



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:41 PM UTC

PDB ID : 1PWW / pdb_00001pww
Title : Crystal structure of Anthrax Lethal Factor active site mutant protein complexed with an optimised peptide substrate in the presence of zinc.
Authors : Wong, T.Y.; Schwarzenbacher, R.; Liddington, R.C.
Deposited on : 2003-07-02
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

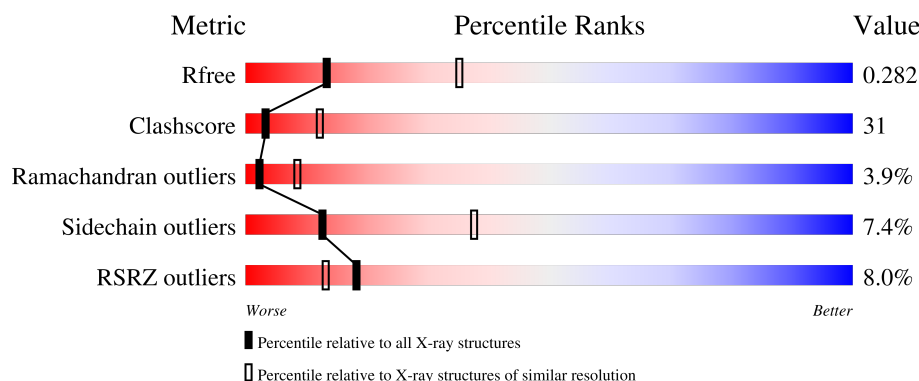
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	776	7% 41% 43% 9% 6%
1	B	776	5% 45% 44% 5% 5%
2	C	20	55% 10% 20% 15% 10% 45%
2	D	20	50% 5% 20% 20% 10% 45%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12185 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 Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5965	3796	1002	1159	8			
1	B	734	Total	C	N	O	S	0	0	0
			6030	3833	1017	1172	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	687	CYS	GLU	engineered mutation	UNP P15917
B	687	CYS	GLU	engineered mutation	UNP P15917

- Molecule 2 is a protein called LF20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	S	0	0	0
			94	64	13	16	1			
2	D	11	Total	C	N	O	S	0	0	0
			94	64	13	16	1			

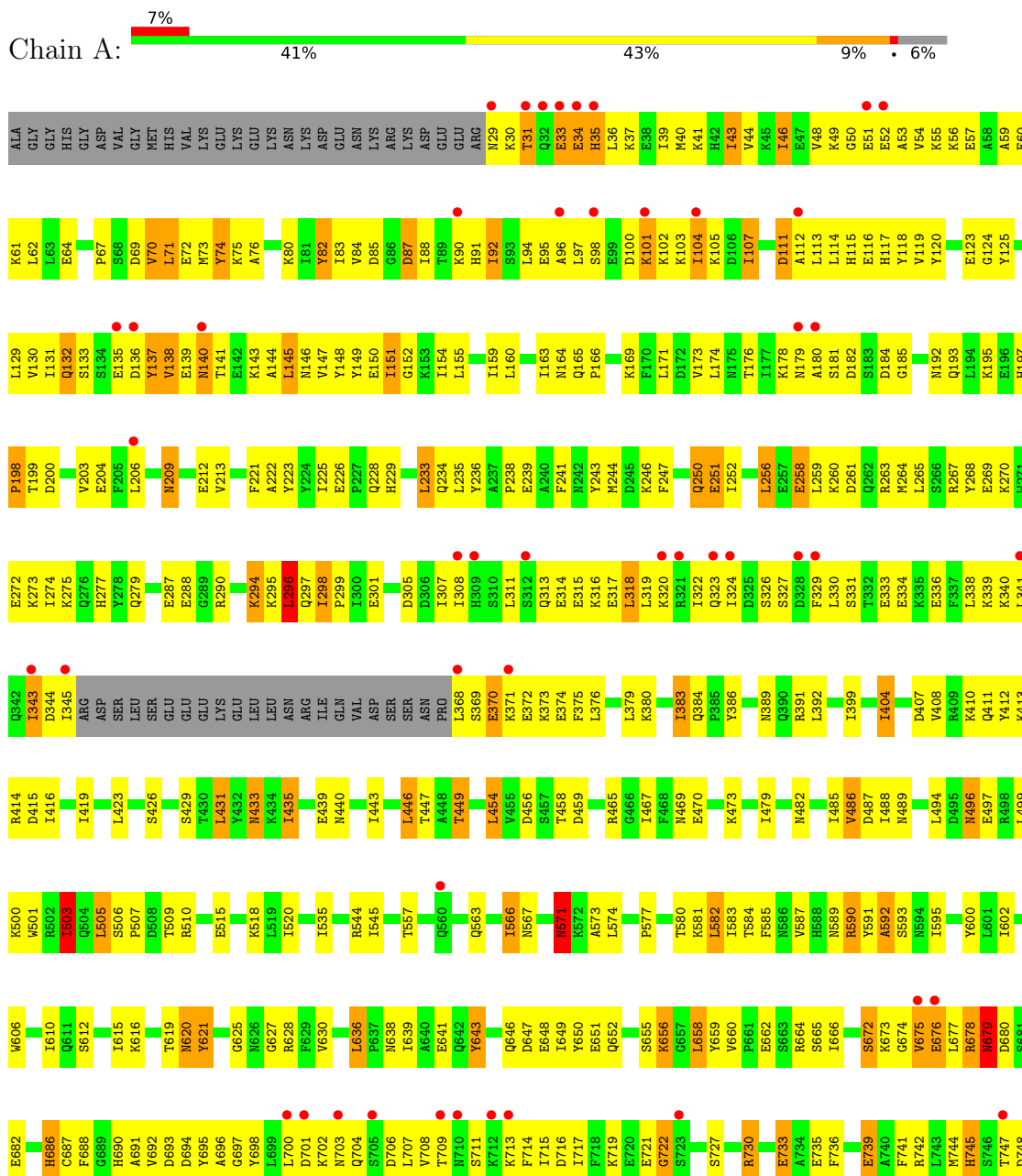
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

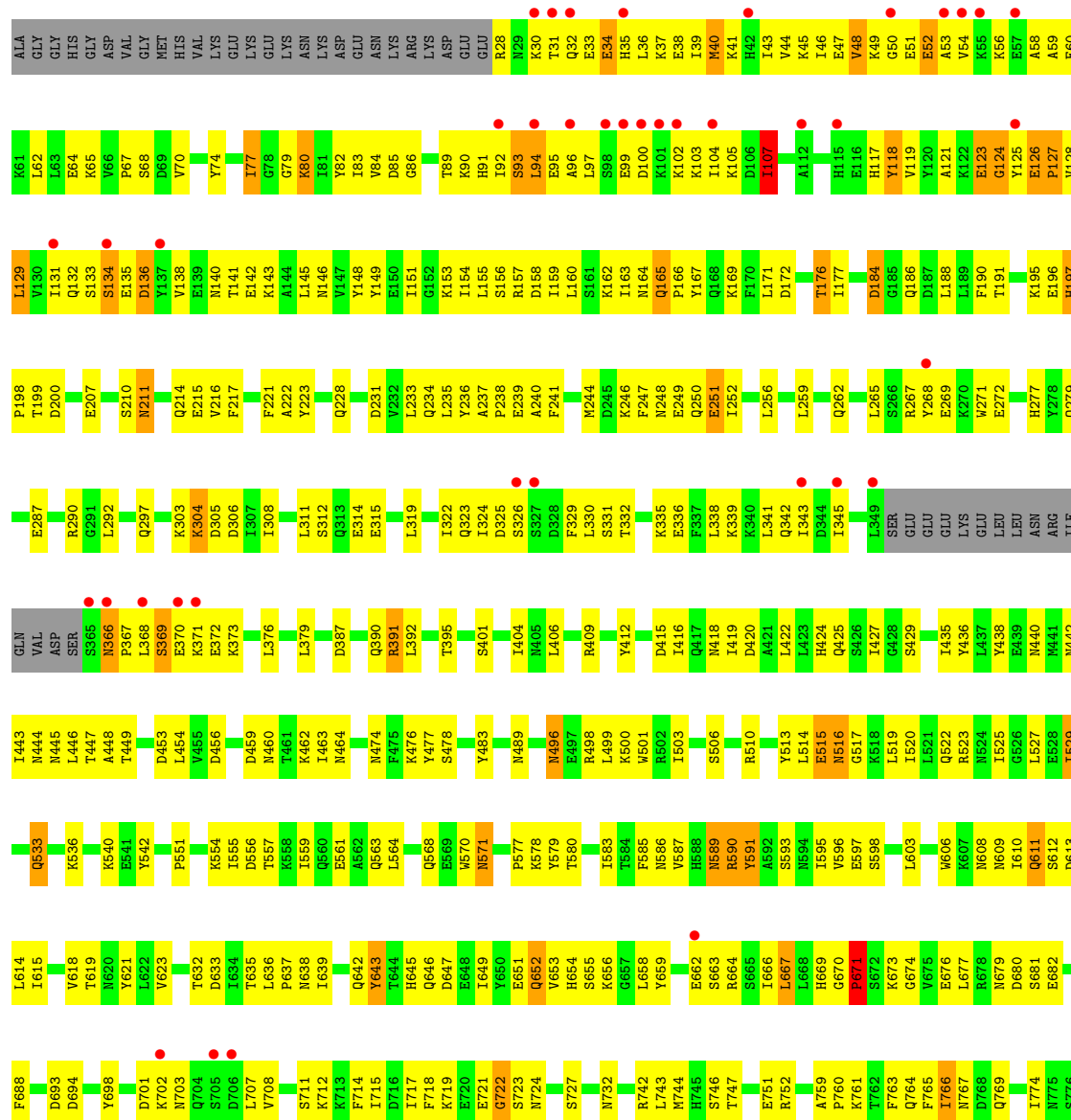
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Lethal factor

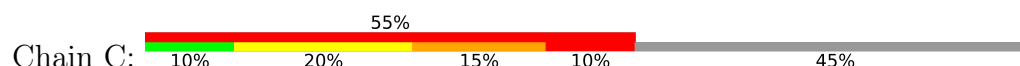




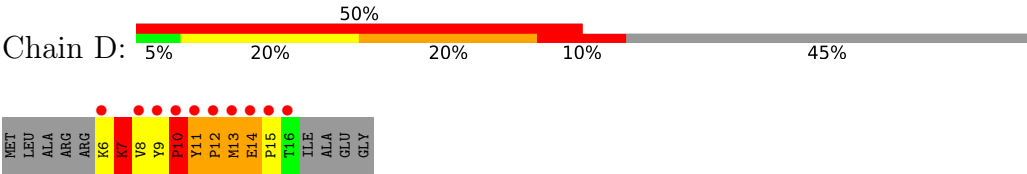
• Molecule 1: Lethal factor



• Molecule 2: LF20



• Molecule 2: LF20



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.70Å 137.40Å 98.30Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	22.69 – 2.80 22.69 – 2.80	Depositor EDS
% Data completeness (in resolution range)	81.7 (22.69-2.80) 81.6 (22.69-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.288 0.237 , 0.282	Depositor DCC
R_{free} test set	2583 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12185	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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 ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/6072	1.00	27/8178 (0.3%)
1	B	0.51	0/6138	1.03	29/8267 (0.4%)
2	C	0.78	0/98	1.67	4/133 (3.0%)
2	D	0.54	0/98	1.63	4/133 (3.0%)
All	All	0.51	0/12406	1.03	64/16711 (0.4%)

