



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:08 AM UTC

PDB ID : 3KYH / pdb_00003kyh
Title : Saccharomyces cerevisiae Cet1-Ceg1 capping apparatus
Authors : Lima, C.D.
Deposited on : 2009-12-06
Resolution : 3.00 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

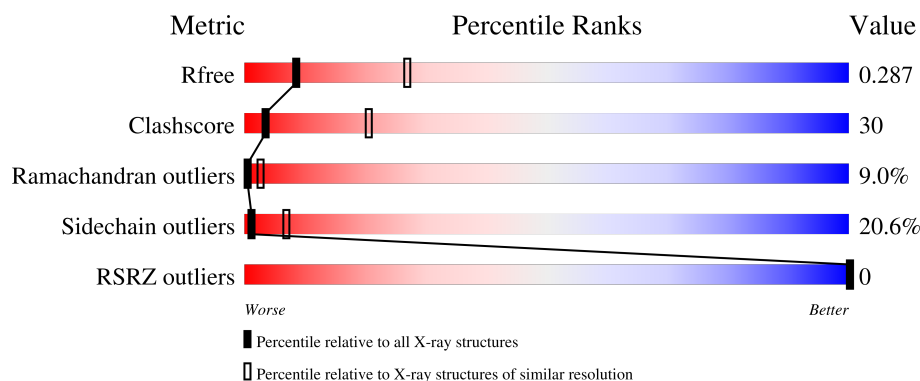
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	310	
1	B	310	
2	C	461	
2	D	461	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10696 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 mRNA-capping enzyme subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2212	1407	375	426	4			
1	B	276	Total	C	N	O	S	0	0	0
			2212	1407	375	426	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	MET	-	initiating methionine	UNP O13297
B	240	MET	-	initiating methionine	UNP O13297

- Molecule 2 is a protein called mRNA-capping enzyme subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	387	Total	C	N	O	S	0	0	0
			3136	2007	528	583	18			
2	D	387	Total	C	N	O	S	0	0	0
			3136	2007	528	583	18			

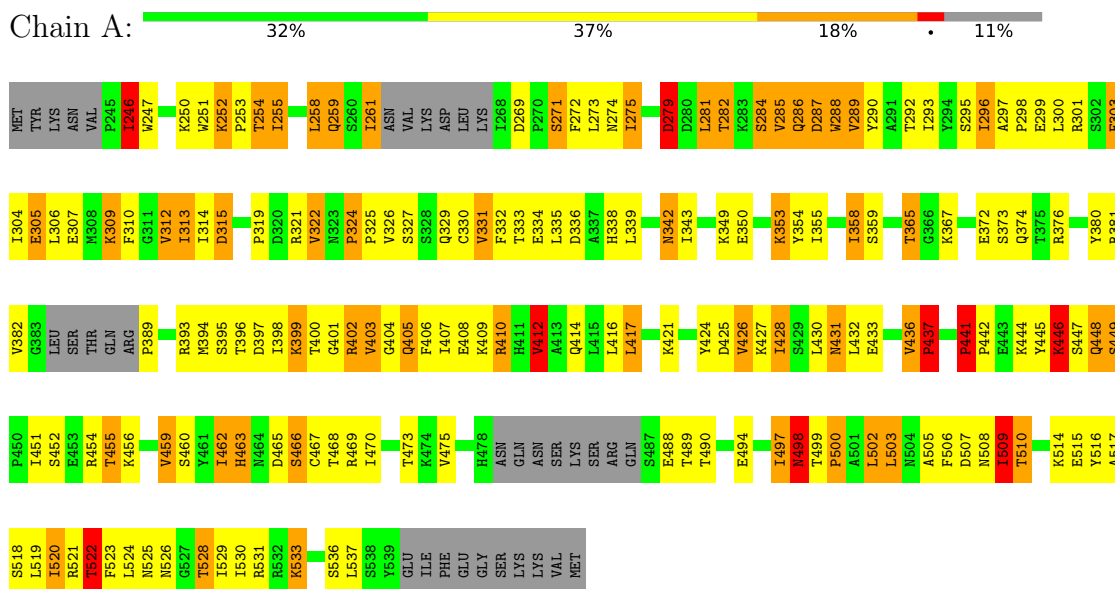
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q01159
C	0	LEU	-	expression tag	UNP Q01159
D	-1	SER	-	expression tag	UNP Q01159
D	0	LEU	-	expression tag	UNP Q01159

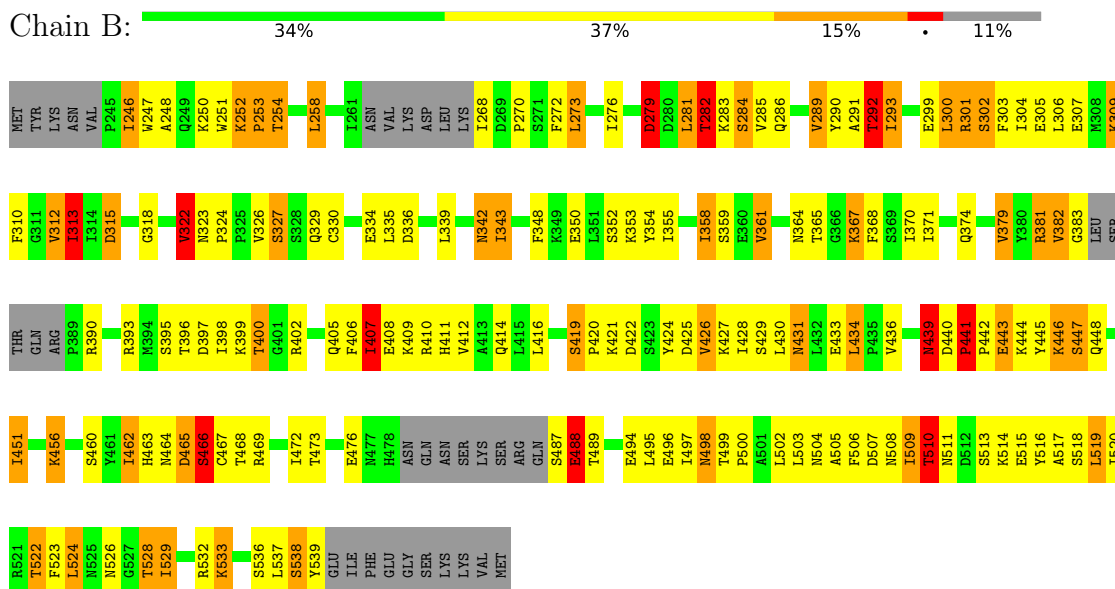
3 Residue-property plots

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.

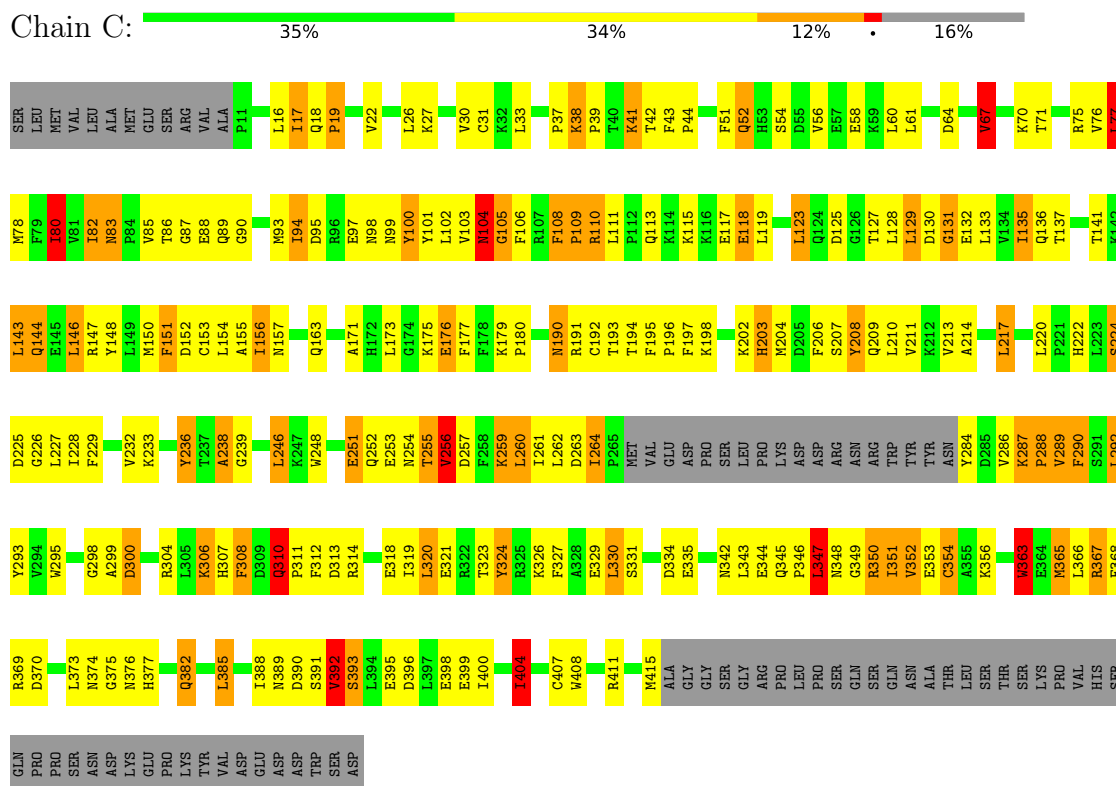
• Molecule 1: mRNA-capping enzyme subunit beta



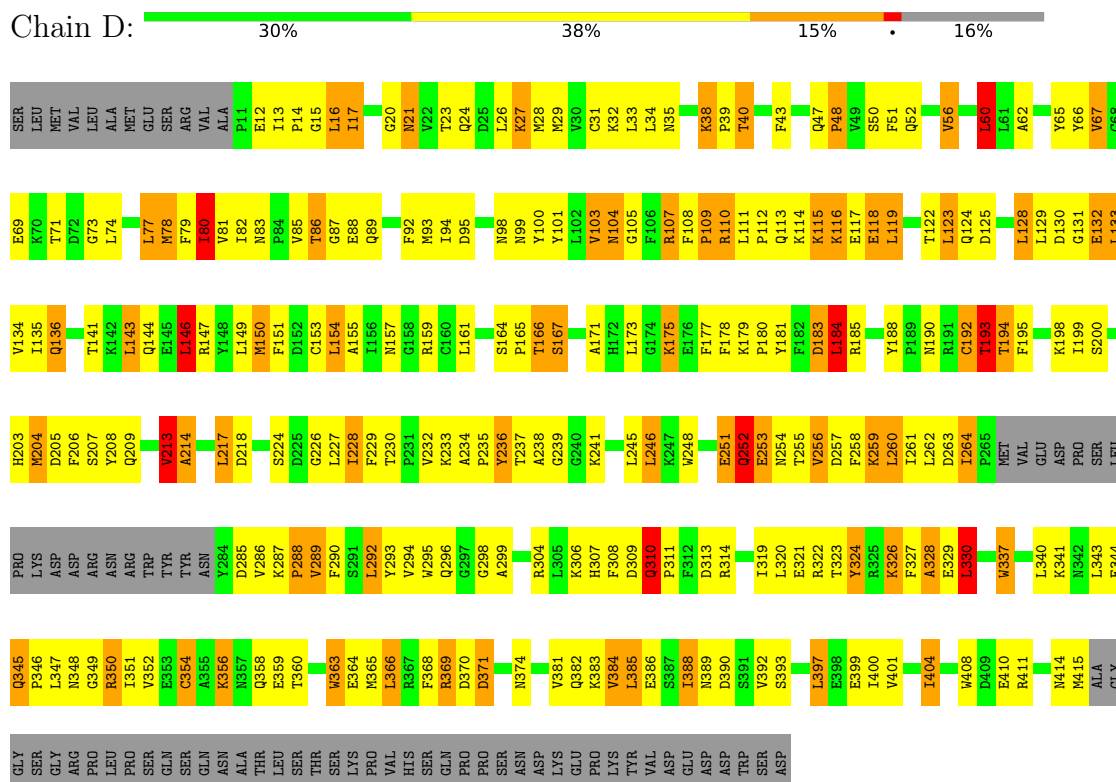
• Molecule 1: mRNA-capping enzyme subunit beta



