



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:48 AM UTC

PDB ID : 5A3F / pdb_00005a3f
Title : Crystal structure of the dynamin tetramer
Authors : Reubold, T.F.; Faelber, K.; Plattner, N.; Posor, Y.; Branz, K.; Curth, U.; Schlegel, J.; Anand, R.; Manstein, D.J.; Noe, F.; Haucke, V.; Daumke, O.; Eschenburg, S.
Deposited on : 2015-05-29
Resolution : 3.70 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

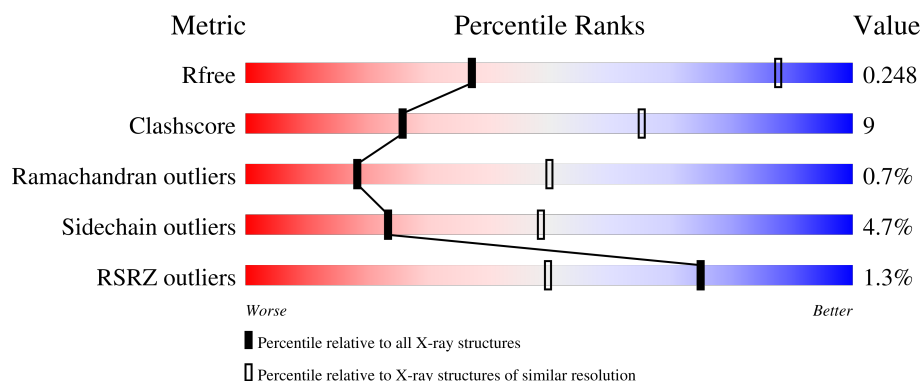
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	754	0.2% 66% 23% 8%
1	B	754	0.2% 64% 9% 26%
1	C	754	0.2% 66% 24% 7%
1	D	754	2% 64% 9% 27%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18654 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 DYNAMIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	0	0
			5548	3520	967	1035	26			
1	B	555	Total	C	N	O	S	0	0	0
			3751	2325	688	724	14			
1	C	700	Total	C	N	O	S	0	0	0
			5616	3557	983	1050	26			
1	D	554	Total	C	N	O	S	0	0	0
			3739	2316	687	722	14			

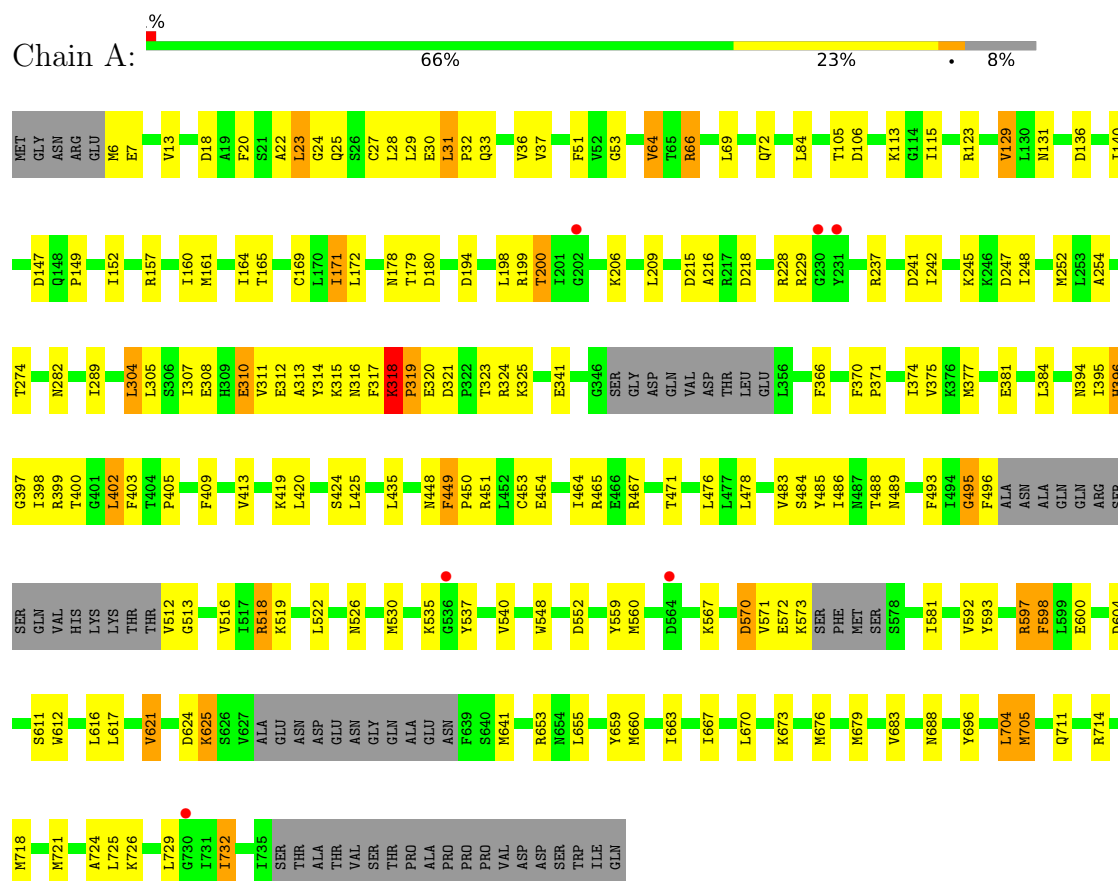
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	361	SER	LYS	engineered mutation	UNP Q9UQ16
B	361	SER	LYS	engineered mutation	UNP Q9UQ16
C	361	SER	LYS	engineered mutation	UNP Q9UQ16
D	361	SER	LYS	engineered mutation	UNP Q9UQ16