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	671	PRO	CA-N-CD	-10.85	96.81	112.00
1	A	137	TYR	N-CA-C	-10.53	100.38	113.01
1	B	279	GLN	OE1-CD-NE2	-9.37	113.23	122.60
1	B	589	ASN	N-CA-C	8.67	121.52	109.29
1	B	126	GLU	CA-C-N	8.39	128.90	119.93
1	B	126	GLU	C-N-CA	8.39	128.90	119.93
1	B	34	GLU	N-CA-C	-8.13	101.69	111.69
1	A	74	TYR	N-CA-C	-7.67	102.85	111.14
2	D	10	PRO	CA-N-CD	-7.55	101.42	112.00
1	B	643	TYR	N-CA-C	7.26	120.06	111.71
1	A	43	ILE	N-CA-C	7.08	117.84	110.62
1	B	435	ILE	N-CA-C	7.06	118.05	108.17
1	A	590	ARG	N-CA-C	6.99	120.91	112.38
1	B	590	ARG	N-CA-C	6.97	121.64	113.20
1	B	747	THR	N-CA-C	-6.93	103.65	111.14
1	B	126	GLU	N-CA-C	-6.93	98.70	109.79
1	A	589	ASN	N-CA-C	6.84	119.80	109.95
1	B	117	HIS	N-CA-C	6.67	119.34	110.53
1	B	680	ASP	N-CA-C	-6.63	104.29	112.38
1	B	279	GLN	CG-CD-NE2	6.47	126.10	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	620	ASN	N-CA-C	-6.37	105.63	113.41
2	D	14	GLU	CA-C-N	6.30	127.71	119.84
2	D	14	GLU	C-N-CA	6.30	127.71	119.84
1	B	506	SER	N-CA-C	-6.23	102.20	109.93
2	C	14	GLU	CA-C-N	6.20	127.59	119.84
2	C	14	GLU	C-N-CA	6.20	127.59	119.84
1	B	197	HIS	CA-C-N	6.15	125.63	119.24
1	B	197	HIS	C-N-CA	6.15	125.63	119.24
1	A	503	ILE	N-CA-C	6.07	117.32	108.58
1	B	591	TYR	N-CA-C	-6.03	103.63	111.71
1	A	287	GLU	N-CA-C	-5.97	104.16	112.45
1	A	679	ASN	N-CA-C	5.96	117.60	108.42
1	A	313	GLN	N-CA-C	-5.94	104.81	111.28
1	A	621	TYR	N-CA-C	-5.91	104.76	111.14
1	B	688	PHE	N-CA-C	-5.84	104.92	111.28
1	A	298	ILE	CA-C-N	5.83	125.74	119.85
1	A	298	ILE	C-N-CA	5.83	125.74	119.85
2	C	6	LYS	CA-C-N	-5.75	113.27	122.53
2	C	6	LYS	C-N-CA	-5.75	113.27	122.53
1	A	151	ILE	N-CA-C	-5.73	104.34	110.36
1	B	312	SER	N-CA-C	-5.71	102.31	110.59
1	A	318	LEU	N-CA-C	-5.70	105.07	111.28
1	A	75	LYS	N-CA-C	-5.59	104.20	111.02
1	A	587	VAL	N-CA-C	5.56	116.10	107.99
1	A	486	VAL	N-CA-C	5.54	116.83	108.96
1	A	747	THR	N-CA-C	-5.53	106.37	113.23
1	B	119	VAL	N-CA-C	5.53	115.14	108.06
1	B	176	THR	N-CA-C	-5.43	105.36	111.28
1	B	92	ILE	N-CA-C	5.38	116.75	110.62
1	A	688	PHE	N-CA-C	-5.35	105.61	111.82
1	B	211	ASN	N-CA-C	5.33	116.77	111.07
1	A	571	ASN	N-CA-C	-5.29	105.68	111.82
2	D	7	LYS	N-CA-C	5.29	115.53	108.38
1	A	643	TYR	N-CA-C	5.23	117.89	111.82
1	B	262	GLN	N-CA-C	-5.23	106.90	113.28
1	A	454	LEU	N-CA-C	5.20	116.94	111.28
1	B	515	GLU	N-CA-C	5.19	118.71	112.38
1	B	612	SER	N-CA-C	5.19	117.61	111.33
1	B	118	TYR	N-CA-C	5.17	120.22	113.30
1	B	127	PRO	N-CA-C	5.16	119.67	111.26
1	A	164	ASN	N-CA-C	5.16	118.70	111.74
1	A	503	ILE	CB-CA-C	-5.14	104.54	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	VAL	N-CA-C	-5.10	105.73	110.53
1	A	82	TYR	N-CA-C	5.05	116.64	108.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5965	0	5957	387	0
1	B	6030	0	6021	350	0
2	C	94	0	95	22	0
2	D	94	0	95	24	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	12185	0	12168	743	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 31.

