W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2017 – 03:20 am GMT

PDB ID	:	2J04
Title	:	THE TAU60-TAU91 SUBCOMPLEX OF YEAST TRANSCRIPTION FACTOR IIIC
Authors	:	Mylona, A.; Fernandez-Tornero, C.; Legrand, P.; Muller, C.W.
Deposited on	:	2006-07-31
Resolution	:	3.20 Å(reported)

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

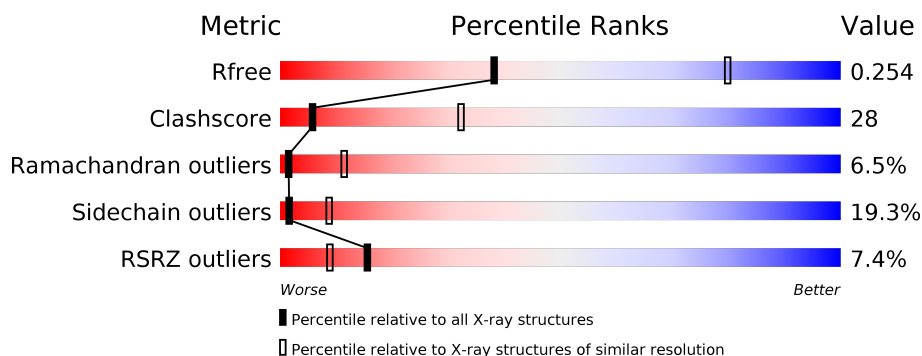|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 3.20 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	Percentile Ranks	Value
Rfree		0.254
Clashscore		28
Ramachandran outliers		6.5%
Sidechain outliers		19.3%
RSRZ outliers		7.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	588	7% — 52% / 34% / 11% / •
1	C	588	7% — 48% / 36% / 13% / •
2	B	524	7% — 43% / 32% / 13% / • / 10%
2	D	524	6% — 43% / 33% / 12% / • / 10%

2 Entity composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 16935 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 HYPOTHETICAL PROTEIN YPL007C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4760	3058	777	902	23			
1	C	586	Total	C	N	O	S	0	0	0
			4751	3052	775	901	23			

- Molecule 2 is a protein called YDR362CP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	472	Total	C	N	O	S	0	0	1
			3715	2384	613	703	15			
2	D	469	Total	C	N	O	S	0	0	1
			3704	2379	609	701	15			

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	1	Total	O	0	0
			1	1		
3	C	1	Total	O	0	0
			1	1		
3	D	1	Total	O	0	0
			1	1		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
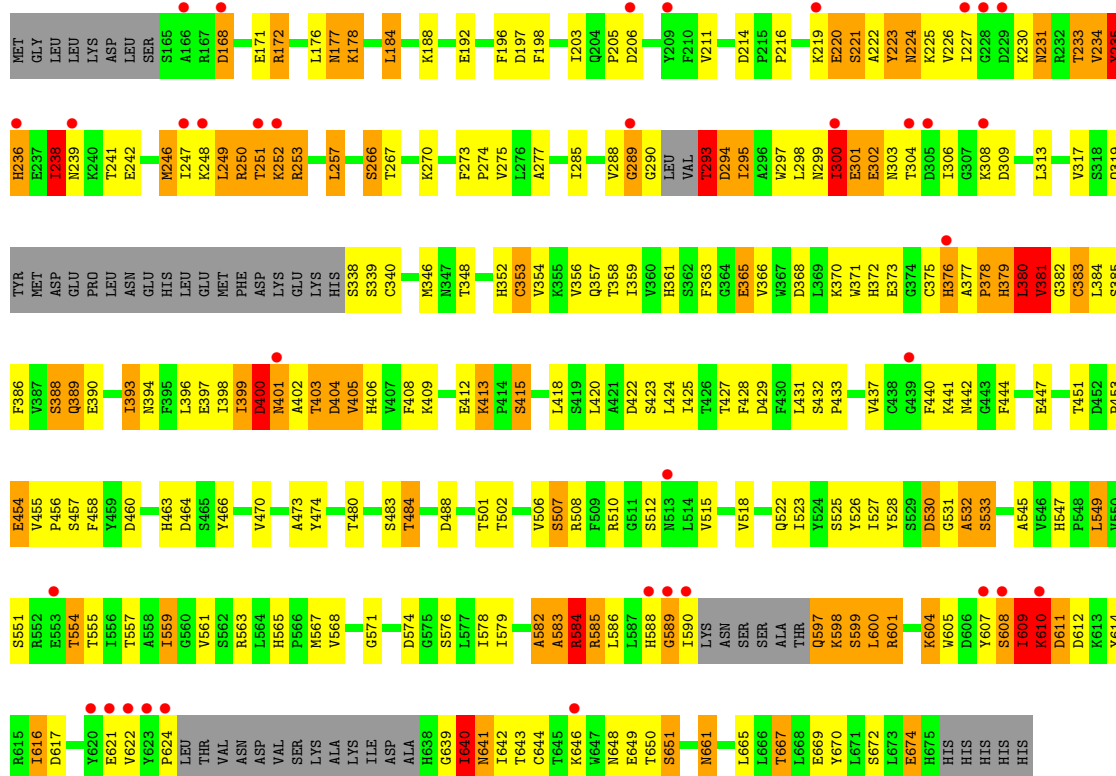
• Molecule 1: HYPOTHETICAL PROTEIN YPL007C
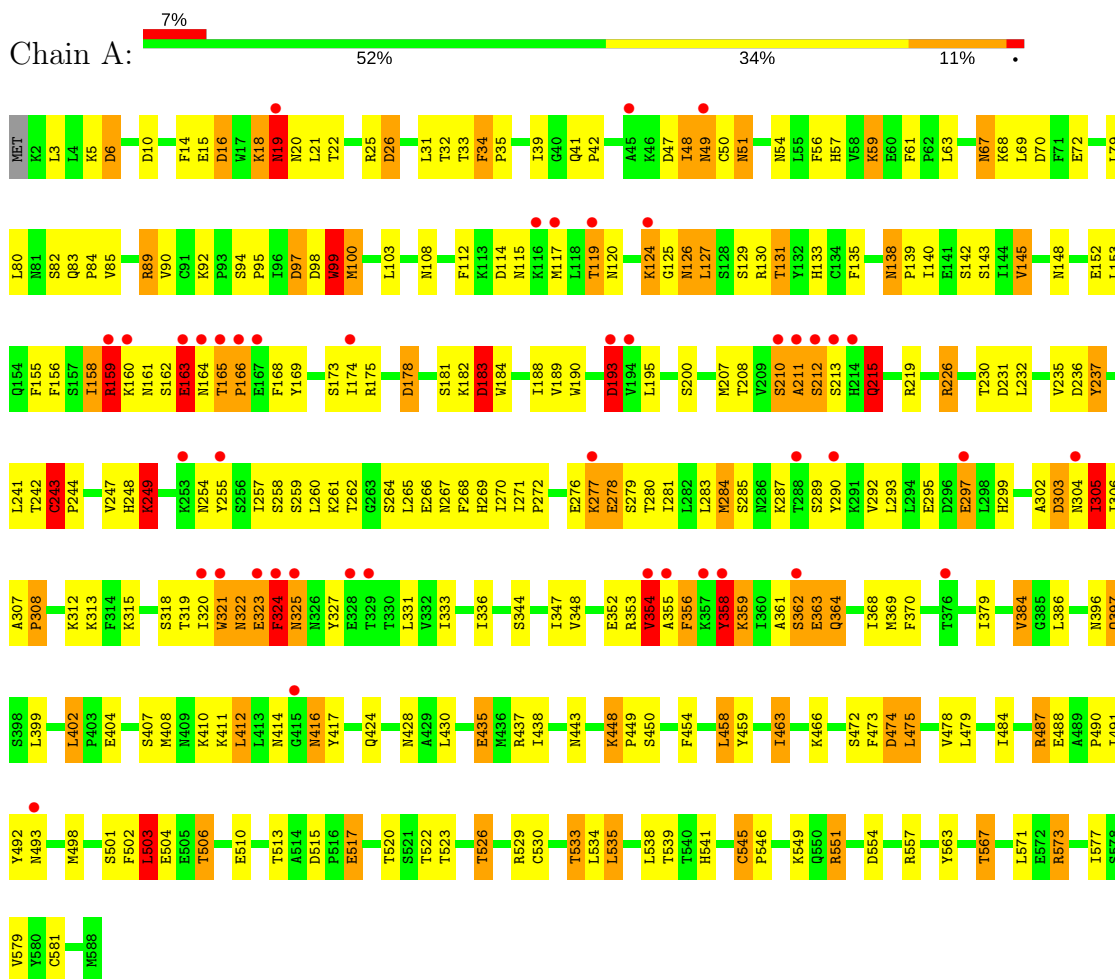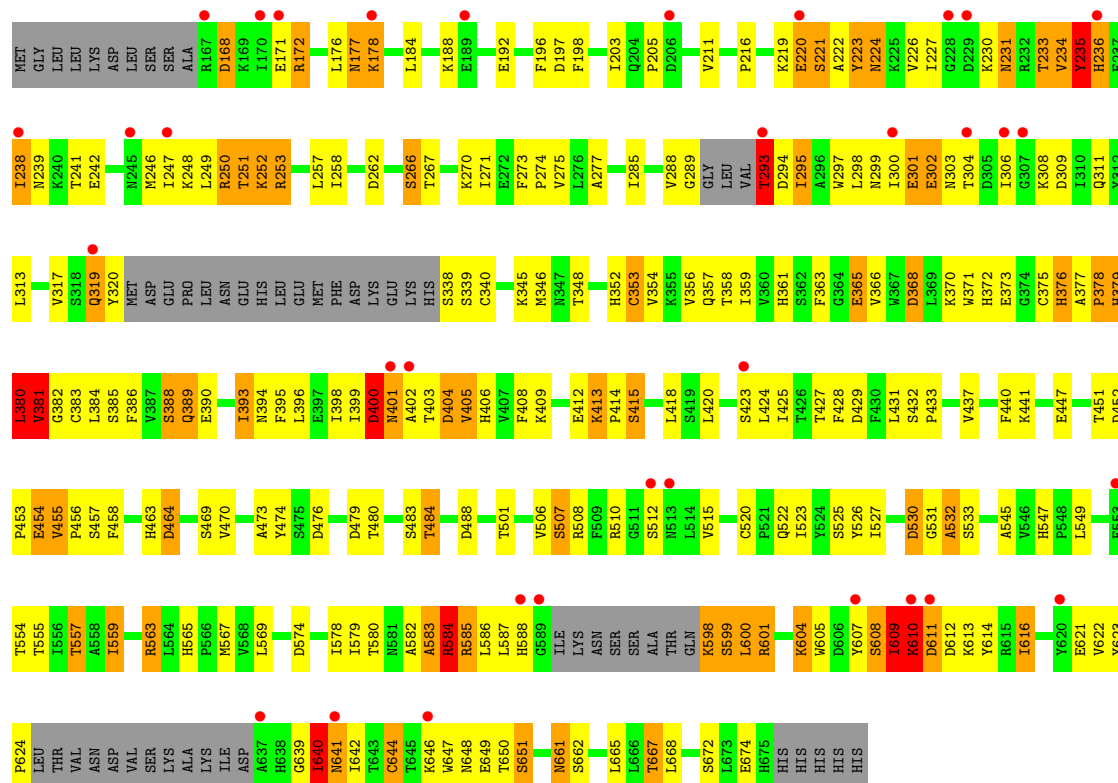

• Molecule 1: HYPOTHETICAL PROTEIN YPL007C

- Molecule 2: YDR362CP

Chain B:

- Molecule 2: YDR362CP

Chain D:
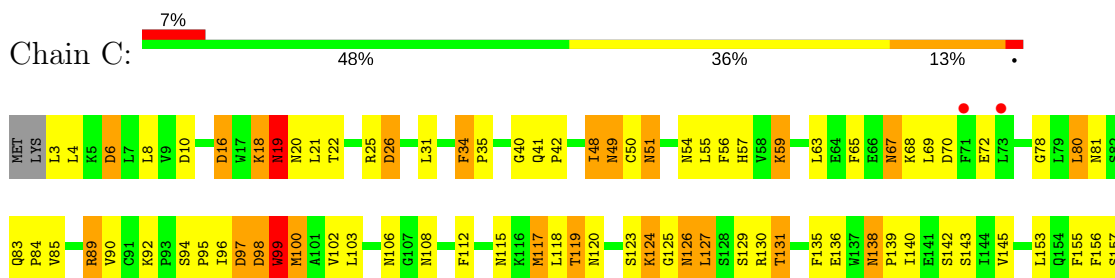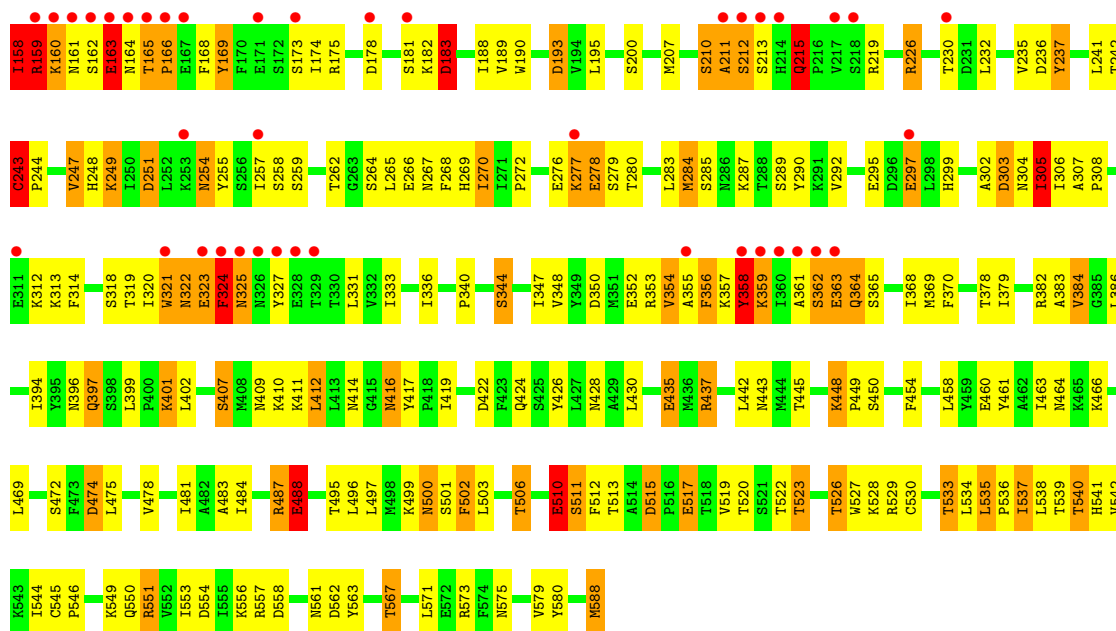
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.42Å 125.80Å 210.47Å 90.00° 94.49° 90.00°	Depositor
Resolution (Å)	208.51 – 3.20 34.91 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (208.51-3.20) 98.8 (34.91-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.212 , 0.257 0.209 , 0.254	Depositor DCC
R_{free} test set	2619 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	77.5	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 130.4	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16935	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.83	5/4872 (0.1%)	0.94	15/6610 (0.2%)
1	C	0.80	5/4863 (0.1%)	0.95	16/6599 (0.2%)
2	B	0.76	4/3798 (0.1%)	0.98	21/5153 (0.4%)
2	D	0.77	4/3788 (0.1%)	0.95	15/5140 (0.3%)
All	All	0.79	18/17321 (0.1%)	0.95	67/23502 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	3
2	B	0	8
2	D	0	7
All	All	0	20

