31:LYS:NZ	2.24	0.52
1:D:21:TYR:CZ	1:D:301:TYR:HB2	2.44	0.52
1:B:73:THR:HB	1:B:74:PRO:HD2	1.92	0.52
1:D:199:ASN:C	1:D:201:GLU:H	2.18	0.52
1:E:102:VAL:HG13	1:E:103:GLU:N	2.23	0.52
1:C:75:ALA:HB1	1:C:97:PRO:CD	2.40	0.52
1:C:214:LEU:HG	1:C:222:ILE:HD11	1.92	0.51
1:D:147:ILE:HD12	1:D:147:ILE:N	2.26	0.51
1:D:199:ASN:O	1:D:201:GLU:N	2.43	0.51
1:D:281:LYS:HA	1:D:290:ILE:O	2.10	0.51
1:C:268:GLY:HA2	1:C:271:GLU:OE1	2.11	0.51
1:D:25:ARG:HH12	1:D:302:GLY:CA	2.22	0.51
1:D:128:ASP:HB3	1:D:130:ASP:OD2	2.10	0.51
1:B:259:LYS:NZ	1:E:286:ASN:ND2	2.59	0.51
1:B:286:ASN:ND2	1:F:259:LYS:NZ	2.59	0.51
1:A:113:ARG:NH1	1:A:113:ARG:HB3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:VAL:HG13	1:B:103:GLU:OE2	2.10	0.51
1:C:106:LYS:HB2	1:C:106:LYS:NZ	2.26	0.51
1:D:110:ALA:CA	1:D:113:ARG:HD2	2.35	0.51
1:B:102:VAL:O	1:B:106:LYS:HG3	2.10	0.51
1:D:61:LEU:HD22	1:D:61:LEU:H	1.74	0.51
1:D:82:ALA:O	1:D:86:ILE:HG12	2.11	0.51
1:E:160:SER:HB3	1:E:161:ILE:HD12	1.92	0.51
1:D:196:ASP:HA	1:D:340:SER:OG	2.11	0.51
1:F:11:GLY:C	1:F:15:ASN:H	2.18	0.51
1:C:46:TYR:O	1:C:51:VAL:HG12	2.11	0.51
1:A:43:ALA:O	1:A:47:GLU:HG3	2.11	0.50
1:D:161:ILE:N	1:D:161:ILE:HD12	2.26	0.50
1:C:8:ILE:HG13	1:C:69:VAL:HG21	1.94	0.50
1:F:192:THR:HA	1:F:346:LEU:HD23	1.93	0.50
1:B:149:ILE:CG1	1:B:239:VAL:HG13	2.41	0.50
1:B:259:LYS:NZ	1:E:286:ASN:HD21	2.09	0.50
1:A:196:ASP:O	1:A:210:PHE:HA	2.11	0.50
1:B:27:ASN:HB3	1:B:309:TYR:CE1	2.47	0.50
1:F:167:LYS:HB2	1:F:173:TYR:CZ	2.46	0.50
1:B:263:MET:HB2	1:B:265:GLU:OE2	2.12	0.50
1:F:134:VAL:HG11	1:F:237:PHE:CB	2.41	0.50
1:F:323:GLU:HA	1:F:326:VAL:HG12	1.93	0.50
1:B:7:PHE:HB2	1:B:33:ILE:HG12	1.94	0.50
1:D:253:GLN:HE22	1:D:256:ASN:HD22	1.60	0.50
1:E:309:TYR:CZ	1:E:313:VAL:HG11	2.45	0.50
1:A:12:LYS:HD2	1:A:12:LYS:H	1.77	0.50
1:A:12:LYS:H	1:A:12:LYS:NZ	2.10	0.50
1:B:131:PHE:CE1	1:B:182:ARG:HB2	2.47	0.50
1:B:322:ASP:O	1:B:326:VAL:HG12	2.11	0.50
1:A:75:ALA:CB	1:A:97:PRO:HD2	2.41	0.50
1:B:138:VAL:HG22	1:B:146:ILE:HD11	1.93	0.50
1:E:298:LEU:HD23	1:E:299:GLY:N	2.27	0.50
1:C:184:ILE:HG23	1:C:188:GLY:O	2.12	0.49
1:D:198:ARG:HH21	1:F:221:LYS:HD2	1.77	0.49
1:E:71:ILE:HD12	1:E:71:ILE:N	2.27	0.49
1:D:210:PHE:O	1:D:210:PHE:CD1	2.65	0.49
1:F:202:VAL:HG23	1:F:205:ALA:HB2	1.93	0.49
1:B:49:ARG:O	1:B:51:VAL:N	2.45	0.49
1:B:196:ASP:HB3	1:B:211:ASP:HB3	1.94	0.49
1:F:150:GLU:OE2	1:F:152:HIS:HE1	1.95	0.49
1:C:94:VAL:HB	1:C:98:PHE:HD1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ILE:CG1	1:C:239:VAL:HG22	2.39	0.49
1:B:19:LEU:HB2	1:B:20:PRO:HD3	1.94	0.49
1:D:69:VAL:CG1	1:D:85:VAL:HG21	2.42	0.49
1:A:147:ILE:HD12	1:E:227:ASN:HD21	1.78	0.49
1:A:203:GLU:OE2	1:E:218:ASN:HB2	2.13	0.49
1:B:172:PHE:CE1	1:B:212:VAL:HG21	2.47	0.49
1:D:6:GLY:C	1:D:69:VAL:HG23	2.38	0.49
1:D:221:LYS:HD2	1:F:198:ARG:NH2	2.25	0.49
1:E:102:VAL:HG13	1:E:103:GLU:H	1.78	0.49
1:F:153:ILE:HD12	1:F:179:THR:HG23	1.95	0.49
1:A:125:ARG:HG3	1:A:178:HIS:CG	2.47	0.49
1:D:110:ALA:C	1:D:112:GLY:H	2.21	0.49
1:D:136:GLN:O	1:D:140:GLN:HG3	2.12	0.49
1:E:104:HIS:O	1:E:108:LEU:HB2	2.12	0.49
1:E:273:SER:HB3	1:F:293:GLN:HB2	1.94	0.49
1:D:89:GLY:C	1:D:117:VAL:HG11	2.37	0.49
1:D:149:ILE:HD12	1:D:187:PHE:CE2	2.48	0.49
1:F:146:ILE:H	1:F:146:ILE:CD1	2.26	0.49
1:A:209:TYR:CD1	1:A:209:TYR:C	2.91	0.48
1:B:124:ASN:C	1:B:126:ARG:H	2.20	0.48
1:C:149:ILE:HG22	1:C:222:ILE:CB	2.39	0.48
1:D:58:ASP:HB3	1:D:62:ASN:ND2	2.28	0.48
1:D:211:ASP:OD2	1:D:225:LYS:HD3	2.12	0.48