All (743) 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:653:VAL:HG11	2:D:10:PRO:HG3	1.34	1.06
1:B:319:LEU:HD23	1:B:345:ILE:HD12	1.39	1.05
1:B:551:PRO:HD2	1:B:554:LYS:HE2	1.36	1.05
1:B:366:ASN:HB3	1:B:367:PRO:HD3	1.38	1.01
1:A:563:GLN:NE2	1:A:585:PHE:H	1.57	1.00
1:A:602:ILE:HD11	1:A:680:ASP:HB3	1.45	0.99
1:B:677:LEU:HD11	2:D:11:TYR:CZ	2.01	0.96
1:A:268:TYR:HB3	1:B:125:TYR:CE2	2.00	0.95
1:B:510:ARG:H	1:B:522:GLN:HE21	0.94	0.92
1:B:496:ASN:HD22	1:B:496:ASN:H	1.13	0.92
2:D:7:LYS:HG2	2:D:8:VAL:H	1.35	0.91
1:B:516:ASN:H	1:B:516:ASN:HD22	1.09	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:ARG:H	1:B:522:GLN:NE2	1.70	0.89
1:A:316:LYS:HE3	1:A:345:ILE:HG21	1.55	0.89
1:B:366:ASN:HB3	1:B:367:PRO:CD	2.03	0.89
1:B:176:THR:HG21	1:B:239:GLU:HG3	1.54	0.88
1:B:658:LEU:HD11	2:D:8:VAL:HG12	1.52	0.88
1:B:677:LEU:HD21	2:D:11:TYR:OH	1.73	0.87
1:B:94:LEU:HB3	1:B:97:LEU:HD12	1.56	0.86
1:A:119:VAL:HG21	1:A:147:VAL:HG22	1.56	0.85
1:B:99:GLU:HG3	1:B:100:ASP:H	1.40	0.85
1:B:85:ASP:HB3	1:B:133:SER:OG	1.77	0.84
1:A:176:THR:HG21	1:A:239:GLU:HG3	1.59	0.84
1:A:92:ILE:HD12	1:A:92:ILE:H	1.42	0.83
1:A:714:PHE:HA	1:A:717:ILE:HD13	1.59	0.83
1:B:424:HIS:HA	1:B:510:ARG:HD2	1.59	0.83
1:B:658:LEU:HD11	2:D:8:VAL:CG1	2.08	0.82
1:A:48:VAL:HG11	1:A:55:LYS:HG2	1.61	0.82
1:A:69:ASP:O	1:A:73:MET:HG3	1.80	0.82
1:B:571:ASN:HD21	1:B:580:THR:HB	1.44	0.82
1:B:510:ARG:N	1:B:522:GLN:HE21	1.75	0.82
1:A:435:ILE:HD12	1:A:435:ILE:H	1.45	0.82
1:A:496:ASN:C	1:A:496:ASN:HD22	1.88	0.82
1:B:585:PHE:CE1	1:B:596:VAL:HG13	2.16	0.81
1:A:308:ILE:HG23	1:A:316:LYS:HE2	1.60	0.80
1:A:771:LYS:HD2	1:A:775:ASN:HD21	1.46	0.80
1:A:440:ASN:ND2	1:A:500:LYS:HZ2	1.80	0.79
1:A:314:GLU:O	1:A:318:LEU:HG	1.82	0.79
1:B:516:ASN:HD22	1:B:516:ASN:N	1.71	0.79
1:A:602:ILE:CD1	1:A:680:ASP:HB3	2.12	0.79
1:B:498:ARG:HH21	1:B:540:LYS:HE2	1.48	0.78
1:A:577:PRO:O	1:A:580:THR:HG23	1.83	0.78
1:B:36:LEU:O	1:B:40:MET:HG2	1.85	0.77
1:A:501:TRP:HB3	1:A:503:ILE:HD11	1.67	0.76
1:A:104:ILE:HG22	1:A:105:LYS:H	1.50	0.76
1:A:435:ILE:HD12	1:A:435:ILE:N	2.01	0.76
1:A:563:GLN:HE21	1:A:585:PHE:H	1.31	0.76
1:B:496:ASN:HD22	1:B:496:ASN:N	1.82	0.76
1:A:233:LEU:HD13	1:A:241:PHE:HB2	1.67	0.76
1:A:636:LEU:HA	1:A:639:ILE:HD13	1.68	0.75
1:B:551:PRO:HD2	1:B:554:LYS:CE	2.15	0.75
1:B:516:ASN:H	1:B:516:ASN:ND2	1.78	0.75
1:B:70:VAL:HG13	1:B:155:LEU:HD13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:SER:O	1:B:715:ILE:HG13	1.86	0.75
1:A:563:GLN:NE2	1:A:584:THR:HA	2.02	0.75
1:A:268:TYR:HB3	1:B:125:TYR:HE2	1.53	0.74
1:B:37:LYS:O	1:B:41:LYS:HG3	1.87	0.74
1:A:566:ILE:HG13	1:A:600:TYR:CE2	2.23	0.74
1:A:581:LYS:HD3	1:A:628:ARG:HH21	1.51	0.74
1:A:648:GLU:HB2	1:A:651:GLU:HG3	1.68	0.74
1:B:387:ASP:HB3	1:B:390:GLN:HB3	1.70	0.74
1:A:113:LEU:HD12	1:A:116:GLU:OE2	1.88	0.73
1:B:156:SER:HB3	1:B:217:PHE:CD2	2.23	0.73
1:A:56:LYS:O	1:A:60:GLU:HG3	1.88	0.73
1:B:49:LYS:HG2	1:B:85:ASP:OD1	1.88	0.73
1:A:449:THR:HA	1:A:673:LYS:HD3	1.70	0.73
1:B:95:GLU:HG3	1:B:96:ALA:H	1.54	0.72
1:B:401:SER:CB	1:B:638:ASN:HD22	2.02	0.72
1:B:77:ILE:HD11	1:B:259:LEU:HD11	1.72	0.72
1:A:686:HIS:HB2	1:A:742:ARG:HD3	1.72	0.72
2:D:7:LYS:HG2	2:D:8:VAL:N	2.04	0.72
1:A:643:TYR:HA	1:A:646:GLN:HG3	1.72	0.71
1:B:483:TYR:HB3	1:B:520:ILE:HD11	1.70	0.71
1:A:368:LEU:N	1:A:373:LYS:HE2	2.05	0.71
1:B:330:LEU:HD11	1:B:376:LEU:HD22	1.72	0.71
1:B:332:THR:O	1:B:336:GLU:HG2	1.91	0.71
1:A:192:ASN:HA	1:A:195:LYS:HB2	1.72	0.71
1:B:99:GLU:HG3	1:B:100:ASP:N	2.06	0.70
1:B:46:ILE:HG13	1:B:56:LYS:HD3	1.73	0.70
1:A:125:TYR:CD1	1:B:269:GLU:HG3	2.25	0.70
1:B:446:LEU:HG	1:B:591:TYR:HB2	1.73	0.70
1:B:571:ASN:ND2	1:B:580:THR:HB	2.06	0.70
1:A:182:ASP:OD2	1:A:184:ASP:HB2	1.92	0.70
1:A:439:GLU:HB2	1:A:486:VAL:HG12	1.72	0.70
2:C:13:MET:HE2	2:C:13:MET:H	1.55	0.70
1:B:645:HIS:CD2	1:B:663:SER:HB3	2.27	0.70
2:D:13:MET:H	2:D:13:MET:HE2	1.57	0.70
1:A:123:GLU:HG2	1:A:124:GLY:H	1.56	0.70
1:B:211:ASN:HA	1:B:214:GLN:HE21	1.55	0.69
1:B:366:ASN:CB	1:B:367:PRO:CD	2.70	0.69
1:B:662:GLU:CD	1:B:662:GLU:H	2.01	0.69
1:B:32:GLN:O	1:B:35:HIS:HB3	1.93	0.69
1:B:308:ILE:HG23	1:B:345:ILE:HD11	1.75	0.69
1:B:60:GLU:O	1:B:64:GLU:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.75	0.69
1:B:107:ILE:HG21	1:B:145:LEU:CD1	2.23	0.68
1:A:707:LEU:HD11	2:C:9:TYR:OH	1.93	0.68
1:B:330:LEU:HB2	1:B:335:LYS:NZ	2.08	0.68
1:B:693:ASP:OD2	1:B:708:VAL:HG12	1.93	0.68
1:A:440:ASN:ND2	1:A:500:LYS:NZ	2.42	0.68
1:B:658:LEU:CD1	2:D:8:VAL:HG12	2.24	0.68
1:A:102:LYS:HA	1:A:114:LEU:HD12	1.74	0.68
1:A:336:GLU:HG3	1:A:340:LYS:HE3	1.74	0.68
1:B:125:TYR:CE2	1:B:162:LYS:HE3	2.29	0.68
1:A:316:LYS:HZ1	1:A:345:ILE:HB	1.59	0.68
1:B:474:ASN:HB3	1:B:597:GLU:HG3	1.76	0.68
1:B:655:SER:HB2	2:D:11:TYR:C	2.19	0.68
1:A:770:ILE:O	1:A:774:ILE:HG12	1.94	0.67
1:A:49:LYS:HD2	1:A:50:GLY:N	2.10	0.67
1:B:449:THR:HA	1:B:673:LYS:HD2	1.76	0.67
1:A:563:GLN:NE2	1:A:585:PHE:N	2.39	0.67
1:A:674:GLY:HA2	2:C:13:MET:HA	1.76	0.67
1:A:31:THR:HG23	1:A:34:GLU:HG2	1.76	0.67
1:A:57:GLU:HA	1:A:60:GLU:OE2	1.95	0.67
1:B:95:GLU:HG3	1:B:96:ALA:N	2.10	0.66
1:A:753:LEU:O	1:A:757:LYS:HG2	1.95	0.66
1:B:84:VAL:O	1:B:132:GLN:HA	1.94	0.66
1:B:611:GLN:NE2	1:B:614:LEU:H	1.92	0.66
1:A:87:ASP:O	1:A:90:LYS:HB3	1.95	0.66
1:B:446:LEU:O	1:B:671:PRO:HG3	1.95	0.66
1:A:204:GLU:OE1	1:A:204:GLU:N	2.27	0.66
1:A:379:LEU:O	1:A:383:ILE:HG12	1.96	0.66
1:B:707:LEU:HD11	2:D:9:TYR:CZ	2.31	0.66
1:A:713:LYS:HE2	1:A:761:LYS:HE2	1.78	0.65
1:A:741:PHE:O	1:A:745:HIS:HD2	1.78	0.65
1:A:67:PRO:O	1:A:70:VAL:HG13	1.95	0.65
1:A:94:LEU:HD11	1:A:130:VAL:HG21	1.77	0.65
1:A:272:GLU:HG3	1:B:125:TYR:CD1	2.31	0.65
1:B:707:LEU:HD11	2:D:9:TYR:OH	1.96	0.65
1:B:401:SER:HB3	1:B:638:ASN:HD22	1.62	0.65
1:B:45:LYS:HB2	1:B:82:TYR:HD2	1.62	0.65
1:B:442:ASN:O	1:B:445:ASN:HB2	1.96	0.65
1:B:611:GLN:HE22	1:B:613:ASP:HB2	1.62	0.64
1:A:80:LYS:HB3	1:A:82:TYR:HE1	1.62	0.64
1:B:440:ASN:ND2	1:B:500:LYS:HG2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:O	1:A:34:GLU:HG3	1.98	0.64
1:A:535:ILE:HD13	1:A:544:ARG:HB2	1.80	0.64
1:B:35:HIS:O	1:B:39:ILE:HG12	1.97	0.64
1:A:298:ILE:O	1:A:298:ILE:HD12	1.98	0.64
1:A:563:GLN:HE22	1:A:585:PHE:H	1.42	0.64
1:B:34:GLU:O	1:B:38:GLU:HB2	1.98	0.64
1:B:769:GLN:HA	1:B:769:GLN:NE2	2.13	0.64
1:A:35:HIS:HD2	1:A:39:ILE:HD11	1.63	0.64
1:A:107:ILE:HG13	1:A:145:LEU:CD1	2.28	0.63
1:B:436:TYR:HA	1:B:503:ILE:O	1.99	0.63
1:A:655:SER:HB2	2:C:11:TYR:C	2.23	0.63
1:A:46:ILE:HD12	1:A:46:ILE:N	2.13	0.63
1:A:256:LEU:HD22	1:A:260:LYS:HE3	1.81	0.63
1:A:163:ILE:HG21	1:A:258:GLU:HG2	1.80	0.63
1:A:327:SER:HB2	1:A:329:PHE:CE2	2.33	0.63
1:A:429:SER:OG	1:A:431:LEU:HG	1.98	0.63
1:B:267:ARG:HB3	1:B:489:ASN:ND2	2.12	0.63
1:A:391:ARG:NH1	1:A:404:ILE:HD12	2.14	0.63
1:B:154:ILE:HD13	1:B:158:ASP:OD1	1.98	0.63
1:B:674:GLY:HA3	1:B:677:LEU:HD12	1.81	0.63
1:B:496:ASN:H	1:B:496:ASN:ND2	1.90	0.63
1:A:87:ASP:OD1	1:A:115:HIS:HB2	1.99	0.63
1:A:443:ILE:HD13	1:A:454:LEU:HD22	1.81	0.63
2:C:11:TYR:N	2:C:12:PRO:HD3	2.14	0.62
1:A:686:HIS:C	1:A:686:HIS:CD2	2.77	0.62
1:A:748:ASP:OD2	1:A:750:ALA:HB3	1.98	0.62
1:A:368:LEU:HD13	1:A:372:GLU:CD	2.24	0.62
1:B:246:LYS:HG3	1:B:250:GLN:HE21	1.64	0.62
1:A:163:ILE:CG2	1:A:258:GLU:HG2	2.29	0.62
1:A:307:ILE:HG21	1:A:341:LEU:HD11	1.80	0.62
1:B:163:ILE:HG13	1:B:165:GLN:HG3	1.81	0.62
1:B:647:ASP:HB2	1:B:651:GLU:OE2	1.99	0.62
1:A:744:MET:O	1:A:752:ARG:HG2	2.01	0.61
1:A:176:THR:CG2	1:A:239:GLU:HG3	2.31	0.61
1:B:184:ASP:HB3	1:B:236:TYR:HB3	1.82	0.61
1:A:658:LEU:HD21	2:C:8:VAL:HG12	1.81	0.61
1:A:647:ASP:HB2	1:A:651:GLU:OE1	2.01	0.60
1:B:551:PRO:CD	1:B:554:LYS:HE2	2.22	0.60
1:B:444:ASN:HD22	1:B:448:ALA:HA	1.67	0.60
1:B:308:ILE:HA	1:B:311:LEU:HD12	1.84	0.60
1:B:235:LEU:HD23	1:B:236:TYR:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLU:HG3	1:A:35:HIS:N	2.17	0.60
1:B:391:ARG:HD3	1:B:391:ARG:C	2.26	0.60
1:A:677:LEU:HD11	2:C:11:TYR:CE2	2.37	0.60
1:B:319:LEU:HD23	1:B:345:ILE:CD1	2.26	0.60
1:B:330:LEU:HB2	1:B:335:LYS:HZ2	1.66	0.60
1:B:415:ASP:O	1:B:419:ILE:HG13	2.02	0.60
2:D:11:TYR:N	2:D:12:PRO:HD3	2.17	0.60
1:A:34:GLU:HG3	1:A:35:HIS:H	1.67	0.59
1:B:188:LEU:HD11	1:B:223:TYR:CE2	2.37	0.59