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	413	LYS	CD-CE	18.55	1.97	1.51
2	B	413	LYS	CD-CE	14.62	1.87	1.51
1	A	249	LYS	CD-CE	13.65	1.85	1.51
1	A	297	GLU	CD-OE1	11.57	1.38	1.25
1	C	249	LYS	CD-CE	11.35	1.79	1.51
2	D	413	LYS	CE-NZ	11.08	1.76	1.49
2	B	413	LYS	CE-NZ	10.30	1.74	1.49
1	A	297	GLU	CD-OE2	9.99	1.36	1.25
2	D	320	TYR	C-O	9.52	1.41	1.23
1	C	297	GLU	CD-OE1	7.97	1.34	1.25
1	C	297	GLU	CD-OE2	7.27	1.33	1.25
2	D	413	LYS	CG-CD	6.40	1.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	ILE	CA-CB	6.39	1.69	1.54
1	A	510	GLU	CD-OE1	6.11	1.32	1.25
2	B	413	LYS	CG-CD	5.47	1.71	1.52
1	C	99	TRP	CB-CG	-5.38	1.40	1.50
1	A	249	LYS	CE-NZ	5.27	1.62	1.49
1	C	488	GLU	CG-CD	5.25	1.59	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	413	LYS	CD-CE-NZ	-8.44	92.29	111.70
2	B	413	LYS	CD-CE-NZ	-8.38	92.42	111.70
2	D	413	LYS	CG-CD-CE	-7.55	89.24	111.90
1	C	6	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	231	ASP	CB-CG-OD2	7.00	124.60	118.30
2	B	168	ASP	CB-CG-OD2	7.00	124.60	118.30
1	C	474	ASP	CB-CG-OD2	6.90	124.51	118.30
1	C	183	ASP	CB-CG-OD2	6.79	124.41	118.30
2	D	429	ASP	CB-CG-OD2	6.71	124.34	118.30
2	D	197	ASP	CB-CG-OD2	6.62	124.26	118.30
1	C	98	ASP	CB-CG-OD2	6.51	124.16	118.30
1	C	554	ASP	CB-CG-OD2	6.41	124.07	118.30
1	C	350	ASP	CB-CG-OD2	6.36	124.02	118.30
1	C	16	ASP	CB-CG-OD2	6.34	124.00	118.30
2	B	599	SER	N-CA-C	6.31	128.04	111.00
2	B	413	LYS	CG-CD-CE	-6.23	93.21	111.90
1	C	558	ASP	CB-CG-OD2	6.20	123.88	118.30
1	C	26	ASP	CB-CG-OD2	6.19	123.87	118.30
2	B	400	ASP	CB-CG-OD2	6.16	123.84	118.30
2	B	197	ASP	CB-CG-OD2	6.11	123.80	118.30
2	D	400	ASP	CB-CG-OD2	5.92	123.62	118.30
2	B	674	GLU	O-C-N	-5.74	113.51	122.70
2	D	368	ASP	CB-CG-OD2	5.69	123.42	118.30
2	B	460	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	193	ASP	CB-CG-OD2	5.61	123.35	118.30
2	B	404	ASP	CB-CG-OD2	5.61	123.34	118.30
2	D	599	SER	N-CA-C	5.57	126.04	111.00
2	B	617	ASP	CB-CG-OD2	5.54	123.29	118.30
2	B	429	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	183	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	422	ASP	CB-CG-OD2	5.53	123.28	118.30
2	D	464	ASP	CB-CG-OD2	5.53	123.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	380	LEU	N-CA-C	5.50	125.85	111.00
2	D	479	ASP	CB-CG-OD2	5.47	123.23	118.30
1	C	562	ASP	CB-CG-OD2	5.47	123.22	118.30
2	B	206	ASP	CB-CG-OD2	5.47	123.22	118.30
2	D	380	LEU	N-CA-C	5.46	125.74	111.00
2	D	476	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	6	ASP	CB-CG-OD2	5.45	123.21	118.30
1	A	503	LEU	CA-CB-CG	5.44	127.81	115.30
2	B	589	GLY	N-CA-C	5.43	126.68	113.10
1	A	193	ASP	CB-CG-OD2	5.43	123.18	118.30
2	D	168	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	515	ASP	CB-CG-OD2	5.39	123.16	118.30
2	B	309	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	10	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	243	CYS	CA-CB-SG	-5.35	104.37	114.00
1	A	114	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	554	ASP	CB-CG-OD2	5.33	123.09	118.30
2	B	585	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	16	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	474	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	510	GLU	CB-CA-C	-5.28	99.83	110.40
2	B	214	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	26	ASP	CB-CG-OD2	5.24	123.01	118.30
2	D	309	ASP	CB-CG-OD2	5.23	123.00	118.30
2	D	530	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	251	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	422	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	178	ASP	CB-CG-OD2	5.14	122.93	118.30
2	B	249	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	47	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	40	GLY	N-CA-C	-5.11	100.32	113.10
2	B	530	ASP	CB-CG-OD2	5.07	122.86	118.30
2	D	452	ASP	CB-CG-OD2	5.04	122.83	118.30
2	B	294	ASP	N-CA-C	5.03	124.58	111.00
1	A	293	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	CYS	Peptide
1	A	98	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	B	277	ALA	Peptide
2	B	293	THR	Peptide
2	B	379	HIS	Peptide
2	B	380	LEU	Peptide
2	B	582	ALA	Peptide
2	B	584	ARG	Peptide
2	B	598	LYS	Peptide
2	B	608	SER	Peptide
1	C	158	ILE	Peptide
1	C	243	CYS	Peptide
1	C	98	ASP	Peptide
2	D	277	ALA	Peptide
2	D	293	THR	Peptide
2	D	379	HIS	Peptide
2	D	380	LEU	Peptide
2	D	584	ARG	Peptide
2	D	598	LYS	Peptide
2	D	608	SER	Peptide

5.2 Too-close contacts (i)

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	4760	0	4722	220	0
1	C	4751	0	4709	244	0
2	B	3715	0	3674	258	0
2	D	3704	0	3660	238	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	16935	0	16765	942	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 28.