1:F:161:ILE:CD1	1:F:208:ASN:HD22	2.26	0.48
1:A:82:ALA:O	1:A:86:ILE:HG13	2.13	0.48
1:C:111:LEU:O	1:C:115:LYS:HB2	2.13	0.48
1:D:199:ASN:HA	1:D:208:ASN:OD1	2.12	0.48
1:E:149:ILE:HA	1:E:238:ILE:O	2.14	0.48
1:C:322:ASP:O	1:C:326:VAL:HG12	2.13	0.48
1:D:96:LYS:HD2	1:D:174:SER:HA	1.95	0.48
1:E:308:ALA:O	1:E:312:ILE:HD13	2.14	0.48
1:B:171:SER:OG	1:B:208:ASN:HA	2.13	0.48
1:C:253:GLN:HA	1:C:253:GLN:HE21	1.77	0.48
1:F:192:THR:HG23	1:F:215:HIS:HB2	1.95	0.48
1:C:146:ILE:HD12	1:C:146:ILE:N	2.28	0.48
1:A:25:ARG:HD2	1:A:306:ASP:OD1	2.13	0.48
1:B:223:LYS:NZ	1:C:223:LYS:NZ	2.62	0.48
1:D:135:LYS:O	1:D:139:GLU:HG3	2.13	0.48
1:E:211:ASP:OD2	1:E:225:LYS:HD3	2.14	0.48
1:E:259:LYS:NZ	1:F:286:ASN:ND2	2.61	0.48
1:F:153:ILE:CD1	1:F:179:THR:HG23	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:209:TYR:CD1	1:F:209:TYR:C	2.92	0.48
1:C:3:LEU:HB3	1:C:28:ILE:HD13	1.95	0.48
1:D:109:LEU:C	1:D:109:LEU:HD23	2.39	0.48
1:E:148:GLU:HA	1:E:221:LYS:O	2.13	0.48
1:D:73:THR:HG21	1:D:81:LEU:CD1	2.44	0.48
1:D:131:PHE:CD1	1:D:182:ARG:HD2	2.48	0.48
1:D:231:ALA:HB3	1:F:245:SER:OG	2.14	0.48
1:E:334:ASN:ND2	1:E:344:TYR:CE1	2.82	0.48
1:D:31:LYS:HB2	1:D:66:ILE:HD11	1.94	0.48
1:D:40:GLU:HA	1:D:43:ALA:HB3	1.95	0.48
1:B:283:ARG:HA	1:B:288:ASP:O	2.14	0.48
1:F:180:MET:HB2	1:F:224:LEU:HD13	1.96	0.48
1:B:102:VAL:HG12	1:B:333:GLU:OE2	2.13	0.47
1:C:283:ARG:HA	1:C:288:ASP:O	2.14	0.47
1:E:150:GLU:OE2	1:E:152:HIS:CE1	2.61	0.47
1:E:172:PHE:CZ	1:E:212:VAL:HG21	2.49	0.47
1:D:39:ASN:HD21	1:D:41:GLU:HB3	1.79	0.47
1:D:39:ASN:ND2	1:D:42:LEU:H	2.12	0.47
1:F:321:LYS:HB2	1:F:324:GLU:CG	2.33	0.47
1:A:122:TYR:CZ	1:A:124:ASN:HB3	2.50	0.47
1:B:136:GLN:O	1:B:140:GLN:HG3	2.13	0.47
1:D:46:TYR:O	1:D:51:VAL:CG1	2.60	0.47
1:E:283:ARG:HA	1:E:288:ASP:O	2.14	0.47
1:E:327:THR:O	1:E:331:ILE:HG12	2.14	0.47
1:A:240:HIS:ND1	1:A:245:SER:HB3	2.28	0.47
1:C:193:VAL:HG21	1:C:331:ILE:HG23	1.95	0.47
1:E:275:MET:HE3	1:E:276:TYR:CZ	2.49	0.47
1:F:214:LEU:HB2	1:F:222:ILE:HG23	1.96	0.47
1:B:235:PRO:HG3	1:B:249:TYR:CZ	2.49	0.47
1:C:71:ILE:HD12	1:C:71:ILE:N	2.29	0.47
1:C:131:PHE:CE1	1:C:182:ARG:HB2	2.49	0.47
1:D:179:THR:HG22	1:D:182:ARG:HH21	1.80	0.47
1:E:273:SER:HB2	1:F:293:GLN:OE1	2.15	0.47
1:A:147:ILE:O	1:A:220:LEU:HA	2.15	0.47
1:D:195:TYR:CE2	1:D:335:GLY:HA2	2.49	0.47
1:F:42:LEU:C	1:F:44:ALA:H	2.23	0.47
1:F:94:VAL:HG12	1:F:95:GLU:N	2.29	0.47
1:A:109:LEU:O	1:A:113:ARG:HG3	2.14	0.47
1:B:25:ARG:NH1	1:B:306:ASP:OD2	2.47	0.47
1:C:153:ILE:HD11	1:C:179:THR:CG2	2.36	0.47
1:D:283:ARG:HA	1:D:288:ASP:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:ASP:HA	1:E:252:ASP:OD2	2.14	0.47
1:A:82:ALA:HB3	1:A:108:LEU:HD21	1.96	0.47
1:A:344:TYR:CE2	1:A:346:LEU:HD13	2.47	0.47
1:C:184:ILE:C	1:C:186:LEU:H	2.23	0.47
1:C:189:ARG:HH22	1:C:330:GLU:CD	2.23	0.47
1:D:209:TYR:CD1	1:D:209:TYR:C	2.93	0.47
1:A:147:ILE:CD1	1:E:227:ASN:HD21	2.28	0.47
1:B:46:TYR:C	1:B:51:VAL:CG1	2.88	0.47
1:B:236:ARG:CZ	1:B:251:GLU:HB2	2.45	0.47
1:F:148:GLU:C	1:F:149:ILE:HG22	2.40	0.47
1:B:149:ILE:O	1:B:222:ILE:HA	2.15	0.47
1:D:111:LEU:HD23	1:D:111:LEU:O	2.15	0.47
1:F:124:ASN:C	1:F:126:ARG:H	2.23	0.47
1:C:69:VAL:CG1	1:C:85:VAL:HG21	2.45	0.46
1:C:253:GLN:HA	1:C:253:GLN:NE2	2.30	0.46
1:D:86:ILE:O	1:D:115:LYS:HE2	2.15	0.46
1:F:134:VAL:HG11	1:F:237:PHE:CG	2.51	0.46
1:A:23:LYS:HE2	1:A:23:LYS:HA	1.97	0.46
1:A:228:HIS:C	1:A:229:ILE:HD12	2.40	0.46
1:B:209:TYR:C	1:B:209:TYR:CD1	2.93	0.46