1:B:442:ASN:ND2	1:B:496:ASN:HB2	2.17	0.59
1:A:415:ASP:O	1:A:419:ILE:HG13	2.02	0.59
1:A:581:LYS:CD	1:A:628:ARG:HH21	2.15	0.59
1:A:123:GLU:HG2	1:A:124:GLY:N	2.18	0.59
1:A:730:ARG:O	1:A:730:ARG:HG2	2.02	0.59
1:B:80:LYS:HZ2	1:B:80:LYS:HB3	1.68	0.59
1:B:476:LYS:O	1:B:529:ILE:HB	2.03	0.59
1:A:465:ARG:O	1:A:469:ASN:OD1	2.21	0.59
1:A:759:ALA:N	1:A:760:PRO:HD3	2.16	0.59
1:B:94:LEU:HB3	1:B:97:LEU:CD1	2.31	0.59
1:B:712:LYS:HA	1:B:715:ILE:HD12	1.85	0.59
1:A:154:ILE:HG22	1:A:159:ILE:HD13	1.85	0.58
1:A:584:THR:CG2	1:A:630:VAL:HG22	2.33	0.58
1:B:287:GLU:HA	1:B:290:ARG:NH1	2.18	0.58
1:B:510:ARG:HH11	1:B:510:ARG:HG3	1.68	0.58
1:B:135:GLU:O	1:B:135:GLU:HG3	2.04	0.58
1:B:483:TYR:CB	1:B:520:ILE:HD11	2.33	0.58
1:A:295:LYS:C	1:A:297:GLN:H	2.11	0.58
1:A:410:LYS:HE3	1:A:414:ARG:NH2	2.18	0.58
1:A:277:HIS:CD2	1:A:429:SER:HB2	2.38	0.58
1:B:151:ILE:O	1:B:151:ILE:HG22	2.04	0.58
1:B:160:LEU:HB3	1:B:165:GLN:HB2	1.84	0.58
1:B:176:THR:CG2	1:B:239:GLU:HG3	2.31	0.58
1:B:338:LEU:HD23	1:B:341:LEU:HD12	1.85	0.58
1:B:564:LEU:O	1:B:568:GLN:HG3	2.04	0.58
1:B:93:SER:O	1:B:95:GLU:HG2	2.04	0.57
1:B:513:TYR:HA	1:B:519:LEU:HD23	1.85	0.57
1:B:308:ILE:O	1:B:311:LEU:HB2	2.04	0.57
1:A:256:LEU:CD2	1:A:260:LYS:HE3	2.33	0.57
1:A:612:SER:O	1:A:616:LYS:HG3	2.04	0.57
1:B:391:ARG:HD3	1:B:391:ARG:O	2.05	0.57
1:A:602:ILE:HD11	1:A:680:ASP:CB	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LYS:HB3	1:B:80:LYS:NZ	2.20	0.57
1:B:292:LEU:HD13	1:B:419:ILE:HG12	1.86	0.57
1:A:97:LEU:HD22	1:A:101:LYS:HD3	1.85	0.57
1:A:487:ASP:OD1	1:A:518:LYS:HG2	2.05	0.57
1:B:608:ASN:C	1:B:609:ASN:HD22	2.12	0.57
1:B:682:GLU:HB3	1:B:742:ARG:HD3	1.85	0.57
1:B:91:HIS:HD2	1:B:93:SER:OG	1.88	0.57
1:B:774:ILE:HG22	1:B:774:ILE:O	2.05	0.57
1:A:100:ASP:C	1:A:102:LYS:H	2.11	0.56
1:A:411:GLN:HE21	1:A:411:GLN:HA	1.70	0.56
1:A:449:THR:HG22	1:A:672:SER:O	2.06	0.56
1:B:395:THR:HG22	1:B:638:ASN:ND2	2.20	0.56
1:B:420:ASP:OD1	1:B:523:ARG:HD3	2.05	0.56
1:A:90:LYS:O	1:A:90:LYS:HG2	2.05	0.56
1:A:264:MET:HE3	1:A:265:LEU:HD12	1.87	0.56
1:A:319:LEU:C	1:A:322:ILE:HG22	2.30	0.56
1:A:322:ILE:HD13	1:A:376:LEU:HD21	1.88	0.56
1:A:717:ILE:CG1	1:A:761:LYS:HD2	2.35	0.56
1:B:51:GLU:C	1:B:53:ALA:H	2.13	0.56
1:B:154:ILE:O	1:B:159:ILE:HG12	2.05	0.56
2:D:8:VAL:HG12	2:D:9:TYR:H	1.70	0.56
1:B:223:TYR:HB3	1:B:233:LEU:HG	1.87	0.56
1:A:658:LEU:HD11	2:C:8:VAL:HG11	1.87	0.56
1:A:426:SER:HA	1:A:510:ARG:HA	1.87	0.56
1:B:267:ARG:CZ	1:B:489:ASN:HB3	2.36	0.56
1:B:338:LEU:HD22	1:B:379:LEU:HD13	1.86	0.56
1:B:765:PHE:O	1:B:769:GLN:HG2	2.06	0.56
1:B:28:ARG:O	1:B:32:GLN:HB2	2.06	0.56
1:B:67:PRO:HB2	1:B:70:VAL:HG23	1.88	0.56
1:B:759:ALA:N	1:B:760:PRO:HD3	2.21	0.56
1:A:772:PHE:C	1:A:772:PHE:CD2	2.84	0.56
1:B:221:PHE:HA	1:B:244:MET:HE2	1.88	0.56
2:C:11:TYR:H	2:C:12:PRO:HD3	1.70	0.56
1:A:711:SER:O	1:A:715:ILE:HG13	2.06	0.56
1:B:701:ASP:C	1:B:703:ASN:H	2.13	0.56
1:B:36:LEU:HG	1:B:40:MET:HE2	1.89	0.55
1:A:92:ILE:H	1:A:92:ILE:CD1	2.15	0.55
1:A:704:GLN:HG3	1:A:704:GLN:O	2.06	0.55
1:A:80:LYS:HB3	1:A:82:TYR:CE1	2.42	0.55
1:B:118:TYR:N	1:B:118:TYR:CD1	2.75	0.55
1:B:401:SER:CB	1:B:638:ASN:ND2	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:SER:HB2	1:B:638:ASN:ND2	2.22	0.55
1:B:339:LYS:O	1:B:343:ILE:HG12	2.06	0.55
1:B:769:GLN:HA	1:B:769:GLN:HE21	1.72	0.55
1:A:693:ASP:OD1	1:A:709:THR:HB	2.06	0.54
1:A:772:PHE:C	1:A:772:PHE:HD2	2.15	0.54
1:A:159:ILE:HD12	1:A:159:ILE:N	2.22	0.54
1:A:176:THR:O	1:A:180:ALA:HB2	2.07	0.54
1:A:296:LEU:HD13	1:A:296:LEU:O	2.06	0.54
1:A:581:LYS:HD3	1:A:628:ARG:NH2	2.19	0.54
1:A:308:ILE:HD11	1:A:341:LEU:HD22	1.89	0.54
1:B:31:THR:O	1:B:34:GLU:HB3	2.07	0.54
1:B:46:ILE:HD13	1:B:83:ILE:HB	1.90	0.54
1:A:171:LEU:HD21	1:A:206:LEU:HB2	1.88	0.54
1:A:392:LEU:HD21	1:A:416:ILE:HD13	1.90	0.54
1:A:691:ALA:O	1:A:694:ASP:HB3	2.08	0.54
1:A:727:SER:O	1:A:730:ARG:HB3	2.08	0.54
1:B:235:LEU:HD23	1:B:236:TYR:CZ	2.42	0.54
1:B:743:LEU:HD22	1:B:751:GLU:OE1	2.08	0.54
1:A:119:VAL:CG2	1:A:147:VAL:HG22	2.31	0.54
1:B:324:ILE:HD13	1:B:338:LEU:HB2	1.89	0.54
1:A:443:ILE:CD1	1:A:454:LEU:HD22	2.37	0.54
1:B:420:ASP:OD2	1:B:523:ARG:NH1	2.41	0.54
1:A:658:LEU:CD2	2:C:8:VAL:HG12	2.37	0.54
1:B:557:THR:O	1:B:561:GLU:HG3	2.08	0.54
1:A:323:GLN:O	1:A:326:SER:N	2.34	0.54
1:A:679:ASN:HD22	1:A:679:ASN:C	2.15	0.54
1:A:717:ILE:HG13	1:A:761:LYS:HD2	1.90	0.54
1:A:51:GLU:C	1:A:53:ALA:H	2.16	0.53
1:A:111:ASP:OD2	1:A:111:ASP:N	2.38	0.53
1:A:178:LYS:HG3	1:A:179:ASN:N	2.22	0.53
1:B:237:ALA:N	1:B:238:PRO:HD3	2.23	0.53
1:B:104:ILE:HG13	1:B:105:LYS:N	2.22	0.53
1:B:404:ILE:HD11	1:B:409:ARG:HA	1.89	0.53
1:B:606:TRP:CZ2	1:B:615:ILE:HG23	2.44	0.53
1:A:496:ASN:C	1:A:496:ASN:ND2	2.59	0.53
1:A:226:GLU:OE1	1:A:229:HIS:ND1	2.32	0.53
1:B:676:GLU:O	1:B:677:LEU:HG	2.08	0.53
1:A:446:LEU:HG	1:A:591:TYR:HB2	1.90	0.53
1:B:477:TYR:HE1	1:B:559:ILE:HD11	1.74	0.53
1:A:244:MET:HE3	1:A:244:MET:HA	1.91	0.53
1:A:343:ILE:HG23	1:A:344:ASP:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:GLU:HB2	1:B:207:GLU:OE1	2.09	0.53
1:A:563:GLN:HE21	1:A:585:PHE:N	2.04	0.53
1:A:102:LYS:O	1:A:114:LEU:HB2	2.09	0.53
1:A:118:TYR:OH	1:A:143:LYS:HA	2.09	0.53
2:D:7:LYS:CG	2:D:8:VAL:H	2.15	0.53
1:B:191:THR:O	1:B:195:LYS:HG3	2.09	0.53
1:A:40:MET:O	1:A:44:VAL:HB	2.08	0.52
1:B:311:LEU:HD22	1:B:315:GLU:HB3	1.90	0.52
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.44	0.52
1:A:90:LYS:O	1:A:90:LYS:CG	2.58	0.52
1:A:290:ARG:O	1:A:294:LYS:HB2	2.09	0.52
1:A:707:LEU:HD11	2:C:9:TYR:CZ	2.44	0.52
1:B:91:HIS:CD2	1:B:93:SER:H	2.27	0.52
1:A:274:ILE:HD12	1:A:488:ILE:HG23	1.91	0.52
1:A:315:GLU:HB3	1:A:375:PHE:CE1	2.45	0.52
1:B:721:GLU:HA	1:B:724:ASN:OD1	2.10	0.52
1:A:31:THR:HG23	1:A:34:GLU:CG	2.39	0.52
1:A:456:ASP:OD2	1:A:456:ASP:C	2.52	0.52
1:A:501:TRP:HB3	1:A:503:ILE:CD1	2.39	0.52
1:A:733:GLU:N	1:A:733:GLU:CD	2.67	0.52
1:A:761:LYS:O	1:A:761:LYS:HD3	2.10	0.52
1:B:210:SER:O	1:B:214:GLN:HG3	2.10	0.52
1:B:304:LYS:HG2	1:B:305:ASP:N	2.24	0.52
1:A:679:ASN:ND2	1:A:682:GLU:H	2.08	0.52
1:B:324:ILE:HD13	1:B:338:LEU:CB	2.40	0.52
1:A:235:LEU:HD23	1:A:236:TYR:CE2	2.45	0.52
1:A:639:ILE:N	1:A:639:ILE:HD12	2.25	0.52
1:B:93:SER:O	1:B:95:GLU:N	2.43	0.52
1:B:121:ALA:HB1	1:B:154:ILE:HD11	1.93	0.51
1:A:656:LYS:HE3	1:A:680:ASP:OD2	2.10	0.51
1:A:36:LEU:O	1:A:40:MET:HG3	2.10	0.51
1:B:460:ASN:O	1:B:498:ARG:NH2	2.40	0.51
1:B:477:TYR:H	1:B:593:SER:HB3	1.75	0.51
1:A:567:ASN:HD21	1:A:583:ILE:H	1.59	0.51
1:A:132:GLN:HG2	1:A:133:SER:H	1.75	0.51
1:A:380:LYS:O	1:A:384:GLN:HG2	2.11	0.51
1:A:411:GLN:HA	1:A:411:GLN:NE2	2.24	0.51
1:B:319:LEU:CD2	1:B:345:ILE:HD12	2.26	0.51
1:A:419:ILE:O	1:A:423:LEU:HG	2.11	0.51
1:A:118:TYR:CD2	1:A:119:VAL:HG23	2.45	0.51
1:A:754:LYS:O	1:A:758:ASN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:MET:HA	1:B:44:VAL:HG23	1.91	0.51
1:A:94:LEU:CD1	1:A:130:VAL:HG21	2.39	0.51
1:B:586:ASN:HB3	1:B:632:THR:HB	1.93	0.51
1:A:61:LYS:HA	1:A:64:GLU:OE2	2.10	0.51
1:A:270:LYS:O	1:A:274:ILE:HG13	2.11	0.51
1:B:65:LYS:HB2	1:B:148:TYR:OH	2.11	0.51
1:B:247:PHE:CE2	1:B:252:ILE:HD13	2.46	0.51
1:B:610:ILE:HB	1:B:615:ILE:HD11	1.93	0.51
1:B:715:ILE:O	1:B:719:LYS:HG2	2.11	0.51
1:A:94:LEU:C	1:A:96:ALA:H	2.19	0.50
1:A:226:GLU:OE1	1:A:228:GLN:HB2	2.11	0.50
1:A:496:ASN:ND2	1:A:497:GLU:HG3	2.25	0.50
1:A:679:ASN:HD21	1:A:682:GLU:HG3	1.76	0.50
1:B:635:THR:HB	1:B:637:PRO:HD2	1.93	0.50
1:A:39:ILE:O	1:A:43:ILE:HG12	2.10	0.50
1:A:76:ALA:O	1:A:263:ARG:NH1	2.44	0.50
1:A:372:GLU:O	1:A:375:PHE:HB3	2.11	0.50
1:A:655:SER:HB2	2:C:11:TYR:O	2.11	0.50
1:B:93:SER:C	1:B:95:GLU:H	2.19	0.50
1:B:236:TYR:C	1:B:238:PRO:HD3	2.36	0.50
1:B:244:MET:HE3	1:B:248:ASN:ND2	2.26	0.50
1:B:653:VAL:CG1	2:D:10:PRO:HG3	2.24	0.50
1:B:666:ILE:C	1:B:667:LEU:HD23	2.37	0.50
1:A:274:ILE:HD12	1:A:488:ILE:CG2	2.42	0.50
1:A:467:ILE:N	1:A:467:ILE:HD12	2.26	0.50
1:A:674:GLY:O	1:A:676:GLU:N	2.45	0.50
1:B:103:LYS:HG3	1:B:103:LYS:O	2.11	0.50
1:B:140:ASN:OD1	1:B:143:LYS:HB2	2.11	0.50
1:B:244:MET:CE	1:B:248:ASN:HD21	2.25	0.50
1:A:114:LEU:C	1:A:116:GLU:H	2.18	0.50
1:A:139:GLU:O	1:A:141:THR:N	2.43	0.50
1:A:141:THR:HG21	1:A:228:GLN:HG3	1.92	0.50