All (942) 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:C:249:LYS:CD	1:C:249:LYS:CE	1.79	1.60
2:B:413:LYS:CD	2:B:413:LYS:CE	1.87	1.52
1:A:249:LYS:CE	1:A:249:LYS:CD	1.85	1.50
2:B:413:LYS:NZ	2:B:413:LYS:CE	1.74	1.47
2:D:413:LYS:CE	2:D:413:LYS:NZ	1.76	1.45
2:D:413:LYS:CE	2:D:413:LYS:CD	1.97	1.43
2:B:608:SER:O	2:B:609:ILE:HG13	1.44	1.16
2:B:601:ARG:HH11	2:B:601:ARG:HG3	0.99	1.16
2:D:601:ARG:HH11	2:D:601:ARG:HG3	1.05	1.13
2:D:608:SER:O	2:D:609:ILE:HG13	1.48	1.12
2:B:584:ARG:HG3	2:B:585:ARG:H	1.01	1.11
1:C:487:ARG:HG2	1:C:487:ARG:HH11	1.14	1.10
2:D:253:ARG:HG3	2:D:253:ARG:HH11	1.17	1.07
2:D:584:ARG:HG3	2:D:585:ARG:H	0.95	1.07
2:D:427:THR:HG22	2:D:470:VAL:HG12	1.38	1.04
2:B:427:THR:HG22	2:B:470:VAL:HG12	1.31	1.04
1:C:533:THR:CG2	1:C:535:LEU:HB2	1.90	1.02
2:D:380:LEU:HD13	2:D:401:ASN:HB3	1.37	1.01
2:B:290:GLY:HA2	2:B:293:THR:N	1.74	1.01
1:C:356:PHE:HZ	2:D:488:ASP:HA	1.25	1.00
2:B:250:ARG:HG2	2:B:267:THR:OG1	1.59	0.99
2:B:253:ARG:HG3	2:B:253:ARG:HH11	1.27	0.98
2:D:250:ARG:HG2	2:D:267:THR:OG1	1.63	0.98
1:C:119:THR:HG21	1:C:168:PHE:H	1.29	0.98
2:D:584:ARG:HG3	2:D:585:ARG:N	1.78	0.97
2:D:584:ARG:CG	2:D:585:ARG:H	1.77	0.97
1:A:100:MET:CE	1:A:112:PHE:HB2	1.93	0.97
1:C:544:ILE:HG13	1:C:588:MET:HG2	1.47	0.97
2:B:301:GLU:HB3	2:B:371:TRP:CD1	2.00	0.96
2:B:463:HIS:NE2	2:B:484:THR:HG23	1.81	0.95
1:C:127:LEU:O	1:C:131:THR:HG22	1.66	0.95
1:C:533:THR:HG22	1:C:535:LEU:HB2	1.47	0.95
2:D:301:GLU:HB3	2:D:371:TRP:CD1	2.01	0.95
2:B:220:GLU:HB2	2:B:433:PRO:HG3	1.48	0.95
2:D:220:GLU:HB2	2:D:433:PRO:HG3	1.47	0.94
1:A:119:THR:HG21	1:A:168:PHE:H	1.31	0.93
1:A:127:LEU:O	1:A:131:THR:HG22	1.68	0.93
2:B:584:ARG:HG3	2:B:585:ARG:N	1.82	0.93
1:C:533:THR:HG22	1:C:535:LEU:H	1.33	0.93
2:B:238:ILE:HA	2:B:408:PHE:HB2	1.47	0.93
1:A:262:THR:HG21	1:A:268:PHE:CZ	2.04	0.93
2:B:299:ASN:HD22	2:B:646:LYS:HZ2	1.16	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:THR:CG2	1:C:535:LEU:HD22	1.99	0.92
2:B:584:ARG:CG	2:B:585:ARG:H	1.82	0.92
2:D:238:ILE:HA	2:D:408:PHE:HB2	1.49	0.92
2:D:198:PHE:CE1	2:D:203:ILE:HD11	2.04	0.91
2:B:236:HIS:HB3	2:B:409:LYS:HG2	1.52	0.91
2:B:250:ARG:HA	2:B:250:ARG:NE	1.83	0.91
2:B:299:ASN:HD22	2:B:646:LYS:NZ	1.69	0.91
2:B:427:THR:CG2	2:B:470:VAL:HG12	2.00	0.91
1:C:100:MET:CE	1:C:112:PHE:HB2	1.99	0.91
1:A:466:LYS:CE	1:A:490:PRO:HB3	2.01	0.91
1:A:533:THR:HG21	1:A:535:LEU:HD22	1.50	0.90
2:B:380:LEU:HD13	2:B:401:ASN:HB3	1.52	0.90
1:A:323:GLU:O	1:A:324:PHE:HB2	1.72	0.90
2:B:601:ARG:HG3	2:B:601:ARG:NH1	1.80	0.90
2:D:188:LYS:O	2:D:192:GLU:HB2	1.71	0.89
2:D:601:ARG:NH1	2:D:601:ARG:HG3	1.85	0.89
2:D:463:HIS:NE2	2:D:484:THR:HG23	1.88	0.89
2:B:188:LYS:O	2:B:192:GLU:HB2	1.71	0.89
2:D:427:THR:HG21	2:D:470:VAL:H	1.39	0.88
1:A:68:LYS:H	1:A:108:ASN:HD21	1.18	0.88
2:B:234:VAL:HG21	2:B:412:GLU:HG2	1.54	0.88
1:C:68:LYS:H	1:C:108:ASN:HD21	1.17	0.88
2:D:563:ARG:HD2	2:D:649:GLU:HB3	1.55	0.88
2:D:250:ARG:NE	2:D:250:ARG:HA	1.87	0.87
1:C:323:GLU:O	1:C:324:PHE:HB2	1.72	0.87
2:D:527:ILE:HG22	2:D:559:ILE:CD1	2.06	0.86
1:C:358:TYR:HB2	2:D:508:ARG:HH22	1.40	0.86
2:B:601:ARG:HH11	2:B:601:ARG:CG	1.88	0.86
1:A:356:PHE:HZ	2:B:488:ASP:HA	1.40	0.86
2:B:295:ILE:O	2:B:295:ILE:HG13	1.76	0.86
2:B:380:LEU:HD22	2:B:401:ASN:HA	1.56	0.85
2:B:598:LYS:HD2	2:B:624:PRO:O	1.75	0.85
1:C:533:THR:HG21	1:C:535:LEU:HD22	1.56	0.85
1:A:289:SER:HB2	1:A:304:ASN:HD21	1.39	0.85
1:A:530:CYS:SG	1:A:533:THR:HB	2.17	0.85
1:C:356:PHE:CZ	2:D:488:ASP:HA	2.11	0.85
2:B:234:VAL:CG2	2:B:412:GLU:HG2	2.07	0.84
1:A:100:MET:HE1	1:A:112:PHE:HB2	1.59	0.84
1:A:466:LYS:HE3	1:A:490:PRO:HB3	1.60	0.84
2:D:234:VAL:HG21	2:D:412:GLU:HG2	1.59	0.84
2:B:236:HIS:CB	2:B:409:LYS:HG2	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:234:VAL:CG2	2:D:412:GLU:HG2	2.08	0.83
1:C:262:THR:HG21	1:C:268:PHE:CZ	2.13	0.83
2:B:361:HIS:HD2	2:B:363:PHE:H	1.26	0.83
1:A:533:THR:CG2	1:A:535:LEU:HD22	2.08	0.83
2:B:301:GLU:HG3	2:B:301:GLU:O	1.79	0.83
1:C:97:ASP:HB2	1:C:99:TRP:CE3	2.14	0.82
1:C:500:ASN:HB2	1:C:539:THR:O	1.80	0.82
1:A:100:MET:HE3	1:A:112:PHE:HB2	1.61	0.82
2:D:380:LEU:HD22	2:D:401:ASN:HA	1.62	0.82
1:C:284:MET:HG2	1:C:289:SER:HB3	1.61	0.81
1:A:533:THR:HG22	1:A:535:LEU:HB2	1.63	0.81
1:A:97:ASP:HB2	1:A:99:TRP:CE3	2.17	0.80
2:D:176:LEU:HG	2:D:177:ASN:H	1.44	0.80
1:C:226:ARG:HG3	2:D:457:SER:OG	1.81	0.80
2:B:384:LEU:HD22	2:B:398:ILE:HD11	1.64	0.80
2:D:427:THR:CG2	2:D:470:VAL:HG12	2.11	0.80
1:A:533:THR:CG2	1:A:535:LEU:HB2	2.11	0.80
1:C:100:MET:HE1	1:C:112:PHE:HB2	1.60	0.80
1:C:487:ARG:NH1	1:C:487:ARG:HG2	1.92	0.80
2:B:413:LYS:CG	2:B:413:LYS:CE	2.60	0.80
1:C:289:SER:HB2	1:C:304:ASN:HD21	1.47	0.80
1:A:226:ARG:HG3	2:B:457:SER:OG	1.81	0.79
1:C:539:THR:HG23	1:C:540:THR:H	1.48	0.79
2:B:427:THR:HG21	2:B:470:VAL:N	1.98	0.79
2:D:198:PHE:HE1	2:D:203:ILE:CD1	1.96	0.79
2:D:585:ARG:HA	2:D:588:HIS:HB3	1.63	0.79
2:B:563:ARG:HD2	2:B:649:GLU:HB3	1.65	0.79
1:C:533:THR:HG21	1:C:535:LEU:HB2	1.65	0.79
1:A:503:LEU:HD12	1:A:504:GLU:N	1.98	0.79
1:C:108:ASN:HD22	1:C:120:ASN:HD21	1.28	0.78
2:B:427:THR:HG21	2:B:470:VAL:H	1.48	0.78
2:B:585:ARG:HA	2:B:588:HIS:HB3	1.65	0.78
2:D:295:ILE:HG13	2:D:295:ILE:O	1.81	0.78
2:D:198:PHE:HE1	2:D:203:ILE:HD11	1.48	0.78
1:A:284:MET:HG2	1:A:289:SER:HB3	1.66	0.78
1:C:249:LYS:CE	1:C:249:LYS:CG	2.61	0.78
2:B:176:LEU:HG	2:B:177:ASN:H	1.49	0.78
2:D:178:LYS:H	2:D:178:LYS:HD2	1.48	0.77
2:D:413:LYS:CE	2:D:413:LYS:CG	2.61	0.77
2:D:601:ARG:HH11	2:D:601:ARG:CG	1.93	0.77
1:A:48:ILE:O	1:A:50:CYS:N	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:LYS:H	2:B:178:LYS:HD2	1.47	0.77
1:A:48:ILE:HG22	1:A:51:ASN:H	1.49	0.76
2:D:640:ILE:HG12	2:D:641:ASN:N	1.99	0.76
1:A:158:ILE:HG22	1:A:159:ARG:N	2.01	0.76
1:A:533:THR:HG22	1:A:535:LEU:H	1.49	0.76
2:D:427:THR:HG21	2:D:470:VAL:N	2.00	0.76
2:D:600:LEU:HG	2:D:601:ARG:N	2.01	0.76
1:A:262:THR:CG2	1:A:268:PHE:HZ	1.99	0.75
2:B:198:PHE:CE1	2:B:203:ILE:HD11	2.21	0.75
2:B:361:HIS:CD2	2:B:363:PHE:H	2.02	0.75
2:D:236:HIS:HB3	2:D:409:LYS:HG2	1.67	0.75
2:B:597:GLN:O	2:B:598:LYS:HG3	1.86	0.75
1:C:487:ARG:CG	1:C:487:ARG:HH11	1.97	0.75
1:A:506:THR:HG23	1:A:522:THR:HG21	1.67	0.74
1:C:159:ARG:HH11	1:C:159:ARG:HB2	1.53	0.74
2:D:288:VAL:HG11	2:D:317:VAL:HG11	1.69	0.74
2:B:381:VAL:HG12	2:B:382:GLY:H	1.53	0.74
2:B:527:ILE:HG22	2:B:559:ILE:CD1	2.18	0.74
1:A:249:LYS:CE	1:A:249:LYS:CG	2.66	0.74
1:A:262:THR:CG2	1:A:268:PHE:CZ	2.71	0.74
1:C:262:THR:CG2	1:C:268:PHE:CZ	2.71	0.73
1:A:474:ASP:OD2	1:A:567:THR:HB	1.88	0.73
2:B:253:ARG:HG2	2:B:266:SER:HB3	1.71	0.72
1:C:21:LEU:HD22	1:C:348:VAL:HG23	1.70	0.72
1:A:159:ARG:HB2	1:A:159:ARG:HH11	1.52	0.72
1:C:67:ASN:O	1:C:70:ASP:HB2	1.89	0.72
2:B:640:ILE:HG12	2:B:641:ASN:N	2.05	0.72
1:C:48:ILE:HG22	1:C:51:ASN:H	1.55	0.72
2:B:239:ASN:HB3	2:B:242:GLU:CG	2.20	0.71
2:D:236:HIS:CB	2:D:409:LYS:HG2	2.20	0.71
2:D:205:PRO:HD3	2:D:651:SER:OG	1.90	0.71
2:B:607:TYR:OH	2:B:612:ASP:OD1	2.08	0.71
1:C:307:ALA:N	1:C:308:PRO:HD2	2.05	0.71
1:C:358:TYR:HB2	2:D:508:ARG:NH2	2.06	0.71
2:B:404:ASP:O	2:B:406:HIS:N	2.24	0.71
2:D:301:GLU:HB3	2:D:371:TRP:CG	2.25	0.71
1:A:466:LYS:HE3	1:A:490:PRO:CB	2.20	0.71
1:A:67:ASN:O	1:A:70:ASP:HB2	1.90	0.71
2:B:288:VAL:O	2:B:290:GLY:N	2.23	0.71
2:D:527:ILE:HG22	2:D:559:ILE:HD11	1.73	0.71
2:B:388:SER:OG	2:B:390:GLU:HG2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:530:CYS:SG	1:C:533:THR:HB	2.30	0.71
1:A:262:THR:HG23	1:A:290:TYR:OH	1.91	0.71
2:B:600:LEU:HG	2:B:601:ARG:N	2.03	0.71
2:B:431:LEU:HG	2:B:437:VAL:CG2	2.21	0.71
1:A:138:ASN:ND2	1:A:140:ILE:H	1.89	0.70
1:A:289:SER:CB	1:A:304:ASN:HD21	2.03	0.70
1:C:302:ALA:O	1:C:304:ASN:N	2.25	0.70
2:D:253:ARG:HH11	2:D:253:ARG:CG	2.00	0.70
2:D:431:LEU:HG	2:D:437:VAL:CG2	2.22	0.70
1:A:473:PHE:HE2	1:A:498:MET:HG3	1.56	0.70
1:C:412:LEU:HD23	1:C:430:LEU:HD22	1.74	0.70
2:D:301:GLU:HG3	2:D:301:GLU:O	1.91	0.70
2:B:301:GLU:HB3	2:B:371:TRP:CG	2.26	0.69
2:B:234:VAL:HG23	2:B:412:GLU:H	1.58	0.69
1:A:563:TYR:HB3	1:A:567:THR:CG2	2.22	0.69
2:D:483:SER:HB3	2:D:526:TYR:CZ	2.27	0.69
1:A:72:GLU:HG2	1:A:127:LEU:HD13	1.75	0.69
2:D:239:ASN:HB3	2:D:242:GLU:CG	2.23	0.69
2:D:512:SER:HB3	2:D:515:VAL:HG23	1.74	0.69
2:B:353:CYS:HA	2:D:275:VAL:HG11	1.73	0.69
1:C:533:THR:HG22	1:C:535:LEU:CB	2.21	0.69
1:C:533:THR:HG23	1:C:535:LEU:HD22	1.74	0.69
2:B:661:ASN:HD21	2:B:665:LEU:H	1.41	0.68
1:C:262:THR:CG2	1:C:268:PHE:HZ	2.04	0.68
2:D:381:VAL:HG12	2:D:382:GLY:H	1.58	0.68
1:A:21:LEU:HD22	1:A:348:VAL:HG23	1.75	0.68
1:C:138:ASN:ND2	1:C:140:ILE:H	1.90	0.68
1:A:412:LEU:HD23	1:A:430:LEU:HD22	1.75	0.68
1:C:247:VAL:HG21	1:C:283:LEU:HD11	1.75	0.68
1:A:356:PHE:CZ	2:B:488:ASP:HA	2.24	0.68
1:C:108:ASN:ND2	1:C:120:ASN:HD21	1.92	0.68
2:D:527:ILE:CG2	2:D:559:ILE:HD11	2.23	0.68
2:D:608:SER:OG	2:D:611:ASP:HB2	1.94	0.68
1:C:142:SER:HB3	1:C:158:ILE:HD12	1.75	0.68
1:A:466:LYS:CE	1:A:490:PRO:CB	2.72	0.68
1:C:474:ASP:OD2	1:C:567:THR:HB	1.93	0.67
2:D:299:ASN:HD22	2:D:646:LYS:HZ2	1.40	0.67
2:B:393:ILE:HD13	2:B:418:LEU:HD12	1.75	0.67
1:C:268:PHE:CG	1:C:285:SER:HB3	2.29	0.67
1:C:355:ALA:O	1:C:356:PHE:HD2	1.77	0.67
1:C:126:ASN:HB2	1:C:129:SER:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:THR:HG21	1:C:535:LEU:CD2	2.24	0.67
1:A:303:ASP:O	1:A:304:ASN:HB3	1.95	0.67
2:B:447:GLU:HB2	2:B:458:PHE:CE2	2.29	0.67
1:C:512:PHE:HE2	1:C:536:PRO:HD3	1.60	0.67
1:C:533:THR:CG2	1:C:535:LEU:CB	2.71	0.67
2:B:288:VAL:HG11	2:B:317:VAL:HG11	1.76	0.66
2:D:299:ASN:HD22	2:D:646:LYS:NZ	1.93	0.66
2:D:661:ASN:HD21	2:D:665:LEU:H	1.44	0.66
2:D:384:LEU:HD22	2:D:398:ILE:HD11	1.78	0.66
2:D:253:ARG:HG2	2:D:266:SER:HB3	1.76	0.66
1:C:72:GLU:HG2	1:C:127:LEU:HD13	1.77	0.66
2:D:640:ILE:HG12	2:D:641:ASN:H	1.58	0.66
2:D:298:LEU:HG	2:D:644:CYS:SG	2.36	0.66
2:B:236:HIS:HB3	2:B:409:LYS:CG	2.24	0.66
2:B:301:GLU:HB3	2:B:371:TRP:NE1	2.11	0.66
1:C:100:MET:HE3	1:C:112:PHE:HB2	1.78	0.66
1:C:42:PRO:HB2	1:C:386:LEU:HD13	1.77	0.66
2:D:234:VAL:HG23	2:D:412:GLU:H	1.59	0.66
1:A:126:ASN:HB2	1:A:129:SER:HB2	1.78	0.65
1:A:459:TYR:OH	1:A:488:GLU:O	2.14	0.65
2:B:295:ILE:HD11	2:B:644:CYS:SG	2.36	0.65
1:C:318:SER:O	1:C:322:ASN:HA	1.95	0.65
2:D:239:ASN:O	2:D:241:THR:N	2.29	0.65
2:B:616:ILE:HD12	2:B:616:ILE:H	1.60	0.65
2:D:554:THR:HG21	2:D:574:ASP:HB3	1.78	0.65
1:A:14:PHE:CD2	1:A:20:ASN:ND2	2.64	0.65
2:B:372:HIS:O	2:B:373:GLU:HB2	1.96	0.65
2:B:643:THR:O	2:B:644:CYS:SG	2.53	0.65
2:D:198:PHE:CE1	2:D:203:ILE:CD1	2.75	0.65
2:B:198:PHE:HE1	2:B:203:ILE:CD1	2.10	0.64
1:C:359:LYS:HG3	1:C:363:GLU:HG3	1.77	0.64
2:D:361:HIS:HD2	2:D:363:PHE:H	1.45	0.64
2:D:361:HIS:CD2	2:D:363:PHE:H	2.14	0.64
2:B:267:THR:HG21	2:B:289:GLY:HA2	1.80	0.64
1:A:363:GLU:O	1:A:364:GLN:CB	2.46	0.64
2:B:413:LYS:CD	2:B:413:LYS:NZ	2.61	0.64
2:D:607:TYR:OH	2:D:612:ASP:OD1	2.15	0.64
2:B:239:ASN:HB3	2:B:242:GLU:HG2	1.80	0.63
2:B:554:THR:HG21	2:B:574:ASP:HB3	1.80	0.63
1:A:304:ASN:C	1:A:306:ILE:H	2.02	0.63
2:B:275:VAL:HG11	2:D:353:CYS:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:SER:CB	1:C:304:ASN:HD21	2.11	0.63
2:D:616:ILE:H	2:D:616:ILE:HD12	1.63	0.63
1:C:25:ARG:HD2	1:C:95:PRO:O	1.97	0.63
1:C:304:ASN:O	1:C:306:ILE:N	2.30	0.63
1:A:215:GLN:H	1:A:215:GLN:NE2	1.97	0.63
1:C:159:ARG:O	1:C:161:ASN:N	2.30	0.63
2:D:640:ILE:O	2:D:661:ASN:HB2	1.99	0.63
2:B:302:GLU:CG	2:B:649:GLU:HB2	2.29	0.63
2:B:641:ASN:O	2:B:642:ILE:HG13	1.99	0.63
1:C:304:ASN:C	1:C:306:ILE:H	2.02	0.63
2:D:523:ILE:HD13	2:D:582:ALA:HB1	1.80	0.63
2:D:302:GLU:CG	2:D:649:GLU:HB2	2.29	0.63
1:A:108:ASN:HD22	1:A:120:ASN:HD21	1.46	0.62
1:A:358:TYR:HB2	2:B:508:ARG:HH22	1.64	0.62
1:C:284:MET:HG2	1:C:289:SER:CB	2.27	0.62
2:B:285:ILE:HG12	2:B:667:THR:HB	1.80	0.62
1:A:359:LYS:HG3	1:A:363:GLU:HG3	1.80	0.62
2:D:220:GLU:CB	2:D:433:PRO:HG3	2.24	0.62
1:C:127:LEU:O	1:C:131:THR:CG2	2.45	0.62
1:C:232:LEU:HD13	1:C:241:LEU:HD23	1.81	0.62
2:D:301:GLU:HB3	2:D:371:TRP:NE1	2.15	0.62
2:D:385:SER:HB3	2:D:428:PHE:HZ	1.64	0.62
2:D:404:ASP:O	2:D:406:HIS:N	2.31	0.62
1:A:268:PHE:CG	1:A:285:SER:HB3	2.35	0.61
2:D:380:LEU:O	2:D:381:VAL:O	2.18	0.61
2:B:506:VAL:HG12	2:B:507:SER:HB3	1.82	0.61
1:C:69:LEU:HD11	1:C:131:THR:HB	1.83	0.61
1:C:363:GLU:O	1:C:364:GLN:CB	2.47	0.61
2:D:527:ILE:CG2	2:D:559:ILE:CD1	2.78	0.61
2:D:641:ASN:O	2:D:642:ILE:HG13	2.00	0.61
1:A:127:LEU:O	1:A:131:THR:CG2	2.46	0.61
1:C:248:HIS:ND1	1:C:259:SER:HB3	2.15	0.61
1:C:6:ASP:OD1	1:C:369:MET:HA	1.99	0.61
1:A:20:ASN:O	1:A:31:LEU:HA	2.00	0.61
1:C:34:PHE:CD2	1:C:35:PRO:HA	2.36	0.61
1:C:48:ILE:HG23	1:C:54:ASN:HB2	1.82	0.61
2:D:605:TRP:CH2	2:D:665:LEU:HD13	2.35	0.61
2:B:176:LEU:O	2:B:177:ASN:CB	2.49	0.61
1:C:533:THR:HG22	1:C:535:LEU:N	2.11	0.61
1:A:119:THR:HG21	1:A:168:PHE:N	2.12	0.61
2:B:523:ILE:HD13	2:B:582:ALA:HB1	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:THR:HG23	1:C:522:THR:HG21	1.82	0.61
1:A:412:LEU:HA	1:A:435:GLU:HG3	1.81	0.61
2:D:483:SER:HB3	2:D:526:TYR:CE1	2.35	0.61
2:B:605:TRP:CH2	2:B:665:LEU:HD13	2.36	0.60
1:A:215:GLN:H	1:A:215:GLN:HE21	1.48	0.60
2:B:545:ALA:O	2:B:547:HIS:HD2	1.84	0.60
1:C:48:ILE:O	1:C:50:CYS:N	2.31	0.60
1:A:473:PHE:CE2	1:A:498:MET:HG3	2.35	0.60
2:B:512:SER:HB3	2:B:515:VAL:HG23	1.83	0.60
2:B:299:ASN:ND2	2:B:646:LYS:NZ	2.45	0.60
2:D:250:ARG:HD2	2:D:252:LYS:O	2.01	0.60
2:D:388:SER:OG	2:D:390:GLU:HG2	2.00	0.60
2:B:220:GLU:CB	2:B:433:PRO:HG3	2.29	0.60
1:A:247:VAL:HG21	1:A:283:LEU:HD11	1.84	0.60
1:A:48:ILE:HG23	1:A:54:ASN:HB2	1.84	0.60
2:B:608:SER:OG	2:B:611:ASP:HB2	2.01	0.60
2:D:239:ASN:HB3	2:D:242:GLU:HG2	1.84	0.60
1:A:533:THR:HG21	1:A:535:LEU:CD2	2.28	0.60
2:B:301:GLU:O	2:B:301:GLU:CG	2.47	0.60
1:C:276:GLU:HB3	1:C:278:GLU:HB2	1.84	0.60
1:A:237:TYR:HD1	1:A:237:TYR:N	1.99	0.60
2:B:604:LYS:NZ	2:B:604:LYS:HB2	2.17	0.60
1:A:355:ALA:O	1:A:356:PHE:HD2	1.85	0.60
2:B:253:ARG:HH11	2:B:253:ARG:CG	2.05	0.60
1:C:359:LYS:HG3	1:C:363:GLU:CG	2.31	0.60
1:A:142:SER:HB3	1:A:158:ILE:HD12	1.83	0.60
1:A:302:ALA:O	1:A:304:ASN:N	2.35	0.60
2:B:205:PRO:HD3	2:B:651:SER:OG	2.01	0.60
1:A:333:ILE:HG21	1:A:336:ILE:HD11	1.83	0.59
2:B:432:SER:HB2	2:B:433:PRO:HD2	1.84	0.59
1:A:211:ALA:O	1:A:213:SER:N	2.35	0.59
1:A:363:GLU:O	1:A:364:GLN:HB2	2.02	0.59
2:D:604:LYS:HB2	2:D:604:LYS:NZ	2.17	0.59
1:C:138:ASN:HD22	1:C:138:ASN:C	2.06	0.59
1:C:533:THR:CG2	1:C:535:LEU:CD2	2.78	0.59
1:C:512:PHE:CE2	1:C:536:PRO:HD3	2.37	0.59
2:D:253:ARG:NH1	2:D:253:ARG:HG3	1.96	0.59
1:A:303:ASP:O	1:A:304:ASN:CB	2.48	0.59
2:D:610:LYS:HA	2:D:610:LYS:NZ	2.17	0.59
2:B:198:PHE:CE1	2:B:203:ILE:CD1	2.84	0.59
1:C:21:LEU:HD22	1:C:348:VAL:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ASN:HD22	1:C:140:ILE:H	1.50	0.59
1:C:333:ILE:HG21	1:C:336:ILE:HD11	1.85	0.59
1:C:25:ARG:HD2	1:C:95:PRO:C	2.23	0.59
2:D:270:LYS:NZ	2:D:353:CYS:O	2.35	0.59
1:A:318:SER:O	1:A:322:ASN:HA	2.03	0.59
1:C:34:PHE:HD2	1:C:35:PRO:CA	2.16	0.59
2:B:250:ARG:NE	2:B:250:ARG:CA	2.63	0.59
1:C:363:GLU:O	1:C:364:GLN:HB2	2.02	0.59
1:C:563:TYR:HB3	1:C:567:THR:CG2	2.32	0.59
1:A:533:THR:HG22	1:A:535:LEU:CB	2.32	0.58
2:B:640:ILE:HG12	2:B:641:ASN:H	1.65	0.58
1:A:289:SER:HB2	1:A:304:ASN:ND2	2.14	0.58
1:C:347:ILE:HD12	1:C:369:MET:HE1	1.85	0.58
2:D:267:THR:HG21	2:D:289:GLY:HA2	1.84	0.58
2:B:250:ARG:CZ	2:B:250:ARG:HA	2.32	0.58
2:B:301:GLU:CB	2:B:371:TRP:CG	2.86	0.58
1:C:211:ALA:O	1:C:213:SER:N	2.35	0.58
1:C:355:ALA:O	1:C:356:PHE:CD2	2.56	0.58
2:D:598:LYS:HD2	2:D:624:PRO:O	2.03	0.58
1:C:249:LYS:CD	1:C:249:LYS:NZ	2.65	0.58
1:A:69:LEU:HD11	1:A:131:THR:HB	1.86	0.58
1:A:138:ASN:HD22	1:A:140:ILE:H	1.50	0.58
1:A:304:ASN:O	1:A:306:ILE:N	2.34	0.58
1:C:237:TYR:N	1:C:237:TYR:HD1	2.01	0.58
2:D:288:VAL:CG1	2:D:317:VAL:HG11	2.33	0.58
2:D:431:LEU:HG	2:D:437:VAL:HG23	1.86	0.58
2:D:506:VAL:HG12	2:D:507:SER:HB3	1.85	0.58
1:A:541:HIS:CE1	1:A:557:ARG:HH21	2.21	0.58
1:A:503:LEU:HD12	1:A:504:GLU:H	1.69	0.58
2:B:301:GLU:CB	2:B:371:TRP:CD1	2.81	0.58
2:D:565:HIS:HD2	2:D:567:MET:H	1.52	0.58
1:A:533:THR:HG21	1:A:535:LEU:HB2	1.86	0.58
2:B:239:ASN:O	2:B:241:THR:N	2.37	0.58
2:B:431:LEU:HG	2:B:437:VAL:HG23	1.86	0.58
1:A:411:LYS:HG2	1:A:417:TYR:OH	2.04	0.57
1:C:528:LYS:O	1:C:537:ILE:HG22	2.04	0.57
1:C:270:ILE:O	1:C:270:ILE:HG13	2.03	0.57
2:D:368:ASP:OD2	2:D:427:THR:HG23	2.04	0.57
1:A:159:ARG:NH1	1:A:159:ARG:HB2	2.19	0.57
2:B:527:ILE:CG2	2:B:559:ILE:HD11	2.33	0.57
2:B:565:HIS:HD2	2:B:567:MET:H	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:ASP:OD1	1:C:517:GLU:N	2.31	0.57
2:B:385:SER:HB3	2:B:428:PHE:HZ	1.68	0.57
1:C:412:LEU:HA	1:C:435:GLU:HG3	1.87	0.57
2:D:611:ASP:O	2:D:612:ASP:HB2	2.03	0.57
1:A:237:TYR:CD1	1:A:237:TYR:N	2.73	0.57
1:C:248:HIS:ND1	1:C:259:SER:CB	2.67	0.57
2:B:608:SER:C	2:B:609:ILE:HG13	2.19	0.57
2:D:301:GLU:CB	2:D:371:TRP:CG	2.87	0.57
1:A:276:GLU:HB3	1:A:278:GLU:HB2	1.87	0.57
1:C:527:TRP:CE2	1:C:538:LEU:HD11	2.40	0.57
2:D:346:MET:HB3	2:D:353:CYS:HB2	1.87	0.56
2:B:176:LEU:CG	2:B:177:ASN:H	2.18	0.56
1:C:215:GLN:H	1:C:215:GLN:HE21	1.53	0.56
1:C:289:SER:HB2	1:C:304:ASN:ND2	2.18	0.56
2:D:250:ARG:NE	2:D:250:ARG:CA	2.66	0.56
2:D:600:LEU:HD12	2:D:621:GLU:H	1.70	0.56
1:C:237:TYR:CD1	1:C:237:TYR:N	2.74	0.56
2:D:301:GLU:CG	2:D:301:GLU:O	2.53	0.56