1:D:110:ALA:C	1:D:112:GLY:N	2.71	0.46
1:D:167:LYS:HG3	1:D:168:GLU:OE2	2.15	0.46
1:E:166:PRO:HG2	1:E:169:GLU:HG2	1.97	0.46
1:D:25:ARG:HH12	1:D:302:GLY:C	2.23	0.46
1:D:96:LYS:HD2	1:D:174:SER:O	2.15	0.46
1:D:214:LEU:O	1:D:216:TYR:HD2	1.97	0.46
1:F:131:PHE:CZ	1:F:182:ARG:HB2	2.50	0.46
1:A:5:MET:HE1	1:A:305:TYR:CE1	2.50	0.46
1:B:78:HIS:CE1	1:B:95:GLU:O	2.68	0.46
1:B:133:ALA:HB2	1:B:297:PRO:HD2	1.97	0.46
1:D:325:ALA:O	1:D:329:ILE:HG12	2.15	0.46
1:F:140:GLN:HE21	1:F:140:GLN:HB3	1.58	0.46
1:F:209:TYR:CD1	1:F:210:PHE:N	2.83	0.46
1:F:343:VAL:HG12	1:F:344:TYR:H	1.80	0.46
1:A:167:LYS:HE3	1:A:168:GLU:OE2	2.16	0.46
1:E:328:ASN:O	1:E:332:LEU:HD13	2.16	0.46
1:B:43:ALA:O	1:B:47:GLU:HG3	2.15	0.46
1:D:13:SER:HB3	1:D:95:GLU:OE2	2.16	0.46
1:D:58:ASP:HB3	1:D:62:ASN:HD22	1.80	0.46
1:D:110:ALA:O	1:D:113:ARG:HG2	2.15	0.46
1:F:131:PHE:CD1	1:F:182:ARG:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ILE:HD12	1:A:229:ILE:N	2.30	0.46
1:D:210:PHE:CD1	1:D:210:PHE:C	2.94	0.46
1:E:177:ILE:HD11	1:E:328:ASN:HD22	1.80	0.46
1:A:51:VAL:O	1:A:51:VAL:HG13	2.15	0.46
1:B:58:ASP:C	1:B:60:LEU:H	2.24	0.46
1:C:75:ALA:HA	1:C:78:HIS:CE1	2.50	0.46
1:E:329:ILE:HD12	1:E:329:ILE:N	2.31	0.46
1:E:350:HIS:O	1:E:351:LEU:HD23	2.16	0.46
1:F:181:ASP:CB	1:F:328:ASN:HD21	2.29	0.46
1:F:234:TYR:HB3	1:F:235:PRO:CD	2.46	0.46
1:C:83:LYS:HB3	1:C:108:LEU:HD11	1.97	0.46
1:D:60:LEU:HD21	1:D:69:VAL:HG21	1.98	0.46
1:D:146:ILE:N	1:D:146:ILE:HD12	2.31	0.46
1:B:283:ARG:HG3	1:B:283:ARG:HH11	1.81	0.45
1:C:103:GLU:CD	1:C:103:GLU:H	2.24	0.45
1:D:134:VAL:O	1:D:138:VAL:HG23	2.16	0.45
1:F:333:GLU:C	1:F:335:GLY:H	2.25	0.45
1:B:44:ALA:HB3	1:B:45:PRO:CD	2.42	0.45
1:B:122:TYR:CZ	1:B:124:ASN:HB3	2.51	0.45
1:B:131:PHE:CG	1:B:182:ARG:HD2	2.51	0.45
1:E:273:SER:CB	1:F:293:GLN:HB2	2.46	0.45
1:B:125:ARG:HD2	1:B:178:HIS:CG	2.51	0.45
1:A:209:TYR:CD1	1:A:210:PHE:N	2.84	0.45
1:D:345:LYS:C	1:D:346:LEU:HD12	2.42	0.45
1:A:47:GLU:C	1:A:49:ARG:N	2.72	0.45
1:B:240:HIS:CE1	1:C:230:VAL:HG13	2.52	0.45
1:D:198:ARG:NH2	1:F:221:LYS:HD2	2.32	0.45
1:D:303:ARG:HA	1:D:306:ASP:OD2	2.16	0.45
1:E:27:ASN:N	1:E:27:ASN:ND2	2.60	0.45
1:A:149:ILE:HA	1:A:238:ILE:O	2.17	0.45
1:A:316:ALA:HB1	1:A:317:PRO:HD2	1.98	0.45
1:E:275:MET:HB2	1:F:293:GLN:OE1	2.17	0.45
1:D:150:GLU:HB3	1:D:238:ILE:HB	1.99	0.45
1:E:325:ALA:O	1:E:329:ILE:HD13	2.17	0.45
1:A:83:LYS:O	1:A:87:LEU:HD22	2.17	0.45
1:E:302:GLY:C	1:E:304:PHE:N	2.75	0.45
1:A:143:LEU:C	1:A:243:ASN:HB2	2.42	0.45
1:F:199:ASN:OD1	1:F:202:VAL:N	2.49	0.45
1:A:192:THR:HG23	1:A:215:HIS:HB2	1.98	0.45
1:B:16:ARG:HH12	1:B:259:LYS:HE2	1.82	0.45
1:C:306:ASP:O	1:C:309:TYR:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:SER:N	1:D:117:VAL:HB	2.31	0.45
1:E:125:ARG:C	1:E:127:PHE:N	2.75	0.45
1:E:141:GLY:HA2	2:E:362:HOH:O	2.16	0.45
1:E:163:HIS:O	1:E:205:ALA:HB1	2.17	0.45
1:A:47:GLU:O	1:A:49:ARG:O	2.35	0.44
1:A:185:SER:HA	1:A:324:GLU:OE2	2.16	0.44
1:B:190:PRO:HB3	1:B:216:TYR:CE2	2.52	0.44
1:B:293:GLN:CD	1:F:275:MET:HB2	2.42	0.44
1:C:195:TYR:HB3	1:C:197:ILE:CD1	2.47	0.44
1:A:275:MET:HE3	1:A:276:TYR:CZ	2.51	0.44
1:B:148:GLU:HA	1:B:221:LYS:O	2.17	0.44
1:C:149:ILE:HD13	1:C:150:GLU:H	1.82	0.44
1:D:76:HIS:ND1	1:D:77:THR:HG23	2.32	0.44
1:E:268:GLY:O	1:E:271:GLU:HB2	2.16	0.44
1:F:11:GLY:HA2	1:F:15:ASN:HD22	1.81	0.44
1:F:227:ASN:OD1	1:F:229:ILE:N	2.38	0.44
1:A:274:PRO:HA	1:A:277:TYR:CE1	2.52	0.44
1:E:209:TYR:CD1	1:E:209:TYR:C	2.94	0.44