• Molecule 2: mRNA-capping enzyme subunit alpha



• Molecule 2: mRNA-capping enzyme subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	165.99Å 165.99Å 172.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.00 19.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.2 (19.98-3.00) 95.3 (19.98-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.249 , 0.298 0.244 , 0.287	Depositor DCC
R_{free} test set	2580 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.458 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.514 for H, K, L 0.486 for h+k,-k,-l	Depositor
Outliers	0 of 50992 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10696	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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	1.12	1/2256 (0.0%)	1.59	26/3058 (0.9%)
1	B	1.19	3/2256 (0.1%)	1.63	31/3058 (1.0%)
2	C	0.81	0/3207	1.41	38/4334 (0.9%)
2	D	0.79	0/3207	1.37	30/4334 (0.7%)
All	All	0.96	4/10926 (0.0%)	1.49	125/14784 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	C	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	ILE	CA-C	6.21	1.59	1.52
1	B	324	PRO	CA-C	5.96	1.57	1.52
1	B	312	VAL	CA-CB	5.43	1.61	1.54
1	B	334	GLU	CA-C	5.12	1.58	1.52

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	VAL	N-CA-C	10.16	122.81	107.77
2	C	131	GLY	N-CA-C	9.94	125.65	111.14
1	B	441	PRO	N-CA-C	9.03	121.72	110.70
1	A	274	ASN	CB-CA-C	8.88	118.63	109.83
1	A	246	ILE	N-CA-C	8.51	119.32	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	347	LEU	N-CA-C	8.48	124.56	114.04
1	A	393	ARG	N-CA-C	-8.26	97.62	110.42
2	C	324	TYR	N-CA-C	8.22	121.82	108.34
2	C	220	LEU	CA-C-N	7.85	127.77	119.05
2	C	220	LEU	C-N-CA	7.85	127.77	119.05
2	D	246	LEU	N-CA-C	7.75	121.58	108.02
2	D	285	ASP	N-CA-C	7.74	122.85	113.41
1	A	441	PRO	N-CA-C	7.69	120.08	110.70
1	B	443	GLU	N-CA-C	-7.67	103.88	113.55
1	B	309	LYS	N-CA-C	7.62	121.81	109.40
1	B	426	VAL	N-CA-C	7.47	119.07	108.17
2	D	65	TYR	N-CA-C	7.39	120.97	109.52
2	C	391	SER	CA-C-N	7.33	134.90	121.70
2	C	391	SER	C-N-CA	7.33	134.90	121.70
1	B	276	ILE	CA-C-N	-7.32	111.23	120.23
1	B	276	ILE	C-N-CA	-7.32	111.23	120.23
2	D	193	THR	N-CA-C	-7.26	104.94	114.31
1	A	305	GLU	N-CA-C	-7.25	97.43	108.96
1	B	419	SER	CA-C-N	7.20	126.46	118.97
1	B	419	SER	C-N-CA	7.20	126.46	118.97
1	B	379	VAL	CB-CA-C	7.13	121.36	111.38
2	D	310	GLN	N-CA-C	7.11	118.86	109.83
1	B	524	LEU	N-CA-C	7.06	119.87	111.33
2	D	324	TYR	N-CA-C	6.98	119.78	108.34
1	A	466	SER	N-CA-C	-6.92	99.42	110.14
2	D	345	GLN	N-CA-C	-6.92	102.00	108.22
2	D	226	GLY	N-CA-C	6.91	120.69	110.60
2	C	239	GLY	N-CA-C	6.91	119.44	111.36
2	D	107	ARG	N-CA-C	6.79	120.53	112.93
1	A	522	THR	N-CA-CB	6.75	120.05	110.12
2	C	354	CYS	N-CA-C	6.75	119.47	108.26
2	D	116	LYS	CA-C-N	6.67	129.77	120.29
2	D	116	LYS	C-N-CA	6.67	129.77	120.29
2	C	193	THR	N-CA-C	-6.63	105.10	113.72
1	A	296	ILE	N-CA-C	-6.62	100.15	108.89
1	A	315	ASP	CA-C-N	6.47	129.60	120.28
1	A	315	ASP	C-N-CA	6.47	129.60	120.28
1	B	407	ILE	N-CA-C	6.45	117.65	108.42
2	D	321	GLU	N-CA-C	6.45	118.84	111.11
2	D	224	SER	N-CA-C	6.43	118.55	107.93
1	B	371	ILE	N-CA-C	6.41	117.34	107.78
1	B	327	SER	N-CA-C	6.41	122.57	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	381	ARG	N-CA-C	6.34	119.85	110.46
2	C	190	ASN	N-CA-C	6.33	118.26	111.36
1	B	310	PHE	N-CA-C	6.33	119.05	108.73
2	C	108	PHE	CA-C-N	6.30	127.72	119.84
2	C	108	PHE	C-N-CA	6.30	127.72	119.84
1	A	324	PRO	CA-C-N	-6.26	112.01	119.84
1	A	324	PRO	C-N-CA	-6.26	112.01	119.84
1	B	318	GLY	N-CA-C	6.25	125.09	112.34
2	D	78	MET	N-CA-C	6.20	118.84	108.73
2	D	363	TRP	N-CA-C	6.18	119.80	107.62
1	B	428	ILE	N-CA-C	-6.16	98.65	107.77
1	B	488	GLU	N-CA-C	6.11	117.80	108.52
2	D	134	VAL	N-CA-C	6.09	118.54	109.17
1	A	428	ILE	N-CA-C	-6.05	99.70	108.17
1	A	432	LEU	N-CA-C	6.04	119.67	109.76
1	A	296	ILE	CB-CA-C	-6.02	103.33	111.15
2	C	313	ASP	N-CA-C	6.01	120.15	112.34
1	B	456	LYS	N-CA-C	5.98	118.48	108.02
1	A	297	ALA	CA-C-N	5.97	125.44	119.24
1	A	297	ALA	C-N-CA	5.97	125.44	119.24
2	C	77	LEU	N-CA-CB	5.94	118.85	110.36
2	C	363	TRP	N-CA-C	5.92	120.07	107.70
2	D	80	ILE	N-CA-C	5.88	116.64	107.28
2	D	133	LEU	N-CA-C	5.87	117.86	108.41
2	D	146	LEU	N-CA-C	-5.84	102.66	110.55
2	C	80	ILE	N-CA-C	5.83	116.26	107.75
2	D	103	VAL	N-CA-C	5.79	117.50	109.45
2	D	326	LYS	N-CA-C	5.78	117.88	108.63
1	A	424	TYR	N-CA-C	5.77	118.61	108.75
1	B	473	THR	N-CA-C	5.76	118.27	108.02
2	C	105	GLY	N-CA-C	5.74	119.92	110.97
1	A	520	ILE	N-CA-CB	5.73	117.91	110.57
2	C	335	GLU	N-CA-C	-5.73	105.95	113.17
2	C	404	ILE	N-CA-C	-5.73	106.72	113.42
2	D	369	ARG	N-CA-C	5.68	117.81	110.65
2	C	217	LEU	CA-CB-CG	5.67	136.16	116.30
2	C	224	SER	N-CA-C	5.67	116.70	107.23
2	C	132	GLU	N-CA-C	5.67	117.94	108.02
2	D	136	GLN	N-CA-C	5.67	118.33	108.76
2	D	128	LEU	N-CA-C	5.62	117.86	108.02
2	C	342	ASN	N-CA-C	5.60	117.38	111.28
1	B	315	ASP	N-CA-CB	-5.60	101.94	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	94	ILE	N-CA-C	5.57	114.75	106.85
2	D	313	ASP	N-CA-C	5.54	119.54	112.34
2	C	287	LYS	N-CA-C	5.53	122.04	109.81
2	C	238	ALA	CA-C-N	5.52	125.22	119.92
2	C	238	ALA	C-N-CA	5.52	125.22	119.92
2	C	353	GLU	N-CA-C	5.49	117.80	108.02
1	B	424	TYR	N-CA-C	5.49	118.36	108.48
1	A	402	ARG	N-CA-C	5.48	117.77	108.02
2	D	328	ALA	N-CA-C	5.47	116.54	107.73
1	A	449	SER	N-CA-C	-5.44	101.64	109.48
2	C	256	VAL	N-CA-C	5.43	117.91	108.90
2	D	256	VAL	N-CA-C	5.43	117.91	108.90
1	B	302	SER	N-CA-C	5.36	120.09	113.50
2	C	58	GLU	N-CA-C	5.34	117.18	111.36
2	D	27	LYS	N-CA-C	-5.32	104.72	111.11
2	C	67	VAL	N-CA-C	5.25	115.83	108.17
2	C	83	ASN	N-CA-C	5.24	121.39	109.81
1	B	342	ASN	N-CA-C	-5.23	99.65	110.80
1	B	439	ASN	N-CA-C	-5.21	100.81	108.99
2	C	246	LEU	N-CA-C	5.21	117.90	109.40
1	A	459	VAL	N-CA-C	5.21	115.47	108.17
1	A	463	HIS	N-CA-C	-5.20	99.73	110.80
1	A	502	LEU	N-CA-CB	5.16	117.55	110.07
2	C	100	TYR	N-CA-C	5.12	116.87	108.52
2	C	177	PHE	N-CA-C	5.11	117.64	111.40
2	C	334	ASP	N-CA-C	5.10	119.35	113.18
1	B	434	LEU	CA-C-N	5.09	125.56	120.52
1	B	434	LEU	C-N-CA	5.09	125.56	120.52
1	B	538	SER	N-CA-C	-5.09	102.37	109.96
1	B	292	THR	CB-CA-C	5.08	119.47	111.39
2	D	217	LEU	N-CA-C	5.07	121.59	110.80
2	C	143	LEU	N-CA-C	5.04	116.41	109.15
2	D	299	ALA	N-CA-C	5.03	119.40	113.16
1	B	536	SER	N-CA-C	5.03	118.90	112.87
1	A	436	VAL	N-CA-C	5.01	113.86	108.95
1	B	466	SER	N-CA-C	-5.01	102.16	109.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	465	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	465	ASP	Peptide
2	C	310	GLN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2212	0	2218	159	0
1	B	2212	0	2218	150	0
2	C	3136	0	3126	157	0
2	D	3136	0	3126	199	0
All	All	10696	0	10688	638	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 30.

