



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:00 PM UTC

PDB ID : 1W26 / pdb_00001w26
Title : Trigger Factor in Complex with the Ribosome forms a Molecular Cradle for Nascent Proteins
Authors : Ferbitz, L.; Maier, T.; Patzelt, H.; Bukau, B.; Deuerling, E.; Ban, N.
Deposited on : 2004-06-28
Resolution : 2.70 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

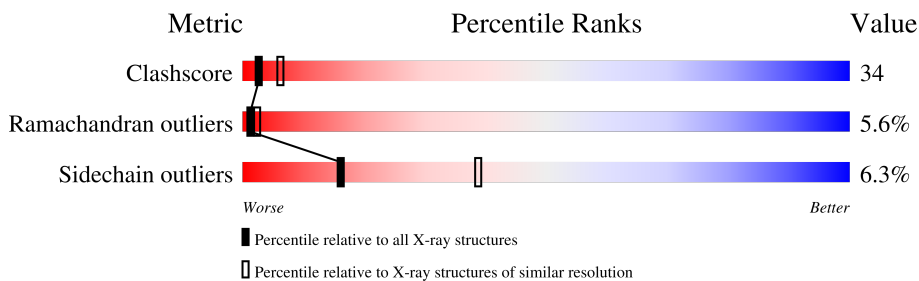
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	432	 53% 39% 7%
1	B	432	 44% 45% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6860 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 TRIGGER FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	Se	0	0	0
			3386	2119	582	674	11			
1	B	432	Total	C	N	O	Se	0	0	0
			3386	2119	582	674	11			

- Molecule 2 is water.

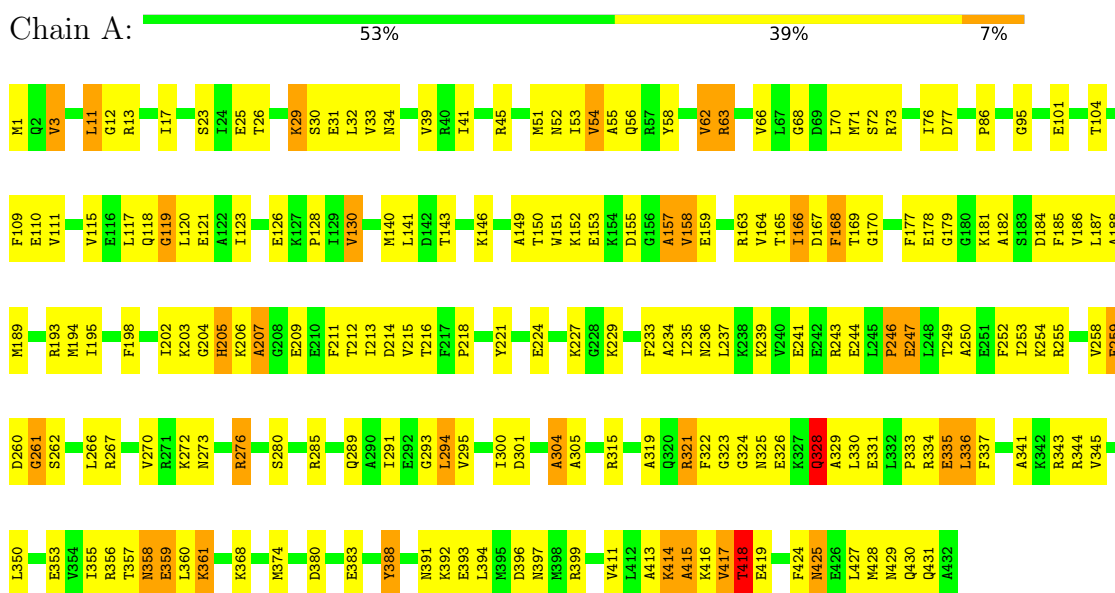
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	55	Total	O	0	0
			55	55		
2	B	33	Total	O	0	0
			33	33		

3 Residue-property plots

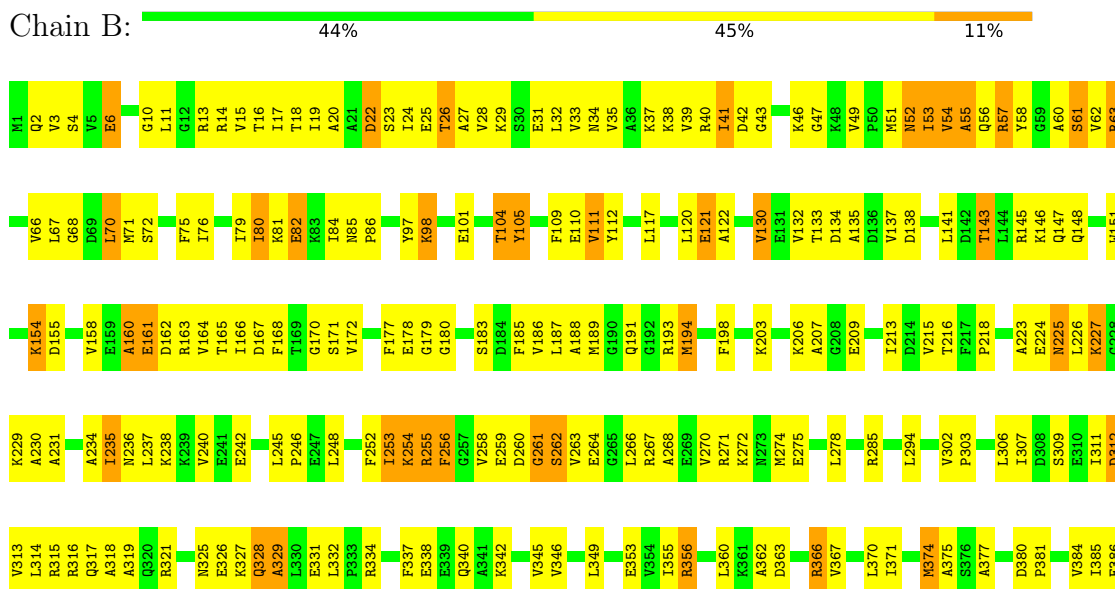
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: TRIGGER FACTOR