1:F:135:LYS:HG2	1:F:139:GLU:OE1	2.17	0.44
1:A:71:ILE:HD13	1:A:81:LEU:HB2	1.99	0.44
1:C:262:ILE:C	1:C:263:MET:HE2	2.43	0.44
1:D:96:LYS:HG3	1:D:177:ILE:HG21	1.98	0.44
1:E:120:MET:HE2	1:E:318:LYS:HG3	1.98	0.44
1:E:165:ALA:HB1	1:E:166:PRO:CD	2.41	0.44
1:C:264:PRO:HA	1:C:269:PHE:CD2	2.52	0.44
1:D:247:ILE:HD13	1:F:232:LYS:HG2	2.00	0.44
1:E:326:VAL:HG13	1:E:349:LEU:HD11	2.00	0.44
1:E:336:PHE:C	1:E:338:ALA:H	2.25	0.44
1:F:14:ALA:O	1:F:18:HIS:HB2	2.18	0.44
1:F:131:PHE:CG	1:F:182:ARG:HD2	2.53	0.44
1:B:49:ARG:C	1:B:51:VAL:H	2.26	0.44
1:D:283:ARG:NH2	1:F:156:PHE:HE2	2.15	0.44
1:E:166:PRO:HG2	1:E:169:GLU:CG	2.48	0.44
1:F:80:GLU:C	1:F:82:ALA:N	2.75	0.44
1:F:300:ASP:HB3	1:F:303:ARG:HG3	2.00	0.44
1:D:80:GLU:O	1:D:83:LYS:HB2	2.17	0.44
1:D:83:LYS:O	1:D:87:LEU:HD13	2.18	0.44
1:D:192:THR:HB	1:D:345:LYS:NZ	2.32	0.44
1:F:264:PRO:HA	1:F:269:PHE:CG	2.53	0.44
1:D:177:ILE:HD13	1:D:177:ILE:C	2.42	0.44
1:F:92:VAL:HG12	1:F:93:ILE:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:GLU:C	1:D:335:GLY:H	2.26	0.43
1:E:95:GLU:HG2	1:E:96:LYS:H	1.82	0.43
1:E:157:ARG:HH21	1:F:288:ASP:CG	2.25	0.43
1:E:302:GLY:O	1:E:304:PHE:N	2.51	0.43
1:F:257:ASP:O	1:F:260:ALA:HB3	2.18	0.43
1:A:121:PRO:HB2	1:A:123:GLN:HE21	1.83	0.43
1:D:327:THR:O	1:D:331:ILE:HG13	2.18	0.43
1:D:333:GLU:C	1:D:335:GLY:N	2.76	0.43
1:E:147:ILE:HD13	1:E:240:HIS:O	2.17	0.43
1:B:153:ILE:HD12	1:B:153:ILE:N	2.33	0.43
1:B:314:ASN:O	1:B:316:ALA:N	2.51	0.43
1:B:338:ALA:O	1:B:339:PRO:C	2.60	0.43
1:D:209:TYR:CD1	1:D:210:PHE:N	2.86	0.43
1:D:223:LYS:NZ	1:F:225:LYS:HZ3	2.16	0.43
1:E:120:MET:O	1:E:120:MET:HG3	2.18	0.43
1:B:183:MET:HG3	1:B:222:ILE:CD1	2.42	0.43
1:B:229:ILE:O	1:B:229:ILE:HG22	2.18	0.43
1:A:180:MET:HG2	1:A:184:ILE:HD12	2.00	0.43
1:C:7:PHE:HB2	1:C:33:ILE:HG12	2.00	0.43
1:D:192:THR:HB	1:D:345:LYS:HZ1	1.83	0.43
1:E:71:ILE:HB	1:E:93:ILE:O	2.18	0.43
1:A:86:ILE:O	1:A:88:ALA:O	2.37	0.43
1:B:242:THR:HA	1:C:229:ILE:HG21	2.00	0.43
1:C:101:THR:HA	1:C:333:GLU:OE1	2.18	0.43
1:D:75:ALA:HA	1:D:78:HIS:ND1	2.34	0.43
1:A:29:LYS:HE2	1:A:31:LYS:HZ1	1.84	0.43
1:A:310:ASP:O	1:A:314:ASN:HB2	2.19	0.43
1:B:164:GLU:HA	1:B:205:ALA:HA	2.00	0.43
1:D:73:THR:HG21	1:D:81:LEU:HD12	2.01	0.43
1:E:121:PRO:HG2	1:E:320:VAL:HG11	2.00	0.43
1:E:196:ASP:HB3	1:E:211:ASP:HB3	1.99	0.43
1:E:334:ASN:C	1:E:336:PHE:H	2.26	0.43
1:A:202:VAL:O	1:A:203:GLU:C	2.61	0.43
1:A:274:PRO:HA	1:A:277:TYR:CD1	2.54	0.43
1:C:88:ALA:O	1:C:90:LYS:N	2.50	0.43
1:C:235:PRO:HG2	1:C:238:ILE:HG13	2.01	0.43
1:C:336:PHE:C	1:C:338:ALA:N	2.76	0.43
1:D:153:ILE:HD13	1:D:236:ARG:CZ	2.48	0.43
1:D:221:LYS:O	1:D:221:LYS:HG2	2.19	0.43
1:E:189:ARG:HH22	1:E:330:GLU:CD	2.25	0.43
1:F:16:ARG:HH11	1:F:259:LYS:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:VAL:HB	1:C:91:SER:HB2	2.01	0.43
1:D:39:ASN:ND2	1:D:42:LEU:HG	2.34	0.43
1:F:16:ARG:HG2	1:F:17:TYR:CE1	2.54	0.43
1:F:181:ASP:HB2	1:F:328:ASN:HD21	1.84	0.43
1:A:22:LEU:C	1:A:24:THR:H	2.27	0.42
1:A:309:TYR:O	1:A:313:VAL:HG12	2.19	0.42
1:D:75:ALA:C	1:D:77:THR:H	2.27	0.42
1:A:193:VAL:HG23	1:A:346:LEU:HD21	2.00	0.42
1:C:246:PHE:C	1:C:247:ILE:HD12	2.43	0.42
1:C:323:GLU:H	1:C:323:GLU:HG2	1.64	0.42
1:D:302:GLY:C	1:D:304:PHE:N	2.77	0.42
1:E:118:VAL:HG21	1:E:312:ILE:CD1	2.49	0.42
1:E:172:PHE:CE1	1:E:212:VAL:HG21	2.54	0.42
1:E:253:GLN:HE22	1:E:256:ASN:ND2	2.06	0.42
1:A:22:LEU:HD23	1:A:22:LEU:HA	1.88	0.42
1:A:197:ILE:O	1:A:198:ARG:HB3	2.19	0.42