All (638) 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:446:LYS:HA	1:B:446:LYS:NZ	1.64	1.13
2:D:109:PRO:HD2	2:D:180:PRO:HB2	1.24	1.13
1:B:497:ILE:HD11	1:B:519:LEU:HD11	1.32	1.12
2:C:390:ASP:O	2:C:392:VAL:HG23	1.55	1.07
1:A:499:THR:HG22	1:A:503:LEU:HD12	1.37	1.07
1:B:518:SER:O	1:B:522:THR:HG22	1.57	1.05
2:D:93:MET:HB2	2:D:101:TYR:HB2	1.38	1.04
2:D:264:ILE:HG12	2:D:288:PRO:HB2	1.38	1.02
1:A:436:VAL:HG11	1:A:441:PRO:HG2	1.44	0.95
2:D:354:CYS:HB3	2:D:365:MET:HA	1.46	0.95
1:A:441:PRO:HD2	1:A:442:PRO:HD3	1.47	0.94
2:C:31:CYS:HB3	2:C:37:PRO:HA	1.51	0.93
2:C:43:PHE:HA	2:C:98:ASN:HD21	1.30	0.93
2:C:135:ILE:H	2:C:135:ILE:HD12	1.35	0.91
2:D:43:PHE:HA	2:D:98:ASN:HD21	1.35	0.91
1:A:255:ILE:HA	1:A:258:LEU:HB3	1.52	0.90
1:B:323:ASN:OD1	1:B:323:ASN:O	1.90	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:MET:HE3	2:C:173:LEU:HD11	1.55	0.89
1:B:446:LYS:HA	1:B:446:LYS:HZ3	1.31	0.89
2:D:385:LEU:HA	2:D:388:ILE:HD11	1.53	0.89
1:B:446:LYS:C	1:B:448:GLN:H	1.76	0.87
2:D:251:GLU:H	2:D:251:GLU:CD	1.82	0.86
1:B:446:LYS:HA	1:B:446:LYS:HZ2	1.40	0.86
2:C:80:ILE:CD1	2:C:127:THR:HB	2.05	0.85
2:D:109:PRO:HD2	2:D:180:PRO:CB	2.07	0.85
2:D:259:LYS:HD2	2:D:261:ILE:HG13	1.56	0.85
2:D:77:LEU:HB2	2:D:94:ILE:HD11	1.56	0.85
2:C:109:PRO:HG2	2:C:180:PRO:HB2	1.59	0.84
1:A:395:SER:O	1:A:403:VAL:HA	1.77	0.84
2:C:97:GLU:HB3	2:C:99:ASN:HD21	1.42	0.83
1:A:394:MET:HG3	1:A:406:PHE:HD2	1.40	0.83
2:C:16:LEU:O	2:C:101:TYR:HA	1.78	0.83
2:C:93:MET:HB2	2:C:101:TYR:HB2	1.61	0.82
1:B:519:LEU:HD12	1:B:519:LEU:O	1.79	0.82
2:D:13:ILE:HG13	2:D:14:PRO:HD2	1.63	0.81
2:D:356:LYS:HA	2:D:363:TRP:HB3	1.62	0.81
2:D:109:PRO:CD	2:D:180:PRO:HB2	2.10	0.81
2:D:131:GLY:HA2	2:D:150:MET:HA	1.62	0.80
2:D:264:ILE:CG1	2:D:288:PRO:HB2	2.12	0.80
2:C:356:LYS:HA	2:C:363:TRP:HB3	1.62	0.79
1:B:339:LEU:HD23	1:B:339:LEU:C	2.08	0.78
2:D:136:GLN:HG3	2:D:147:ARG:HD2	1.63	0.78
2:C:77:LEU:HB2	2:C:94:ILE:CG1	2.15	0.77
2:C:77:LEU:HG	2:C:130:ASP:HA	1.65	0.77
2:C:77:LEU:HB2	2:C:94:ILE:HG12	1.67	0.77
2:C:135:ILE:HD12	2:C:135:ILE:N	1.99	0.77
2:D:78:MET:HB3	2:D:129:LEU:HG	1.65	0.77
1:B:309:LYS:HG2	1:B:494:GLU:HG2	1.65	0.76
2:C:150:MET:CE	2:C:173:LEU:HD11	2.15	0.76
2:C:259:LYS:NZ	2:C:349:GLY:C	2.44	0.76
1:B:497:ILE:HD11	1:B:519:LEU:CD1	2.14	0.76
2:C:259:LYS:NZ	2:C:349:GLY:O	2.19	0.76
2:D:295:TRP:HA	2:D:323:THR:O	1.85	0.76
2:C:80:ILE:HD12	2:C:127:THR:HB	1.67	0.75
1:A:394:MET:HE1	1:A:446:LYS:HD3	1.68	0.75
1:A:305:GLU:HB3	1:A:431:ASN:ND2	2.02	0.75
1:B:292:THR:CG2	1:B:430:LEU:HD13	2.16	0.75
2:C:125:ASP:O	2:C:157:ASN:HA	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:259:LYS:HZ1	2:C:349:GLY:C	1.94	0.74
1:B:246:ILE:HD12	1:B:247:TRP:H	1.51	0.74
1:B:494:GLU:C	1:B:495:LEU:HD12	2.12	0.74
1:B:305:GLU:HG3	1:B:496:GLU:OE1	1.87	0.74
1:A:380:TYR:CE2	1:A:445:TYR:O	2.41	0.74
1:A:498:ASN:HD21	1:A:500:PRO:HG2	1.52	0.74
2:C:43:PHE:HA	2:C:98:ASN:ND2	2.02	0.74
1:A:326:VAL:HG21	1:A:330:CYS:SG	2.28	0.74
2:D:115:LYS:HG3	2:D:118:GLU:HB2	1.68	0.74
2:C:350:ARG:HD3	2:C:351:ILE:H	1.53	0.73
2:D:27:LYS:NZ	2:D:98:ASN:HB3	2.04	0.72
2:D:132:GLU:HB2	2:D:151:PHE:HE1	1.55	0.72
2:C:61:LEU:HD12	2:C:407:CYS:SG	2.30	0.72
1:A:499:THR:HG22	1:A:503:LEU:CD1	2.18	0.72
1:B:309:LYS:CG	1:B:494:GLU:HG2	2.19	0.72
2:C:299:ALA:HB3	2:C:323:THR:HB	1.70	0.72
1:A:445:TYR:C	1:A:447:SER:H	1.95	0.72
1:A:300:LEU:O	1:A:303:PHE:HD1	1.73	0.71
1:A:441:PRO:CD	1:A:442:PRO:HD3	2.21	0.71
2:D:251:GLU:CD	2:D:251:GLU:N	2.49	0.71
1:B:505:ALA:HA	1:B:515:GLU:OE1	1.91	0.70
2:C:263:ASP:OD2	2:C:289:VAL:HB	1.91	0.70
1:A:309:LYS:O	1:A:426:VAL:HG12	1.91	0.70
1:B:446:LYS:C	1:B:448:GLN:N	2.48	0.70
2:D:43:PHE:O	2:D:239:GLY:HA2	1.92	0.70
2:C:151:PHE:HB3	2:C:202:LYS:HD3	1.73	0.69
1:B:509:ILE:HG23	1:B:510:THR:H	1.57	0.69
2:C:56:VAL:HG11	2:C:400:ILE:HD13	1.74	0.69
2:D:92:PHE:HA	2:D:101:TYR:O	1.92	0.69
2:C:52:GLN:HB3	2:C:54:SER:OG	1.91	0.69
1:A:380:TYR:CD2	1:A:445:TYR:HB3	2.27	0.69
1:A:255:ILE:HA	1:A:258:LEU:CB	2.21	0.69
2:D:153:CYS:HB2	2:D:173:LEU:HD22	1.75	0.69
1:A:436:VAL:HG11	1:A:441:PRO:CG	2.22	0.69
1:A:299:GLU:HG2	1:A:300:LEU:H	1.58	0.68
1:A:306:LEU:HB3	1:A:497:ILE:CG2	2.24	0.68
2:D:354:CYS:HB3	2:D:365:MET:CA	2.21	0.68
1:A:448:GLN:HA	1:A:448:GLN:HE21	1.59	0.67
2:D:181:TYR:CE1	2:D:199:ILE:HD13	2.29	0.67
1:A:298:PRO:O	1:A:301:ARG:HB2	1.95	0.67
1:A:468:THR:HG21	1:A:526:ASN:HD22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:SER:HB2	1:A:404:GLY:H	1.59	0.66
1:A:498:ASN:ND2	1:A:500:PRO:HG2	2.09	0.66
1:B:313:ILE:HD13	1:B:416:LEU:HB3	1.76	0.66
2:C:390:ASP:O	2:C:392:VAL:CG2	2.39	0.66
2:C:80:ILE:HG22	2:C:90:GLY:O	1.94	0.66
2:D:128:LEU:O	2:D:154:LEU:HD12	1.95	0.66
1:A:394:MET:HG3	1:A:406:PHE:CD2	2.29	0.66
2:D:213:VAL:HG12	2:D:214:ALA:N	2.08	0.66
2:D:337:TRP:HA	2:D:337:TRP:CE3	2.31	0.66
1:B:292:THR:HG22	1:B:430:LEU:HD13	1.79	0.65
2:D:304:ARG:HD2	2:D:307:HIS:HD2	1.60	0.65
1:B:488:GLU:OE2	1:B:488:GLU:HA	1.95	0.65
2:C:127:THR:HG23	2:C:156:ILE:HD12	1.78	0.65
2:D:27:LYS:NZ	2:D:98:ASN:CB	2.59	0.65
2:D:385:LEU:HA	2:D:388:ILE:CD1	2.25	0.65
1:B:300:LEU:O	1:B:302:SER:N	2.29	0.65
2:C:82:ILE:HD11	2:C:125:ASP:HB2	1.78	0.65
2:C:129:LEU:HD23	2:C:129:LEU:H	1.61	0.65
2:C:257:ASP:HB2	2:C:375:GLY:O	1.95	0.65
2:D:83:ASN:HD22	2:D:85:VAL:HB	1.62	0.64
1:B:445:TYR:C	1:B:446:LYS:HD2	2.22	0.64
2:C:41:LYS:HG2	2:C:42:THR:N	2.13	0.64
1:A:451:ILE:C	1:A:451:ILE:HD12	2.23	0.64
2:C:408:TRP:HA	2:C:411:ARG:HE	1.61	0.64
1:A:520:ILE:O	1:A:523:PHE:HB3	1.98	0.64
1:B:292:THR:HG21	1:B:430:LEU:HD13	1.79	0.64
2:C:17:ILE:HA	2:C:100:TYR:O	1.97	0.64
1:A:261:ILE:HD11	1:B:464:ASN:HB3	1.80	0.63
1:B:306:LEU:HB3	1:B:497:ILE:CG2	2.27	0.63
2:D:89:GLN:HB2	2:D:123:LEU:HD11	1.81	0.63
1:A:529:ILE:HG21	1:B:273:LEU:HD12	1.81	0.63
1:B:306:LEU:HB3	1:B:497:ILE:HG22	1.79	0.63
1:B:350:GLU:HB3	1:B:537:LEU:HD22	1.80	0.63
1:B:307:GLU:OE1	1:B:494:GLU:HB3	1.98	0.63
2:D:256:VAL:HG13	2:D:257:ASP:H	1.63	0.63
2:C:356:LYS:CA	2:C:363:TRP:HB3	2.29	0.63
2:C:153:CYS:HB2	2:C:173:LEU:HD22	1.80	0.62
2:D:78:MET:O	2:D:128:LEU:HD12	2.00	0.62
1:A:350:GLU:HB3	1:A:537:LEU:HD22	1.82	0.62
1:A:412:VAL:HG23	1:A:431:ASN:HA	1.81	0.61
2:C:260:LEU:C	2:C:260:LEU:HD12	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:CYS:CB	2:C:37:PRO:HA	2.28	0.61
1:B:322:VAL:O	1:B:323:ASN:HB2	1.99	0.61
1:A:397:ASP:O	1:A:401:GLY:HA2	2.00	0.61
2:D:23:THR:HG23	2:D:100:TYR:HB2	1.83	0.60
2:D:27:LYS:HD3	2:D:40:THR:O	2.00	0.60
1:A:372:GLU:HA	1:A:459:VAL:HG22	1.83	0.60
1:A:456:LYS:HG2	1:A:475:VAL:HB	1.83	0.60
2:C:264:ILE:CG1	2:C:288:PRO:HB2	2.31	0.60
2:D:82:ILE:HA	2:D:88:GLU:O	2.02	0.60
2:D:337:TRP:HA	2:D:337:TRP:HE3	1.64	0.60
1:B:286:GLN:HG2	1:B:520:ILE:HG21	1.84	0.60
2:C:259:LYS:HG2	2:C:324:TYR:CZ	2.37	0.60
2:D:15:GLY:O	2:D:16:LEU:HB3	2.02	0.60
2:C:251:GLU:OE2	2:C:393:SER:HA	2.02	0.60
2:C:295:TRP:HZ3	2:C:298:GLY:HA2	1.67	0.59
1:A:421:LYS:NZ	1:B:284:SER:OG	2.35	0.59
1:A:462:ILE:HG22	1:A:463:HIS:H	1.66	0.59
1:B:246:ILE:HD13	2:C:344:GLU:HG3	1.83	0.59
2:D:292:LEU:HG	2:D:328:ALA:HB3	1.83	0.59
1:A:314:ILE:HG22	1:A:314:ILE:O	2.01	0.59
1:A:436:VAL:CG1	1:A:441:PRO:HG2	2.26	0.59
1:B:300:LEU:HD23	1:B:434:LEU:HD21	1.83	0.59
1:B:313:ILE:CD1	1:B:416:LEU:HB3	2.32	0.59
2:C:307:HIS:O	2:C:310:GLN:HB3	2.03	0.59
2:D:177:PHE:O	2:D:177:PHE:CD2	2.56	0.59
2:C:80:ILE:HD11	2:C:127:THR:HB	1.85	0.59
2:D:256:VAL:CG1	2:D:257:ASP:N	2.66	0.59
2:D:229:PHE:HB2	2:D:246:LEU:HB2	1.84	0.58
2:D:259:LYS:HE3	2:D:349:GLY:HA2	1.83	0.58
1:B:396:THR:HG22	1:B:397:ASP:O	2.03	0.58
1:B:250:LYS:HD3	2:C:310:GLN:HG3	1.84	0.58
1:B:411:HIS:CD2	1:B:431:ASN:HB3	2.38	0.58
2:D:78:MET:HB3	2:D:129:LEU:CG	2.34	0.58
2:D:264:ILE:HG12	2:D:288:PRO:CB	2.23	0.58
1:B:407:ILE:HD12	1:B:433:GLU:HG2	1.86	0.58
1:B:411:HIS:HD2	1:B:431:ASN:HB3	1.69	0.58
2:D:261:ILE:HB	2:D:293:TYR:CE1	2.39	0.58
2:C:261:ILE:HB	2:C:293:TYR:CE1	2.39	0.58
1:B:382:VAL:HG12	1:B:383:GLY:N	2.19	0.58
1:A:381:ARG:NH1	1:A:389:PRO:HB3	2.19	0.58
2:C:404:ILE:O	2:C:408:TRP:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LEU:HD23	1:B:339:LEU:O	2.04	0.57
2:C:83:ASN:ND2	2:C:86:THR:H	2.01	0.57
1:B:446:LYS:HD2	1:B:446:LYS:N	2.19	0.57
2:D:129:LEU:H	2:D:129:LEU:HD23	1.67	0.57
1:A:313:ILE:CD1	1:A:416:LEU:HB3	2.35	0.57
1:B:246:ILE:CD1	2:C:344:GLU:HG3	2.35	0.57
2:C:41:LYS:HG2	2:C:42:THR:H	1.68	0.57
2:C:350:ARG:HD3	2:C:351:ILE:N	2.20	0.57
2:D:13:ILE:HG13	2:D:14:PRO:CD	2.33	0.57
2:D:206:PHE:HB3	2:D:408:TRP:CH2	2.39	0.57
1:A:310:PHE:CE2	1:A:426:VAL:HG11	2.39	0.57
2:D:77:LEU:HB2	2:D:94:ILE:CD1	2.31	0.56
2:D:115:LYS:C	2:D:117:GLU:N	2.62	0.56
1:A:300:LEU:O	1:A:303:PHE:CD1	2.57	0.56
1:A:250:LYS:HB2	1:A:252:LYS:HE3	1.86	0.56
1:A:310:PHE:HE2	1:A:531:ARG:HB2	1.70	0.56
1:A:454:ARG:HD3	1:A:475:VAL:HG21	1.86	0.56
1:B:285:VAL:HG11	1:B:524:LEU:HD11	1.87	0.56
1:B:393:ARG:HD2	1:B:409:LYS:HB2	1.87	0.56
2:C:27:LYS:NZ	2:C:98:ASN:HB3	2.20	0.56
2:C:399:GLU:HG3	2:C:400:ILE:HG13	1.87	0.56
2:C:44:PRO:HD3	2:C:98:ASN:HD21	1.69	0.56
1:A:462:ILE:CG1	1:A:469:ARG:HG3	2.35	0.56
1:B:282:THR:O	1:B:283:LYS:C	2.49	0.56
1:B:289:VAL:HG11	1:B:520:ILE:HD11	1.86	0.56
1:B:252:LYS:C	1:B:254:THR:H	2.14	0.56
1:B:252:LYS:N	1:B:253:PRO:HD2	2.21	0.56
2:D:347:LEU:CD2	2:D:350:ARG:HG2	2.36	0.56
1:A:445:TYR:C	1:A:447:SER:N	2.61	0.56
2:C:128:LEU:H	2:C:155:ALA:HB3	1.70	0.56
2:D:350:ARG:O	2:D:351:ILE:HD13	2.06	0.56
1:A:286:GLN:HG2	1:A:520:ILE:HG21	1.87	0.56