• Molecule 1: TRIGGER FACTOR



F387	Y388	S389	K392	E393	L394	M395	D396	N397	M398	R399	M400	V401	A402	L403	E404	E405	Q406	L412	A413	K414	T422	T423	F424	M425	E426	L427	M428	M429	Q430	Q431	A432
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.25Å 47.41Å 114.83Å 90.00° 113.66° 90.00°	Depositor
Resolution (Å)	45.91 – 2.70	Depositor
% Data completeness (in resolution range)	100.0 (45.91-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.324	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6860	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

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	0.49	0/3416	1.03	19/4575 (0.4%)
1	B	0.46	0/3416	0.96	10/4575 (0.2%)
All	All	0.48	0/6832	0.99	29/9150 (0.3%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	VAL	N-CA-C	-11.52	102.44	112.12
1	A	328	GLN	N-CA-C	-10.98	97.14	113.61
1	A	54	VAL	N-CA-C	-7.75	102.89	110.72
1	B	38	LYS	N-CA-C	-7.33	103.94	113.17
1	A	424	PHE	N-CA-C	-7.29	103.26	111.14
1	A	95	GLY	N-CA-C	-7.21	99.86	112.55
1	A	3	VAL	N-CA-C	6.58	117.50	107.77
1	B	235	ILE	N-CA-C	6.39	117.05	108.11
1	A	330	LEU	N-CA-C	-6.14	105.64	113.01
1	A	255	ARG	N-CA-C	-6.10	105.33	112.89
1	A	77	ASP	N-CA-C	-6.09	104.27	111.03
1	B	393	GLU	N-CA-C	6.09	117.59	111.07
1	B	97	TYR	N-CA-C	5.88	117.38	110.97
1	A	321	ARG	N-CA-C	-5.54	106.66	113.41
1	B	238	LYS	N-CA-C	5.54	118.24	111.82
1	B	52	ASN	N-CA-C	-5.52	106.62	113.19
1	B	384	VAL	N-CA-C	-5.49	105.37	110.53
1	B	82	GLU	N-CA-C	-5.42	106.65	113.20
1	A	23	SER	N-CA-C	-5.39	105.57	111.82
1	A	399	ARG	N-CA-C	-5.36	104.86	111.40
1	A	168	PHE	N-CA-C	5.34	117.31	109.24
1	A	415	ALA	N-CA-C	5.30	117.88	109.50
1	A	119	GLY	N-CA-C	5.13	125.35	113.18
1	B	388	TYR	N-CA-C	-5.13	104.76	111.02
1	A	304	ALA	N-CA-C	5.10	116.53	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	ARG	N-CA-C	-5.09	105.42	111.69
1	A	417	VAL	N-CA-C	5.08	113.91	106.55
1	A	229	LYS	N-CA-C	5.06	116.82	110.24
1	A	166	ILE	N-CA-C	5.04	116.26	108.44