1:B:260:ALA:O	1:B:262:ILE:HG13	2.19	0.42
1:D:46:TYR:C	1:D:51:VAL:CG1	2.92	0.42
1:D:85:VAL:HG22	1:D:92:VAL:HG22	2.00	0.42
1:D:99:CYS:SG	1:D:105:ALA:HA	2.60	0.42
1:D:254:GLN:O	1:D:258:LEU:HD22	2.19	0.42
1:F:264:PRO:HA	1:F:269:PHE:CD2	2.54	0.42
1:B:313:VAL:O	1:B:313:VAL:HG22	2.19	0.42
1:C:190:PRO:O	1:C:346:LEU:HB2	2.19	0.42
1:C:273:SER:HB3	1:D:293:GLN:HB2	2.02	0.42
1:D:18:HIS:CE1	1:D:122:TYR:CE2	3.08	0.42
1:D:172:PHE:CE2	1:D:332:LEU:HD12	2.54	0.42
1:D:309:TYR:CE2	1:D:313:VAL:HG11	2.54	0.42
1:F:134:VAL:HG11	1:F:237:PHE:HB3	2.01	0.42
1:A:183:MET:HE2	1:A:183:MET:HA	2.00	0.42
1:B:120:MET:HA	1:B:121:PRO:HD3	1.84	0.42
1:B:134:VAL:O	1:B:138:VAL:HG23	2.19	0.42
1:D:44:ALA:N	1:D:45:PRO:HD2	2.34	0.42
1:D:214:LEU:HD12	1:D:222:ILE:CD1	2.49	0.42
1:F:49:ARG:O	1:F:51:VAL:N	2.43	0.42
1:A:14:ALA:HB2	1:A:72:CYS:SG	2.59	0.42
1:C:22:LEU:C	1:C:24:THR:H	2.27	0.42
1:C:152:HIS:HD2	1:C:154:ASP:OD2	2.02	0.42
1:D:161:ILE:HD12	1:D:161:ILE:H	1.85	0.42
1:E:253:GLN:HE21	1:F:292:LYS:HZ1	1.68	0.42
1:E:334:ASN:C	1:E:336:PHE:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:TYR:O	1:F:277:TYR:C	2.63	0.42
1:F:344:TYR:CE2	1:F:346:LEU:HD13	2.54	0.42
1:B:220:LEU:HD12	1:B:221:LYS:N	2.34	0.42
1:D:316:ALA:HB1	1:D:317:PRO:HD2	2.01	0.42
1:F:246:PHE:HA	1:F:279:ILE:O	2.19	0.42
1:D:131:PHE:CG	1:D:182:ARG:HD2	2.55	0.42
1:E:208:ASN:O	1:E:228:HIS:HD2	2.03	0.42
1:E:309:TYR:O	1:E:313:VAL:HG12	2.20	0.42
1:C:283:ARG:HG3	1:C:283:ARG:NH1	2.34	0.42
1:B:76:HIS:CE1	1:B:77:THR:HG23	2.54	0.42
1:B:109:LEU:HD13	1:B:322:ASP:HB3	2.02	0.42
1:D:47:GLU:C	1:D:49:ARG:N	2.78	0.42
1:D:83:LYS:O	1:D:86:ILE:HB	2.20	0.42
1:D:253:GLN:NE2	1:D:256:ASN:HD22	2.17	0.42
1:B:265:GLU:HG2	1:B:266:SER:N	2.34	0.41
1:E:25:ARG:HH11	1:E:25:ARG:HG2	1.85	0.41
1:E:118:VAL:HG21	1:E:312:ILE:HD11	2.01	0.41
1:F:125:ARG:HD2	1:F:178:HIS:CG	2.55	0.41
1:A:130:ASP:OD1	1:A:130:ASP:N	2.52	0.41
1:A:153:ILE:HG13	1:A:179:THR:HG21	2.02	0.41
1:A:157:ARG:HB3	1:A:160:SER:HB2	2.01	0.41
1:A:259:LYS:NZ	1:C:286:ASN:HD21	2.18	0.41
1:C:92:VAL:HG23	1:C:119:VAL:HG22	2.01	0.41
1:D:6:GLY:O	1:D:69:VAL:HA	2.21	0.41
1:D:333:GLU:O	1:D:335:GLY:N	2.53	0.41
1:F:149:ILE:HD12	1:F:149:ILE:C	2.45	0.41
1:F:192:THR:OG1	1:F:193:VAL:N	2.53	0.41
1:F:228:HIS:C	1:F:229:ILE:HD13	2.45	0.41
1:F:152:HIS:HD2	1:F:154:ASP:OD2	2.03	0.41
1:A:328:ASN:O	1:A:332:LEU:HB2	2.20	0.41
1:B:165:ALA:HB1	1:B:166:PRO:CD	2.46	0.41
1:B:248:LYS:HD3	1:B:248:LYS:C	2.46	0.41
1:D:32:THR:HG23	1:D:60:LEU:HD13	2.01	0.41
1:E:191:ASN:HD22	1:E:217:GLY:N	2.16	0.41
1:A:292:LYS:HZ2	1:D:253:GLN:HE21	1.66	0.41
1:B:57:LEU:O	1:B:61:LEU:HD23	2.21	0.41
1:C:68:VAL:HA	1:C:91:SER:O	2.20	0.41
1:C:195:TYR:O	1:C:341:PRO:HA	2.21	0.41
1:E:73:THR:O	1:E:74:PRO:C	2.64	0.41
1:F:167:LYS:H	1:F:167:LYS:HD3	1.84	0.41
1:A:196:ASP:HB3	1:A:211:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:GLU:O	1:D:96:LYS:C	2.64	0.41
1:D:180:MET:O	1:D:184:ILE:HG13	2.20	0.41
1:D:214:LEU:HB2	1:D:222:ILE:CG1	2.50	0.41
1:A:68:VAL:HG23	1:A:91:SER:HB2	2.03	0.41
1:A:284:ASN:OD1	1:A:284:ASN:C	2.64	0.41
1:B:153:ILE:O	1:B:226:THR:HG23	2.20	0.41
1:B:293:GLN:OE1	1:F:273:SER:HB3	2.21	0.41
1:D:19:LEU:HD13	1:D:46:TYR:CZ	2.54	0.41
1:D:302:GLY:O	1:D:304:PHE:N	2.54	0.41
1:F:168:GLU:HA	1:F:173:TYR:CD2	2.56	0.41
1:B:210:PHE:CE2	1:B:226:THR:HB	2.56	0.41
1:B:223:LYS:HZ1	1:C:223:LYS:NZ	2.19	0.41
1:C:69:VAL:HG22	1:C:70:THR:N	2.36	0.41
1:F:275:MET:HE3	1:F:276:TYR:CZ	2.56	0.41