2:D:393:ILE:HD13	2:D:418:LEU:HD12	1.87	0.56
1:A:90:VAL:HG22	1:A:103:LEU:HB3	1.88	0.56
2:D:223:TYR:HD2	2:D:224:ASN:HD22	1.53	0.56
2:D:563:ARG:HD2	2:D:649:GLU:CB	2.31	0.56
1:A:359:LYS:HG3	1:A:363:GLU:CG	2.35	0.56
1:A:479:LEU:HD21	1:A:492:TYR:CD2	2.40	0.56
1:C:20:ASN:O	1:C:31:LEU:HA	2.06	0.56
1:A:289:SER:CB	1:A:304:ASN:ND2	2.68	0.56
1:A:356:PHE:CD2	1:A:356:PHE:C	2.78	0.56
2:B:527:ILE:HG22	2:B:559:ILE:HD11	1.88	0.56
2:B:611:ASP:O	2:B:612:ASP:HB2	2.05	0.56
1:A:232:LEU:HD13	1:A:241:LEU:HD23	1.88	0.56
1:A:97:ASP:CB	1:A:99:TRP:CE3	2.89	0.56
1:C:123:SER:O	1:C:130:ARG:HD3	2.05	0.56
1:C:419:ILE:HD12	1:C:464:ASN:ND2	2.21	0.56
2:B:640:ILE:O	2:B:661:ASN:HB2	2.05	0.55
2:D:298:LEU:O	2:D:646:LYS:HD2	2.06	0.55
2:D:211:VAL:HG12	2:D:522:GLN:HE21	1.72	0.55
2:D:223:TYR:HB2	2:D:375:CYS:HA	1.88	0.55
2:B:301:GLU:HB3	2:B:371:TRP:CE2	2.42	0.55
1:C:356:PHE:CD2	1:C:356:PHE:C	2.80	0.55
2:D:352:HIS:O	2:D:353:CYS:HB3	2.06	0.55
2:D:413:LYS:NZ	2:D:413:LYS:CD	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:HD13	1:A:241:LEU:CD2	2.36	0.55
1:A:6:ASP:OD1	1:A:369:MET:HA	2.05	0.55
2:D:295:ILE:HD11	2:D:644:CYS:SG	2.46	0.55
1:A:163:GLU:O	1:A:165:THR:N	2.39	0.55
1:A:68:LYS:H	1:A:108:ASN:ND2	1.98	0.55
2:B:384:LEU:CD2	2:B:398:ILE:HD11	2.35	0.55
2:B:483:SER:HB3	2:B:526:TYR:CZ	2.42	0.55
1:C:264:SER:HB3	1:C:268:PHE:HE2	1.71	0.55
2:D:248:LYS:H	2:D:319:GLN:HE21	1.54	0.55
1:C:292:VAL:HA	1:C:299:HIS:O	2.06	0.55
1:A:48:ILE:HG21	1:A:51:ASN:O	2.07	0.55
1:C:519:VAL:HG11	1:C:536:PRO:HG3	1.88	0.55
2:B:393:ILE:HG23	2:B:418:LEU:HB2	1.89	0.55
1:C:215:GLN:H	1:C:215:GLN:NE2	2.05	0.55
2:B:483:SER:HB3	2:B:526:TYR:CE1	2.42	0.54
1:A:34:PHE:CD2	1:A:35:PRO:HA	2.42	0.54
1:C:412:LEU:HD22	1:C:454:PHE:HA	1.89	0.54
1:C:158:ILE:HG22	1:C:159:ARG:N	2.22	0.54
1:A:25:ARG:HD2	1:A:95:PRO:O	2.07	0.54
1:C:527:TRP:CD2	1:C:538:LEU:HD11	2.42	0.54
2:B:363:PHE:HB3	2:B:388:SER:HB2	1.89	0.54
2:B:565:HIS:CD2	2:B:567:MET:HB2	2.41	0.54
2:D:365:GLU:HG3	2:D:389:GLN:NE2	2.22	0.54
2:D:363:PHE:HB3	2:D:388:SER:HB2	1.89	0.54
2:B:253:ARG:HG3	2:B:253:ARG:NH1	2.05	0.54
2:B:532:ALA:HA	2:B:555:THR:HG22	1.88	0.54
1:C:138:ASN:HD22	1:C:139:PRO:N	2.06	0.54
2:D:176:LEU:O	2:D:177:ASN:CB	2.56	0.54
1:A:159:ARG:O	1:A:161:ASN:N	2.40	0.54
1:A:25:ARG:HD2	1:A:95:PRO:C	2.28	0.54
1:A:248:HIS:ND1	1:A:259:SER:HB3	2.22	0.54
2:B:431:LEU:HG	2:B:437:VAL:HG22	1.89	0.54
2:D:285:ILE:HG12	2:D:667:THR:HB	1.90	0.54
2:D:301:GLU:CB	2:D:371:TRP:CD1	2.84	0.54
2:B:211:VAL:HG12	2:B:522:GLN:HE21	1.72	0.54
2:B:297:TRP:HD1	2:B:298:LEU:O	1.91	0.54
1:A:502:PHE:CZ	1:A:503:LEU:HD23	2.43	0.53
2:D:236:HIS:HB3	2:D:409:LYS:CG	2.34	0.53
2:D:545:ALA:O	2:D:547:HIS:HD2	1.91	0.53
1:A:266:GLU:O	1:A:268:PHE:HD2	1.92	0.53
2:B:585:ARG:HB2	2:B:585:ARG:HH11	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:297:TRP:HD1	2:D:298:LEU:H	1.57	0.53
2:D:447:GLU:HB2	2:D:458:PHE:CE2	2.44	0.53
1:A:304:ASN:O	1:A:305:ILE:HG12	2.08	0.53
2:D:234:VAL:HG21	2:D:412:GLU:CG	2.35	0.53
2:D:288:VAL:HG11	2:D:317:VAL:CG1	2.37	0.53
2:D:289:GLY:O	2:D:293:THR:N	2.42	0.53
2:D:231:ASN:O	2:D:415:SER:HA	2.07	0.53
2:D:605:TRP:CZ3	2:D:616:ILE:HG13	2.43	0.53
1:A:264:SER:HB3	1:A:268:PHE:HE2	1.73	0.53
2:D:297:TRP:HD1	2:D:298:LEU:N	2.07	0.53
2:D:399:ILE:O	2:D:400:ASP:HB2	2.08	0.53
1:A:466:LYS:HE2	1:A:490:PRO:HB3	1.90	0.53
2:B:250:ARG:HD2	2:B:252:LYS:O	2.09	0.53
2:D:302:GLU:HG3	2:D:649:GLU:HB2	1.90	0.53
2:B:527:ILE:CG2	2:B:559:ILE:CD1	2.86	0.53
1:C:379:ILE:HG22	1:C:437:ARG:HD2	1.90	0.53
1:A:248:HIS:ND1	1:A:259:SER:CB	2.72	0.53
2:B:616:ILE:N	2:B:616:ILE:HD12	2.24	0.53
2:B:289:GLY:O	2:B:293:THR:N	2.42	0.53
1:C:232:LEU:HD13	1:C:241:LEU:CD2	2.39	0.53
1:C:520:THR:OG1	1:C:526:THR:HB	2.09	0.53
2:B:473:ALA:HB2	2:B:526:TYR:CZ	2.44	0.52
1:C:289:SER:CB	1:C:304:ASN:ND2	2.72	0.52
2:B:610:LYS:NZ	2:B:610:LYS:HA	2.25	0.52
2:D:431:LEU:HG	2:D:437:VAL:HG22	1.92	0.52
2:D:432:SER:HB2	2:D:433:PRO:HD2	1.91	0.52
1:A:428:ASN:OD1	1:A:573:ARG:NH1	2.42	0.52
2:B:220:GLU:O	2:B:221:SER:HB3	2.10	0.52
2:D:610:LYS:HA	2:D:610:LYS:CE	2.40	0.52
1:A:517:GLU:C	1:A:529:ARG:HD2	2.29	0.52
2:B:441:LYS:HG2	2:B:441:LYS:O	2.10	0.52
2:B:380:LEU:O	2:B:381:VAL:O	2.28	0.52
1:C:544:ILE:HD11	1:C:588:MET:SD	2.50	0.52
1:A:284:MET:HG2	1:A:289:SER:CB	2.37	0.52
1:A:563:TYR:HB3	1:A:567:THR:HG22	1.92	0.52
1:A:193:ASP:O	1:A:208:THR:HG23	2.10	0.52
1:A:248:HIS:HA	1:A:259:SER:HB3	1.92	0.52
1:A:292:VAL:HA	1:A:299:HIS:O	2.09	0.52
2:D:385:SER:HB3	2:D:428:PHE:CZ	2.45	0.51
2:B:368:ASP:OD2	2:B:427:THR:HG23	2.10	0.51
2:B:454:GLU:O	2:B:456:PRO:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:TYR:HB2	2:B:508:ARG:NH2	2.25	0.51
1:C:303:ASP:OD1	1:C:305:ILE:HG23	2.10	0.51
1:C:443:ASN:OD1	1:C:449:PRO:HA	2.10	0.51
2:B:203:ILE:O	2:B:651:SER:OG	2.27	0.51
1:A:307:ALA:N	1:A:308:PRO:HD2	2.26	0.51
2:B:298:LEU:O	2:B:299:ASN:HB2	2.11	0.51
2:B:365:GLU:HG3	2:B:389:GLN:NE2	2.25	0.51
2:B:585:ARG:HH11	2:B:585:ARG:CB	2.23	0.51
2:B:588:HIS:HE1	2:B:590:ILE:CD1	2.24	0.51
2:B:604:LYS:HG3	2:B:604:LYS:O	2.10	0.51
2:D:301:GLU:HB3	2:D:371:TRP:CE2	2.45	0.51
1:A:533:THR:CG2	1:A:535:LEU:CD2	2.87	0.51
2:B:405:VAL:HG13	2:B:406:HIS:N	2.26	0.51
2:D:176:LEU:CG	2:D:177:ASN:H	2.18	0.51
1:C:327:TYR:CD2	1:C:353:ARG:HD3	2.45	0.51
1:C:541:HIS:CE1	1:C:557:ARG:HE	2.28	0.51
1:A:125:GLY:O	1:A:130:ARG:HG3	2.11	0.51
2:B:614:TYR:HE2	2:B:639:GLY:O	1.94	0.51
2:D:250:ARG:HA	2:D:250:ARG:CZ	2.41	0.51
2:D:196:PHE:HE2	2:D:599:SER:HA	1.76	0.51
1:A:155:PHE:HE1	1:A:174:ILE:HD12	1.76	0.50
1:A:277:LYS:O	1:A:278:GLU:HG2	2.10	0.50
2:B:288:VAL:CG1	2:B:317:VAL:HG11	2.41	0.50
1:C:407:SER:HB3	1:C:410:LYS:HG3	1.93	0.50
2:D:578:ILE:HD13	2:D:601:ARG:HB2	1.93	0.50
1:A:297:GLU:HA	1:A:297:GLU:OE2	2.11	0.50
1:A:424:GLN:OE1	1:A:573:ARG:HB2	2.10	0.50
1:C:159:ARG:NH1	1:C:159:ARG:HB2	2.22	0.50
1:C:307:ALA:N	1:C:308:PRO:CD	2.74	0.50
1:C:347:ILE:HD12	1:C:369:MET:CE	2.42	0.50
1:A:355:ALA:O	1:A:356:PHE:CD2	2.64	0.50
1:C:153:LEU:O	1:C:173:SER:HA	2.12	0.50
1:C:483:ALA:HB2	1:C:513:THR:HG22	1.94	0.50
2:B:176:LEU:O	2:B:177:ASN:HB3	2.11	0.50
1:A:108:ASN:ND2	1:A:120:ASN:HD21	2.10	0.50
1:A:79:LEU:HD23	2:B:502:THR:HB	1.93	0.50
2:D:273:PHE:N	2:D:274:PRO:CD	2.75	0.50
2:D:345:LYS:HB2	2:D:356:VAL:HG21	1.94	0.50
1:A:379:ILE:HG22	1:A:437:ARG:HD2	1.94	0.50
1:C:264:SER:C	1:C:266:GLU:H	2.15	0.50
1:C:537:ILE:HG23	1:C:537:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:SER:O	1:A:363:GLU:CB	2.60	0.50
2:B:607:TYR:CG	2:B:608:SER:N	2.80	0.50
1:A:89:ARG:CG	1:A:89:ARG:HH11	2.24	0.49
2:B:239:ASN:CB	2:B:242:GLU:HG2	2.41	0.49
2:D:176:LEU:O	2:D:177:ASN:HB3	2.12	0.49
2:D:233:THR:O	2:D:234:VAL:HG13	2.12	0.49
1:A:466:LYS:HE2	1:A:490:PRO:CB	2.43	0.49
1:A:249:LYS:NZ	1:A:249:LYS:CD	2.72	0.49
1:C:362:SER:O	1:C:363:GLU:CB	2.60	0.49
2:D:247:ILE:HG22	2:D:247:ILE:O	2.12	0.49
1:A:94:SER:HB3	1:A:97:ASP:O	2.12	0.49
2:B:223:TYR:HB2	2:B:375:CYS:HA	1.95	0.49
2:B:588:HIS:HE1	2:B:590:ILE:HD12	1.77	0.49
1:C:268:PHE:CD2	1:C:285:SER:HB3	2.46	0.49
2:B:377:ALA:HB1	2:B:378:PRO:HD2	1.93	0.49
2:B:527:ILE:HD13	2:B:568:VAL:HG21	1.94	0.49
1:C:321:TRP:HZ2	1:C:325:ASN:HD22	1.61	0.49
1:C:48:ILE:HG21	1:C:51:ASN:O	2.12	0.49
2:D:168:ASP:HA	2:D:171:GLU:HB2	1.94	0.49
1:A:138:ASN:HD22	1:A:139:PRO:N	2.10	0.49
1:A:264:SER:C	1:A:266:GLU:H	2.14	0.49
2:B:302:GLU:HG3	2:B:649:GLU:HB2	1.95	0.49
2:B:610:LYS:HA	2:B:610:LYS:CE	2.42	0.49
1:C:16:ASP:N	1:C:16:ASP:OD1	2.44	0.49
1:C:537:ILE:HD11	1:C:542:VAL:HG11	1.94	0.49
2:D:616:ILE:N	2:D:616:ILE:HD12	2.27	0.49
2:B:198:PHE:HE1	2:B:203:ILE:HD12	1.76	0.49
2:B:233:THR:O	2:B:234:VAL:HG13	2.13	0.49
2:B:527:ILE:HD12	2:B:561:VAL:HG11	1.95	0.49
2:B:399:ILE:O	2:B:400:ASP:HB2	2.12	0.49
1:C:304:ASN:O	1:C:305:ILE:HG12	2.13	0.49
1:A:18:LYS:HE2	1:A:90:VAL:HG12	1.94	0.48
1:A:563:TYR:HB3	1:A:567:THR:HG23	1.93	0.48
1:C:262:THR:HG21	1:C:268:PHE:CE2	2.47	0.48
1:C:428:ASN:OD1	1:C:573:ARG:NH1	2.46	0.48
2:B:370:LYS:O	2:B:385:SER:HB2	2.13	0.48
2:D:405:VAL:HG13	2:D:406:HIS:N	2.28	0.48
1:A:3:LEU:HD11	1:A:370:PHE:O	2.13	0.48
1:C:322:ASN:O	1:C:323:GLU:O	2.31	0.48
1:C:344:SER:HB3	1:C:394:ILE:HG21	1.95	0.48
2:D:239:ASN:CB	2:D:242:GLU:HG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASN:C	1:A:138:ASN:HD22	2.17	0.48
2:B:216:PRO:O	2:B:433:PRO:HD3	2.12	0.48
2:B:605:TRP:CZ3	2:B:616:ILE:HG13	2.48	0.48
1:C:94:SER:HB3	1:C:97:ASP:O	2.13	0.48
2:D:340:CYS:HB2	2:D:359:ILE:O	2.13	0.48
2:D:357:GLN:OE1	2:D:400:ASP:HB3	2.13	0.48
2:D:532:ALA:HA	2:D:555:THR:HG22	1.94	0.48
2:B:235:TYR:CG	2:B:236:HIS:N	2.81	0.48
2:B:253:ARG:HG2	2:B:266:SER:CB	2.43	0.48
2:B:384:LEU:HD22	2:B:398:ILE:CD1	2.37	0.48
1:C:243:CYS:HB3	1:C:244:PRO:CD	2.42	0.48
1:C:553:ILE:HB	1:C:571:LEU:HD22	1.96	0.48
1:C:378:THR:HG22	1:C:401:LYS:HB2	1.95	0.48
1:C:242:THR:HG21	1:C:268:PHE:O	2.14	0.48
2:B:385:SER:HB3	2:B:428:PHE:CZ	2.48	0.48
2:B:533:SER:O	2:B:551:SER:HA	2.14	0.48
1:A:183:ASP:HB3	1:A:200:SER:HB2	1.96	0.48
2:B:223:TYR:HD2	2:B:224:ASN:HD22	1.60	0.48
1:A:159:ARG:O	1:A:166:PRO:O	2.32	0.47
2:B:234:VAL:CB	2:B:412:GLU:HG2	2.44	0.47
2:B:601:ARG:NH1	2:B:604:LYS:HB3	2.29	0.47
2:D:301:GLU:HB3	2:D:371:TRP:CD2	2.49	0.47
1:A:42:PRO:HB2	1:A:386:LEU:HD13	1.94	0.47
1:A:520:THR:OG1	1:A:526:THR:HB	2.14	0.47
1:A:68:LYS:N	1:A:108:ASN:HD21	2.00	0.47
2:D:231:ASN:N	2:D:231:ASN:OD1	2.47	0.47
2:D:235:TYR:CG	2:D:236:HIS:N	2.80	0.47
1:A:322:ASN:O	1:A:323:GLU:O	2.33	0.47
1:C:448:LYS:HB3	1:C:448:LYS:HE3	1.55	0.47
1:C:500:ASN:O	1:C:502:PHE:N	2.47	0.47
2:D:384:LEU:HD22	2:D:398:ILE:CD1	2.44	0.47
1:A:515:ASP:OD1	1:A:517:GLU:N	2.41	0.47
2:B:597:GLN:C	2:B:598:LYS:HG3	2.35	0.47
1:C:21:LEU:HD13	1:C:31:LEU:CD2	2.45	0.47
1:C:496:LEU:HA	1:C:496:LEU:HD12	1.51	0.47
1:C:550:GLN:HG2	1:C:580:TYR:CE1	2.49	0.47
2:D:454:GLU:O	2:D:456:PRO:HD3	2.14	0.47
1:C:466:LYS:HA	1:C:469:LEU:HD12	1.96	0.47
1:A:89:ARG:HG2	1:A:89:ARG:HH11	1.80	0.47
1:C:230:THR:CG2	1:C:267:ASN:HB2	2.45	0.47
1:C:424:GLN:OE1	1:C:573:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:297:TRP:HD1	2:D:298:LEU:O	1.98	0.47
2:B:267:THR:CG2	2:B:289:GLY:HA2	2.43	0.47
2:B:299:ASN:HD22	2:B:646:LYS:HZ3	1.60	0.47
2:B:352:HIS:O	2:B:353:CYS:HB3	2.15	0.47
2:B:600:LEU:HD12	2:B:621:GLU:H	1.79	0.47
2:D:346:MET:CB	2:D:353:CYS:HB2	2.44	0.47
1:A:34:PHE:HD2	1:A:35:PRO:CA	2.28	0.47
1:A:402:LEU:HD22	1:A:438:ILE:HG23	1.96	0.47
2:B:361:HIS:HB2	2:B:363:PHE:CD1	2.49	0.47
2:D:230:LYS:HD3	2:D:230:LYS:HA	1.65	0.47
2:D:607:TYR:CG	2:D:608:SER:N	2.79	0.47
1:A:260:LEU:HG	1:A:261:LYS:O	2.15	0.46
1:A:412:LEU:HD22	1:A:454:PHE:HA	1.97	0.46
1:A:41:GLN:O	1:A:56:PHE:HA	2.14	0.46
2:B:273:PHE:N	2:B:274:PRO:CD	2.78	0.46
2:B:661:ASN:HD22	2:B:661:ASN:C	2.18	0.46
1:C:163:GLU:O	1:C:165:THR:N	2.47	0.46
1:C:268:PHE:HB2	1:C:284:MET:O	2.15	0.46
1:C:314:PHE:CD1	1:C:314:PHE:O	2.68	0.46
1:C:357:LYS:O	1:C:359:LYS:N	2.48	0.46
2:D:178:LYS:HD2	2:D:178:LYS:N	2.25	0.46
2:D:361:HIS:HB2	2:D:363:PHE:CD1	2.49	0.46
2:D:604:LYS:HG3	2:D:604:LYS:O	2.14	0.46
1:A:59:LYS:HD2	1:A:59:LYS:HA	1.69	0.46
1:C:125:GLY:O	1:C:130:ARG:HG3	2.14	0.46
1:C:517:GLU:C	1:C:529:ARG:HD2	2.36	0.46
2:B:357:GLN:OE1	2:B:400:ASP:HB3	2.16	0.46
2:B:247:ILE:HG22	2:B:247:ILE:O	2.15	0.46
2:B:642:ILE:HA	2:B:661:ASN:HA	1.96	0.46
2:D:520:CYS:HB2	2:D:527:ILE:HD12	1.98	0.46
2:D:648:ASN:ND2	2:D:650:THR:H	2.13	0.46
1:A:264:SER:O	1:A:266:GLU:N	2.48	0.46
2:B:230:LYS:HA	2:B:230:LYS:HD3	1.58	0.46
1:C:124:LYS:HG3	1:C:125:GLY:H	1.81	0.46
1:A:188:ILE:HG23	1:A:195:LEU:HD11	1.97	0.46
2:B:578:ILE:HD13	2:B:601:ARG:HB2	1.98	0.46
1:C:183:ASP:HB3	1:C:200:SER:HB2	1.98	0.46
1:C:264:SER:O	1:C:266:GLU:N	2.48	0.46
2:D:239:ASN:HB3	2:D:242:GLU:HB2	1.97	0.46
2:D:250:ARG:C	2:D:250:ARG:HD3	2.36	0.46
2:D:372:HIS:O	2:D:373:GLU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:579:ILE:O	2:D:599:SER:HB3	2.15	0.46
2:D:601:ARG:NH1	2:D:604:LYS:HB3	2.31	0.46
1:C:159:ARG:O	1:C:166:PRO:O	2.33	0.46
1:C:481:ILE:HG12	1:C:534:LEU:HD12	1.97	0.46
2:D:585:ARG:HB2	2:D:585:ARG:HH11	1.81	0.46
1:A:278:GLU:O	1:A:279:SER:C	2.54	0.46
1:C:117:MET:HG3	1:C:118:LEU:N	2.30	0.46
1:C:21:LEU:HD13	1:C:31:LEU:HD23	1.98	0.46
1:C:18:LYS:HE2	1:C:90:VAL:HG12	1.98	0.46
2:D:298:LEU:HD12	2:D:298:LEU:C	2.37	0.46
2:B:239:ASN:HB3	2:B:242:GLU:HB2	1.98	0.46
2:B:297:TRP:HD1	2:B:298:LEU:H	1.64	0.46
2:B:301:GLU:HB3	2:B:371:TRP:CD2	2.50	0.46
2:B:545:ALA:O	2:B:547:HIS:CD2	2.66	0.46
2:D:545:ALA:O	2:D:547:HIS:CD2	2.69	0.46
2:B:298:LEU:C	2:B:298:LEU:HD12	2.37	0.46
1:C:230:THR:HG21	1:C:267:ASN:HB2	1.97	0.46
1:C:541:HIS:CE1	1:C:557:ARG:HG3	2.50	0.46
2:D:247:ILE:CD1	2:D:340:CYS:HB3	2.46	0.46
1:A:18:LYS:O	1:A:18:LYS:HG2	2.16	0.45
1:A:443:ASN:OD1	1:A:449:PRO:HA	2.17	0.45
2:B:356:VAL:O	2:B:406:HIS:HA	2.17	0.45
1:C:303:ASP:O	1:C:304:ASN:HB3	2.16	0.45
1:C:537:ILE:O	1:C:538:LEU:HD23	2.16	0.45
2:B:288:VAL:HG11	2:B:317:VAL:CG1	2.44	0.45
2:D:311:GLN:HE22	2:D:650:THR:HG21	1.82	0.45
2:D:377:ALA:HB1	2:D:378:PRO:HD2	1.97	0.45
2:D:234:VAL:CB	2:D:412:GLU:HG2	2.45	0.45
2:D:473:ALA:HB2	2:D:526:TYR:CZ	2.51	0.45
2:D:608:SER:C	2:D:609:ILE:HG13	2.25	0.45
1:A:18:LYS:O	1:A:19:ASN:CB	2.64	0.45
1:A:303:ASP:OD1	1:A:305:ILE:HG23	2.16	0.45
2:B:607:TYR:OH	2:B:612:ASP:HA	2.15	0.45
1:C:537:ILE:CG1	1:C:542:VAL:HG11	2.46	0.45
2:D:393:ILE:HG23	2:D:418:LEU:HB2	1.98	0.45
2:B:172:ARG:HD3	2:B:172:ARG:HA	1.79	0.45
2:B:361:HIS:CD2	2:B:363:PHE:HB2	2.51	0.45
2:B:376:HIS:HB2	2:B:377:ALA:H	1.56	0.45
1:C:262:THR:HG22	1:C:262:THR:O	2.17	0.45
1:C:96:ILE:HG22	1:C:97:ASP:OD2	2.16	0.45
1:A:435:GLU:H	1:A:435:GLU:CD	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:231:ASN:O	2:B:415:SER:HA	2.16	0.45
2:B:231:ASN:N	2:B:231:ASN:OD1	2.50	0.45
2:B:584:ARG:CG	2:B:585:ARG:N	2.54	0.45
1:C:18:LYS:O	1:C:19:ASN:CB	2.63	0.45
1:C:3:LEU:HD11	1:C:370:PHE:O	2.17	0.45
1:C:90:VAL:HG22	1:C:103:LEU:HB3	1.99	0.45
2:D:198:PHE:HE1	2:D:203:ILE:HD12	1.77	0.45
1:A:533:THR:CG2	1:A:535:LEU:CB	2.88	0.45
1:C:4:LEU:HA	1:C:4:LEU:HD23	1.72	0.45
1:C:510:GLU:O	1:C:512:PHE:N	2.50	0.45
2:D:642:ILE:HA	2:D:661:ASN:HA	1.99	0.45
1:A:268:PHE:HB2	1:A:284:MET:O	2.17	0.45
2:B:579:ILE:O	2:B:599:SER:HB3	2.17	0.45
2:B:270:LYS:NZ	2:B:353:CYS:O	2.49	0.45
2:B:361:HIS:HD2	2:B:363:PHE:N	2.04	0.45
2:B:661:ASN:ND2	2:B:661:ASN:C	2.70	0.45
2:D:297:TRP:CD1	2:D:298:LEU:N	2.83	0.45
1:A:92:LYS:HB2	1:A:135:PHE:CE1	2.52	0.45
1:A:235:VAL:CG2	1:A:272:PRO:HB3	2.47	0.45
1:C:539:THR:HG23	1:C:540:THR:N	2.24	0.45
1:C:563:TYR:HB3	1:C:567:THR:HG23	1.98	0.45
1:C:97:ASP:CB	1:C:99:TRP:CE3	2.95	0.45
2:D:203:ILE:O	2:D:651:SER:OG	2.34	0.45
2:D:250:ARG:HG2	2:D:267:THR:HG1	1.75	0.45
2:D:303:ASN:H	2:D:650:THR:HG21	1.81	0.45
1:A:26:ASP:HA	1:A:384:VAL:HG23	1.99	0.44
1:A:15:GLU:HG3	1:A:34:PHE:CD1	2.52	0.44
1:C:210:SER:C	1:C:212:SER:H	2.20	0.44
1:C:243:CYS:CB	1:C:244:PRO:CD	2.95	0.44
2:D:370:LYS:O	2:D:385:SER:HB2	2.17	0.44
2:B:216:PRO:HD3	2:B:474:TYR:CG	2.52	0.44
2:D:569:LEU:HG	2:D:647:TRP:CZ2	2.51	0.44
1:A:155:PHE:CE1	1:A:174:ILE:HD12	2.51	0.44
2:B:234:VAL:HG21	2:B:412:GLU:CG	2.37	0.44
2:B:247:ILE:CD1	2:B:340:CYS:HB3	2.47	0.44
1:C:34:PHE:CD2	1:C:35:PRO:CA	2.96	0.44
2:D:235:TYR:CD1	2:D:236:HIS:N	2.85	0.44
1:C:157:SER:HB2	1:C:169:TYR:CE2	2.52	0.44
1:C:297:GLU:OE2	1:C:297:GLU:HA	2.17	0.44
1:A:242:THR:HG21	1:A:268:PHE:O	2.17	0.44
1:A:402:LEU:HD22	1:A:438:ILE:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:ILE:HG12	2:B:440:PHE:CE2	2.52	0.44
2:D:376:HIS:O	2:D:377:ALA:HB3	2.17	0.44
1:A:20:ASN:HB3	1:A:32:THR:OG1	2.17	0.44
2:B:563:ARG:HD2	2:B:649:GLU:CB	2.40	0.44
2:B:648:ASN:ND2	2:B:650:THR:H	2.15	0.44
2:D:216:PRO:HD3	2:D:474:TYR:CG	2.53	0.44
2:B:401:ASN:O	2:B:403:THR:N	2.47	0.44
2:B:512:SER:HB2	2:B:531:GLY:HA2	2.00	0.44
1:C:304:ASN:OD1	1:C:306:ILE:HB	2.18	0.44
1:C:92:LYS:HB2	1:C:135:PHE:CE1	2.53	0.44
2:D:262:ASP:OD1	2:D:613:LYS:HE2	2.17	0.44
1:A:458:LEU:HD12	1:A:458:LEU:HA	1.71	0.44
2:B:299:ASN:ND2	2:B:646:LYS:HZ3	2.16	0.44
2:B:640:ILE:CG1	2:B:641:ASN:H	2.26	0.44
2:D:557:THR:HB	2:D:642:ILE:O	2.18	0.44
1:A:412:LEU:HA	1:A:435:GLU:CG	2.48	0.44
2:B:427:THR:HG22	2:B:428:PHE:N	2.32	0.44
2:B:582:ALA:O	2:B:583:ALA:HB2	2.18	0.44
1:C:235:VAL:CG2	1:C:272:PRO:HB3	2.47	0.44
1:C:266:GLU:O	1:C:268:PHE:HD2	2.00	0.44
1:C:89:ARG:HD3	2:D:501:THR:HA	2.00	0.44
2:D:512:SER:HB2	2:D:531:GLY:HA2	2.00	0.44
1:A:21:LEU:HD22	1:A:348:VAL:CG2	2.47	0.43
1:A:39:ILE:HD12	1:A:61:PHE:CD1	2.53	0.43
2:B:346:MET:HB3	2:B:353:CYS:HB2	1.99	0.43
2:B:473:ALA:HB2	2:B:526:TYR:OH	2.18	0.43
1:C:136:GLU:HG2	1:C:190:TRP:H	1.83	0.43
1:C:262:THR:HG23	1:C:290:TYR:OH	2.18	0.43
1:C:412:LEU:HA	1:C:435:GLU:CG	2.48	0.43
2:B:225:LYS:O	2:B:451:THR:HG22	2.18	0.43
1:C:155:PHE:HE1	1:C:174:ILE:HD12	1.82	0.43
1:C:175:ARG:HA	1:C:175:ARG:HD2	1.84	0.43
1:A:230:THR:CG2	1:A:267:ASN:HB2	2.48	0.43
1:A:533:THR:HG22	1:A:535:LEU:N	2.26	0.43
2:B:248:LYS:H	2:B:319:GLN:HE21	1.66	0.43
1:C:126:ASN:O	1:C:127:LEU:CB	2.65	0.43
1:C:188:ILE:HG23	1:C:195:LEU:HD11	2.00	0.43
1:C:18:LYS:HG2	1:C:18:LYS:O	2.18	0.43
1:A:545:CYS:HA	1:A:546:PRO:HD3	1.82	0.43
2:B:297:TRP:HD1	2:B:298:LEU:N	2.15	0.43
2:B:381:VAL:HG12	2:B:382:GLY:N	2.27	0.43

Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:LYS:HG2	1:C:417:TYR:OH	2.19	0.43
2:D:585:ARG:CB	2:D:585:ARG:HH11	2.31	0.43
2:D:661:ASN:HD22	2:D:661:ASN:C	2.21	0.43
1:A:210:SER:C	1:A:212:SER:H	2.22	0.43
1:A:530:CYS:O	1:A:551:ARG:O	2.37	0.43
2:D:220:GLU:O	2:D:221:SER:HB3	2.18	0.43
2:D:661:ASN:ND2	2:D:661:ASN:C	2.72	0.43
2:B:290:GLY:CA	2:B:293:THR:N	2.63	0.43
2:B:571:GLY:HA2	2:B:576:SER:O	2.19	0.43
1:C:41:GLN:O	1:C:56:PHE:HA	2.18	0.43
1:A:304:ASN:C	1:A:305:ILE:HG12	2.38	0.43
2:B:239:ASN:HB3	2:B:242:GLU:CB	2.49	0.43
2:B:585:ARG:NH1	2:B:585:ARG:CB	2.81	0.43
1:A:321:TRP:CG	1:A:321:TRP:O	2.71	0.43
1:A:271:ILE:HD11	1:A:284:MET:HE2	2.00	0.43
1:A:268:PHE:CD2	1:A:285:SER:HB3	2.53	0.43
2:B:418:LEU:HD23	2:B:453:PRO:HB3	2.00	0.43
1:C:284:MET:HA	1:C:289:SER:HB3	2.01	0.43
1:C:460:GLU:HA	1:C:460:GLU:OE2	2.19	0.43
1:C:55:LEU:HD23	1:C:55:LEU:HA	1.71	0.43
2:D:233:THR:HG23	2:D:414:PRO:HA	2.01	0.43
1:A:34:PHE:CD2	1:A:35:PRO:CA	3.01	0.43
2:B:340:CYS:HB2	2:B:359:ILE:O	2.19	0.43
2:B:372:HIS:O	2:B:373:GLU:CB	2.61	0.43
1:C:251:ASP:HB3	1:C:254:ASN:OD1	2.19	0.43
1:C:426:TYR:CE2	1:C:461:TYR:HB2	2.54	0.43
1:C:59:LYS:HA	1:C:59:LYS:HD2	1.59	0.43
1:A:133:HIS:ND1	2:B:501:THR:HG21	2.34	0.42
1:A:262:THR:O	1:A:262:THR:HG22	2.19	0.42
1:A:272:PRO:HA	1:A:281:ILE:HG22	2.01	0.42
1:C:226:ARG:HG3	2:D:457:SER:HG	1.81	0.42
1:C:396:ASN:O	1:C:397:GLN:HB2	2.19	0.42
2:D:294:ASP:HB3	2:D:662:SER:O	2.19	0.42
1:C:126:ASN:O	1:C:127:LEU:HB3	2.19	0.42
1:C:26:ASP:HA	1:C:384:VAL:HG23	2.01	0.42
2:D:614:TYR:HE2	2:D:639:GLY:O	2.03	0.42
1:A:262:THR:HG21	1:A:268:PHE:CE2	2.50	0.42
2:B:358:THR:OG1	2:B:406:HIS:HE1	2.02	0.42
1:C:553:ILE:HB	1:C:571:LEU:CD2	2.49	0.42
1:A:396:ASN:O	1:A:397:GLN:HB2	2.18	0.42
2:B:303:ASN:H	2:B:650:THR:HG21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ILE:HD12	2:B:428:PHE:CD1	2.54	0.42
1:C:247:VAL:HG21	1:C:283:LEU:CD1	2.48	0.42
1:C:530:CYS:O	1:C:551:ARG:O	2.38	0.42
1:C:65:PHE:CE2	1:C:102:VAL:HG11	2.54	0.42
2:D:172:ARG:HA	2:D:172:ARG:HD3	1.84	0.42
2:D:239:ASN:CG	2:D:242:GLU:HG2	2.40	0.42
1:A:315:LYS:O	1:A:318:SER:HB3	2.19	0.42
1:A:5:LYS:HD3	1:A:51:ASN:ND2	2.34	0.42
2:B:297:TRP:CD1	2:B:298:LEU:O	2.73	0.42
2:B:549:LEU:HD12	2:B:549:LEU:HA	1.94	0.42
2:B:669:GLU:HG2	2:B:670:TYR:N	2.34	0.42
1:C:278:GLU:O	1:C:279:SER:C	2.58	0.42
1:C:321:TRP:O	1:C:322:ASN:C	2.58	0.42
1:C:226:ARG:NH1	2:D:455:VAL:O	2.51	0.42
1:A:347:ILE:HD12	1:A:369:MET:CE	2.50	0.42
2:B:242:GLU:O	2:B:246:MET:HB2	2.20	0.42
2:B:376:HIS:O	2:B:377:ALA:HB3	2.20	0.42
2:B:470:VAL:O	2:B:470:VAL:HG13	2.18	0.42
2:D:405:VAL:HG13	2:D:406:HIS:H	1.84	0.42
2:D:425:ILE:HG12	2:D:440:PHE:CE2	2.54	0.42
2:D:608:SER:HG	2:D:611:ASP:HB2	1.84	0.42
1:A:303:ASP:CG	1:A:305:ILE:HG23	2.40	0.42
2:B:235:TYR:CD1	2:B:236:HIS:N	2.87	0.42
2:B:366:VAL:HG13	2:B:386:PHE:HB2	2.01	0.42
2:B:373:GLU:OE2	2:B:563:ARG:NH2	2.52	0.42
1:C:303:ASP:O	1:C:304:ASN:CB	2.68	0.42
2:D:512:SER:HB3	2:D:515:VAL:CG2	2.46	0.42
2:D:640:ILE:CG1	2:D:641:ASN:H	2.21	0.42
2:B:528:TYR:N	2:B:528:TYR:CD2	2.87	0.42
1:C:143:SER:HB2	1:C:156:PHE:O	2.20	0.42
2:D:641:ASN:HD21	2:D:662:SER:HB3	1.85	0.42
1:A:148:ASN:OD1	1:A:152:GLU:HB3	2.20	0.42
1:A:459:TYR:CE2	1:A:487:ARG:HG2	2.55	0.42
1:C:277:LYS:O	1:C:278:GLU:HG2	2.19	0.42
1:C:442:LEU:O	1:C:445:THR:HB	2.20	0.42
1:C:522:THR:HG23	1:C:523:THR:N	2.35	0.42
1:A:325:ASN:HA	1:A:325:ASN:HD22	1.72	0.42
1:A:327:TYR:CD2	1:A:353:ARG:HD3	2.54	0.42
2:B:196:PHE:CZ	2:B:622:VAL:HG13	2.55	0.42
1:C:321:TRP:CG	1:C:321:TRP:O	2.73	0.42
2:D:610:LYS:HA	2:D:610:LYS:HZ1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:PHE:CZ	2:D:622:VAL:HG13	2.54	0.42
1:A:153:LEU:O	1:A:173:SER:HA	2.20	0.41
1:A:475:LEU:HD13	1:A:475:LEU:HA	1.76	0.41
2:B:298:LEU:HG	2:B:644:CYS:SG	2.60	0.41
1:C:528:LYS:HB2	1:C:537:ILE:HG21	2.01	0.41
2:D:420:LEU:HA	2:D:420:LEU:HD12	1.82	0.41
1:A:126:ASN:O	1:A:127:LEU:CB	2.68	0.41
1:A:347:ILE:HD12	1:A:369:MET:HE2	2.01	0.41
1:C:48:ILE:CG2	1:C:54:ASN:HB2	2.50	0.41
2:D:451:THR:H	2:D:451:THR:HG1	1.63	0.41
2:B:405:VAL:HG13	2:B:406:HIS:H	1.85	0.41
2:B:196:PHE:HE2	2:B:599:SER:HA	1.84	0.41
1:C:321:TRP:CD1	1:C:327:TYR:HB2	2.56	0.41
1:C:519:VAL:CG1	1:C:536:PRO:HG3	2.51	0.41
1:C:545:CYS:HA	1:C:546:PRO:HD3	1.87	0.41
1:C:358:TYR:CB	2:D:508:ARG:NH2	2.79	0.41
1:A:354:VAL:HB	1:A:355:ALA:H	1.51	0.41
1:A:571:LEU:HD23	1:A:571:LEU:HA	1.85	0.41
1:A:89:ARG:CG	1:A:89:ARG:NH1	2.83	0.41
2:B:168:ASP:HA	2:B:171:GLU:HB2	2.02	0.41
2:B:250:ARG:HD3	2:B:252:LYS:N	2.36	0.41
1:C:112:PHE:CD2	1:C:117:MET:HA	2.55	0.41
1:C:3:LEU:HD12	1:C:4:LEU:H	1.86	0.41
1:C:41:GLN:HA	1:C:42:PRO:HD3	1.87	0.41
2:D:239:ASN:HB3	2:D:242:GLU:CB	2.49	0.41
2:D:216:PRO:O	2:D:433:PRO:HD3	2.20	0.41
2:D:584:ARG:HH21	2:D:585:ARG:HD3	1.85	0.41
1:A:321:TRP:HZ2	1:A:325:ASN:HD22	1.67	0.41
1:A:529:ARG:NH1	1:A:534:LEU:O	2.53	0.41
2:B:257:LEU:O	2:B:616:ILE:HD12	2.21	0.41
1:C:78:GLY:C	1:C:80:LEU:H	2.23	0.41
2:D:302:GLU:HA	2:D:302:GLU:OE2	2.21	0.41
2:D:418:LEU:HD23	2:D:453:PRO:HB3	2.02	0.41
2:D:427:THR:HG21	2:D:469:SER:HA	2.01	0.41
2:D:580:THR:HB	2:D:599:SER:CB	2.51	0.41
2:D:623:TYR:HA	2:D:624:PRO:HD3	1.74	0.41
2:B:239:ASN:CG	2:B:242:GLU:HG2	2.41	0.41
2:B:300:ILE:HG21	2:B:300:ILE:HD12	1.88	0.41
2:D:258:ILE:CD1	2:D:271:ILE:HG21	2.50	0.41
1:A:16:ASP:OD1	1:A:16:ASP:N	2.54	0.41
1:A:175:ARG:HD2	1:A:175:ARG:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:SER:HB3	1:A:410:LYS:HD2	2.02	0.41
1:A:143:SER:HB2	1:A:156:PHE:O	2.21	0.41
2:B:585:ARG:HB3	2:B:585:ARG:NH1	2.36	0.41
2:D:358:THR:OG1	2:D:406:HIS:HE1	2.04	0.41
2:D:366:VAL:HG13	2:D:386:PHE:HB2	2.02	0.41
2:D:582:ALA:O	2:D:583:ALA:HB2	2.20	0.41
1:A:138:ASN:HD22	1:A:139:PRO:HD2	1.86	0.41
1:A:448:LYS:HE3	1:A:448:LYS:HB3	1.41	0.41
1:A:459:TYR:OH	1:A:463:ILE:HD11	2.20	0.41
2:D:273:PHE:N	2:D:274:PRO:HD3	2.36	0.41
2:D:395:PHE:N	2:D:395:PHE:CD2	2.88	0.41
2:D:441:LYS:HG2	2:D:441:LYS:O	2.20	0.41
2:D:661:ASN:HD22	2:D:661:ASN:H	1.69	0.41
1:A:230:THR:HG21	1:A:267:ASN:HB2	2.01	0.41
2:B:253:ARG:CG	2:B:253:ARG:NH1	2.74	0.41
2:B:383:CYS:HB2	2:B:397:GLU:HA	2.02	0.41
2:B:559:ILE:HD13	2:B:559:ILE:HG21	1.81	0.41
1:C:382:ARG:HH11	1:C:382:ARG:HG2	1.86	0.41
2:D:203:ILE:HG22	2:D:651:SER:HA	2.03	0.41
1:A:138:ASN:HD22	1:A:139:PRO:CD	2.34	0.40
1:A:145:VAL:HG22	1:A:190:TRP:CZ3	2.56	0.40
2:B:588:HIS:HE1	2:B:590:ILE:CG1	2.34	0.40
1:C:10:ASP:OD1	1:C:365:SER:HB3	2.22	0.40
1:C:155:PHE:HE1	1:C:174:ILE:CD1	2.34	0.40
1:C:563:TYR:HB3	1:C:567:THR:HG22	2.02	0.40
1:A:124:LYS:HG3	1:A:125:GLY:H	1.85	0.40
1:C:340:PRO:HB2	1:C:383:ALA:HB2	2.02	0.40
1:C:81:ASN:HA	1:C:106:ASN:ND2	2.37	0.40
1:A:243:CYS:HB3	1:A:244:PRO:CD	2.50	0.40
1:A:5:LYS:HB3	1:A:51:ASN:HA	2.04	0.40
2:B:442:ASN:OD1	2:B:444:PHE:HD1	2.04	0.40
2:B:661:ASN:ND2	2:B:665:LEU:H	2.14	0.40
1:C:556:LYS:HD2	1:C:575:ASN:ND2	2.36	0.40
2:B:184:LEU:HA	2:B:184:LEU:HD12	1.93	0.40
1:A:100:MET:HE2	1:A:100:MET:HB3	1.69	0.40
2:B:420:LEU:HA	2:B:420:LEU:HD12	1.92	0.40
2:B:641:ASN:HD22	2:B:642:ILE:N	2.20	0.40
1:C:499:LYS:O	1:C:561:ASN:ND2	2.53	0.40
2:D:196:PHE:O	2:D:579:ILE:HD13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	585/588 (100%)	475 (81%)	74 (13%)	36 (6%)	2	13
1	C	584/588 (99%)	475 (81%)	69 (12%)	40 (7%)	1	10
2	B	462/524 (88%)	362 (78%)	68 (15%)	32 (7%)	1	9
2	D	459/524 (88%)	356 (78%)	76 (17%)	27 (6%)	2	15
All	All	2090/2224 (94%)	1668 (80%)	287 (14%)	135 (6%)	1	11