1:A:733:GLU:CD	1:A:733:GLU:H	2.18	0.50
1:B:97:LEU:O	1:B:102:LYS:HE3	2.12	0.50
1:B:303:LYS:HB3	1:B:306:ASP:OD2	2.11	0.50
1:B:169:LYS:O	1:B:172:ASP:HB2	2.11	0.50
1:B:249:GLU:C	1:B:250:GLN:HG2	2.37	0.50
1:A:94:LEU:O	1:A:96:ALA:N	2.45	0.50
1:A:456:ASP:OD2	1:A:458:THR:N	2.41	0.50
1:A:43:ILE:HG13	1:A:44:VAL:N	2.27	0.50
1:A:125:TYR:HA	1:B:268:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:LEU:HD11	2:D:11:TYR:CE1	2.45	0.50
1:A:31:THR:HA	1:A:34:GLU:HG2	1.94	0.50
1:A:140:ASN:HD22	1:A:143:LYS:NZ	2.08	0.50
1:A:771:LYS:HD2	1:A:775:ASN:ND2	2.22	0.50
1:A:440:ASN:HD21	1:A:500:LYS:NZ	2.10	0.49
1:A:678:ARG:HG3	1:A:678:ARG:HH11	1.76	0.49
1:A:690:HIS:CE1	2:C:9:TYR:HB3	2.46	0.49
1:A:706:ASP:OD1	1:A:707:LEU:N	2.45	0.49
1:A:49:LYS:CD	1:A:50:GLY:N	2.75	0.49
1:A:129:LEU:HD13	1:A:154:ILE:HD11	1.93	0.49
1:A:223:TYR:CD2	1:A:229:HIS:HB3	2.48	0.49
1:A:100:ASP:C	1:A:102:LYS:N	2.71	0.49
1:A:136:ASP:C	1:A:138:VAL:N	2.70	0.49
1:A:165:GLN:HB3	1:A:166:PRO:HA	1.95	0.49
1:B:135:GLU:O	1:B:135:GLU:CG	2.60	0.49
1:B:391:ARG:HG3	1:B:412:TYR:CD1	2.47	0.49
1:B:610:ILE:O	1:B:611:GLN:C	2.54	0.49
1:A:340:LYS:O	1:A:343:ILE:HG22	2.11	0.49
1:A:221:PHE:CE2	1:A:225:ILE:HG13	2.47	0.49
1:A:389:ASN:OD1	1:A:482:ASN:HB2	2.11	0.49
1:B:125:TYR:CZ	1:B:162:LYS:HE3	2.47	0.49
1:B:440:ASN:HD21	1:B:500:LYS:NZ	2.11	0.49
1:B:459:ASP:C	1:B:459:ASP:OD2	2.55	0.49
1:B:221:PHE:HD1	1:B:244:MET:HE1	1.78	0.49
1:B:323:GLN:HE21	1:B:325:ASP:HB2	1.77	0.49
1:A:173:VAL:HG21	1:A:243:TYR:CD2	2.47	0.49
1:A:658:LEU:HD23	2:C:10:PRO:HA	1.93	0.49
1:B:167:TYR:O	1:B:171:LEU:HG	2.13	0.49
1:A:103:LYS:O	1:A:103:LYS:HD3	2.13	0.48
1:A:410:LYS:HE3	1:A:414:ARG:HH21	1.76	0.48
1:B:444:ASN:ND2	1:B:448:ALA:HA	2.27	0.48
1:B:54:VAL:O	1:B:58:ALA:HB2	2.12	0.48
1:A:308:ILE:CD1	1:A:341:LEU:HD22	2.42	0.48
2:C:9:TYR:HA	2:C:10:PRO:HD3	1.64	0.48
1:A:33:GLU:O	1:A:37:LYS:HG3	2.12	0.48
1:A:739:GLU:HA	1:A:739:GLU:OE1	2.13	0.48
1:A:766:ILE:O	1:A:770:ILE:HG13	2.14	0.48
1:B:157:ARG:HA	1:B:214:GLN:OE1	2.11	0.48
1:A:113:LEU:O	1:A:116:GLU:HB2	2.14	0.48
1:A:412:TYR:O	1:A:416:ILE:HG13	2.14	0.48
1:A:479:ILE:O	1:A:590:ARG:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ASP:HB3	1:B:140:ASN:HD22	1.79	0.48
1:B:570:TRP:CZ2	1:B:603:LEU:HB3	2.48	0.48
1:A:46:ILE:HD12	1:A:46:ILE:H	1.79	0.48
1:A:316:LYS:HE3	1:A:345:ILE:CG2	2.35	0.48
1:A:368:LEU:HD13	1:A:372:GLU:HB3	1.95	0.48
1:A:745:HIS:CD2	1:A:745:HIS:N	2.82	0.48
1:B:34:GLU:O	1:B:38:GLU:CB	2.62	0.48
1:B:45:LYS:HB2	1:B:82:TYR:CD2	2.46	0.48
1:B:477:TYR:CD1	1:B:555:ILE:HG23	2.49	0.48
1:A:83:ILE:O	1:A:83:ILE:HG22	2.13	0.48
1:B:56:LYS:C	1:B:58:ALA:N	2.71	0.48
1:A:322:ILE:HG13	1:A:368:LEU:HD12	1.94	0.48
1:A:658:LEU:HD21	2:C:8:VAL:CG1	2.43	0.48
1:B:438:TYR:CD1	1:B:438:TYR:N	2.81	0.48
1:A:295:LYS:C	1:A:297:GLN:N	2.72	0.48
1:B:392:LEU:HD21	1:B:416:ILE:HD13	1.95	0.48
1:A:119:VAL:HG12	1:A:120:TYR:N	2.29	0.47
1:A:567:ASN:ND2	1:A:582:LEU:H	2.12	0.47
1:A:741:PHE:C	1:A:741:PHE:CD2	2.92	0.47
1:B:444:ASN:HA	1:B:448:ALA:HA	1.95	0.47
1:B:677:LEU:HD11	2:D:11:TYR:CE2	2.47	0.47
1:A:100:ASP:O	1:A:102:LYS:N	2.47	0.47
1:A:330:LEU:HD13	1:A:338:LEU:CD1	2.44	0.47
1:A:715:ILE:O	1:A:719:LYS:HD3	2.14	0.47
1:B:636:LEU:N	1:B:636:LEU:HD12	2.29	0.47
2:D:8:VAL:HG12	2:D:9:TYR:N	2.29	0.47
1:B:135:GLU:CD	1:B:138:VAL:HG23	2.40	0.47
2:D:11:TYR:H	2:D:12:PRO:HD3	1.78	0.47
1:B:165:GLN:HB3	1:B:166:PRO:HA	1.97	0.47
1:B:249:GLU:O	1:B:250:GLN:HG2	2.14	0.47
1:B:613:ASP:HB2	1:B:774:ILE:HG23	1.97	0.47
1:A:399:ILE:HD12	1:A:413:LYS:HG3	1.97	0.47
1:B:96:ALA:O	1:B:97:LEU:C	2.57	0.47
1:B:556:ASP:O	1:B:559:ILE:HB	2.15	0.47
1:B:48:VAL:CG2	1:B:52:GLU:HG2	2.45	0.47
1:B:77:ILE:HD13	1:B:259:LEU:HD21	1.95	0.47
1:A:87:ASP:CG	1:A:115:HIS:HB2	2.40	0.47
1:A:107:ILE:HG13	1:A:145:LEU:HD11	1.97	0.47
1:A:308:ILE:CG2	1:A:316:LYS:HE2	2.39	0.47
1:B:136:ASP:O	1:B:140:ASN:HB2	2.15	0.47
2:C:11:TYR:N	2:C:12:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:TYR:O	1:A:698:TYR:HB3	2.15	0.47
1:A:104:ILE:HD11	1:A:114:LEU:HG	1.95	0.46
1:A:234:GLN:O	1:A:238:PRO:HG3	2.15	0.46
1:A:368:LEU:HB3	1:A:372:GLU:CB	2.46	0.46
1:A:722:GLY:HA2	1:A:736:PHE:CZ	2.49	0.46
1:A:50:GLY:O	1:A:51:GLU:C	2.57	0.46
1:B:427:ILE:O	1:B:427:ILE:HG13	2.15	0.46
1:B:698:TYR:CD1	1:B:698:TYR:C	2.94	0.46
1:A:371:LYS:HG3	1:A:372:GLU:N	2.29	0.46
1:A:615:ILE:O	1:A:619:THR:HG23	2.16	0.46
1:A:659:TYR:O	2:C:8:VAL:CG1	2.63	0.46
1:A:717:ILE:HG23	1:A:721:GLU:OE1	2.15	0.46
1:B:231:ASP:O	1:B:235:LEU:HB2	2.15	0.46
1:B:619:THR:O	1:B:623:VAL:HG23	2.15	0.46
1:A:92:ILE:HD12	1:A:92:ILE:N	2.20	0.46
1:A:323:GLN:HB3	1:A:326:SER:OG	2.15	0.46
1:B:287:GLU:HA	1:B:290:ARG:HH12	1.80	0.46
1:A:677:LEU:O	1:A:679:ASN:N	2.47	0.46
1:B:99:GLU:CG	1:B:100:ASP:H	2.19	0.46
1:B:515:GLU:C	1:B:517:GLY:H	2.23	0.46
1:A:154:ILE:HG22	1:A:159:ILE:CD1	2.46	0.46
1:B:463:ILE:HG22	1:B:464:ASN:O	2.15	0.46
1:B:587:VAL:HG22	1:B:595:ILE:HG21	1.97	0.46
1:A:369:SER:O	1:A:373:LYS:HG2	2.15	0.46
1:A:485:ILE:HG12	1:A:520:ILE:HG12	1.97	0.46
1:B:48:VAL:HB	1:B:85:ASP:OD2	2.15	0.46
1:B:107:ILE:HG12	1:B:149:TYR:CG	2.51	0.46
1:B:714:PHE:HA	1:B:717:ILE:HG13	1.98	0.46
1:A:146:ASN:O	1:A:149:TYR:HB3	2.16	0.46
1:A:716:ASP:HA	1:A:719:LYS:HB2	1.97	0.46
1:A:592:ALA:O	1:A:593:SER:C	2.59	0.46
1:A:54:VAL:O	1:A:57:GLU:HB3	2.16	0.45
1:A:228:GLN:OE1	1:A:228:GLN:HA	2.16	0.45
1:A:505:LEU:HD12	1:A:509:THR:HG21	1.97	0.45
1:A:318:LEU:O	1:A:322:ILE:HB	2.15	0.45
1:A:625:GLY:HA3	1:A:664:ARG:HD2	1.98	0.45
1:B:46:ILE:HG22	1:B:46:ILE:O	2.16	0.45
1:B:94:LEU:HD22	1:B:97:LEU:HD11	1.98	0.45
1:B:331:SER:O	1:B:332:THR:C	2.59	0.45
1:B:368:LEU:O	1:B:369:SER:O	2.35	0.45
1:B:578:LYS:O	1:B:579:TYR:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:MET:HA	1:A:44:VAL:HG23	1.98	0.45
1:A:636:LEU:C	1:A:638:ASN:H	2.24	0.45
1:B:129:LEU:HD13	1:B:131:ILE:HD11	1.98	0.45
1:B:297:GLN:NE2	1:B:514:LEU:HD13	2.32	0.45
1:A:118:TYR:CZ	1:A:143:LYS:HG2	2.51	0.45
1:A:319:LEU:O	1:A:322:ILE:HG22	2.17	0.45
1:B:583:ILE:N	1:B:583:ILE:HD12	2.32	0.45
1:B:656:LYS:NZ	1:B:670:GLY:O	2.50	0.45
1:A:62:LEU:HD22	1:A:137:TYR:CD1	2.52	0.45
1:A:275:LYS:NZ	1:A:279:GLN:HE22	2.14	0.45
1:B:58:ALA:O	1:B:59:ALA:C	2.60	0.45
1:B:319:LEU:HD12	1:B:319:LEU:O	2.17	0.45
1:B:746:SER:O	1:B:752:ARG:NH1	2.49	0.45
1:A:87:ASP:OD2	1:A:115:HIS:HA	2.17	0.45
1:A:112:ALA:O	1:A:113:LEU:HD23	2.17	0.45
1:A:660:VAL:HA	2:C:8:VAL:HG13	1.97	0.45
1:B:79:GLY:HA2	1:B:127:PRO:HG2	1.98	0.45
1:B:123:GLU:O	1:B:124:GLY:C	2.58	0.45
1:B:135:GLU:OE1	1:B:138:VAL:HG23	2.17	0.45
1:B:326:SER:C	1:B:368:LEU:HD11	2.42	0.45
1:B:501:TRP:HB3	1:B:503:ILE:CD1	2.46	0.45
1:B:718:PHE:O	1:B:722:GLY:HA3	2.17	0.45
1:A:59:ALA:HB2	1:A:83:ILE:HG12	1.99	0.45
1:A:331:SER:OG	1:A:334:GLU:HG3	2.17	0.45
1:A:499:LEU:HG	1:A:545:ILE:HD11	1.99	0.45
1:A:679:ASN:HD21	1:A:682:GLU:H	1.63	0.45
1:B:86:GLY:O	1:B:132:GLN:NE2	2.49	0.45
1:B:177:ILE:HD11	1:B:240:ALA:HB2	1.98	0.45
1:B:164:ASN:OD1	1:B:536:LYS:HG2	2.17	0.45
1:A:97:LEU:HB3	1:A:101:LYS:HB2	1.99	0.45
1:A:221:PHE:O	1:A:225:ILE:HG12	2.17	0.45
1:A:679:ASN:C	1:A:679:ASN:ND2	2.75	0.45
1:A:759:ALA:N	1:A:760:PRO:CD	2.80	0.45
1:B:330:LEU:HB2	1:B:335:LYS:HZ3	1.80	0.45
1:A:241:PHE:CD1	1:A:241:PHE:C	2.95	0.44
1:B:153:LYS:O	1:B:157:ARG:HB3	2.17	0.44
1:A:71:LEU:HD12	1:A:71:LEU:HA	1.80	0.44
1:A:386:TYR:OH	1:A:411:GLN:HG3	2.17	0.44
1:B:246:LYS:O	1:B:251:GLU:HG3	2.17	0.44
1:B:456:ASP:HB3	1:B:462:LYS:O	2.18	0.44
1:B:603:LEU:O	1:B:606:TRP:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:GLN:HE22	1:B:652:GLN:HB3	1.81	0.44
1:A:107:ILE:HG13	1:A:145:LEU:HD12	1.99	0.44
1:A:330:LEU:HD11	1:A:376:LEU:HD13	1.98	0.44
1:B:322:ILE:O	1:B:342:GLN:NE2	2.50	0.44
1:A:506:SER:O	1:A:507:PRO:C	2.60	0.44
1:A:567:ASN:O	1:A:571:ASN:HB2	2.17	0.44
1:A:748:ASP:OD2	1:A:751:GLU:HG3	2.17	0.44
1:B:613:ASP:CB	1:B:774:ILE:HG23	2.48	0.44
1:A:118:TYR:CD1	1:A:118:TYR:N	2.85	0.44
1:A:144:ALA:O	1:A:148:TYR:CD1	2.71	0.44
1:A:246:LYS:O	1:A:250:GLN:HG2	2.17	0.44
1:B:80:LYS:O	1:B:128:VAL:HA	2.17	0.44
1:B:719:LYS:HA	1:B:719:LYS:HD3	1.76	0.44
1:A:269:GLU:HG2	1:A:273:LYS:HE3	1.99	0.44
1:B:125:TYR:C	1:B:127:PRO:HD3	2.42	0.44
1:B:304:LYS:HD2	1:B:304:LYS:N	2.33	0.44