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	3386	0	3403	200	0
1	B	3386	0	3403	258	0
2	A	55	0	0	3	0
2	B	33	0	0	3	0
All	All	6860	0	6806	458	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (458) 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:53:ILE:HG21	1:B:58:TYR:CB	1.89	1.02
1:B:53:ILE:HG21	1:B:58:TYR:HB3	1.00	0.99
1:B:53:ILE:CG2	1:B:58:TYR:HB3	1.93	0.98
1:B:133:THR:HG22	1:B:135:ALA:H	1.28	0.97
1:A:168:PHE:H	1:A:182:ALA:HB3	1.28	0.96
1:B:32:LEU:HD13	1:B:53:ILE:HG23	1.44	0.95
1:B:355:ILE:HA	1:B:360:LEU:HD12	1.52	0.91
1:A:140:MSE:HE3	1:A:143:THR:HB	1.53	0.90
1:B:146:LYS:HG2	1:B:245:LEU:HD11	1.51	0.90
1:A:164:VAL:HG11	1:A:237:LEU:HD11	1.62	0.82
1:A:425:ASN:N	1:A:425:ASN:HD22	1.77	0.82
1:A:152:LYS:HG2	1:A:153:GLU:H	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:VAL:HG21	1:B:46:LYS:HD3	1.61	0.81
1:A:164:VAL:HG13	1:A:239:LYS:O	1.81	0.80
1:B:133:THR:HG22	1:B:135:ALA:N	1.95	0.80
1:B:194:MSE:HE2	1:B:194:MSE:HA	1.61	0.80
1:B:207:ALA:HA	1:B:237:LEU:HG	1.63	0.80
1:A:167:ASP:HB2	1:A:236:ASN:HB2	1.64	0.80
1:B:158:VAL:CG1	1:B:189:MSE:HE2	2.13	0.79
1:B:158:VAL:HG11	1:B:189:MSE:HE2	1.63	0.79
1:B:18:THR:HG23	1:B:104:THR:HG22	1.64	0.79
1:B:363:ASP:H	1:B:406:GLN:HE22	1.27	0.79
1:A:361:LYS:HD2	1:A:361:LYS:O	1.83	0.78
1:B:366:ARG:HD3	1:B:405:GLU:OE1	1.83	0.78
1:A:187:LEU:HA	1:A:193:ARG:HH21	1.48	0.78
1:B:6:GLU:HG3	1:B:14:ARG:HB3	1.66	0.77
1:B:386:GLU:O	1:B:389:SER:HB3	1.84	0.77
1:A:193:ARG:O	1:A:194:MSE:HE2	1.84	0.77
1:A:358:ASN:N	1:A:358:ASN:HD22	1.80	0.77
1:A:335:GLU:CD	1:A:335:GLU:H	1.94	0.76
1:B:254:LYS:HG3	1:B:255:ARG:H	1.50	0.76
1:B:60:ALA:C	1:B:62:VAL:H	1.94	0.76
1:B:303:PRO:HG2	1:B:306:LEU:HD12	1.68	0.76
1:B:342:LYS:O	1:B:346:VAL:HG23	1.87	0.75
1:B:215:VAL:HG12	1:B:216:THR:H	1.52	0.75
1:B:120:LEU:C	1:B:122:ALA:H	1.95	0.74
1:B:254:LYS:HZ1	1:B:255:ARG:CZ	2.00	0.74
1:A:260:ASP:O	1:A:262:SER:N	2.20	0.74
1:B:326:GLU:HG3	1:B:327:LYS:N	2.02	0.74
1:B:49:VAL:HG11	1:B:54:VAL:HG13	1.69	0.74
1:B:2:GLN:HB2	1:B:18:THR:HB	1.68	0.73
1:B:6:GLU:CD	1:B:14:ARG:HD2	2.14	0.72
1:A:73:ARG:HB3	1:A:73:ARG:HH11	1.53	0.72
1:A:150:THR:HA	2:A:2027:HOH:O	1.88	0.72
1:A:250:ALA:O	1:A:254:LYS:HG2	1.90	0.72
1:A:45:ARG:HG3	1:A:45:ARG:HH11	1.54	0.71
1:B:63:ARG:HB2	1:B:63:ARG:HH11	1.54	0.71
1:B:168:PHE:HA	1:B:234:ALA:O	1.91	0.71
1:B:32:LEU:HD12	1:B:53:ILE:HD12	1.71	0.70
1:B:207:ALA:HB2	1:B:240:VAL:HG23	1.73	0.70
1:B:4:SER:HB2	2:B:2001:HOH:O	1.92	0.70
1:A:13:ARG:HH11	1:A:13:ARG:HG3	1.56	0.70
1:A:118:GLN:O	1:A:120:LEU:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG21	1:A:427:LEU:HD22	1.72	0.69
1:B:49:VAL:CG1	1:B:54:VAL:HG22	2.22	0.69
1:B:164:VAL:HG12	1:B:166:ILE:HG23	1.74	0.69
1:B:311:ILE:O	1:B:315:ARG:HG2	1.92	0.69
1:B:60:ALA:O	1:B:62:VAL:N	2.23	0.69
1:A:206:LYS:O	1:A:237:LEU:HD23	1.92	0.69
1:B:41:ILE:C	1:B:43:GLY:H	2.00	0.69
1:A:51:MSE:SE	1:A:54:VAL:HG21	2.43	0.69
1:A:187:LEU:HA	1:A:193:ARG:NH2	2.08	0.69
1:A:164:VAL:HG11	1:A:237:LEU:CD1	2.23	0.68
1:A:62:VAL:HG13	1:A:66:VAL:CG2	2.23	0.68
1:B:41:ILE:HD11	1:B:46:LYS:HD3	1.75	0.68
1:B:31:GLU:O	1:B:35:VAL:HG23	1.93	0.67
1:B:312:ASP:HB3	1:B:316:ARG:HH12	1.59	0.67
1:A:357:THR:HG22	1:A:358:ASN:ND2	2.09	0.67
1:A:325:ASN:O	1:A:328:GLN:HB2	1.94	0.67
1:B:32:LEU:CD1	1:B:53:ILE:HD12	2.24	0.67
1:B:145:ARG:HD3	1:B:248:LEU:HD21	1.77	0.67
1:B:206:LYS:O	1:B:209:GLU:HG2	1.93	0.67
1:B:76:ILE:O	1:B:79:ILE:HG12	1.94	0.67
1:B:253:ILE:HD12	1:B:266:LEU:HD12	1.76	0.66
1:B:389:SER:HA	1:B:395:MSE:HE3	1.77	0.66
1:A:388:TYR:CE1	1:A:394:LEU:HD23	2.30	0.66
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.59	0.66
1:B:171:SER:O	1:B:231:ALA:HB1	1.95	0.66
1:A:291:ILE:O	1:A:295:VAL:HG23	1.96	0.66
1:A:425:ASN:HD22	1:A:425:ASN:H	1.44	0.66
1:A:357:THR:HG22	1:A:358:ASN:HD22	1.60	0.65
1:B:178:GLU:HG2	1:B:179:GLY:N	2.12	0.65
1:B:80:ILE:O	1:B:80:ILE:HG22	1.95	0.65
1:B:371:ILE:HD13	1:B:395:MSE:HE1	1.78	0.65
1:A:213:ILE:HD12	1:A:214:ASP:H	1.61	0.65
1:B:254:LYS:HG3	1:B:255:ARG:N	2.10	0.65
1:B:49:VAL:HG11	1:B:54:VAL:HG22	1.78	0.65
1:A:1:MSE:HE3	1:A:3:VAL:HG11	1.79	0.65
1:A:166:ILE:HG21	1:A:235:ILE:HG23	1.79	0.65
1:A:149:ALA:HA	1:A:246:PRO:CD	2.27	0.65
1:A:165:THR:HG22	1:A:186:VAL:HG12	1.77	0.64
1:B:397:ASN:O	1:B:401:VAL:HG23	1.97	0.64
1:A:72:SER:O	1:A:76:ILE:HG22	1.97	0.64
1:B:253:ILE:HG23	1:B:266:LEU:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:HB2	1:A:29:LYS:NZ	2.12	0.63
1:B:54:VAL:C	1:B:56:GLN:H	2.05	0.63
1:B:17:ILE:HB	1:B:105:TYR:CE2	2.34	0.63
1:B:120:LEU:HD21	1:B:294:LEU:HD13	1.81	0.63
1:B:193:ARG:O	1:B:194:MSE:HE3	1.99	0.63
1:A:41:ILE:HG22	1:A:41:ILE:O	1.98	0.63
1:B:141:LEU:O	1:B:145:ARG:HG3	1.99	0.62
1:B:389:SER:CA	1:B:395:MSE:HE3	2.29	0.62
1:B:430:GLN:OE1	1:B:430:GLN:HA	1.98	0.62
1:A:62:VAL:HG13	1:A:66:VAL:HG21	1.81	0.62
1:A:165:THR:OG1	1:A:239:LYS:HB2	1.99	0.62
1:B:303:PRO:CG	1:B:306:LEU:HD12	2.29	0.62
1:A:361:LYS:HD2	1:A:361:LYS:C	2.25	0.61
1:A:168:PHE:N	1:A:182:ALA:HB3	2.09	0.61
1:A:272:LYS:HE2	1:A:276:ARG:NH2	2.14	0.61