1:A:519:LEU:HA	1:A:522:THR:HG23	1.86	0.56
1:B:282:THR:HG22	1:B:283:LYS:N	2.21	0.56
2:D:80:ILE:HG21	2:D:108:PHE:CE1	2.41	0.56
2:D:351:ILE:CD1	2:D:374:ASN:HA	2.35	0.56
2:D:16:LEU:CA	2:D:101:TYR:HD2	2.19	0.55
1:A:354:TYR:HD2	1:A:355:ILE:HD13	1.72	0.55
2:D:340:LEU:O	2:D:340:LEU:HD23	2.07	0.55
2:D:206:PHE:HB3	2:D:408:TRP:HH2	1.72	0.55
2:C:17:ILE:HG23	2:C:100:TYR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:350:ARG:HD3	2:D:351:ILE:N	2.21	0.55
2:C:60:LEU:HD11	2:C:404:ILE:HG12	1.88	0.55
2:D:27:LYS:HZ3	2:D:98:ASN:HB3	1.71	0.55
2:D:261:ILE:HD13	2:D:320:LEU:HD21	1.88	0.55
1:A:272:PHE:HA	1:B:463:HIS:CE1	2.41	0.55
1:A:460:SER:HA	1:A:470:ILE:O	2.07	0.55
1:B:446:LYS:NZ	1:B:446:LYS:CA	2.55	0.54
1:B:528:THR:O	1:B:529:ILE:C	2.51	0.54
2:D:80:ILE:HD13	2:D:124:GLN:HG2	1.88	0.54
2:C:89:GLN:HE22	2:C:108:PHE:H	1.53	0.54
1:A:518:SER:O	1:A:522:THR:HG22	2.07	0.54
1:B:313:ILE:HG13	1:B:425:ASP:HB3	1.90	0.54
2:C:306:LYS:HE2	2:C:319:ILE:HD13	1.88	0.54
1:A:284:SER:O	1:A:285:VAL:C	2.51	0.54
1:A:330:CYS:HB3	1:B:330:CYS:HB3	1.89	0.54
1:B:374:GLN:O	1:B:398:ILE:HG13	2.06	0.54
2:C:147:ARG:HH22	2:C:198:LYS:HD3	1.72	0.54
2:C:382:GLN:HA	2:C:385:LEU:HD23	1.89	0.54
2:D:80:ILE:HG21	2:D:108:PHE:CD1	2.42	0.54
2:D:177:PHE:CD2	2:D:177:PHE:C	2.86	0.54
1:A:436:VAL:CG1	1:A:441:PRO:CG	2.85	0.54
1:B:359:SER:HA	1:B:368:PHE:CD1	2.43	0.54
2:C:70:LYS:HE2	2:C:225:ASP:OD1	2.08	0.54
1:A:525:ASN:O	1:A:529:ILE:HD12	2.07	0.54
2:C:26:LEU:O	2:C:30:VAL:HG23	2.06	0.54
2:C:351:ILE:HG21	2:C:374:ASN:O	2.08	0.54
2:D:43:PHE:CA	2:D:98:ASN:HD21	2.14	0.54
1:A:247:TRP:HZ2	2:D:341:LYS:HA	1.72	0.54
1:B:301:ARG:O	1:B:503:LEU:HD21	2.07	0.54
2:C:395:GLU:HA	2:C:398:GLU:HB2	1.90	0.54
2:D:257:ASP:OD1	2:D:369:ARG:HG3	2.08	0.54
2:D:260:LEU:HD23	2:D:352:VAL:HG21	1.88	0.54
1:A:251:TRP:HA	2:D:346:PRO:HB2	1.90	0.53
2:C:18:GLN:HB3	2:C:19:PRO:HD2	1.90	0.53
2:D:83:ASN:O	2:D:87:GLY:N	2.35	0.53
1:A:246:ILE:O	2:D:346:PRO:HA	2.07	0.53
1:A:455:THR:O	1:A:475:VAL:HA	2.09	0.53
1:B:379:VAL:HG12	1:B:451:ILE:HD11	1.91	0.53
2:C:133:LEU:HD21	2:C:146:LEU:HD11	1.90	0.53
1:A:247:TRP:HH2	2:D:341:LYS:HG2	1.72	0.53
2:C:290:PHE:O	2:C:292:LEU:HD23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:LEU:HA	2:D:200:SER:O	2.08	0.53
2:C:78:MET:O	2:C:128:LEU:HD12	2.08	0.53
2:C:345:GLN:HB2	2:C:346:PRO:HD2	1.90	0.53
2:D:179:LYS:N	2:D:180:PRO:HD2	2.24	0.53
2:C:129:LEU:HB3	2:C:153:CYS:SG	2.49	0.53
1:A:258:LEU:HG	1:B:464:ASN:ND2	2.24	0.53
1:B:367:LYS:HD3	1:B:465:ASP:OD1	2.10	0.52
2:D:79:PHE:HB3	2:D:92:PHE:HB2	1.89	0.52
1:B:355:ILE:HA	1:B:358:ILE:HG22	1.91	0.52
2:C:77:LEU:CB	2:C:94:ILE:HG12	2.38	0.52
2:D:292:LEU:HG	2:D:328:ALA:CB	2.40	0.52
2:D:27:LYS:HZ3	2:D:98:ASN:CB	2.21	0.52
2:D:83:ASN:C	2:D:85:VAL:H	2.18	0.52
1:A:462:ILE:HG13	1:A:469:ARG:HG3	1.91	0.52
1:A:509:ILE:HG23	1:A:510:THR:H	1.75	0.52
2:C:197:PHE:CD1	2:C:197:PHE:C	2.87	0.52
2:D:190:ASN:C	2:D:192:CYS:H	2.18	0.52
1:A:395:SER:OG	1:A:405:GLN:HB3	2.08	0.52
2:C:129:LEU:N	2:C:129:LEU:CD2	2.73	0.52
1:A:306:LEU:HB3	1:A:497:ILE:HG21	1.90	0.52
1:B:506:PHE:C	1:B:506:PHE:CD2	2.88	0.52
2:C:264:ILE:HG13	2:C:288:PRO:HB2	1.90	0.52
2:D:27:LYS:HZ1	2:D:98:ASN:CB	2.21	0.52
2:D:107:ARG:O	2:D:109:PRO:HD3	2.10	0.52
2:C:129:LEU:HD23	2:C:129:LEU:N	2.23	0.52
2:D:95:ASP:OD2	2:D:99:ASN:HB2	2.10	0.52
1:B:467:CYS:HB3	1:B:498:ASN:HB3	1.92	0.51
2:D:67:VAL:HA	2:D:228:ILE:O	2.10	0.51
1:A:451:ILE:C	1:A:451:ILE:CD1	2.83	0.51
2:D:17:ILE:HG23	2:D:100:TYR:O	2.11	0.51
2:D:125:ASP:O	2:D:157:ASN:HA	2.10	0.51
1:B:462:ILE:HG22	1:B:463:HIS:H	1.75	0.51
1:A:258:LEU:HG	1:B:464:ASN:HD21	1.75	0.51
1:A:305:GLU:HB3	1:A:431:ASN:HD22	1.72	0.51
1:B:299:GLU:HG2	1:B:300:LEU:HD12	1.93	0.51
1:B:300:LEU:C	1:B:302:SER:H	2.18	0.51
2:D:17:ILE:HG13	2:D:101:TYR:CE2	2.45	0.51
1:A:305:GLU:OE2	1:A:409:LYS:HE3	2.11	0.51
1:A:402:ARG:HB2	1:A:402:ARG:CZ	2.40	0.51
1:B:315:ASP:HB2	1:B:322:VAL:HG23	1.92	0.51
1:B:414:GLN:HE21	1:B:416:LEU:HD21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:LYS:HB2	2:D:117:GLU:HB2	1.91	0.51
1:A:407:ILE:HD12	1:A:433:GLU:HG2	1.93	0.51
2:C:133:LEU:HD11	2:C:146:LEU:CD1	2.41	0.50
2:C:156:ILE:HG12	2:C:176:GLU:HB3	1.93	0.50
2:D:21:ASN:HA	2:D:24:GLN:CD	2.36	0.50
1:A:394:MET:CE	1:A:446:LYS:HD3	2.39	0.50
1:B:329:GLN:HG3	1:B:330:CYS:N	2.26	0.50
1:A:299:GLU:HG2	1:A:300:LEU:N	2.25	0.50
1:A:444:LYS:O	1:A:447:SER:HB3	2.12	0.50
2:D:256:VAL:HG13	2:D:257:ASP:N	2.26	0.50
1:A:301:ARG:O	1:A:304:ILE:HG13	2.11	0.50
2:C:206:PHE:H	2:C:209:GLN:HE22	1.60	0.50
2:C:229:PHE:HB2	2:C:246:LEU:HB2	1.93	0.50
1:B:283:LYS:O	1:B:286:GLN:HB2	2.10	0.50
1:A:430:LEU:C	1:A:430:LEU:HD23	2.37	0.50
1:A:451:ILE:HD12	1:A:452:SER:N	2.26	0.50
1:A:509:ILE:HG13	1:A:510:THR:N	2.26	0.50
1:B:390:ARG:HD2	1:B:408:GLU:OE2	2.12	0.50
2:C:256:VAL:HG13	2:C:257:ASP:N	2.27	0.50
2:C:323:THR:HG23	2:C:324:TYR:CD1	2.47	0.50
2:C:110:ARG:HD2	2:C:123:LEU:O	2.12	0.50
2:D:286:VAL:HG12	2:D:287:LYS:H	1.77	0.50
1:B:463:HIS:ND1	1:B:466:SER:OG	2.44	0.49
1:B:281:LEU:O	1:B:282:THR:C	2.54	0.49
2:C:259:LYS:HZ2	2:C:349:GLY:C	2.20	0.49
2:D:356:LYS:CA	2:D:363:TRP:HB3	2.38	0.49
2:D:51:PHE:HD2	2:D:248:TRP:HD1	1.60	0.49
2:D:51:PHE:HE2	2:D:397:LEU:HD11	1.77	0.49
2:D:147:ARG:NH1	2:D:200:SER:HB2	2.27	0.49
2:C:352:VAL:HG13	2:C:368:PHE:CD2	2.48	0.49
1:A:285:VAL:O	1:A:289:VAL:HG23	2.13	0.49
1:B:398:ILE:HD12	1:B:399:LYS:N	2.28	0.49
1:B:409:LYS:O	1:B:410:ARG:HD3	2.12	0.49
1:B:505:ALA:HB1	1:B:516:TYR:HA	1.94	0.49
2:C:105:GLY:HA3	2:C:194:THR:HB	1.95	0.49
2:C:115:LYS:HG3	2:C:118:GLU:HB2	1.95	0.49
2:D:294:VAL:HG21	2:D:327:PHE:HE2	1.78	0.49
1:B:352:SER:HB2	1:B:472:ILE:HG21	1.95	0.48
1:B:526:ASN:HA	1:B:529:ILE:HD12	1.95	0.48
2:D:347:LEU:O	2:D:349:GLY:N	2.45	0.48
2:D:390:ASP:O	2:D:392:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:304:ARG:HA	2:C:307:HIS:HB2	1.93	0.48
2:C:367:ARG:HD2	2:C:369:ARG:NH1	2.28	0.48
2:D:66:TYR:CE1	2:D:232:VAL:HG22	2.49	0.48
1:A:279:ASP:CG	1:A:282:THR:HB	2.38	0.48
1:A:315:ASP:OD2	1:A:334:GLU:OE2	2.30	0.48
2:D:114:LYS:O	2:D:115:LYS:C	2.57	0.48
1:A:310:PHE:CD2	1:A:426:VAL:CG1	2.97	0.48
1:A:519:LEU:HB2	1:B:268:ILE:HD11	1.94	0.48
2:D:293:TYR:CB	2:D:324:TYR:CD2	2.96	0.48
1:A:259:GLN:H	1:A:259:GLN:HE21	1.61	0.48
1:A:271:SER:C	1:A:273:LEU:H	2.21	0.48
1:A:289:VAL:HG12	1:A:516:TYR:OH	2.14	0.48
1:A:307:GLU:OE2	1:A:494:GLU:HB3	2.13	0.48
1:B:495:LEU:HD12	1:B:495:LEU:N	2.28	0.48
2:C:77:LEU:HB2	2:C:94:ILE:CD1	2.43	0.48
2:D:105:GLY:HA3	2:D:194:THR:OG1	2.13	0.48
2:C:287:LYS:HA	2:C:288:PRO:HD3	1.74	0.48
2:C:290:PHE:CE2	2:C:330:LEU:HB3	2.49	0.48
2:C:300:ASP:CG	2:C:374:ASN:HD22	2.22	0.48
2:D:27:LYS:HB3	2:D:39:PRO:O	2.14	0.48
2:D:112:PRO:HB2	2:D:113:GLN:HE21	1.79	0.48
2:D:213:VAL:HG12	2:D:214:ALA:H	1.79	0.48
2:D:264:ILE:CD1	2:D:288:PRO:HB2	2.44	0.48
1:A:462:ILE:HG22	1:A:463:HIS:N	2.28	0.48
2:C:136:GLN:HG3	2:C:147:ARG:HE	1.78	0.48
2:D:180:PRO:O	2:D:184:LEU:HB2	2.14	0.48
2:D:263:ASP:O	2:D:289:VAL:HB	2.14	0.48
1:B:354:TYR:O	1:B:358:ILE:HB	2.14	0.48
2:D:47:GLN:HB2	2:D:241:LYS:HA	1.96	0.48
2:D:198:LYS:HG2	2:D:199:ILE:H	1.77	0.48
1:A:431:ASN:HD22	1:A:431:ASN:C	2.22	0.47
2:D:327:PHE:O	2:D:328:ALA:HB2	2.13	0.47
1:B:248:ALA:O	2:C:312:PHE:HD1	1.97	0.47
2:D:28:MET:HA	2:D:31:CYS:SG	2.54	0.47
1:A:330:CYS:SG	1:B:326:VAL:HG11	2.54	0.47
1:A:448:GLN:HG3	1:A:449:SER:O	2.14	0.47
1:A:380:TYR:CG	1:A:445:TYR:HB3	2.50	0.47
1:B:462:ILE:HG23	1:B:469:ARG:HB2	1.95	0.47
1:B:497:ILE:HG23	1:B:497:ILE:O	2.13	0.47
2:C:261:ILE:HG22	2:C:262:LEU:N	2.29	0.47
2:D:193:THR:C	2:D:195:PHE:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:PHE:CD1	2:C:246:LEU:HD13	2.50	0.47
2:D:34:LEU:HD22	2:D:238:ALA:HB2	1.96	0.47
2:D:115:LYS:C	2:D:117:GLU:H	2.20	0.47
2:D:255:THR:O	2:D:256:VAL:HG23	2.14	0.47
1:A:259:GLN:HA	1:B:464:ASN:OD1	2.15	0.47
1:A:307:GLU:CD	1:A:494:GLU:HB3	2.39	0.47
1:A:408:GLU:OE1	1:A:410:ARG:HD3	2.15	0.47
1:B:416:LEU:CD2	1:B:427:LYS:HG3	2.44	0.47
2:D:62:ALA:HA	2:D:411:ARG:HH12	1.80	0.47
2:D:166:THR:O	2:D:167:SER:C	2.57	0.47
2:D:60:LEU:CD1	2:D:404:ILE:HG12	2.45	0.47
1:B:323:ASN:OD1	1:B:323:ASN:C	2.56	0.46
2:C:77:LEU:HB2	2:C:94:ILE:HD11	1.98	0.46
2:C:109:PRO:CG	2:C:180:PRO:HB2	2.37	0.46
2:D:153:CYS:HB2	2:D:173:LEU:HD13	1.97	0.46
1:A:310:PHE:CE2	1:A:426:VAL:CG1	2.99	0.46
1:A:397:ASP:HB3	1:A:402:ARG:H	1.79	0.46
1:A:462:ILE:HG12	1:A:469:ARG:HG3	1.97	0.46
1:A:530:ILE:HD11	1:B:272:PHE:CZ	2.50	0.46
2:C:131:GLY:HA3	2:C:148:TYR:CZ	2.50	0.46
2:D:27:LYS:NZ	2:D:98:ASN:HB2	2.29	0.46
2:D:56:VAL:HG11	2:D:400:ILE:HD13	1.96	0.46
2:D:77:LEU:HG	2:D:130:ASP:OD1	2.16	0.46
2:D:183:ASP:OD2	2:D:183:ASP:N	2.49	0.46
1:A:279:ASP:OD2	1:A:279:ASP:N	2.49	0.46
2:C:44:PRO:HG2	2:C:94:ILE:HD12	1.97	0.46
2:C:78:MET:HB3	2:C:129:LEU:CD2	2.45	0.46
2:D:252:GLN:O	2:D:253:GLU:C	2.58	0.46
2:D:293:TYR:HB3	2:D:324:TYR:CD2	2.51	0.46
1:B:282:THR:O	1:B:286:GLN:HG3	2.16	0.46
1:B:446:LYS:HZ2	1:B:446:LYS:CA	2.21	0.46
2:C:136:GLN:O	2:C:144:GLN:HA	2.16	0.46
2:D:351:ILE:HD11	2:D:374:ASN:HA	1.98	0.46
1:B:370:ILE:HA	1:B:460:SER:O	2.16	0.46
1:B:520:ILE:O	1:B:523:PHE:N	2.48	0.46
2:C:290:PHE:CD2	2:C:330:LEU:HB3	2.51	0.46
2:D:16:LEU:HA	2:D:101:TYR:HD2	1.80	0.46
2:D:38:LYS:HB2	2:D:39:PRO:HD3	1.97	0.46
2:D:133:LEU:HD21	2:D:146:LEU:HD11	1.98	0.46
1:B:292:THR:O	1:B:293:ILE:C	2.58	0.45
1:B:343:ILE:HD11	1:B:348:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:VAL:HG12	1:B:383:GLY:H	1.79	0.45