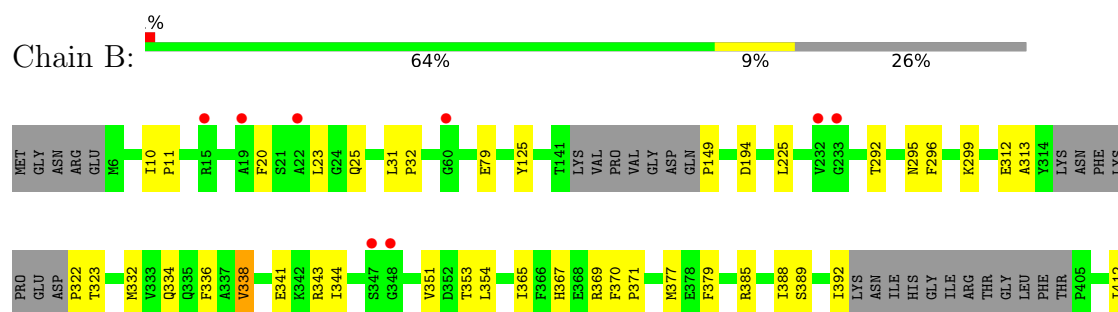
3 Residue-property plots [i](#)

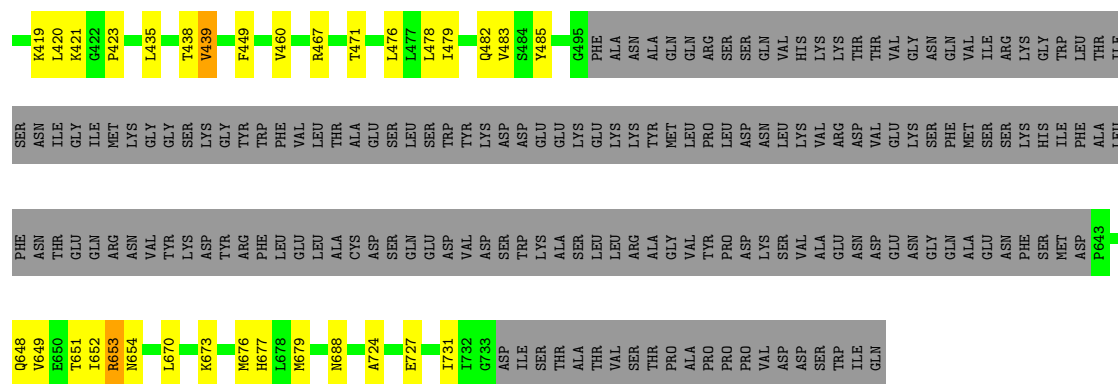
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DYNAMIN 3