1:A:195:ILE:HD11	1:A:221:TYR:HE1	1.65	0.60
1:A:168:PHE:HA	1:A:234:ALA:O	2.02	0.60
1:A:315:ARG:HG2	1:A:337:PHE:CE1	2.37	0.60
1:B:40:ARG:HG3	1:B:40:ARG:HH11	1.67	0.60
1:A:253:ILE:HG21	1:A:261:GLY:O	2.02	0.60
1:A:355:ILE:HA	1:A:360:LEU:HD12	1.84	0.60
1:B:53:ILE:O	1:B:53:ILE:HG22	2.01	0.59
1:B:328:GLN:O	1:B:332:LEU:HD13	2.02	0.59
1:A:146:LYS:HE2	1:A:243:ARG:HH11	1.68	0.59
1:B:252:PHE:O	1:B:254:LYS:HG2	2.02	0.59
1:A:166:ILE:HG22	1:A:167:ASP:N	2.16	0.59
1:A:126:GLU:HA	1:A:418:THR:HG23	1.83	0.59
1:B:194:MSE:HA	1:B:194:MSE:CE	2.32	0.59
1:A:368:LYS:HE3	2:A:2040:HOH:O	2.01	0.59
1:B:326:GLU:HG3	1:B:327:LYS:H	1.66	0.58
1:A:325:ASN:OD1	1:A:328:GLN:HG3	2.04	0.58
1:B:63:ARG:O	1:B:67:LEU:HB2	2.03	0.58
1:B:112:TYR:CE2	1:B:306:LEU:HD11	2.38	0.58
1:B:327:LYS:C	1:B:329:ALA:H	2.12	0.58
1:B:198:PHE:CD1	1:B:213:ILE:HD11	2.38	0.58
1:A:429:ASN:HA	1:A:431:GLN:HE22	1.69	0.58
1:B:66:VAL:O	1:B:70:LEU:HD13	2.03	0.58
1:A:68:GLY:HA2	1:A:71:MSE:HE2	1.85	0.57
1:A:166:ILE:CG2	1:A:167:ASP:N	2.67	0.57
1:A:333:PRO:O	1:A:336:LEU:HB2	2.04	0.57
1:B:13:ARG:HG3	1:B:13:ARG:HH11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ILE:O	1:B:311:ILE:HG23	2.05	0.57
1:B:401:VAL:O	1:B:404:GLU:HG3	2.04	0.57
1:A:188:ALA:H	1:A:193:ARG:NH2	2.02	0.57
1:B:68:GLY:O	1:B:71:MSE:HB2	2.05	0.57
1:B:198:PHE:HD1	1:B:213:ILE:HD11	1.70	0.57
1:B:40:ARG:O	1:B:42:ASP:N	2.35	0.57
1:B:325:ASN:OD1	1:B:328:GLN:HG2	2.05	0.57
1:B:15:VAL:HG21	1:B:75:PHE:HE1	1.70	0.56
1:B:55:ALA:HA	1:B:58:TYR:CD2	2.40	0.56
1:B:137:VAL:HG11	1:B:267:ARG:HG3	1.87	0.56
1:B:34:ASN:O	1:B:37:LYS:HG3	2.04	0.56
1:B:172:VAL:HG11	1:B:229:LYS:HD3	1.86	0.56
1:A:31:GLU:HG3	1:A:62:VAL:CG2	2.36	0.56
1:B:23:SER:O	1:B:27:ALA:HB2	2.06	0.56
1:B:315:ARG:HB3	1:B:337:PHE:CE2	2.40	0.56
1:B:120:LEU:HD21	1:B:294:LEU:CD1	2.36	0.56
1:A:54:VAL:HG23	1:A:55:ALA:N	2.20	0.55
1:A:30:SER:O	1:A:33:VAL:HG12	2.07	0.55
1:A:425:ASN:N	1:A:425:ASN:ND2	2.49	0.55
1:B:13:ARG:HG3	1:B:13:ARG:NH1	2.22	0.55
1:A:358:ASN:N	1:A:358:ASN:ND2	2.49	0.55
1:B:40:ARG:HG3	1:B:40:ARG:O	2.07	0.55
1:B:427:LEU:O	1:B:430:GLN:HG2	2.07	0.55
1:A:358:ASN:O	1:A:359:GLU:C	2.49	0.55
1:B:22:ASP:O	1:B:26:THR:HG23	2.07	0.55
1:B:29:LYS:HG2	1:B:53:ILE:HD11	1.88	0.55
1:B:392:LYS:NZ	1:B:393:GLU:HG3	2.21	0.55
1:B:271:ARG:O	1:B:275:GLU:HG3	2.07	0.55
1:B:68:GLY:HA2	1:B:71:MSE:HE3	1.89	0.55
1:B:172:VAL:HG23	1:B:177:PHE:CD2	2.42	0.55
1:A:356:ARG:HG2	1:A:356:ARG:NH1	2.21	0.54
1:A:260:ASP:C	1:A:262:SER:H	2.14	0.54
1:A:205:HIS:HB2	1:A:237:LEU:HD22	1.89	0.54
1:A:428:MSE:HE3	1:A:430:GLN:HG3	1.89	0.54
1:B:302:VAL:HG23	1:B:307:ILE:HD11	1.89	0.54
1:A:3:VAL:HG12	1:A:17:ILE:HG12	1.89	0.54
1:A:396:ASP:OD1	1:A:397:ASN:N	2.41	0.54
1:B:388:TYR:C	1:B:395:MSE:CE	2.81	0.54
1:B:41:ILE:HG22	1:B:41:ILE:O	2.08	0.53
1:B:165:THR:HA	1:B:185:PHE:O	2.08	0.53
1:B:423:THR:OG1	1:B:426:GLU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HG3	1:A:45:ARG:NH1	2.23	0.53
1:A:428:MSE:HE1	1:A:430:GLN:HE21	1.72	0.53
1:B:309:SER:O	1:B:313:VAL:HG23	2.07	0.53
1:B:39:VAL:HG13	1:B:39:VAL:O	2.08	0.53
1:A:140:MSE:HG2	1:A:270:VAL:HG13	1.90	0.53
1:B:40:ARG:HG3	1:B:40:ARG:NH1	2.24	0.53
1:B:164:VAL:CG1	1:B:166:ILE:HG23	2.37	0.53
1:B:198:PHE:CE1	1:B:235:ILE:HD11	2.43	0.53
1:B:266:LEU:O	1:B:270:VAL:HG23	2.09	0.53
1:B:11:LEU:HD22	1:B:111:VAL:O	2.08	0.53
1:A:153:GLU:HG2	1:A:241:GLU:HG2	1.91	0.53
1:A:151:TRP:CH2	1:A:163:ARG:HB2	2.45	0.53
1:B:268:ALA:O	1:B:272:LYS:HG3	2.09	0.53
1:B:353:GLU:OE1	1:B:356:ARG:HD3	2.08	0.53
1:A:29:LYS:HB2	1:A:29:LYS:HZ2	1.72	0.52
1:B:61:SER:HA	2:B:2010:HOH:O	2.09	0.52
1:A:418:THR:OG1	1:A:419:GLU:N	2.42	0.52
1:B:362:ALA:N	1:B:403:LEU:HD21	2.24	0.52
1:B:189:MSE:O	1:B:191:GLN:HG3	2.10	0.52
1:A:126:GLU:HB3	1:A:289:GLN:HE22	1.75	0.52
1:B:60:ALA:O	1:B:62:VAL:HG13	2.10	0.52
1:B:198:PHE:HE1	1:B:235:ILE:HD11	1.75	0.52
1:A:13:ARG:HG3	1:A:13:ARG:NH1	2.19	0.52
1:B:57:ARG:HG3	1:B:57:ARG:O	2.10	0.52
1:B:363:ASP:N	1:B:406:GLN:HE22	2.02	0.52
1:B:24:ILE:O	1:B:27:ALA:HB3	2.09	0.52
1:B:302:VAL:HG22	1:B:342:LYS:HE3	1.91	0.52
1:A:31:GLU:HG3	1:A:62:VAL:HG22	1.92	0.52
1:A:62:VAL:HG13	1:A:66:VAL:HG23	1.92	0.52
1:B:254:LYS:HZ1	1:B:255:ARG:NH1	2.08	0.52
1:A:300:ILE:HG13	1:A:301:ASP:N	2.25	0.52
1:B:3:VAL:HG12	1:B:4:SER:H	1.75	0.51
1:B:143:THR:O	1:B:147:GLN:HG2	2.09	0.51
1:A:253:ILE:HG13	1:A:266:LEU:HB2	1.92	0.51
1:A:429:ASN:HA	1:A:431:GLN:NE2	2.26	0.51
1:B:3:VAL:HG12	1:B:4:SER:N	2.25	0.51
1:A:141:LEU:HD11	1:A:267:ARG:HG2	1.92	0.51
1:A:166:ILE:HD13	1:A:235:ILE:CG2	2.41	0.51
1:A:224:GLU:HA	1:A:227:LYS:HD2	1.92	0.51
1:B:53:ILE:C	1:B:55:ALA:H	2.18	0.51
1:B:215:VAL:HG12	1:B:216:THR:N	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:VAL:O	1:B:349:LEU:HD13	2.10	0.51
1:A:253:ILE:HD13	1:A:261:GLY:O	2.10	0.51
1:B:39:VAL:HG22	1:B:41:ILE:HG12	1.93	0.51
1:B:327:LYS:O	1:B:331:GLU:HG2	2.10	0.51
1:A:149:ALA:HA	1:A:246:PRO:HD3	1.93	0.51
1:B:253:ILE:O	1:B:254:LYS:C	2.53	0.51
1:B:325:ASN:CG	1:B:328:GLN:HG2	2.36	0.51
1:B:120:LEU:O	1:B:122:ALA:N	2.44	0.51
1:B:158:VAL:HG22	1:B:240:VAL:HG11	1.93	0.51