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	124	LYS
1	A	159	ARG
1	A	164	ASN
1	A	166	PRO
1	A	212	SER
1	A	278	GLU
1	A	303	ASP
1	A	305	ILE
1	A	320	ILE
1	A	321	TRP
1	A	323	GLU
1	A	324	PHE
1	A	354	VAL
1	A	358	TYR
1	A	361	ALA
1	A	363	GLU
1	A	364	GLN
2	B	177	ASN
2	B	222	ALA
2	B	223	TYR
2	B	235	TYR

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type
2	B	238	ILE
2	B	289	GLY
2	B	379	HIS
2	B	380	LEU
2	B	381	VAL
2	B	400	ASP
2	B	405	VAL
2	B	583	ALA
2	B	584	ARG
2	B	610	LYS
2	B	640	ILE
2	B	674	GLU
1	C	80	LEU
1	C	124	LYS
1	C	126	ASN
1	C	127	LEU
1	C	159	ARG
1	C	164	ASN
1	C	166	PRO
1	C	212	SER
1	C	278	GLU
1	C	303	ASP
1	C	305	ILE
1	C	320	ILE
1	C	321	TRP
1	C	323	GLU
1	C	324	PHE
1	C	354	VAL
1	C	358	TYR
1	C	361	ALA
1	C	363	GLU
1	C	364	GLN
1	C	501	SER
2	D	222	ALA
2	D	223	TYR
2	D	235	TYR
2	D	238	ILE
2	D	379	HIS
2	D	380	LEU
2	D	381	VAL
2	D	400	ASP
2	D	405	VAL