2:C:70:LYS:O	2:C:224:SER:HA	2.15	0.45
2:C:206:PHE:H	2:C:209:GLN:NE2	2.14	0.45
2:D:32:LYS:C	2:D:35:ASN:H	2.23	0.45
2:D:388:ILE:H	2:D:388:ILE:HG13	1.47	0.45
1:A:331:VAL:HG22	1:A:417:LEU:CD1	2.46	0.45
2:C:354:CYS:HB3	2:C:365:MET:HA	1.99	0.45
1:A:394:MET:CG	1:A:406:PHE:HD2	2.21	0.45
1:B:293:ILE:HD13	1:B:304:ILE:HD13	1.98	0.45
2:D:256:VAL:CG1	2:D:257:ASP:H	2.27	0.45
2:D:350:ARG:HD3	2:D:351:ILE:C	2.41	0.45
1:A:304:ILE:HD12	1:A:503:LEU:HG	1.98	0.45
1:A:312:VAL:HB	1:A:321:ARG:HG3	1.98	0.45
1:B:400:THR:HB	1:B:402:ARG:HG2	1.98	0.45
2:C:95:ASP:OD2	2:C:97:GLU:O	2.34	0.45
2:C:106:PHE:CZ	2:C:196:PRO:HD2	2.52	0.45
2:D:128:LEU:HB3	2:D:154:LEU:CD1	2.46	0.45
2:D:204:MET:HG3	2:D:205:ASP:H	1.80	0.45
2:D:207:SER:O	2:D:209:GLN:N	2.49	0.45
1:A:252:LYS:N	1:A:253:PRO:CD	2.79	0.45
1:A:292:THR:CG2	1:A:430:LEU:HD13	2.47	0.45
1:A:517:ALA:HB1	1:A:521:ARG:NH2	2.32	0.45
2:C:19:PRO:HB2	2:C:22:VAL:HG23	1.98	0.45
2:C:141:THR:HG22	2:C:143:LEU:HG	1.98	0.45
2:D:132:GLU:HB2	2:D:151:PHE:CE1	2.44	0.45
1:A:252:LYS:C	1:A:254:THR:H	2.25	0.45
1:B:379:VAL:HG12	1:B:451:ILE:CD1	2.47	0.45
2:C:127:THR:CG2	2:C:156:ILE:HD12	2.46	0.45
2:D:66:TYR:O	2:D:229:PHE:HA	2.16	0.45
2:C:192:CYS:HB2	2:C:195:PHE:CD2	2.52	0.45
2:C:295:TRP:HA	2:C:323:THR:O	2.17	0.45
1:A:499:THR:O	1:A:503:LEU:HB2	2.17	0.45
2:D:180:PRO:HG2	2:D:181:TYR:H	1.81	0.45
2:D:252:GLN:O	2:D:254:ASN:O	2.35	0.45
1:A:488:GLU:HG3	1:A:489:THR:H	1.82	0.45
1:B:504:ASN:O	1:B:507:ASP:N	2.49	0.45
1:A:305:GLU:OE2	1:A:409:LYS:CE	2.64	0.45
2:C:108:PHE:HA	2:C:109:PRO:HD3	1.58	0.44
2:D:165:PRO:O	2:D:166:THR:C	2.59	0.44
2:D:179:LYS:HD3	2:D:183:ASP:OD1	2.16	0.44
2:D:207:SER:C	2:D:209:GLN:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:257:ASP:HA	2:D:352:VAL:O	2.17	0.44
2:D:351:ILE:HD12	2:D:374:ASN:HA	1.98	0.44
1:A:354:TYR:CD2	1:A:355:ILE:HD13	2.52	0.44
1:A:520:ILE:HD13	1:A:520:ILE:HA	1.83	0.44
1:B:406:PHE:CD1	1:B:406:PHE:C	2.96	0.44
1:B:252:LYS:C	1:B:254:THR:N	2.75	0.44
1:B:464:ASN:C	1:B:466:SER:O	2.60	0.44
2:C:264:ILE:HD11	2:C:288:PRO:HB2	1.98	0.44
1:B:406:PHE:CZ	1:B:445:TYR:CE1	3.05	0.44
2:D:293:TYR:HB2	2:D:324:TYR:CD2	2.53	0.44
1:A:281:LEU:CD2	1:A:329:GLN:HG2	2.48	0.44
1:A:292:THR:HG22	1:A:430:LEU:HD13	1.99	0.44
2:C:176:GLU:O	2:C:180:PRO:HG3	2.18	0.44
2:C:253:GLU:O	2:C:255:THR:HG22	2.17	0.44
2:D:293:TYR:HB3	2:D:324:TYR:HD2	1.83	0.44
2:D:383:LYS:O	2:D:386:GLU:HB3	2.18	0.44
1:A:332:PHE:CE2	1:A:334:GLU:HB2	2.52	0.44
2:C:104:ASN:HB3	2:C:105:GLY:H	1.59	0.44
2:C:347:LEU:O	2:C:349:GLY:N	2.50	0.44
1:A:259:GLN:H	1:A:259:GLN:NE2	2.15	0.44
1:A:269:ASP:C	1:A:271:SER:H	2.26	0.44
1:A:528:THR:O	1:A:529:ILE:C	2.61	0.44
2:D:154:LEU:HD23	2:D:236:TYR:CD2	2.52	0.44
2:D:308:PHE:C	2:D:310:GLN:H	2.26	0.44
2:C:197:PHE:C	2:C:197:PHE:HD1	2.25	0.44
2:D:48:PRO:HB3	2:D:245:LEU:HG	1.99	0.44
2:D:109:PRO:HB2	2:D:110:ARG:H	1.56	0.44
2:D:141:THR:HG22	2:D:143:LEU:HG	1.99	0.44
1:A:247:TRP:CH2	2:D:341:LYS:HG2	2.51	0.43
1:B:406:PHE:CD2	1:B:442:PRO:HG3	2.53	0.43
2:C:214:ALA:HA	2:C:217:LEU:HB2	1.99	0.43
2:C:226:GLY:HA3	2:C:248:TRP:O	2.18	0.43
2:C:295:TRP:O	2:C:377:HIS:HA	2.17	0.43
2:D:73:GLY:O	2:D:132:GLU:OE2	2.36	0.43
1:A:394:MET:CG	1:A:406:PHE:CD2	2.99	0.43
1:B:407:ILE:HG13	1:B:409:LYS:N	2.33	0.43
1:A:284:SER:O	1:A:287:ASP:N	2.52	0.43
1:B:272:PHE:O	1:B:272:PHE:CG	2.72	0.43
1:B:339:LEU:C	1:B:339:LEU:CD2	2.81	0.43
2:C:17:ILE:HD13	2:C:99:ASN:HB3	1.98	0.43
2:C:135:ILE:N	2:C:135:ILE:CD1	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LYS:O	1:A:353:LYS:HG2	2.18	0.43
1:B:487:SER:O	1:B:488:GLU:HB2	2.18	0.43
2:D:352:VAL:HG13	2:D:368:PHE:CD2	2.52	0.43
1:A:462:ILE:HD11	1:B:258:LEU:HD21	2.01	0.43
2:C:259:LYS:NZ	2:C:349:GLY:HA2	2.33	0.43
2:C:319:ILE:HG13	2:C:320:LEU:H	1.83	0.43
1:A:250:LYS:HG3	2:D:310:GLN:HG3	2.00	0.43
1:A:255:ILE:CA	1:A:258:LEU:HB3	2.36	0.43
1:B:273:LEU:HD23	1:B:273:LEU:HA	1.41	0.43
2:C:129:LEU:HA	2:C:153:CYS:HA	2.01	0.43
1:A:313:ILE:HG12	1:A:339:LEU:HD12	2.01	0.43
1:B:445:TYR:HD2	1:B:445:TYR:HA	1.72	0.43
1:B:513:SER:O	1:B:514:LYS:C	2.61	0.43
2:C:318:GLU:O	2:C:321:GLU:CG	2.66	0.43
2:D:13:ILE:HD12	2:D:74:LEU:HD21	2.00	0.43
2:D:366:LEU:HD23	2:D:366:LEU:N	2.33	0.43
1:A:436:VAL:HA	1:A:437:PRO:HD2	1.94	0.43
2:C:67:VAL:HG21	2:C:210:LEU:HD23	2.01	0.43
2:C:156:ILE:HG12	2:C:176:GLU:CB	2.49	0.43
2:D:358:GLN:C	2:D:360:THR:H	2.27	0.43
1:A:395:SER:HB2	1:A:404:GLY:N	2.31	0.42
1:B:300:LEU:C	1:B:302:SER:N	2.77	0.42
2:C:259:LYS:HZ3	2:C:351:ILE:CD1	2.32	0.42
2:D:13:ILE:CG1	2:D:14:PRO:HD2	2.42	0.42
2:D:129:LEU:HD23	2:D:129:LEU:N	2.34	0.42
1:A:467:CYS:HB3	1:A:498:ASN:HB3	2.00	0.42
2:C:128:LEU:N	2:C:155:ALA:HB3	2.32	0.42
2:D:20:GLY:O	2:D:23:THR:HB	2.18	0.42
2:D:128:LEU:HD23	2:D:154:LEU:HD11	2.02	0.42
2:D:326:LYS:HD2	2:D:326:LYS:O	2.19	0.42
2:D:347:LEU:HA	2:D:347:LEU:HD23	1.84	0.42
1:A:488:GLU:CG	1:A:489:THR:H	2.32	0.42
1:B:246:ILE:HD13	2:C:344:GLU:CG	2.49	0.42
1:B:301:ARG:HG2	1:B:503:LEU:HD21	2.00	0.42
1:B:329:GLN:CG	1:B:330:CYS:N	2.82	0.42
1:A:288:TRP:O	1:A:289:VAL:C	2.62	0.42
1:A:417:LEU:CD2	1:A:428:ILE:HD12	2.49	0.42
1:B:420:PRO:C	1:B:422:ASP:H	2.28	0.42
2:C:207:SER:C	2:C:209:GLN:H	2.26	0.42
2:D:26:LEU:HA	2:D:29:MET:HB2	2.01	0.42
2:D:119:LEU:HD13	2:D:184:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:241:LYS:H	2:D:241:LYS:HG3	1.69	0.42
2:D:397:LEU:C	2:D:399:GLU:H	2.27	0.42
1:B:307:GLU:CD	1:B:494:GLU:HB3	2.45	0.42
1:B:439:ASN:C	1:B:441:PRO:HD2	2.45	0.42
1:B:509:ILE:CG2	1:B:510:THR:H	2.26	0.42
2:D:290:PHE:CE2	2:D:330:LEU:HB3	2.54	0.42
1:A:285:VAL:H	1:A:285:VAL:HG23	1.47	0.42
1:A:305:GLU:HB3	1:A:431:ASN:HD21	1.79	0.42
1:A:466:SER:HB2	1:A:522:THR:OG1	2.20	0.42
1:B:374:GLN:HA	1:B:456:LYS:O	2.19	0.42
1:B:502:LEU:HA	1:B:519:LEU:HD21	2.02	0.42
1:A:285:VAL:HG11	1:A:524:LEU:HD21	2.02	0.42
1:B:251:TRP:CE3	2:C:350:ARG:HB2	2.55	0.42
1:B:393:ARG:HD2	1:B:409:LYS:CB	2.50	0.42
1:B:498:ASN:ND2	1:B:500:PRO:HD2	2.35	0.42
2:D:183:ASP:C	2:D:185:ARG:H	2.27	0.42
2:D:188:TYR:C	2:D:190:ASN:H	2.28	0.42
1:A:376:ARG:NH2	1:A:398:ILE:HG22	2.35	0.42
2:C:80:ILE:HG21	2:C:108:PHE:CD1	2.55	0.42
2:C:259:LYS:NZ	2:C:349:GLY:CA	2.83	0.42
1:B:313:ILE:HG12	1:B:339:LEU:HD12	2.01	0.42
2:D:26:LEU:HD21	2:D:92:PHE:CZ	2.55	0.42
2:D:234:ALA:HA	2:D:235:PRO:HD3	1.89	0.42
1:B:315:ASP:HB2	1:B:322:VAL:CG2	2.50	0.41
2:C:400:ILE:HG22	2:C:400:ILE:O	2.20	0.41
2:D:23:THR:O	2:D:24:GLN:C	2.62	0.41
2:D:119:LEU:HA	2:D:122:THR:OG1	2.20	0.41
2:D:155:ALA:HA	2:D:161:LEU:H	1.85	0.41
2:D:198:LYS:C	2:D:199:ILE:HD12	2.45	0.41
2:D:256:VAL:HG11	2:D:381:VAL:HG22	2.02	0.41
2:D:293:TYR:CD2	2:D:324:TYR:HB3	2.54	0.41
1:A:342:ASN:CG	1:A:490:THR:HG23	2.45	0.41
1:A:462:ILE:CG2	1:A:463:HIS:H	2.32	0.41
1:A:533:LYS:HG3	1:A:537:LEU:CD1	2.50	0.41
1:B:246:ILE:HD12	1:B:247:TRP:N	2.28	0.41
1:B:509:ILE:HG23	1:B:510:THR:N	2.31	0.41
2:C:85:VAL:HG12	2:C:86:THR:HG23	2.02	0.41
2:D:287:LYS:HA	2:D:288:PRO:HD3	1.84	0.41
1:A:463:HIS:CE1	1:B:272:PHE:HA	2.55	0.41
2:D:166:THR:HB	2:D:232:VAL:O	2.20	0.41
2:D:344:GLU:HG2	2:D:345:GLN:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ILE:HG13	1:A:425:ASP:HB3	2.02	0.41
1:B:252:LYS:HG2	2:C:308:PHE:CZ	2.55	0.41
1:B:538:SER:O	1:B:539:TYR:CG	2.74	0.41
1:A:397:ASP:OD1	1:A:399:LYS:HG3	2.21	0.41
1:B:251:TRP:CD2	1:B:253:PRO:HG2	2.56	0.41
2:C:208:TYR:HD1	2:C:208:TYR:O	2.03	0.41
2:D:258:PHE:HE2	2:D:294:VAL:HG13	1.85	0.41
2:D:351:ILE:CG2	2:D:374:ASN:O	2.69	0.41
2:D:384:VAL:O	2:D:388:ILE:HG13	2.20	0.41
1:A:273:LEU:HB3	1:A:275:ILE:HG12	2.02	0.41
1:A:321:ARG:NH2	1:A:425:ASP:OD1	2.54	0.41
2:D:171:ALA:O	2:D:175:LYS:HG2	2.21	0.41
1:B:279:ASP:OD2	1:B:279:ASP:N	2.54	0.41
1:B:312:VAL:O	1:B:313:ILE:C	2.64	0.41
1:B:519:LEU:HD12	1:B:519:LEU:C	2.42	0.41
2:C:38:LYS:H	2:C:38:LYS:HG2	1.69	0.41
1:B:532:ARG:O	1:B:533:LYS:C	2.64	0.41
2:C:262:LEU:HD12	2:C:348:ASN:HA	2.02	0.41
2:D:213:VAL:CG1	2:D:214:ALA:N	2.77	0.41
1:A:286:GLN:O	1:A:287:ASP:C	2.62	0.41
2:C:71:THR:HG22	2:C:222:HIS:CD2	2.56	0.41
2:D:83:ASN:C	2:D:85:VAL:N	2.79	0.41
1:A:414:GLN:NE2	1:A:427:LYS:HD2	2.36	0.41
1:B:250:LYS:O	1:B:252:LYS:HD2	2.20	0.41
1:B:476:GLU:HA	1:B:489:THR:HG22	2.01	0.41
2:C:44:PRO:HD3	2:C:98:ASN:ND2	2.36	0.41
2:C:152:ASP:OD2	2:C:236:TYR:CD1	2.74	0.41
2:C:190:ASN:C	2:C:192:CYS:H	2.29	0.41
2:D:410:GLU:HG2	2:D:414:ASN:ND2	2.36	0.41
1:A:271:SER:HB2	1:B:529:ILE:HD11	2.02	0.40
1:A:355:ILE:HA	1:A:358:ILE:HG22	2.03	0.40
1:A:355:ILE:O	1:A:359:SER:HB3	2.21	0.40
1:B:252:LYS:O	1:B:254:THR:N	2.54	0.40
1:B:354:TYR:CD2	1:B:533:LYS:HD2	2.56	0.40
2:D:350:ARG:HD3	2:D:351:ILE:O	2.20	0.40
1:A:290:TYR:HB2	1:A:516:TYR:HE2	1.84	0.40
2:C:106:PHE:CE2	2:C:196:PRO:HD2	2.56	0.40
2:C:347:LEU:CD2	2:C:350:ARG:HG2	2.51	0.40
2:D:178:PHE:O	2:D:179:LYS:C	2.64	0.40
2:D:295:TRP:HZ3	2:D:298:GLY:HA2	1.87	0.40
1:A:251:TRP:NE1	1:A:253:PRO:C	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ALA:HB2	1:A:515:GLU:HG2	2.04	0.40
1:B:406:PHE:HZ	1:B:445:TYR:CE1	2.39	0.40
1:A:506:PHE:CD2	1:A:506:PHE:C	3.00	0.40
1:B:374:GLN:O	1:B:398:ILE:CG1	2.69	0.40
2:C:256:VAL:CG1	2:C:257:ASP:N	2.85	0.40
2:D:60:LEU:HD11	2:D:404:ILE:HG12	2.04	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	268/310 (86%)	195 (73%)	46 (17%)	27 (10%)	0	2
1	B	268/310 (86%)	192 (72%)	48 (18%)	28 (10%)	0	2
2	C	383/461 (83%)	287 (75%)	68 (18%)	28 (7%)	1	4
2	D	383/461 (83%)	280 (73%)	69 (18%)	34 (9%)	0	3
All	All	1302/1542 (84%)	954 (73%)	231 (18%)	117 (9%)	0	3