1:A:157:ALA:O	1:A:159:GLU:N	2.45	0.50
1:A:259:GLU:CD	1:A:259:GLU:H	2.20	0.50
1:A:165:THR:HA	1:A:185:PHE:O	2.11	0.50
1:A:167:ASP:HB2	1:A:236:ASN:CB	2.40	0.50
1:B:76:ILE:O	1:B:79:ILE:CG1	2.59	0.50
1:A:29:LYS:HG3	1:A:51:MSE:HG3	1.93	0.50
1:A:425:ASN:H	1:A:425:ASN:ND2	2.07	0.50
1:B:120:LEU:C	1:B:122:ALA:N	2.62	0.50
1:B:224:GLU:O	1:B:226:LEU:N	2.45	0.50
1:B:172:VAL:HG23	1:B:177:PHE:CE2	2.46	0.50
1:B:374:MSE:HE2	1:B:398:MSE:SE	2.61	0.50
1:A:167:ASP:OD1	1:A:184:ASP:N	2.35	0.50
1:B:254:LYS:CG	1:B:255:ARG:H	2.23	0.50
1:A:221:TYR:O	1:A:227:LYS:HE3	2.12	0.49
1:A:202:ILE:O	1:A:202:ILE:HG22	2.12	0.49
1:A:246:PRO:O	1:A:247:GLU:O	2.30	0.49
1:A:294:LEU:HD22	1:A:350:LEU:HD13	1.93	0.49
1:A:152:LYS:HG2	1:A:153:GLU:N	2.20	0.49
1:B:302:VAL:CG2	1:B:307:ILE:HD11	2.43	0.49
1:A:319:ALA:HB2	1:A:329:ALA:HB2	1.95	0.49
1:B:62:VAL:HG23	1:B:63:ARG:N	2.28	0.49
1:B:172:VAL:CG1	1:B:229:LYS:HD3	2.42	0.49
1:B:258:VAL:C	1:B:260:ASP:H	2.21	0.49
1:A:1:MSE:HE3	1:A:3:VAL:CG1	2.42	0.49
1:B:25:GLU:HG2	2:B:2005:HOH:O	2.13	0.49
1:A:374:MSE:HE1	1:A:388:TYR:CE1	2.48	0.49
1:A:73:ARG:HB3	1:A:73:ARG:NH1	2.26	0.48
1:A:117:LEU:HG	1:A:353:GLU:HG2	1.94	0.48
1:A:249:THR:O	1:A:253:ILE:HG22	2.12	0.48
1:B:285:ARG:HD2	1:B:285:ARG:O	2.13	0.48
1:A:322:PHE:CG	1:A:322:PHE:O	2.65	0.48
1:B:20:ALA:O	1:B:24:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:VAL:C	1:B:56:GLN:N	2.70	0.48
1:A:170:GLY:HA3	1:A:177:PHE:CZ	2.49	0.48
1:A:272:LYS:CE	1:A:276:ARG:NH2	2.77	0.48
1:A:328:GLN:O	1:A:331:GLU:HB3	2.13	0.48
1:B:170:GLY:N	1:B:180:GLY:O	2.45	0.48
1:A:39:VAL:O	1:A:39:VAL:HG12	2.12	0.48
1:A:146:LYS:CE	1:A:243:ARG:HH11	2.26	0.48
1:B:76:ILE:HG22	1:B:80:ILE:HD12	1.96	0.48
1:A:115:VAL:HG12	1:A:353:GLU:HG2	1.96	0.48
1:B:31:GLU:HA	1:B:31:GLU:OE1	2.12	0.48
1:B:39:VAL:HB	1:B:46:LYS:HZ3	1.78	0.48
1:B:313:VAL:O	1:B:317:GLN:HG3	2.14	0.48
1:A:52:ASN:OD1	1:A:53:ILE:HG13	2.14	0.48
1:B:133:THR:CG2	1:B:135:ALA:H	2.12	0.48
1:B:428:MSE:O	1:B:430:GLN:N	2.44	0.48
1:B:35:VAL:C	1:B:37:LYS:H	2.22	0.47
1:A:169:THR:OG1	1:A:234:ALA:HB3	2.13	0.47
1:B:253:ILE:CD1	1:B:266:LEU:HD12	2.43	0.47
1:B:75:PHE:O	1:B:76:ILE:C	2.57	0.47
1:B:363:ASP:H	1:B:406:GLN:NE2	2.04	0.47
1:A:243:ARG:O	1:A:243:ARG:HG3	2.13	0.47
1:B:41:ILE:C	1:B:43:GLY:N	2.63	0.47
1:B:261:GLY:O	1:B:262:SER:C	2.57	0.47
1:A:428:MSE:HE3	1:A:428:MSE:HA	1.97	0.47
1:B:52:ASN:O	1:B:53:ILE:HG12	2.14	0.47
1:B:253:ILE:HG22	1:B:258:VAL:HB	1.97	0.47
1:A:272:LYS:NZ	1:A:276:ARG:NH2	2.63	0.47
1:B:388:TYR:CD2	1:B:394:LEU:HB3	2.50	0.47
1:A:155:ASP:HA	1:A:207:ALA:HB2	1.97	0.47
1:B:51:MSE:C	1:B:53:ILE:H	2.23	0.47
1:A:168:PHE:CE1	1:A:182:ALA:HB2	2.50	0.47
1:A:333:PRO:HG2	1:A:336:LEU:HG	1.96	0.47
1:B:398:MSE:HE3	1:B:398:MSE:HA	1.97	0.47
1:A:341:ALA:O	1:A:345:VAL:HG23	2.15	0.47
1:B:58:TYR:C	1:B:60:ALA:H	2.22	0.46
1:A:32:LEU:CD1	1:A:55:ALA:HA	2.44	0.46
1:B:380:ASP:O	1:B:381:PRO:C	2.58	0.46
1:A:117:LEU:HG	1:A:353:GLU:CG	2.45	0.46
1:B:110:GLU:HB3	1:B:303:PRO:HB3	1.96	0.46
1:B:327:LYS:C	1:B:329:ALA:N	2.74	0.46
1:A:41:ILE:O	1:A:41:ILE:CG2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:VAL:HG23	1:B:51:MSE:SE	2.66	0.46
1:B:388:TYR:C	1:B:395:MSE:HE2	2.41	0.46
1:A:123:ILE:HG23	1:A:293:GLY:HA3	1.98	0.46
1:A:31:GLU:OE1	1:A:31:GLU:HA	2.15	0.46
1:B:254:LYS:O	1:B:256:PHE:N	2.49	0.46
1:B:355:ILE:CD1	1:B:403:LEU:HB3	2.46	0.46
1:A:391:ASN:OD1	1:A:393:GLU:HB3	2.16	0.46
1:B:19:ILE:HD13	1:B:70:LEU:HB3	1.97	0.46
1:A:195:ILE:HG23	1:A:218:PRO:HD3	1.98	0.45
1:A:380:ASP:OD2	1:A:383:GLU:HB3	2.15	0.45
1:A:429:ASN:HB3	1:A:431:GLN:OE1	2.16	0.45
1:B:168:PHE:CD1	1:B:168:PHE:C	2.94	0.45
1:B:319:ALA:C	1:B:321:ARG:H	2.24	0.45
1:A:321:ARG:C	1:A:323:GLY:H	2.24	0.45
1:A:168:PHE:CZ	1:A:182:ALA:HB2	2.52	0.45
1:B:254:LYS:CG	1:B:255:ARG:N	2.79	0.45
1:B:52:ASN:O	1:B:53:ILE:HB	2.17	0.45
1:B:105:TYR:N	1:B:105:TYR:CD2	2.85	0.45
1:B:133:THR:CG2	1:B:134:ASP:N	2.79	0.45
1:A:205:HIS:CE1	1:A:211:PHE:HB3	2.52	0.45
1:B:412:LEU:C	1:B:414:LYS:H	2.25	0.45
1:A:244:GLU:O	1:A:246:PRO:HD3	2.16	0.45
1:A:427:LEU:C	1:A:429:ASN:H	2.24	0.45
1:A:272:LYS:HE3	1:A:272:LYS:HB2	1.68	0.45
1:A:415:ALA:O	1:A:417:VAL:HG23	2.17	0.45
1:B:223:ALA:O	1:B:227:LYS:HB2	2.16	0.45
1:A:12:GLY:O	1:A:13:ARG:HG3	2.16	0.45
1:B:40:ARG:C	1:B:42:ASP:N	2.75	0.45
1:B:371:ILE:CD1	1:B:395:MSE:HE1	2.45	0.45
1:A:121:GLU:HA	1:A:414:LYS:O	2.17	0.45
1:A:253:ILE:HG23	1:A:261:GLY:HA2	1.98	0.45
1:A:151:TRP:CZ2	1:A:163:ARG:HB2	2.52	0.44
1:A:158:VAL:HG21	1:A:237:LEU:HD21	1.97	0.44
1:A:206:LYS:H	1:A:209:GLU:HG2	1.82	0.44
1:B:84:ILE:HG22	1:B:86:PRO:HD3	1.99	0.44
1:B:388:TYR:CE2	1:B:394:LEU:HB3	2.52	0.44
1:A:121:GLU:H	1:A:121:GLU:CD	2.25	0.44
1:B:138:ASP:CG	1:B:267:ARG:HH22	2.25	0.44
1:B:404:GLU:HG3	1:B:405:GLU:H	1.82	0.44
1:A:128:PRO:CG	1:A:427:LEU:HD21	2.47	0.44
1:B:216:THR:HA	1:B:230:ALA:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:PHE:O	1:B:388:TYR:C	2.59	0.44
1:A:29:LYS:NZ	1:A:29:LYS:CB	2.80	0.44
1:A:272:LYS:HG3	1:A:273:ASN:N	2.32	0.44
1:B:52:ASN:O	1:B:53:ILE:CB	2.65	0.44