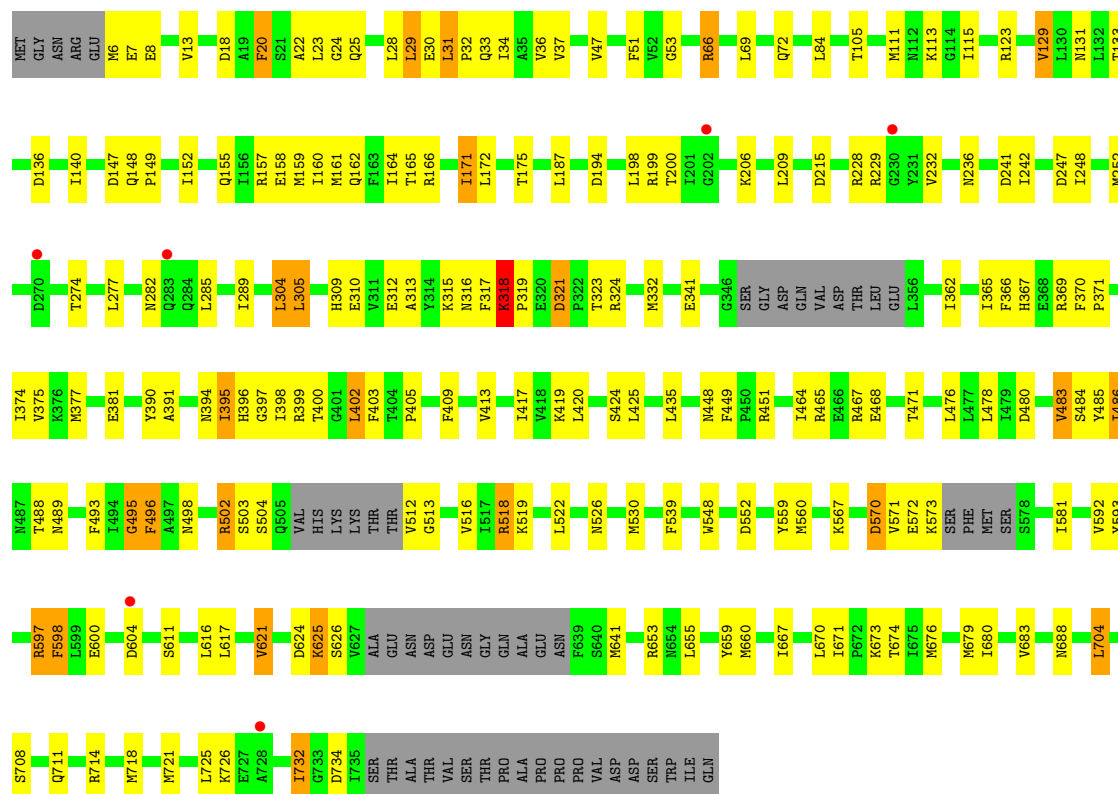


• Molecule 1: DYNAMIN 3

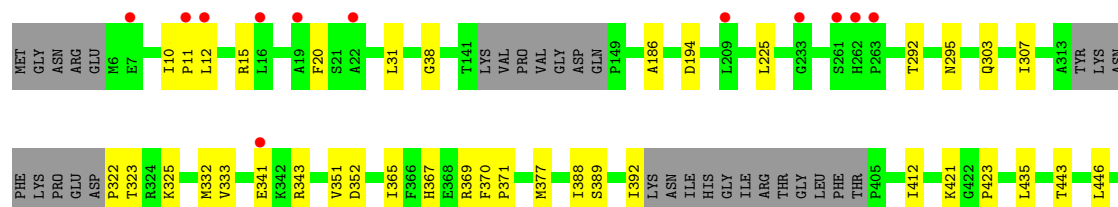


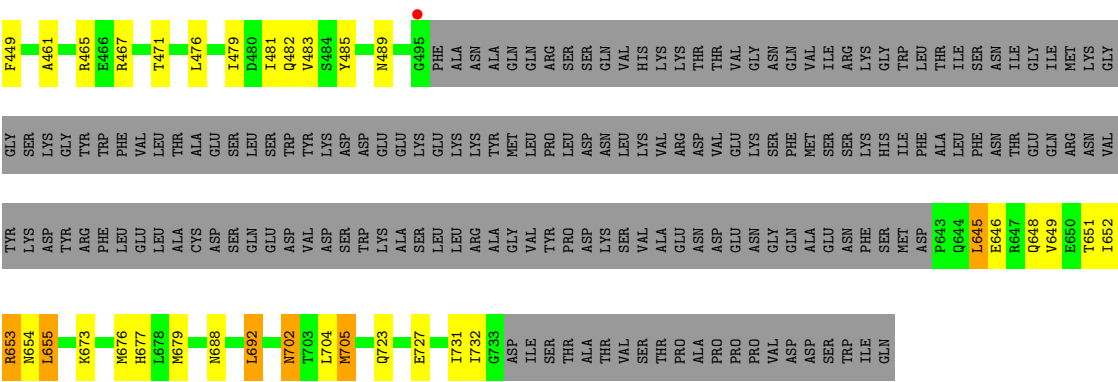


• Molecule 1: DYNAMIN 3



• Molecule 1: DYNAMIN 3





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.70Å 98.00Å 401.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 3.70 49.47 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.47-3.70) 98.8 (49.47-3.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.232 , 0.278 0.238 , 0.248	Depositor DCC
R_{free} test set	2472 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	142.0	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 240.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.368 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18654	wwPDB-VP
Average B, all atoms (Å ²)	211.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/5635	0.82	6/7588 (0.1%)
1	B	0.36	0/3782	0.90	6/5134 (0.1%)
1	C	0.34	0/5703	0.81	7/7679 (0.1%)
1	D	0.36	0/3769	0.89	4/5116 (0.1%)
All	All	0.35	0/18889	0.85	23/25517 (0.1%)

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

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

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	225	LEU	CA-C-N	9.47	131.67	119.84
1	D	225	LEU	C-N-CA	9.47	131.67	119.84
1	B	225	LEU	CA-C-N	9.46	131.67	119.84
1	B	225	LEU	C-N-CA	9.46	131.67	119.84
1	A	27	CYS	N-CA-C	-8.90	103.53	114.75
1	A	318	LYS	CA-C-N	-8.71	108.95	119.84
1	A	318	LYS	C-N-CA	-8.71	108.95	119.84
1	C	318	LYS	CA-C-N	-7.62	110.31	119.84
1	C	318	LYS	C-N-CA	-7.62	110.31	119.84