All (117) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	ASP
1	A	286	GLN
1	A	336	ASP
1	A	342	ASN
1	B	279	ASP
1	B	289	VAL
1	B	291	ALA
1	B	301	ARG
1	B	342	ASN

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Mol	Chain	Res	Type
1	B	440	ASP
1	B	447	SER
1	B	509	ILE
1	B	510	THR
2	C	109	PRO
2	C	118	GLU
2	C	203	HIS
2	C	232	VAL
2	C	233	LYS
2	C	238	ALA
2	C	376	ASN
2	C	392	VAL
2	D	16	LEU
2	D	104	ASN
2	D	109	PRO
2	D	118	GLU
2	D	194	THR
2	D	217	LEU
2	D	348	ASN
2	D	401	VAL
1	A	271	SER
1	A	285	VAL
1	A	289	VAL
1	A	322	VAL
1	A	325	PRO
1	A	446	LYS
1	A	509	ILE
1	B	254	THR
1	B	290	TYR
1	B	336	ASP
2	C	19	PRO
2	C	87	GLY
2	C	88	GLU
2	C	176	GLU
2	C	288	PRO
2	C	311	PRO
2	C	320	LEU
2	C	330	LEU
2	C	331	SER
2	D	86	THR
2	D	167	SER
2	D	208	TYR