1:A:151:ILE:O	1:A:152:GLY:C	2.60	0.44
1:A:259:LEU:HD23	1:A:259:LEU:HA	1.83	0.44
1:A:261:ASP:O	1:A:267:ARG:HD2	2.18	0.44
1:B:406:LEU:O	1:B:406:LEU:HD12	2.18	0.44
1:B:443:ILE:CD1	1:B:454:LEU:HD22	2.47	0.44
1:A:94:LEU:C	1:A:96:ALA:N	2.74	0.44
1:A:192:ASN:O	1:A:193:GLN:C	2.60	0.44
1:A:268:TYR:CB	1:B:125:TYR:HE2	2.25	0.44
1:A:592:ALA:O	1:A:595:ILE:N	2.50	0.44
1:B:62:LEU:O	1:B:148:TYR:OH	2.29	0.44
1:B:247:PHE:HE2	1:B:252:ILE:HD13	1.83	0.44
1:A:49:LYS:HD2	1:A:49:LYS:C	2.43	0.44
2:D:11:TYR:N	2:D:12:PRO:CD	2.80	0.44
1:A:197:HIS:ND1	1:A:198:PRO:HD2	2.33	0.43
1:A:322:ILE:HG13	1:A:368:LEU:CD1	2.48	0.43
1:A:606:TRP:CD1	1:A:610:ILE:HD12	2.53	0.43
1:B:271:TRP:CZ2	1:B:517:GLY:HA3	2.53	0.43
1:B:477:TYR:CZ	1:B:593:SER:HA	2.53	0.43
1:B:636:LEU:HD11	1:B:669:HIS:HB2	2.00	0.43
1:B:718:PHE:CZ	1:B:732:ASN:HA	2.53	0.43
1:A:135:GLU:OE1	1:A:135:GLU:N	2.49	0.43
1:A:458:THR:OG1	1:A:459:ASP:N	2.51	0.43
1:A:662:GLU:OE2	1:A:662:GLU:N	2.38	0.43
1:A:701:ASP:O	1:A:703:ASN:N	2.50	0.43
1:A:33:GLU:O	1:A:36:LEU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LYS:NZ	1:A:251:GLU:OE2	2.51	0.43
1:A:368:LEU:HB3	1:A:369:SER:H	1.69	0.43
1:A:767:ASN:HD22	1:A:767:ASN:HA	1.66	0.43
1:B:107:ILE:HD13	1:B:107:ILE:O	2.18	0.43
1:B:211:ASN:HA	1:B:214:GLN:HG3	2.00	0.43
1:B:233:LEU:C	1:B:235:LEU:H	2.24	0.43
1:B:658:LEU:HD11	2:D:8:VAL:HG11	1.96	0.43
1:A:31:THR:O	1:A:34:GLU:CG	2.64	0.43
1:A:70:VAL:HG12	1:A:252:ILE:HD11	1.99	0.43
1:A:91:HIS:ND1	1:A:92:ILE:N	2.67	0.43
1:A:155:LEU:O	1:A:160:LEU:HG	2.19	0.43
1:B:679:ASN:C	1:B:681:SER:N	2.75	0.43
1:A:199:THR:OG1	1:A:200:ASP:N	2.50	0.43
1:A:674:GLY:O	1:A:675:VAL:C	2.60	0.43
1:A:672:SER:HB2	1:A:673:LYS:H	1.61	0.43
1:A:697:GLY:N	1:A:708:VAL:HB	2.34	0.43
1:A:758:ASN:C	1:A:760:PRO:HD3	2.44	0.43
1:A:174:LEU:HD11	1:A:213:VAL:HG13	2.00	0.43
1:B:149:TYR:HA	1:B:222:ALA:HB2	2.00	0.43
1:B:234:GLN:HB2	1:B:241:PHE:CD2	2.54	0.43
1:B:368:LEU:O	1:B:373:LYS:HG3	2.18	0.43
1:B:370:GLU:HG3	1:B:371:LYS:N	2.33	0.43
1:B:637:PRO:HA	1:B:642:GLN:NE2	2.34	0.43
1:A:37:LYS:O	1:A:41:LYS:N	2.49	0.43
1:A:159:ILE:N	1:A:159:ILE:CD1	2.81	0.43
1:A:295:LYS:O	1:A:297:GLN:N	2.51	0.43
1:A:322:ILE:HD11	1:A:376:LEU:HD11	2.00	0.43
1:B:444:ASN:HD22	1:B:448:ALA:CA	2.29	0.43
1:A:30:LYS:HB3	1:A:31:THR:H	1.58	0.43
1:B:74:TYR:CE2	1:B:79:GLY:HA3	2.54	0.43
1:B:462:LYS:HE2	1:B:462:LYS:HB3	1.78	0.43
1:A:298:ILE:HA	1:A:299:PRO:HD3	1.84	0.43
1:A:320:LYS:HA	1:A:320:LYS:HD2	1.84	0.43
1:A:435:ILE:N	1:A:435:ILE:CD1	2.66	0.43
1:A:581:LYS:HE2	1:A:628:ARG:HE	1.84	0.43
1:B:136:ASP:O	1:B:140:ASN:CB	2.67	0.43
1:B:244:MET:CE	1:B:248:ASN:ND2	2.82	0.43
1:B:277:HIS:CD2	1:B:429:SER:HB2	2.53	0.43
1:B:563:GLN:HE21	1:B:585:PHE:HB2	1.83	0.43
1:B:611:GLN:HE21	1:B:614:LEU:H	1.64	0.43
1:A:744:MET:HE3	1:A:763:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:MET:HE3	1:A:159:ILE:HG21	2.01	0.42
1:A:146:ASN:O	1:A:147:VAL:C	2.61	0.42
1:A:267:ARG:NH1	1:A:489:ASN:HB3	2.34	0.42
1:A:308:ILE:HA	1:A:311:LEU:HD12	2.01	0.42
1:B:39:ILE:O	1:B:43:ILE:HG12	2.18	0.42
1:A:264:MET:HE2	1:A:264:MET:HB3	1.88	0.42
1:A:327:SER:OG	1:A:330:LEU:HD12	2.19	0.42
1:B:233:LEU:C	1:B:235:LEU:N	2.76	0.42
1:B:744:MET:SD	1:B:766:ILE:HG21	2.59	0.42
1:A:107:ILE:HG12	1:A:149:TYR:CG	2.54	0.42
1:A:694:ASP:OD1	1:A:694:ASP:C	2.62	0.42
1:B:34:GLU:O	1:B:38:GLU:N	2.52	0.42
1:B:368:LEU:O	1:B:369:SER:C	2.61	0.42
1:B:721:GLU:OE1	1:B:761:LYS:HB2	2.19	0.42
1:B:165:GLN:HA	1:B:166:PRO:C	2.44	0.42
1:B:304:LYS:CG	1:B:305:ASP:N	2.82	0.42
1:B:744:MET:HE3	1:B:763:PHE:CD1	2.54	0.42
1:A:39:ILE:HD13	1:A:72:GLU:HB2	2.00	0.42
1:A:114:LEU:HD21	1:A:120:TYR:HB2	2.01	0.42
1:A:125:TYR:CE1	1:B:269:GLU:HG3	2.55	0.42
1:B:268:TYR:O	1:B:272:GLU:HG2	2.19	0.42
1:B:420:ASP:C	1:B:422:LEU:H	2.27	0.42
1:A:233:LEU:HD13	1:A:241:PHE:CB	2.42	0.42
1:A:627:GLY:HA3	1:A:664:ARG:O	2.20	0.42
1:B:33:GLU:O	1:B:37:LYS:HG2	2.20	0.42
1:B:151:ILE:O	1:B:151:ILE:CG2	2.66	0.42
1:B:498:ARG:HD3	1:B:498:ARG:HA	1.73	0.42
1:B:589:ASN:HB3	1:B:590:ARG:H	1.68	0.42
1:B:632:THR:OG1	1:B:633:ASP:N	2.53	0.42
2:D:13:MET:H	2:D:13:MET:CE	2.28	0.42
1:B:89:THR:HG21	1:B:102:LYS:NZ	2.34	0.42
1:B:329:PHE:O	1:B:330:LEU:HD23	2.19	0.42
1:A:339:LYS:C	1:A:339:LYS:HD2	2.45	0.42
1:A:407:ASP:CG	1:A:408:VAL:H	2.28	0.42
1:B:107:ILE:HG21	1:B:145:LEU:HD12	1.99	0.42
1:B:186:GLN:HG3	1:B:190:PHE:CD1	2.55	0.42
1:B:215:GLU:O	1:B:216:VAL:C	2.60	0.42
1:B:292:LEU:HD11	1:B:418:ASN:HB2	2.01	0.42
1:A:322:ILE:O	1:A:322:ILE:HG23	2.19	0.41
1:A:339:LYS:HD2	1:A:339:LYS:O	2.20	0.41
1:A:573:ALA:O	1:A:574:LEU:HD12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:TYR:HA	1:A:222:ALA:HB2	2.01	0.41
1:A:247:PHE:O	1:A:252:ILE:HB	2.20	0.41
1:B:51:GLU:C	1:B:53:ALA:N	2.77	0.41
1:B:662:GLU:CD	1:B:662:GLU:N	2.76	0.41
1:A:407:ASP:CG	1:A:408:VAL:N	2.78	0.41
1:B:621:TYR:CE1	1:B:664:ARG:CZ	3.03	0.41
1:A:343:ILE:CG2	1:A:344:ASP:N	2.82	0.41
1:A:621:TYR:CE1	1:A:664:ARG:NH2	2.89	0.41
1:A:628:ARG:O	1:A:665:SER:HB3	2.21	0.41
1:A:649:ILE:O	1:A:652:GLN:HG2	2.20	0.41
1:B:653:VAL:HG12	1:B:654:HIS:N	2.35	0.41
1:A:209:ASN:O	1:A:212:GLU:HB2	2.19	0.41
1:A:496:ASN:HD22	1:A:497:GLU:HG3	1.85	0.41
1:A:571:ASN:HD22	1:A:571:ASN:HA	1.58	0.41
1:A:659:TYR:O	2:C:8:VAL:HG12	2.20	0.41
1:B:369:SER:OG	1:B:372:GLU:HG3	2.20	0.41
1:B:453:ASP:O	1:B:464:ASN:ND2	2.45	0.41
1:B:611:GLN:CD	1:B:774:ILE:HD13	2.46	0.41
1:A:151:ILE:O	1:A:154:ILE:HB	2.21	0.41
1:A:307:ILE:HG21	1:A:341:LEU:CD1	2.49	0.41
1:A:368:LEU:CD1	1:A:372:GLU:HB3	2.51	0.41
1:A:505:LEU:CD1	1:A:509:THR:HG21	2.51	0.41
1:A:673:LYS:HG3	2:C:14:GLU:OE2	2.21	0.41
1:B:250:GLN:HB2	1:B:251:GLU:H	1.63	0.41
1:B:498:ARG:NH2	1:B:540:LYS:HE2	2.24	0.41
1:A:584:THR:HG23	1:A:630:VAL:HG22	2.03	0.41
1:A:717:ILE:N	1:A:717:ILE:HD12	2.35	0.41
1:B:163:ILE:CG1	1:B:165:GLN:HG3	2.50	0.41
1:A:131:ILE:O	1:A:132:GLN:O	2.39	0.41
1:A:370:GLU:O	1:A:371:LYS:C	2.63	0.41
1:A:675:VAL:HG23	2:C:12:PRO:O	2.20	0.41
1:B:129:LEU:HD22	1:B:131:ILE:HD11	2.03	0.41
1:B:197:HIS:HA	1:B:198:PRO:HD2	1.86	0.41
1:B:440:ASN:HD21	1:B:500:LYS:HZ3	1.66	0.41
1:A:34:GLU:CG	1:A:35:HIS:N	2.84	0.41
1:A:375:PHE:CE2	1:A:379:LEU:HD11	2.56	0.41
1:A:482:ASN:OD1	1:A:482:ASN:C	2.64	0.41
1:B:250:GLN:O	1:B:252:ILE:N	2.53	0.41
1:B:478:SER:HB3	1:B:527:LEU:HB2	2.03	0.41
1:B:563:GLN:NE2	1:B:585:PHE:H	2.19	0.41
1:B:597:GLU:O	1:B:598:SER:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:ASP:OD1	1:B:694:ASP:O	2.39	0.41
1:A:125:TYR:CG	1:B:269:GLU:HG3	2.55	0.41
1:A:243:TYR:CD1	1:A:243:TYR:C	2.99	0.41
1:A:333:GLU:O	1:A:336:GLU:HB3	2.21	0.41
1:A:666:ILE:HG23	1:A:687:CYS:HB3	2.03	0.41
1:A:749:HIS:O	1:A:750:ALA:C	2.63	0.41
1:B:214:GLN:O	1:B:217:PHE:HB3	2.20	0.41
1:B:500:LYS:HD2	1:B:542:TYR:CG	2.56	0.41
1:B:659:TYR:O	2:D:8:VAL:HG13	2.20	0.41
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.92	0.40
1:A:184:ASP:O	1:A:185:GLY:C	2.64	0.40
1:A:433:ASN:O	1:A:435:ILE:HG13	2.21	0.40
1:A:648:GLU:HB3	1:A:650:TYR:CD2	2.56	0.40
1:A:769:GLN:O	1:A:772:PHE:HB3	2.21	0.40
1:B:589:ASN:HB2	1:B:633:ASP:OD2	2.21	0.40
1:A:46:ILE:N	1:A:46:ILE:CD1	2.84	0.40
1:A:74:TYR:HD2	1:A:74:TYR:HA	1.78	0.40
1:A:101:LYS:O	1:A:114:LEU:HD12	2.21	0.40
1:B:48:VAL:O	1:B:49:LYS:HD3	2.21	0.40
1:B:118:TYR:CE2	1:B:143:LYS:HG2	2.56	0.40
1:B:133:SER:O	1:B:134:SER:HB3	2.22	0.40
1:B:424:HIS:CA	1:B:510:ARG:HD2	2.42	0.40
1:B:589:ASN:N	1:B:633:ASP:OD2	2.50	0.40
1:B:701:ASP:C	1:B:703:ASN:N	2.73	0.40
1:B:47:GLU:O	1:B:84:VAL:HG23	2.20	0.40
1:B:643:TYR:CD1	1:B:643:TYR:C	2.99	0.40
1:B:721:GLU:O	1:B:723:SER:N	2.55	0.40
1:A:150:GLU:O	1:A:151:ILE:C	2.63	0.40
1:A:690:HIS:CE1	1:A:735:GLU:OE2	2.75	0.40
1:B:50:GLY:O	1:B:51:GLU:HB2	2.22	0.40
1:B:533:GLN:HE21	1:B:533:GLN:HB2	1.73	0.40
1:B:618:VAL:O	1:B:621:TYR:HB3	2.21	0.40
1:B:649:ILE:O	1:B:649:ILE:HG22	2.21	0.40
1:B:676:GLU:OE1	1:B:676:GLU:HA	2.20	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	722/776 (93%)	617 (86%)	74 (10%)	31 (4%)	2	7
1	B	730/776 (94%)	635 (87%)	76 (10%)	19 (3%)	4	15
2	C	9/20 (45%)	4 (44%)	1 (11%)	4 (44%)	0	0
2	D	9/20 (45%)	4 (44%)	1 (11%)	4 (44%)	0	0
All	All	1470/1592 (92%)	1260 (86%)	152 (10%)	58 (4%)	2	8