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Mol	Chain	Res	Type
2	D	583	ALA
2	D	584	ARG
2	D	610	LYS
2	D	640	ILE
1	A	49	ASN
1	A	126	ASN
1	A	127	LEU
1	A	322	ASN
2	B	339	SER
2	B	402	ALA
2	B	611	ASP
1	C	322	ASN
1	C	416	ASN
2	D	177	ASN
2	D	339	SER
2	D	424	LEU
2	D	611	ASP
1	A	99	TRP
1	A	210	SER
1	A	416	ASN
2	B	233	THR
2	B	378	PRO
2	B	423	SER
2	B	589	GLY
2	B	641	ASN
2	B	672	SER
1	C	160	LYS
1	C	163	GLU
1	C	402	LEU
1	C	488	GLU
2	D	233	THR
2	D	378	PRO
2	D	402	ALA
2	D	423	SER
2	D	641	ASN
2	D	672	SER
1	A	19	ASN
1	A	163	GLU
2	B	251	THR
2	B	424	LEU
2	B	532	ALA
1	C	49	ASN

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Mol	Chain	Res	Type
1	C	99	TRP
1	C	210	SER
1	C	211	ALA
1	C	215	GLN
1	C	236	ASP
1	C	265	LEU
1	C	359	LYS
2	D	251	THR
2	D	530	ASP
2	D	532	ALA
1	A	158	ILE
1	A	211	ALA
1	A	215	GLN
1	A	236	ASP
1	A	359	LYS
1	A	402	LEU
2	B	530	ASP
1	C	19	ASN
1	C	158	ILE
1	C	243	CYS
1	A	84	PRO
1	A	265	LEU
2	B	308	LYS
2	B	466	TYR
1	C	511	SER
1	C	84	PRO
2	B	609	ILE
2	D	609	ILE
1	A	243	CYS

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	543/544 (100%)	434 (80%)	109 (20%)	1	7
1	C	542/544 (100%)	434 (80%)	108 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
2	B	415/465 (89%)	340 (82%)	75 (18%)		2	10
2	D	414/465 (89%)	336 (81%)	78 (19%)		2	9
All	All	1914/2018 (95%)	1544 (81%)	370 (19%)		1	9

All (370) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	19	ASN
1	A	22	THR
1	A	33	THR
1	A	34	PHE
1	A	48	ILE
1	A	49	ASN
1	A	51	ASN
1	A	57	HIS
1	A	59	LYS
1	A	63	LEU
1	A	67	ASN
1	A	82	SER
1	A	83	GLN
1	A	85	VAL
1	A	89	ARG
1	A	97	ASP
1	A	99	TRP
1	A	100	MET
1	A	115	ASN
1	A	117	MET
1	A	119	THR
1	A	131	THR
1	A	138	ASN
1	A	145	VAL
1	A	159	ARG
1	A	160	LYS
1	A	162	SER
1	A	163	GLU
1	A	165	THR
1	A	169	TYR
1	A	178	ASP
1	A	181	SER
1	A	182	LYS