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Mol	Chain	Res	Type
2	D	214	ALA
2	D	311	PRO
1	A	288	TRP
1	A	498	ASN
1	B	253	PRO
1	B	273	LEU
1	B	313	ILE
1	B	498	ASN
1	B	511	ASN
2	C	39	PRO
2	C	104	ASN
2	C	208	TYR
2	C	236	TYR
2	C	373	LEU
2	C	396	ASP
2	D	116	LYS
2	D	166	THR
2	D	252	GLN
2	D	288	PRO
2	D	314	ARG
2	D	330	LEU
2	D	356	LYS
2	D	359	GLU
2	D	393	SER
1	A	324	PRO
1	A	333	THR
1	A	405	GLN
1	A	441	PRO
1	A	528	THR
1	B	281	LEU
1	B	282	THR
1	B	421	LYS
1	B	517	ALA
1	B	528	THR
2	C	113	GLN
2	C	171	ALA
2	C	314	ARG
2	D	184	LEU
2	D	192	CYS
2	D	203	HIS
2	D	253	GLU
2	D	371	ASP

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Mol	Chain	Res	Type
1	A	284	SER
1	A	319	PRO
1	A	365	THR
1	A	437	PRO
1	A	510	THR
1	B	382	VAL
2	C	213	VAL
2	C	367	ARG
2	D	309	ASP
2	D	322	ARG
1	A	382	VAL
1	B	270	PRO
2	D	60	LEU
2	D	115	LYS
2	D	213	VAL
2	D	236	TYR
1	A	412	VAL
1	B	529	ILE
1	A	403	VAL
1	B	361	VAL
1	B	412	VAL
2	D	48	PRO
1	B	322	VAL
1	A	500	PRO