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	181	SER
1	A	370	GLU
1	A	473	LYS
1	A	675	VAL
1	A	678	ARG
1	B	30	LYS
1	B	94	LEU
1	B	200	ASP
1	B	366	ASN
1	B	369	SER
2	C	15	PRO
2	D	15	PRO
1	A	31	THR
1	A	98	SER
1	A	101	LYS
1	A	140	ASN
1	A	296	LEU
1	A	592	ALA
1	A	676	GLU
1	A	696	ALA
1	A	700	LEU

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Mol	Chain	Res	Type
1	A	702	LYS
1	B	48	VAL
1	B	93	SER
1	B	123	GLU
1	B	134	SER
1	B	251	GLU
1	B	722	GLY
2	C	10	PRO
1	A	52	GLU
1	A	87	ASP
1	A	95	GLU
1	A	209	ASN
1	A	250	GLN
1	A	641	GLU
1	B	141	THR
1	B	652	GLN
2	D	10	PRO
1	A	198	PRO
1	A	251	GLU
1	A	324	ILE
1	A	672	SER
1	B	52	GLU
1	B	196	GLU
1	B	702	LYS
2	C	11	TYR
1	A	760	PRO
1	B	124	GLY
2	D	11	TYR
2	D	12	PRO
1	A	722	GLY
1	B	577	PRO
1	A	92	ILE
1	A	88	ILE
2	C	12	PRO
1	A	383	ILE
1	B	107	ILE