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Mol	Chain	Res	Type
1	A	183	ASP
1	A	184	TRP
1	A	189	VAL
1	A	193	ASP
1	A	207	MET
1	A	215	GLN
1	A	219	ARG
1	A	226	ARG
1	A	237	TYR
1	A	249	LYS
1	A	254	ASN
1	A	255	TYR
1	A	257	ILE
1	A	258	SER
1	A	269	HIS
1	A	270	ILE
1	A	277	LYS
1	A	280	THR
1	A	284	MET
1	A	287	LYS
1	A	295	GLU
1	A	305	ILE
1	A	308	PRO
1	A	312	LYS
1	A	313	LYS
1	A	319	THR
1	A	324	PHE
1	A	325	ASN
1	A	331	LEU
1	A	344	SER
1	A	352	GLU
1	A	354	VAL
1	A	356	PHE
1	A	358	TYR
1	A	362	SER
1	A	368	ILE
1	A	384	VAL
1	A	397	GLN
1	A	399	LEU
1	A	404	GLU
1	A	408	MET
1	A	412	LEU

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Mol	Chain	Res	Type
1	A	414	ASN
1	A	416	ASN
1	A	435	GLU
1	A	448	LYS
1	A	450	SER
1	A	458	LEU
1	A	463	ILE
1	A	472	SER
1	A	475	LEU
1	A	478	VAL
1	A	484	ILE
1	A	487	ARG
1	A	491	ILE
1	A	493	ASN
1	A	501	SER
1	A	503	LEU
1	A	506	THR
1	A	513	THR
1	A	517	GLU
1	A	523	THR
1	A	526	THR
1	A	533	THR
1	A	535	LEU
1	A	538	LEU
1	A	539	THR
1	A	545	CYS
1	A	549	LYS
1	A	551	ARG
1	A	567	THR
1	A	573	ARG
1	A	577	ILE
1	A	579	VAL
1	A	581	CYS
2	B	172	ARG
2	B	178	LYS
2	B	184	LEU
2	B	219	LYS
2	B	220	GLU
2	B	221	SER
2	B	224	ASN
2	B	226	VAL
2	B	227	ILE

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Mol	Chain	Res	Type
2	B	231	ASN
2	B	234	VAL
2	B	235	TYR
2	B	236	HIS
2	B	238	ILE
2	B	246	MET
2	B	249	LEU
2	B	250	ARG
2	B	251	THR
2	B	252	LYS
2	B	253	ARG
2	B	257	LEU
2	B	266	SER
2	B	293	THR
2	B	294	ASP
2	B	295	ILE
2	B	300	ILE
2	B	301	GLU
2	B	302	GLU
2	B	304	THR
2	B	306	ILE
2	B	313	LEU
2	B	338	SER
2	B	348	THR
2	B	353	CYS
2	B	354	VAL
2	B	365	GLU
2	B	376	HIS
2	B	381	VAL
2	B	383	CYS
2	B	388	SER
2	B	389	GLN
2	B	393	ILE
2	B	394	ASN
2	B	396	LEU
2	B	399	ILE
2	B	401	ASN
2	B	403	THR
2	B	415	SER
2	B	454	GLU
2	B	455	VAL
2	B	464	ASP

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Mol	Chain	Res	Type
2	B	480	THR
2	B	484	THR
2	B	507	SER
2	B	510	ARG
2	B	518	VAL
2	B	525	SER
2	B	533	SER
2	B	549	LEU
2	B	554	THR
2	B	557	THR
2	B	559	ILE
2	B	584	ARG
2	B	586	LEU
2	B	597	GLN
2	B	600	LEU
2	B	601	ARG
2	B	604	LYS
2	B	609	ILE
2	B	610	LYS
2	B	616	ILE
2	B	640	ILE
2	B	651	SER
2	B	661	ASN
2	B	667	THR
1	C	8	LEU
1	C	18	LYS
1	C	19	ASN
1	C	22	THR
1	C	34	PHE
1	C	48	ILE
1	C	49	ASN
1	C	51	ASN
1	C	57	HIS
1	C	59	LYS
1	C	63	LEU
1	C	67	ASN
1	C	83	GLN
1	C	85	VAL
1	C	89	ARG
1	C	97	ASP
1	C	100	MET
1	C	115	ASN

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Mol	Chain	Res	Type
1	C	117	MET
1	C	119	THR
1	C	131	THR
1	C	138	ASN
1	C	145	VAL
1	C	159	ARG
1	C	160	LYS
1	C	162	SER
1	C	163	GLU
1	C	165	THR
1	C	169	TYR
1	C	178	ASP
1	C	181	SER
1	C	182	LYS
1	C	183	ASP
1	C	189	VAL
1	C	193	ASP
1	C	207	MET
1	C	215	GLN
1	C	219	ARG
1	C	226	ARG
1	C	237	TYR
1	C	243	CYS
1	C	247	VAL
1	C	254	ASN
1	C	255	TYR
1	C	257	ILE
1	C	258	SER
1	C	269	HIS
1	C	270	ILE
1	C	277	LYS
1	C	280	THR
1	C	284	MET
1	C	287	LYS
1	C	295	GLU
1	C	305	ILE
1	C	312	LYS
1	C	313	LYS
1	C	319	THR
1	C	324	PHE
1	C	325	ASN
1	C	331	LEU

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Mol	Chain	Res	Type
1	C	344	SER
1	C	352	GLU
1	C	354	VAL
1	C	356	PHE
1	C	358	TYR
1	C	362	SER
1	C	368	ILE
1	C	384	VAL
1	C	397	GLN
1	C	399	LEU
1	C	401	LYS
1	C	407	SER
1	C	409	ASN
1	C	412	LEU
1	C	414	ASN
1	C	416	ASN
1	C	435	GLU
1	C	437	ARG
1	C	448	LYS
1	C	450	SER
1	C	458	LEU
1	C	463	ILE
1	C	472	SER
1	C	475	LEU
1	C	478	VAL
1	C	484	ILE
1	C	487	ARG
1	C	488	GLU
1	C	495	THR
1	C	497	LEU
1	C	500	ASN
1	C	502	PHE
1	C	503	LEU
1	C	506	THR
1	C	510	GLU
1	C	511	SER
1	C	517	GLU
1	C	523	THR
1	C	526	THR
1	C	533	THR
1	C	535	LEU
1	C	537	ILE

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Mol	Chain	Res	Type
1	C	540	THR
1	C	549	LYS
1	C	551	ARG
1	C	567	THR
1	C	579	VAL
1	C	588	MET
2	D	172	ARG
2	D	178	LYS
2	D	184	LEU
2	D	219	LYS
2	D	220	GLU
2	D	221	SER
2	D	224	ASN
2	D	226	VAL
2	D	227	ILE
2	D	231	ASN
2	D	234	VAL
2	D	235	TYR
2	D	236	HIS
2	D	246	MET
2	D	249	LEU
2	D	250	ARG
2	D	251	THR
2	D	252	LYS
2	D	253	ARG
2	D	257	LEU
2	D	266	SER
2	D	293	THR
2	D	295	ILE
2	D	300	ILE
2	D	301	GLU
2	D	302	GLU
2	D	304	THR
2	D	306	ILE
2	D	308	LYS
2	D	313	LEU
2	D	319	GLN
2	D	338	SER
2	D	348	THR
2	D	353	CYS
2	D	354	VAL
2	D	365	GLU

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Mol	Chain	Res	Type
2	D	376	HIS
2	D	381	VAL
2	D	383	CYS
2	D	388	SER
2	D	389	GLN
2	D	393	ILE
2	D	394	ASN
2	D	396	LEU
2	D	401	ASN
2	D	403	THR
2	D	404	ASP
2	D	415	SER
2	D	454	GLU
2	D	455	VAL
2	D	464	ASP
2	D	480	THR
2	D	484	THR
2	D	507	SER
2	D	510	ARG
2	D	525	SER
2	D	533	SER
2	D	549	LEU
2	D	557	THR
2	D	559	ILE
2	D	563	ARG
2	D	584	ARG
2	D	585	ARG
2	D	586	LEU
2	D	587	LEU
2	D	600	LEU
2	D	601	ARG
2	D	604	LYS
2	D	609	ILE
2	D	610	LYS
2	D	616	ILE
2	D	640	ILE
2	D	644	CYS
2	D	651	SER
2	D	661	ASN
2	D	667	THR
2	D	668	LEU
2	D	674	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	51	ASN
1	A	67	ASN
1	A	106	ASN
1	A	108	ASN
1	A	138	ASN
1	A	161	ASN
1	A	187	HIS
1	A	215	GLN
1	A	304	ASN
1	A	325	ASN
1	A	397	GLN
1	A	416	ASN
1	A	541	HIS
1	A	575	ASN
2	B	224	ASN
2	B	287	ASN
2	B	299	ASN
2	B	357	GLN
2	B	361	HIS
2	B	389	GLN
2	B	401	ASN
2	B	406	HIS
2	B	522	GLN
2	B	547	HIS
2	B	588	HIS
2	B	597	GLN
2	B	641	ASN
2	B	648	ASN
2	B	661	ASN
1	C	41	GLN
1	C	51	ASN
1	C	67	ASN
1	C	106	ASN
1	C	108	ASN
1	C	138	ASN
1	C	161	ASN
1	C	215	GLN
1	C	304	ASN
1	C	325	ASN
1	C	397	GLN

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Mol	Chain	Res	Type
1	C	416	ASN
1	C	541	HIS
1	C	575	ASN
2	D	224	ASN
2	D	245	ASN
2	D	299	ASN
2	D	311	GLN
2	D	357	GLN
2	D	361	HIS
2	D	389	GLN
2	D	401	ASN
2	D	406	HIS
2	D	522	GLN
2	D	547	HIS
2	D	565	HIS
2	D	638	HIS
2	D	641	ASN
2	D	648	ASN
2	D	661	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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(Å²)	Q<0.9
1	A	587/588 (99%)	0.43	44 (7%)	15	8	61, 71, 71, 81	0
1	C	586/588 (99%)	0.49	42 (7%)	16	10	60, 71, 71, 87	0
2	B	472/524 (90%)	0.63	36 (7%)	15	8	70, 71, 71, 72	0
2	D	469/524 (89%)	0.60	34 (7%)	16	10	71, 71, 71, 75	0
All	All	2114/2224 (95%)	0.53	156 (7%)	15	9	60, 71, 71, 87	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	211	ALA	6.5
2	D	589	GLY	6.1
1	C	325	ASN	5.8
1	A	328	GLU	5.7
1	C	324	PHE	5.7
1	C	212	SER	5.5
2	D	588	HIS	5.2
1	A	214	HIS	4.9
1	C	71	PHE	4.7
1	C	163	GLU	4.7
2	D	229	ASP	4.6
1	C	160	LYS	4.2
2	B	401	ASN	4.2
1	C	362	SER	4.2
1	C	165	THR	4.2
1	C	161	ASN	4.1
1	A	166	PRO	4.0
1	A	297	GLU	4.0
2	D	293	THR	4.0
1	A	159	ARG	4.0
1	C	213	SER	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	229	ASP	3.9
1	A	210	SER	3.9
1	C	326	ASN	3.8
1	A	212	SER	3.8
1	A	213	SER	3.8
1	A	329	THR	3.8
1	A	323	GLU	3.7
1	A	164	ASN	3.6
1	C	214	HIS	3.6
1	A	193	ASP	3.5
1	A	165	THR	3.5
1	C	328	GLU	3.5
1	A	362	SER	3.4
2	D	307	GLY	3.4
1	A	325	ASN	3.4
1	C	164	ASN	3.4
1	C	159	ARG	3.4
2	D	513	ASN	3.3
1	C	253	LYS	3.3
2	B	304	THR	3.3
2	D	553	GLU	3.3
1	C	321	TRP	3.3
1	A	357	LYS	3.3
1	A	354	VAL	3.3
1	A	324	PHE	3.2
1	C	361	ALA	3.2
2	B	553	GLU	3.1
1	A	255	TYR	3.1
1	A	304	ASN	3.1
1	C	358	TYR	3.1
2	D	178	LYS	3.1
2	B	376	HIS	3.1
1	A	19	ASN	3.1
2	B	621	GLU	3.0
2	D	236	HIS	3.0
1	C	327	TYR	3.0
1	C	166	PRO	3.0
2	B	646	LYS	3.0
2	B	227	ILE	3.0
1	C	73	LEU	3.0
1	C	230	THR	3.0
2	B	247	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	181	SER	2.9
2	D	512	SER	2.9
2	D	620	TYR	2.9
2	D	306	ILE	2.9
1	A	124	LYS	2.9
1	A	45	ALA	2.8
1	C	167	GLU	2.8
1	A	116	LYS	2.8
1	A	194	VAL	2.8
2	B	624	PRO	2.8
2	B	590	ILE	2.8
1	C	218	SER	2.8
2	B	239	ASN	2.8
2	B	300	ILE	2.8
2	B	219	LYS	2.8
2	D	220	GLU	2.8
1	C	162	SER	2.7
2	D	245	ASN	2.7
2	D	611	ASP	2.7
1	A	358	TYR	2.7
2	D	228	GLY	2.7
1	A	167	GLU	2.7
1	A	355	ALA	2.7
2	D	238	ILE	2.6
2	D	641	ASN	2.6
1	A	253	LYS	2.6
2	B	588	HIS	2.6
2	D	189	GLU	2.6
2	B	623	TYR	2.6
2	D	300	ILE	2.6
2	D	319	GLN	2.6
2	B	228	GLY	2.6
2	B	251	THR	2.6
2	D	423	SER	2.6
2	D	401	ASN	2.6
2	B	513	ASN	2.6
1	A	211	ALA	2.5
1	A	320	ILE	2.5
2	D	637	ALA	2.5
2	B	439	GLY	2.5
1	A	163	GLU	2.5
1	A	376	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	355	ALA	2.4
2	B	622	VAL	2.4
1	C	360	ILE	2.4
2	B	305	ASP	2.4
1	C	311	GLU	2.4
1	C	323	GLU	2.4
1	C	217	VAL	2.4
1	A	493	ASN	2.4
1	C	277	LYS	2.4
2	B	209	TYR	2.3
2	D	206	ASP	2.3
1	C	257	ILE	2.3
2	D	304	THR	2.3
1	A	290	TYR	2.3
2	B	620	TYR	2.3
2	B	248	LYS	2.3
2	D	170	ILE	2.3
1	C	171	GLU	2.3
1	C	178	ASP	2.2
2	D	610	LYS	2.2
1	A	277	LYS	2.2
1	A	321	TRP	2.2
1	A	288	THR	2.2
1	C	363	GLU	2.2
2	B	308	LYS	2.2
2	B	607	TYR	2.2
2	B	252	LYS	2.2
2	B	589	GLY	2.2
1	C	359	LYS	2.2
2	B	289	GLY	2.2
1	A	160	LYS	2.2
1	C	173	SER	2.2
2	B	168	ASP	2.1
1	C	297	GLU	2.1
1	A	174	ILE	2.1
2	D	171	GLU	2.1
2	B	608	SER	2.1
2	B	236	HIS	2.1
2	B	206	ASP	2.1
2	D	167	ARG	2.1
2	D	607	TYR	2.1
2	D	402	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	415	GLY	2.1
1	A	117	MET	2.1
2	B	166	ALA	2.1
1	C	329	THR	2.1
1	A	119	THR	2.1
1	A	49	ASN	2.0
2	B	610	LYS	2.0
2	D	247	ILE	2.0
2	D	646	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.