1:B:328:GLN:HA	1:B:331:GLU:HG3	2.00	0.44
1:A:86:PRO:HB3	1:A:109:PHE:CD1	2.52	0.44
1:A:178:GLU:O	1:A:181:LYS:HE3	2.17	0.44
1:A:272:LYS:HZ3	1:A:276:ARG:HH22	1.65	0.44
1:A:319:ALA:HA	1:A:322:PHE:HB3	2.00	0.44
1:B:40:ARG:C	1:B:42:ASP:H	2.22	0.44
1:B:138:ASP:OD1	1:B:267:ARG:NH2	2.51	0.44
1:B:160:ALA:O	1:B:162:ASP:N	2.51	0.44
1:B:375:ALA:C	1:B:377:ALA:H	2.24	0.44
1:B:367:VAL:HA	1:B:370:LEU:HD12	2.00	0.44
1:B:245:LEU:HA	1:B:246:PRO:HD3	1.81	0.44
1:B:381:PRO:O	1:B:385:ILE:HG13	2.16	0.44
1:A:17:ILE:O	1:A:104:THR:HG23	2.17	0.44
1:A:357:THR:C	1:A:358:ASN:HD22	2.26	0.44
1:B:19:ILE:HG22	1:B:20:ALA:N	2.33	0.44
1:A:198:PHE:CD1	1:A:198:PHE:C	2.96	0.44
1:B:252:PHE:O	1:B:253:ILE:C	2.59	0.43
1:A:325:ASN:CG	1:A:328:GLN:HG3	2.42	0.43
1:A:253:ILE:HD13	1:A:261:GLY:C	2.44	0.43
1:B:314:LEU:HD21	1:B:340:GLN:NE2	2.33	0.43
1:A:195:ILE:HD11	1:A:221:TYR:CE1	2.50	0.43
1:B:41:ILE:O	1:B:43:GLY:N	2.47	0.43
1:B:392:LYS:HZ2	1:B:393:GLU:HG3	1.83	0.43
1:B:224:GLU:C	1:B:226:LEU:N	2.76	0.43
1:B:254:LYS:HE3	1:B:255:ARG:NH1	2.33	0.43
1:A:11:LEU:HG	1:A:111:VAL:O	2.19	0.43
1:A:126:GLU:H	1:A:289:GLN:NE2	2.15	0.43
1:B:32:LEU:O	1:B:33:VAL:C	2.60	0.43
1:B:312:ASP:HB3	1:B:316:ARG:NH1	2.30	0.43
1:B:47:GLY:C	1:B:49:VAL:H	2.25	0.43
1:B:121:GLU:O	1:B:121:GLU:HG2	2.18	0.43
1:B:137:VAL:CG1	1:B:267:ARG:HG3	2.48	0.43
1:B:167:ASP:HB2	1:B:236:ASN:HB2	2.01	0.43
1:B:332:LEU:N	1:B:332:LEU:HD12	2.33	0.43
1:B:32:LEU:O	1:B:35:VAL:HB	2.18	0.43
1:B:49:VAL:HG11	1:B:54:VAL:CG1	2.46	0.43
1:B:79:ILE:HG13	1:B:80:ILE:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HG	1:B:353:GLU:CG	2.48	0.43
1:B:371:ILE:HD11	1:B:395:MSE:SE	2.69	0.43
1:B:117:LEU:HG	1:B:353:GLU:HG3	2.01	0.42
1:B:370:LEU:O	1:B:371:ILE:C	2.63	0.42
1:A:272:LYS:NZ	1:A:276:ARG:HH22	2.17	0.42
1:B:53:ILE:CG2	1:B:53:ILE:O	2.67	0.42
1:B:72:SER:O	1:B:75:PHE:N	2.50	0.42
1:B:261:GLY:O	1:B:262:SER:O	2.36	0.42
1:A:45:ARG:HH11	1:A:45:ARG:CG	2.28	0.42
1:A:110:GLU:OE1	1:A:304:ALA:N	2.46	0.42
1:A:258:VAL:O	1:A:259:GLU:C	2.62	0.42
1:A:325:ASN:O	1:A:326:GLU:C	2.63	0.42
1:B:4:SER:HB3	1:B:16:THR:HB	2.01	0.42
1:B:161:GLU:N	1:B:189:MSE:HB2	2.35	0.42
1:B:262:SER:O	1:B:263:VAL:C	2.63	0.42
1:B:121:GLU:HA	1:B:414:LYS:O	2.19	0.42
1:B:151:TRP:CZ3	1:B:163:ARG:HB2	2.55	0.42
1:A:39:VAL:O	1:A:39:VAL:CG1	2.67	0.42
1:B:255:ARG:HH11	1:B:255:ARG:HG3	1.85	0.42
1:B:399:ARG:O	1:B:402:ALA:HB3	2.20	0.42
1:A:233:PHE:HB3	1:A:235:ILE:HD11	2.01	0.41
1:A:247:GLU:HB3	1:A:252:PHE:HB2	2.02	0.41
1:B:51:MSE:HE3	1:B:53:ILE:HD13	2.02	0.41
1:A:153:GLU:HA	1:A:241:GLU:HA	2.01	0.41
1:A:253:ILE:HD11	1:A:262:SER:O	2.19	0.41
1:B:154:LYS:HZ2	1:B:242:GLU:CD	2.29	0.41
1:B:337:PHE:O	1:B:338:GLU:C	2.61	0.41
1:A:54:VAL:CG2	1:A:55:ALA:N	2.84	0.41
1:A:128:PRO:HG3	1:A:427:LEU:HD21	2.03	0.41
1:A:193:ARG:C	1:A:194:MSE:HE2	2.42	0.41
1:A:319:ALA:O	1:A:322:PHE:N	2.53	0.41
1:A:417:VAL:C	1:A:418:THR:O	2.63	0.41
1:B:82:GLU:OE1	1:B:82:GLU:N	2.54	0.41
1:B:187:LEU:HD12	1:B:188:ALA:N	2.35	0.41
1:A:344:ARG:HH11	1:A:344:ARG:HG2	1.86	0.41
1:B:54:VAL:O	1:B:56:GLN:N	2.54	0.41
1:B:315:ARG:HA	1:B:318:ALA:HB3	2.03	0.41
1:A:427:LEU:HD12	1:A:427:LEU:N	2.35	0.41
1:B:274:MSE:HE2	1:B:424:PHE:CE2	2.56	0.41
1:B:329:ALA:C	1:B:331:GLU:N	2.79	0.41
1:A:68:GLY:HA2	1:A:71:MSE:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ASP:C	1:A:262:SER:N	2.78	0.41
1:A:329:ALA:C	1:A:331:GLU:N	2.77	0.41
1:B:164:VAL:HG13	1:B:237:LEU:CD1	2.51	0.41
1:B:311:ILE:HD13	1:B:334:ARG:HD3	2.03	0.41
1:A:30:SER:O	1:A:34:ASN:ND2	2.54	0.41
1:A:215:VAL:HG12	1:A:216:THR:N	2.35	0.41
1:B:63:ARG:HB2	1:B:63:ARG:NH1	2.27	0.41
1:B:325:ASN:OD1	1:B:327:LYS:HB2	2.21	0.41
1:A:140:MSE:O	1:A:143:THR:HB	2.21	0.41
1:A:155:ASP:CG	1:A:207:ALA:HB3	2.46	0.41
1:A:304:ALA:O	1:A:305:ALA:C	2.63	0.41
1:A:328:GLN:HE22	1:A:331:GLU:CD	2.29	0.41
1:A:329:ALA:C	1:A:331:GLU:H	2.28	0.41
1:A:368:LYS:CE	2:A:2040:HOH:O	2.66	0.41
1:A:374:MSE:HE1	1:A:388:TYR:CD1	2.56	0.41
1:B:167:ASP:HB2	1:B:236:ASN:CB	2.51	0.41
1:A:413:ALA:C	1:A:415:ALA:H	2.29	0.41
1:B:105:TYR:H	1:B:105:TYR:HD2	1.67	0.41
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.91	0.40
1:A:334:ARG:C	1:A:336:LEU:H	2.29	0.40
1:B:17:ILE:HG22	1:B:18:THR:N	2.35	0.40
1:B:98:LYS:HE3	1:B:101:GLU:OE1	2.21	0.40
1:A:62:VAL:O	1:A:66:VAL:HG23	2.21	0.40
1:A:54:VAL:O	1:A:58:TYR:N	2.50	0.40
1:A:70:LEU:HD23	1:A:70:LEU:HA	1.90	0.40
1:A:212:THR:HA	1:A:233:PHE:O	2.21	0.40
1:B:130:VAL:HG13	1:B:422:THR:O	2.21	0.40
1:B:146:LYS:C	1:B:148:GLN:N	2.77	0.40
1:B:260:ASP:O	1:B:261:GLY:C	2.62	0.40
1:B:375:ALA:C	1:B:377:ALA:N	2.79	0.40
1:B:66:VAL:HG12	1:B:70:LEU:HD22	2.03	0.40
1:B:75:PHE:HZ	1:B:109:PHE:CE2	2.39	0.40
1:B:132:VAL:HG23	1:B:278:LEU:HD23	2.02	0.40
1:B:167:ASP:OD1	1:B:183:SER:HA	2.21	0.40
1:A:179:GLY:O	1:A:181:LYS:HG3	2.21	0.40
1:B:85:ASN:CG	1:B:111:VAL:HG22	2.47	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	430/432 (100%)	368 (86%)	43 (10%)	19 (4%)	2	4
1	B	430/432 (100%)	339 (79%)	62 (14%)	29 (7%)	1	1
All	All	860/864 (100%)	707 (82%)	105 (12%)	48 (6%)	1	2