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	254/290 (88%)	200 (79%)	54 (21%)	1	6
1	B	254/290 (88%)	206 (81%)	48 (19%)	1	9
2	C	352/421 (84%)	278 (79%)	74 (21%)	1	6
2	D	352/421 (84%)	278 (79%)	74 (21%)	1	6
All	All	1212/1422 (85%)	962 (79%)	250 (21%)	1	7

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	ILE
1	A	252	LYS
1	A	254	THR
1	A	255	ILE
1	A	258	LEU
1	A	259	GLN
1	A	261	ILE
1	A	279	ASP
1	A	281	LEU
1	A	282	THR
1	A	287	ASP
1	A	293	ILE
1	A	295	SER
1	A	296	ILE
1	A	303	PHE
1	A	309	LYS
1	A	312	VAL
1	A	313	ILE
1	A	322	VAL
1	A	327	SER
1	A	331	VAL
1	A	335	LEU
1	A	338	HIS
1	A	343	ILE
1	A	353	LYS
1	A	358	ILE
1	A	365	THR
1	A	367	LYS
1	A	373	SER
1	A	374	GLN
1	A	396	THR
1	A	399	LYS
1	A	400	THR
1	A	410	ARG
1	A	412	VAL
1	A	417	LEU
1	A	431	ASN
1	A	437	PRO
1	A	446	LYS
1	A	448	GLN
1	A	455	THR
1	A	462	ILE

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Mol	Chain	Res	Type
1	A	473	THR
1	A	497	ILE
1	A	498	ASN
1	A	502	LEU
1	A	503	LEU
1	A	507	ASP
1	A	508	ASN
1	A	509	ILE
1	A	514	LYS
1	A	522	THR
1	A	533	LYS
1	A	536	SER
1	B	246	ILE
1	B	252	LYS
1	B	258	LEU
1	B	279	ASP
1	B	282	THR
1	B	284	SER
1	B	292	THR
1	B	293	ILE
1	B	300	LEU
1	B	303	PHE
1	B	313	ILE
1	B	322	VAL
1	B	327	SER
1	B	335	LEU
1	B	343	ILE
1	B	353	LYS
1	B	358	ILE
1	B	361	VAL
1	B	364	ASN
1	B	365	THR
1	B	367	LYS
1	B	381	ARG
1	B	395	SER
1	B	400	THR
1	B	405	GLN
1	B	407	ILE
1	B	419	SER
1	B	426	VAL
1	B	429	SER
1	B	431	ASN

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Mol	Chain	Res	Type
1	B	436	VAL
1	B	439	ASN
1	B	441	PRO
1	B	443	GLU
1	B	444	LYS
1	B	446	LYS
1	B	447	SER
1	B	451	ILE
1	B	462	ILE
1	B	466	SER
1	B	468	THR
1	B	488	GLU
1	B	499	THR
1	B	508	ASN
1	B	510	THR
1	B	519	LEU
1	B	522	THR
1	B	533	LYS
2	C	17	ILE
2	C	33	LEU
2	C	38	LYS
2	C	41	LYS
2	C	52	GLN
2	C	64	ASP
2	C	67	VAL
2	C	75	ARG
2	C	76	VAL
2	C	77	LEU
2	C	80	ILE
2	C	82	ILE
2	C	102	LEU
2	C	103	VAL
2	C	104	ASN
2	C	110	ARG
2	C	111	LEU
2	C	117	GLU
2	C	119	LEU
2	C	123	LEU
2	C	129	LEU
2	C	135	ILE
2	C	137	THR
2	C	144	GLN

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Mol	Chain	Res	Type
2	C	146	LEU
2	C	151	PHE
2	C	154	LEU
2	C	156	ILE
2	C	163	GLN
2	C	175	LYS
2	C	179	LYS
2	C	191	ARG
2	C	203	HIS
2	C	204	MET
2	C	211	VAL
2	C	227	LEU
2	C	228	ILE
2	C	251	GLU
2	C	252	GLN
2	C	254	ASN
2	C	255	THR
2	C	256	VAL
2	C	259	LYS
2	C	260	LEU
2	C	264	ILE
2	C	284	TYR
2	C	286	VAL
2	C	289	VAL
2	C	290	PHE
2	C	292	LEU
2	C	300	ASP
2	C	306	LYS
2	C	308	PHE
2	C	310	GLN
2	C	326	LYS
2	C	327	PHE
2	C	329	GLU
2	C	343	LEU
2	C	347	LEU
2	C	350	ARG
2	C	351	ILE
2	C	352	VAL
2	C	363	TRP
2	C	365	MET
2	C	366	LEU
2	C	370	ASP

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Mol	Chain	Res	Type
2	C	382	GLN
2	C	385	LEU
2	C	388	ILE
2	C	389	ASN
2	C	392	VAL
2	C	393	SER
2	C	404	ILE
2	C	415	MET
2	D	12	GLU
2	D	17	ILE
2	D	21	ASN
2	D	33	LEU
2	D	38	LYS
2	D	40	THR
2	D	50	SER
2	D	52	GLN
2	D	56	VAL
2	D	60	LEU
2	D	67	VAL
2	D	69	GLU
2	D	71	THR
2	D	77	LEU
2	D	80	ILE
2	D	81	VAL
2	D	86	THR
2	D	103	VAL
2	D	104	ASN
2	D	110	ARG
2	D	111	LEU
2	D	119	LEU
2	D	123	LEU
2	D	132	GLU
2	D	135	ILE
2	D	143	LEU
2	D	144	GLN
2	D	146	LEU
2	D	150	MET
2	D	154	LEU
2	D	159	ARG
2	D	164	SER
2	D	175	LYS
2	D	183	ASP

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Mol	Chain	Res	Type
2	D	184	LEU
2	D	193	THR
2	D	204	MET
2	D	213	VAL
2	D	218	ASP
2	D	227	LEU
2	D	228	ILE
2	D	230	THR
2	D	233	LYS
2	D	237	THR
2	D	251	GLU
2	D	252	GLN
2	D	259	LYS
2	D	260	LEU
2	D	262	LEU
2	D	264	ILE
2	D	289	VAL
2	D	292	LEU
2	D	296	GLN
2	D	306	LYS
2	D	310	GLN
2	D	319	ILE
2	D	329	GLU
2	D	330	LEU
2	D	337	TRP
2	D	343	LEU
2	D	350	ARG
2	D	354	CYS
2	D	364	GLU
2	D	366	LEU
2	D	370	ASP
2	D	371	ASP
2	D	382	GLN
2	D	384	VAL
2	D	385	LEU
2	D	388	ILE
2	D	389	ASN
2	D	397	LEU
2	D	404	ILE
2	D	415	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	GLN
1	A	274	ASN
1	A	286	GLN
1	A	374	GLN
1	A	405	GLN
1	A	411	HIS
1	A	414	GLN
1	A	431	ASN
1	A	448	GLN
1	A	498	ASN
1	A	508	ASN
1	B	323	ASN
1	B	405	GLN
1	B	414	GLN
1	B	431	ASN
1	B	464	ASN
1	B	498	ASN
2	C	35	ASN
2	C	47	GLN
2	C	63	HIS
2	C	83	ASN
2	C	89	GLN
2	C	98	ASN
2	C	99	ASN
2	C	209	GLN
2	C	252	GLN
2	C	339	ASN
2	C	374	ASN
2	C	382	GLN
2	D	21	ASN
2	D	47	GLN
2	D	83	ASN
2	D	98	ASN
2	D	104	ASN
2	D	113	GLN
2	D	163	GLN
2	D	252	GLN
2	D	339	ASN
2	D	357	ASN
2	D	414	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	276/310 (89%)	-1.27	0 100 100	24, 55, 112, 145	0
1	B	276/310 (89%)	-1.28	0 100 100	19, 53, 100, 156	0
2	C	387/461 (83%)	-1.20	0 100 100	46, 92, 123, 154	0
2	D	387/461 (83%)	-1.18	0 100 100	50, 91, 124, 155	0
All	All	1326/1542 (85%)	-1.22	0 100 100	19, 80, 121, 156	0

There are no RSRZ outliers to report.

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.