1:B:23:LYS:HD3	1:B:49:ARG:NH2	2.36	0.41
1:B:147:ILE:HD11	1:C:229:ILE:HB	2.03	0.41
1:B:157:ARG:O	1:B:160:SER:HB2	2.21	0.41
1:C:229:ILE:HG22	1:C:229:ILE:O	2.20	0.41
1:C:253:GLN:HE21	1:C:253:GLN:CA	2.33	0.41
1:D:3:LEU:HD23	1:D:3:LEU:C	2.46	0.41
1:D:199:ASN:C	1:D:201:GLU:N	2.78	0.41
1:E:210:PHE:CD1	1:E:210:PHE:C	2.99	0.41
1:E:253:GLN:O	1:E:254:GLN:C	2.63	0.41
1:E:269:PHE:C	1:E:271:GLU:H	2.29	0.41
1:F:146:ILE:N	1:F:146:ILE:CD1	2.83	0.41
1:F:322:ASP:O	1:F:325:ALA:HB3	2.20	0.41
1:B:47:GLU:C	1:B:49:ARG:N	2.72	0.41
1:D:96:LYS:HB3	1:D:96:LYS:HZ2	1.84	0.41
1:E:91:SER:HB3	1:E:118:VAL:HG23	2.03	0.41
1:B:102:VAL:HG13	1:B:103:GLU:CD	2.45	0.40
1:B:286:ASN:HD21	1:F:259:LYS:NZ	2.19	0.40
1:E:12:LYS:HD3	1:E:12:LYS:N	2.30	0.40
1:F:147:ILE:C	1:F:147:ILE:HD12	2.46	0.40
1:A:149:ILE:HG23	1:A:222:ILE:CG1	2.51	0.40
1:B:35:VAL:O	1:B:55:THR:HG22	2.21	0.40
1:B:49:ARG:C	1:B:51:VAL:N	2.79	0.40
1:B:296:THR:HA	1:B:297:PRO:HD3	1.88	0.40
1:C:3:LEU:HD23	1:C:28:ILE:CD1	2.45	0.40
1:C:96:LYS:NZ	1:C:178:HIS:NE2	2.66	0.40
1:C:221:LYS:HE2	1:C:223:LYS:HG2	2.02	0.40
1:D:268:GLY:O	1:D:271:GLU:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:PRO:HG2	1:E:169:GLU:CD	2.46	0.40
1:B:59:GLU:O	1:B:59:GLU:HG2	2.21	0.40
1:B:189:ARG:NH2	1:B:330:GLU:OE2	2.54	0.40
1:C:5:MET:HA	1:C:68:VAL:O	2.21	0.40
1:D:102:VAL:HG12	1:D:333:GLU:OE1	2.22	0.40
1:D:214:LEU:O	1:D:216:TYR:CD2	2.75	0.40
1:F:214:LEU:O	1:F:216:TYR:HD2	2.05	0.40
1:A:180:MET:HB2	1:A:224:LEU:HD13	2.02	0.40
1:C:113:ARG:HH11	1:C:113:ARG:HB2	1.85	0.40
1:C:313:VAL:C	1:C:314:ASN:HD22	2.30	0.40
1:C:315:GLY:O	1:C:316:ALA:C	2.64	0.40
1:E:99:CYS:SG	1:E:104:HIS:HB3	2.61	0.40
1:E:101:THR:HA	1:E:333:GLU:OE1	2.20	0.40
1:F:11:GLY:CA	1:F:15:ASN:HD22	2.34	0.40
1:F:195:TYR:OH	1:F:331:ILE:HG23	2.22	0.40
1:A:277:TYR:CE2	1:A:295:LYS:HG2	2.57	0.40
1:B:150:GLU:HG2	1:B:152:HIS:CE1	2.57	0.40
1:C:47:GLU:C	1:C:49:ARG:H	2.29	0.40
1:C:177:ILE:HD13	1:C:177:ILE:O	2.22	0.40
1:C:253:GLN:NE2	1:C:256:ASN:HD22	2.16	0.40
1:C:310:ASP:O	1:C:316:ALA:HB3	2.22	0.40
1:D:147:ILE:HD11	1:D:242:THR:CG2	2.46	0.40
1:D:313:VAL:CG1	1:D:314:ASN:N	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	348/353 (99%)	325 (93%)	22 (6%)	1 (0%)	36	58
1	B	348/353 (99%)	316 (91%)	26 (8%)	6 (2%)	7	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	334/353 (95%)	290 (87%)	39 (12%)	5 (2%)	8	18
1	D	340/353 (96%)	292 (86%)	39 (12%)	9 (3%)	4	7
1	E	291/353 (82%)	252 (87%)	31 (11%)	8 (3%)	4	7
1	F	280/353 (79%)	227 (81%)	42 (15%)	11 (4%)	2	3
All	All	1941/2118 (92%)	1702 (88%)	199 (10%)	40 (2%)	5	11

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	203	GLU
1	C	160	SER
1	D	196	ASP
1	D	200	ASN
1	E	31	LYS
1	E	32	THR
1	F	337	ALA
1	A	203	GLU
1	B	125	ARG
1	C	10	PHE
1	C	153	ILE
1	C	174	SER
1	C	203	GLU
1	D	98	PHE
1	D	153	ILE
1	D	160	SER
1	E	12	LYS
1	E	203	GLU
1	F	34	PHE
1	F	153	ILE
1	B	50	GLY
1	B	160	SER
1	B	315	GLY
1	E	33	ILE
1	F	24	THR
1	F	38	ILE
1	D	303	ARG
1	D	334	ASN
1	E	303	ARG
1	F	125	ARG
1	D	219	GLN
1	E	23	LYS

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Mol	Chain	Res	Type
1	E	74	PRO
1	F	8	ILE
1	F	27	ASN
1	F	334	ASN
1	D	88	ALA
1	B	153	ILE
1	F	141	GLY
1	F	50	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	291/301 (97%)	264 (91%)	27 (9%)	8	18
1	B	294/301 (98%)	274 (93%)	20 (7%)	14	32
1	C	276/301 (92%)	250 (91%)	26 (9%)	8	18
1	D	290/301 (96%)	278 (96%)	12 (4%)	27	54
1	E	232/301 (77%)	211 (91%)	21 (9%)	9	19