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	GLY
1	A	247	GLU
1	A	261	GLY
1	B	53	ILE
1	B	54	VAL
1	B	61	SER
1	B	161	GLU
1	B	253	ILE
1	B	254	LYS
1	B	255	ARG
1	B	262	SER
1	B	329	ALA
1	A	158	VAL
1	A	189	MSE
1	B	10	GLY
1	B	41	ILE
1	B	121	GLU
1	B	154	LYS
1	B	225	ASN
1	B	259	GLU
1	B	261	GLY
1	B	389	SER
1	B	413	ALA
1	A	205	HIS
1	A	207	ALA

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Mol	Chain	Res	Type
1	A	414	LYS
1	A	416	LYS
1	B	57	ARG
1	B	155	ASP
1	A	259	GLU
1	A	324	GLY
1	A	392	LYS
1	A	418	THR
1	B	80	ILE
1	B	81	LYS
1	B	160	ALA
1	B	328	GLN
1	B	356	ARG
1	A	157	ALA
1	A	203	LYS
1	A	204	GLY
1	A	359	GLU
1	B	98	LYS
1	A	63	ARG
1	A	246	PRO
1	B	55	ALA
1	B	227	LYS
1	B	218	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/348 (103%)	337 (94%)	22 (6%)	17	40
1	B	359/348 (103%)	336 (94%)	23 (6%)	16	38
All	All	718/696 (103%)	673 (94%)	45 (6%)	16	39