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	665/710 (94%)	609 (92%)	56 (8%)	10	32
1	B	673/710 (95%)	636 (94%)	37 (6%)	19	51
2	C	11/17 (65%)	8 (73%)	3 (27%)	0	1
2	D	11/17 (65%)	6 (54%)	5 (46%)	0	0
All	All	1360/1454 (94%)	1259 (93%)	101 (7%)	13	37

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	33	GLU
1	A	34	GLU
1	A	35	HIS
1	A	46	ILE
1	A	70	VAL
1	A	71	LEU
1	A	84	VAL
1	A	85	ASP
1	A	104	ILE
1	A	107	ILE
1	A	111	ASP
1	A	117	HIS
1	A	145	LEU
1	A	203	VAL
1	A	233	LEU
1	A	256	LEU
1	A	258	GLU
1	A	288	GLU
1	A	294	LYS
1	A	296	LEU
1	A	301	GLU
1	A	305	ASP
1	A	317	GLU
1	A	343	ILE
1	A	374	GLU
1	A	404	ILE
1	A	431	LEU
1	A	433	ASN
1	A	435	ILE

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Mol	Chain	Res	Type
1	A	446	LEU
1	A	447	THR
1	A	449	THR
1	A	470	GLU
1	A	494	LEU
1	A	496	ASN
1	A	503	ILE
1	A	505	LEU
1	A	557	THR
1	A	566	ILE
1	A	571	ASN
1	A	582	LEU
1	A	620	ASN
1	A	636	LEU
1	A	656	LYS
1	A	658	LEU
1	A	679	ASN
1	A	686	HIS
1	A	692	VAL
1	A	730	ARG
1	A	733	GLU
1	A	739	GLU
1	A	745	HIS
1	A	761	LYS
1	A	767	ASN
1	A	772	PHE
1	B	40	MET
1	B	68	SER
1	B	77	ILE
1	B	80	LYS
1	B	90	LYS
1	B	107	ILE
1	B	126	GLU
1	B	129	LEU
1	B	136	ASP
1	B	142	GLU
1	B	146	ASN
1	B	165	GLN
1	B	184	ASP
1	B	199	THR
1	B	228	GLN
1	B	256	LEU

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Mol	Chain	Res	Type
1	B	265	LEU
1	B	304	LYS
1	B	314	GLU
1	B	391	ARG
1	B	425	GLN
1	B	447	THR
1	B	496	ASN
1	B	499	LEU
1	B	516	ASN
1	B	525	ILE
1	B	529	ILE
1	B	533	GLN
1	B	571	ASN
1	B	611	GLN
1	B	639	ILE
1	B	667	LEU
1	B	671	PRO
1	B	727	SER
1	B	764	GLN
1	B	766	ILE
1	B	767	ASN
2	C	11	TYR
2	C	13	MET
2	C	14	GLU
2	D	6	LYS
2	D	7	LYS
2	D	10	PRO
2	D	13	MET
2	D	14	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	35	HIS
1	A	140	ASN
1	A	164	ASN
1	A	192	ASN
1	A	193	GLN
1	A	209	ASN
1	A	242	ASN
1	A	248	ASN

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Mol	Chain	Res	Type
1	A	253	ASN
1	A	276	GLN
1	A	277	HIS
1	A	279	GLN
1	A	390	GLN
1	A	411	GLN
1	A	417	GLN
1	A	425	GLN
1	A	440	ASN
1	A	496	ASN
1	A	504	GLN
1	A	524	ASN
1	A	560	GLN
1	A	563	GLN
1	A	567	ASN
1	A	571	ASN
1	A	589	ASN
1	A	608	ASN
1	A	611	GLN
1	A	646	GLN
1	A	679	ASN
1	A	745	HIS
1	A	767	ASN
1	A	775	ASN
1	B	35	HIS
1	B	91	HIS
1	B	132	GLN
1	B	140	ASN
1	B	165	GLN
1	B	193	GLN
1	B	197	HIS
1	B	209	ASN
1	B	214	GLN
1	B	242	ASN
1	B	250	GLN
1	B	253	ASN
1	B	262	GLN
1	B	277	HIS
1	B	297	GLN
1	B	309	HIS
1	B	313	GLN
1	B	323	GLN

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Mol	Chain	Res	Type
1	B	390	GLN
1	B	440	ASN
1	B	444	ASN
1	B	489	ASN
1	B	496	ASN
1	B	504	GLN
1	B	516	ASN
1	B	522	GLN
1	B	524	ASN
1	B	533	GLN
1	B	537	GLN
1	B	563	GLN
1	B	571	ASN
1	B	589	ASN
1	B	608	ASN
1	B	609	ASN
1	B	611	GLN
1	B	638	ASN
1	B	654	HIS
1	B	710	ASN
1	B	749	HIS
1	B	756	GLN
1	B	769	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	726/776 (93%)	0.38	58 (7%) 18 13	14, 40, 88, 94	0
1	B	734/776 (94%)	0.22	40 (5%) 31 24	12, 39, 85, 123	0
2	C	11/20 (55%)	4.30	11 (100%) 0 0	89, 98, 108, 108	0
2	D	11/20 (55%)	3.77	10 (90%) 0 0	88, 98, 108, 108	0
All	All	1482/1592 (93%)	0.35	119 (8%) 18 13	12, 40, 88, 123	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	11	TYR	7.9
2	C	12	PRO	6.4
1	B	349	LEU	5.4
2	D	11	TYR	5.3
2	D	9	TYR	4.9
2	C	9	TYR	4.8
2	C	15	PRO	4.7
1	A	703	ASN	4.4
2	D	12	PRO	4.3
2	D	6	LYS	4.2
1	B	365	SER	4.2
2	C	16	THR	4.1
1	A	29	ASN	4.0
2	D	16	THR	3.9
1	A	312	SER	3.9
2	D	14	GLU	3.8
1	A	32	GLN	3.8
2	D	15	PRO	3.8
2	C	14	GLU	3.8
2	C	13	MET	3.7
1	A	34	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	6	LYS	3.4
1	A	31	THR	3.4
1	A	345	ILE	3.4
1	A	98	SER	3.4
1	B	115	HIS	3.4
2	D	10	PRO	3.4
1	B	30	LYS	3.3
1	B	345	ILE	3.3
2	C	10	PRO	3.3
2	D	13	MET	3.3
1	A	754	LYS	3.2
1	B	702	LYS	3.2
1	B	31	THR	3.2
1	A	33	GLU	3.2
1	A	760	PRO	3.2
1	B	35	HIS	3.1
1	A	757	LYS	3.1
2	C	8	VAL	3.1
1	A	343	ILE	3.0
1	B	104	ILE	3.0
1	B	54	VAL	3.0
1	A	112	ALA	3.0
1	A	320	LYS	3.0
1	A	324	ILE	2.9
1	A	323	GLN	2.9
1	B	50	GLY	2.9
2	D	8	VAL	2.9
1	B	134	SER	2.8
1	A	700	LEU	2.8
1	A	755	VAL	2.8
1	A	104	ILE	2.8
1	B	101	LYS	2.7
1	B	706	ASP	2.7
1	A	52	GLU	2.7
1	A	140	ASN	2.7
1	B	99	GLU	2.7
1	A	180	ALA	2.6
1	A	101	LYS	2.6
1	A	675	VAL	2.6
1	B	370	GLU	2.6
1	A	368	LEU	2.5
1	B	96	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	761	LYS	2.5
1	B	327	SER	2.5
1	B	57	GLU	2.5
1	A	321	ARG	2.5
1	B	368	LEU	2.5
1	B	92	ILE	2.5
1	B	98	SER	2.5
1	B	55	LYS	2.5
1	B	137	TYR	2.4
1	A	328	ASP	2.4
1	B	343	ILE	2.4
1	A	676	GLU	2.4
1	A	560	GLN	2.4
1	A	90	LYS	2.4
1	A	705	SER	2.4
1	B	705	SER	2.4
1	A	206	LEU	2.4
1	A	341	LEU	2.4
1	A	710	ASN	2.3
1	A	758	ASN	2.3
1	A	179	ASN	2.3
1	A	701	ASP	2.3
1	A	309	HIS	2.3
1	B	131	ILE	2.3
1	A	135	GLU	2.3
1	B	326	SER	2.3
1	B	32	GLN	2.2
1	A	35	HIS	2.2
2	C	7	LYS	2.2
1	A	723	SER	2.2
1	A	713	LYS	2.2
1	A	750	ALA	2.2
1	A	756	GLN	2.2
1	B	366	ASN	2.2
1	A	709	THR	2.2
1	B	125	TYR	2.2
1	B	94	LEU	2.2
1	B	112	ALA	2.1
1	B	662	GLU	2.1
1	A	769	GLN	2.1
1	A	329	PHE	2.1
1	A	51	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	763	PHE	2.1
1	A	770	ILE	2.1
1	B	53	ALA	2.1
1	A	371	LYS	2.1
1	B	102	LYS	2.1
1	A	308	ILE	2.1
1	B	42	HIS	2.0
1	A	136	ASP	2.0
1	B	100	ASP	2.0
1	B	268	TYR	2.0
1	A	96	ALA	2.0
1	A	747	THR	2.0
1	A	712	LYS	2.0
1	B	371	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	9001	1/1	0.99	0.09	45,45,45,45	0
3	ZN	B	9002	1/1	0.99	0.09	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.