1	F	208/301 (69%)	196 (94%)	12 (6%)	18	39
All	All	1591/1806 (88%)	1473 (93%)	118 (7%)	13	29

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	24	THR
1	A	32	THR
1	A	48	GLU
1	A	54	THR
1	A	73	THR
1	A	83	LYS
1	A	87	LEU
1	A	90	LYS
1	A	92	VAL

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Mol	Chain	Res	Type
1	A	102	VAL
1	A	106	LYS
1	A	108	LEU
1	A	115	LYS
1	A	134	VAL
1	A	163	HIS
1	A	192	THR
1	A	194	THR
1	A	218	ASN
1	A	222	ILE
1	A	225	LYS
1	A	245	SER
1	A	247	ILE
1	A	258	LEU
1	A	295	LYS
1	A	332	LEU
1	A	345	LYS
1	B	12	LYS
1	B	26	ASN
1	B	32	THR
1	B	36	ARG
1	B	55	THR
1	B	69	VAL
1	B	85	VAL
1	B	87	LEU
1	B	92	VAL
1	B	100	ASP
1	B	108	LEU
1	B	130	ASP
1	B	134	VAL
1	B	139	GLU
1	B	153	ILE
1	B	184	ILE
1	B	222	ILE
1	B	258	LEU
1	B	265	GLU
1	B	345	LYS
1	C	2	THR
1	C	12	LYS
1	C	32	THR
1	C	61	LEU
1	C	87	LEU

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Mol	Chain	Res	Type
1	C	92	VAL
1	C	96	LYS
1	C	103	GLU
1	C	106	LYS
1	C	108	LEU
1	C	111	LEU
1	C	115	LYS
1	C	130	ASP
1	C	134	VAL
1	C	139	GLU
1	C	149	ILE
1	C	177	ILE
1	C	192	THR
1	C	203	GLU
1	C	209	TYR
1	C	219	GLN
1	C	225	LYS
1	C	229	ILE
1	C	258	LEU
1	C	281	LYS
1	C	295	LYS
1	D	41	GLU
1	D	84	LYS
1	D	85	VAL
1	D	96	LYS
1	D	134	VAL
1	D	177	ILE
1	D	192	THR
1	D	258	LEU
1	D	295	LYS
1	D	298	LEU
1	D	310	ASP
1	D	342	SER
1	E	12	LYS
1	E	27	ASN
1	E	71	ILE
1	E	130	ASP
1	E	134	VAL
1	E	147	ILE
1	E	149	ILE
1	E	163	HIS
1	E	184	ILE

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Mol	Chain	Res	Type
1	E	192	THR
1	E	194	THR
1	E	203	GLU
1	E	222	ILE
1	E	225	LYS
1	E	271	GLU
1	E	273	SER
1	E	283	ARG
1	E	290	ILE
1	E	295	LYS
1	E	298	LEU
1	E	310	ASP
1	F	94	VAL
1	F	130	ASP
1	F	139	GLU
1	F	140	GLN
1	F	149	ILE
1	F	167	LYS
1	F	192	THR
1	F	203	GLU
1	F	222	ILE
1	F	225	LYS
1	F	248	LYS
1	F	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	152	HIS
1	A	191	ASN
1	A	253	GLN
1	A	286	ASN
1	A	314	ASN
1	A	334	ASN
1	B	26	ASN
1	B	104	HIS
1	B	152	HIS
1	B	163	HIS
1	B	191	ASN
1	B	200	ASN
1	B	228	HIS

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Mol	Chain	Res	Type
1	B	253	GLN
1	B	286	ASN
1	B	314	ASN
1	B	334	ASN
1	C	67	GLN
1	C	152	HIS
1	C	228	HIS
1	C	253	GLN
1	C	286	ASN
1	C	314	ASN
1	C	334	ASN
1	D	39	ASN
1	D	62	ASN
1	D	67	GLN
1	D	123	GLN
1	D	136	GLN
1	D	152	HIS
1	D	163	HIS
1	D	191	ASN
1	D	218	ASN
1	D	219	GLN
1	D	228	HIS
1	D	253	GLN
1	D	256	ASN
1	D	286	ASN
1	E	27	ASN
1	E	136	GLN
1	E	152	HIS
1	E	191	ASN
1	E	228	HIS
1	E	253	GLN
1	E	286	ASN
1	E	328	ASN
1	E	334	ASN
1	F	15	ASN
1	F	26	ASN
1	F	136	GLN
1	F	140	GLN
1	F	152	HIS
1	F	191	ASN
1	F	200	ASN
1	F	208	ASN

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Mol	Chain	Res	Type
1	F	218	ASN
1	F	219	GLN
1	F	243	ASN
1	F	253	GLN
1	F	286	ASN
1	F	328	ASN
1	F	334	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 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	350/353 (99%)	0.16	11 (3%) 51 45	23, 45, 69, 87	0
1	B	350/353 (99%)	0.38	10 (2%) 53 48	36, 56, 75, 94	0
1	C	340/353 (96%)	0.86	38 (11%) 10 8	32, 65, 91, 97	0
1	D	344/353 (97%)	0.83	37 (10%) 11 8	34, 67, 90, 97	0
1	E	297/353 (84%)	0.70	39 (13%) 7 5	26, 58, 97, 99	0
1	F	294/353 (83%)	1.34	68 (23%) 2 1	41, 80, 98, 99	0
All	All	1975/2118 (93%)	0.69	203 (10%) 12 9	23, 60, 95, 99	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	60	LEU	5.7
1	C	26	ASN	5.3
1	C	57	LEU	5.2
1	D	89	GLY	5.1
1	F	14	ALA	4.9
1	F	63	ASP	4.6