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	25	GLU
1	A	26	THR
1	A	29	LYS
1	A	56	GLN
1	A	62	VAL
1	A	63	ARG
1	A	101	GLU
1	A	130	VAL
1	A	276	ARG
1	A	280	SER
1	A	285	ARG
1	A	294	LEU
1	A	328	GLN
1	A	335	GLU
1	A	336	LEU
1	A	343	ARG
1	A	358	ASN
1	A	361	LYS
1	A	388	TYR
1	A	418	THR
1	A	425	ASN
1	B	6	GLU
1	B	22	ASP
1	B	26	THR
1	B	28	VAL
1	B	63	ARG
1	B	70	LEU
1	B	104	THR
1	B	105	TYR
1	B	111	VAL
1	B	130	VAL
1	B	143	THR
1	B	186	VAL
1	B	194	MSE
1	B	203	LYS
1	B	225	ASN
1	B	256	PHE
1	B	264	GLU
1	B	312	ASP
1	B	374	MSE
1	B	404	GLU
1	B	422	THR

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Mol	Chain	Res	Type
1	B	428	MSE
1	B	430	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	56	GLN
1	A	205	HIS
1	A	236	ASN
1	A	284	ASN
1	A	289	GLN
1	A	328	GLN
1	A	358	ASN
1	A	400	ASN
1	A	425	ASN
1	A	430	GLN
1	B	222	HIS
1	B	289	GLN
1	B	298	ASN
1	B	358	ASN
1	B	397	ASN
1	B	406	GLN
1	B	429	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.