1	E	34	PHE	4.6
1	E	33	ILE	4.3
1	F	32	THR	4.3
1	C	348	ALA	4.0
1	D	346	LEU	3.9
1	F	54	THR	3.9
1	E	71	ILE	3.8
1	B	351	LEU	3.8
1	F	90	LYS	3.8
1	E	351	LEU	3.8
1	C	205	ALA	3.8
1	E	81	LEU	3.7
1	F	36	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	313	VAL	3.7
1	C	40	GLU	3.7
1	C	68	VAL	3.7
1	C	54	THR	3.7
1	F	11	GLY	3.6
1	F	9	GLY	3.6
1	A	162	THR	3.6
1	F	307	ALA	3.6
1	F	95	GLU	3.6
1	E	76	HIS	3.5
1	A	345	LYS	3.5
1	E	77	THR	3.5
1	C	80	GLU	3.5
1	F	80	GLU	3.4
1	F	161	ILE	3.4
1	D	311	THR	3.4
1	C	30	VAL	3.4
1	D	85	VAL	3.3
1	F	216	TYR	3.3
1	F	329	ILE	3.3
1	F	347	GLU	3.3
1	E	309	TYR	3.3
1	C	41	GLU	3.2
1	E	94	VAL	3.2
1	D	74	PRO	3.2
1	F	45	PRO	3.2
1	E	319	LEU	3.2
1	E	116	GLY	3.2
1	F	217	GLY	3.1
1	C	161	ILE	3.1
1	E	163	HIS	3.1
1	C	337	ALA	3.1
1	F	91	SER	3.0
1	D	312	ILE	3.0
1	F	30	VAL	3.0
1	F	47	GLU	3.0
1	F	92	VAL	3.0
1	A	163	HIS	3.0
1	F	37	GLN	3.0
1	F	39	ASN	2.9
1	E	32	THR	2.9
1	E	109	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	270	GLY	2.9
1	E	73	THR	2.9
1	F	35	VAL	2.9
1	D	243	ASN	2.8
1	F	268	GLY	2.8
1	D	75	ALA	2.8
1	D	111	LEU	2.8
1	F	8	ILE	2.8
1	D	217	GLY	2.8
1	F	81	LEU	2.8
1	C	218	ASN	2.8
1	D	205	ALA	2.8
1	E	174	SER	2.8
1	F	43	ALA	2.8
1	D	120	MET	2.7
1	F	85	VAL	2.7
1	C	60	LEU	2.7
1	C	56	ASP	2.7
1	A	99	CYS	2.7
1	F	331	ILE	2.7
1	F	89	GLY	2.7
1	D	192	THR	2.7
1	D	222	ILE	2.6
1	E	113	ARG	2.6
1	C	27	ASN	2.6
1	C	35	VAL	2.6
1	F	51	VAL	2.6
1	C	38	ILE	2.6
1	D	287	GLY	2.6
1	C	34	PHE	2.6
1	F	332	LEU	2.6
1	E	328	ASN	2.6
1	E	29	LYS	2.5
1	E	20	PRO	2.5
1	B	164	GLU	2.5
1	C	61	LEU	2.5
1	C	46	TYR	2.5
1	D	50	GLY	2.5
1	B	219	GLN	2.5
1	F	325	ALA	2.5
1	F	21	TYR	2.5
1	F	202	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	38	ILE	2.4
1	C	42	LEU	2.4
1	F	19	LEU	2.4
1	E	350	HIS	2.4
1	D	30	VAL	2.4
1	F	34	PHE	2.4
1	D	116	GLY	2.4
1	E	97	PRO	2.4
1	D	92	VAL	2.4
1	D	308	ALA	2.4
1	E	75	ALA	2.4
1	F	53	PHE	2.4
1	F	7	PHE	2.4
1	F	49	ARG	2.4
1	B	161	ILE	2.4
1	B	288	ASP	2.4
1	D	69	VAL	2.4
1	D	337	ALA	2.4
1	F	57	LEU	2.3
1	D	161	ILE	2.3
1	F	187	PHE	2.3
1	B	87	LEU	2.3
1	D	79	TYR	2.3
1	F	301	TYR	2.3
1	D	77	THR	2.3
1	D	80	GLU	2.3
1	E	268	GLY	2.3
1	D	105	ALA	2.3
1	F	40	GLU	2.3
1	D	204	GLY	2.3
1	F	302	GLY	2.3
1	D	99	CYS	2.3
1	D	313	VAL	2.3
1	D	53	PHE	2.3
1	D	88	ALA	2.3
1	E	17	TYR	2.3
1	F	58	ASP	2.3
1	F	158	PRO	2.3
1	D	119	VAL	2.3
1	E	117	VAL	2.3
1	F	87	LEU	2.3
1	F	238	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	77	THR	2.2
1	F	173	TYR	2.2
1	F	342	SER	2.2
1	A	51	VAL	2.2
1	C	98	PHE	2.2
1	C	165	ALA	2.2
1	E	312	ILE	2.2
1	C	101	THR	2.2
1	E	91	SER	2.2
1	C	12	LYS	2.2
1	C	102	VAL	2.2
1	A	88	ALA	2.2
1	A	351	LEU	2.2
1	C	3	LEU	2.2
1	E	28	ILE	2.2
1	F	10	PHE	2.2
1	F	82	ALA	2.2
1	E	72	CYS	2.2
1	F	341	PRO	2.2
1	B	50	GLY	2.2
1	E	112	GLY	2.2
1	F	214	LEU	2.2
1	E	30	VAL	2.2
1	F	171	SER	2.2
1	F	222	ILE	2.2
1	C	88	ALA	2.1
1	C	347	GLU	2.1
1	E	115	LYS	2.1
1	F	257	ASP	2.1
1	E	98	PHE	2.1
1	D	209	TYR	2.1
1	F	46	TYR	2.1
1	C	87	LEU	2.1
1	B	326	VAL	2.1
1	C	69	VAL	2.1
1	F	118	VAL	2.1
1	B	347	GLU	2.1
1	F	6	GLY	2.1
1	C	309	TYR	2.1
1	C	23	LYS	2.0
1	D	329	ILE	2.0
1	D	202	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	68	VAL	2.0
1	F	320	VAL	2.0
1	E	269	PHE	2.0
1	A	56	ASP	2.0
1	B	338	ALA	2.0
1	D	338	ALA	2.0
1	E	165	ALA	2.0
1	C	55	THR	2.0
1	F	5	MET	2.0
1	E	346	LEU	2.0
1	A	39	ASN	2.0
1	A	161	ILE	2.0
1	C	312	ILE	2.0
1	C	92	VAL	2.0
1	E	320	VAL	2.0
1	F	326	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.