1	B	194	ASP	CA-C-N	7.55	127.93	119.32
1	B	194	ASP	C-N-CA	7.55	127.93	119.32
1	C	495	GLY	N-CA-C	-6.36	98.10	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	626	SER	N-CA-C	6.32	119.65	110.42
1	D	194	ASP	CA-C-N	6.28	126.47	119.32
1	D	194	ASP	C-N-CA	6.28	126.47	119.32
1	C	449	PHE	CA-C-N	6.18	125.39	118.97
1	C	449	PHE	C-N-CA	6.18	125.39	118.97
1	A	495	GLY	N-CA-C	-5.72	99.62	113.18
1	A	449	PHE	CA-C-N	5.40	124.58	118.97
1	A	449	PHE	C-N-CA	5.40	124.58	118.97
1	B	149	PRO	CA-C-N	5.32	124.83	119.19
1	B	149	PRO	C-N-CA	5.32	124.83	119.19
1	C	498	ASN	CB-CA-C	-5.14	110.23	117.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	625	LYS	Peptide
1	C	625	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5548	0	5670	127	0
1	B	3751	0	3183	48	0
1	C	5616	0	5733	142	0
1	D	3739	0	3174	47	0
All	All	18654	0	17760	344	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 9.

All (344) 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:A:22:ALA:HB2	1:A:84:LEU:HD21	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:ARG:HD2	1:C:704:LEU:HA	1.64	0.80
1:A:23:LEU:O	1:A:25:GLN:N	2.16	0.77
1:C:6:MET:HG3	1:C:7:GLU:H	1.50	0.76
1:A:451:ARG:HD2	1:A:704:LEU:HA	1.68	0.74
1:C:66:ARG:HD3	1:C:113:LYS:HB3	1.70	0.74
1:A:31:LEU:HB2	1:A:32:PRO:HD2	1.70	0.72
1:A:20:PHE:HE2	1:A:28:LEU:HB2	1.55	0.72
1:C:478:LEU:HD21	1:C:670:LEU:HD23	1.72	0.72
1:D:388:ILE:HG21	1:D:652:ILE:HD13	1.72	0.71
1:A:6:MET:HG3	1:A:7:GLU:H	1.54	0.70
1:A:199:ARG:HA	1:A:229:ARG:HE	1.55	0.70
1:B:20:PHE:HD2	1:B:31:LEU:HD21	1.56	0.70
1:C:28:LEU:HD11	1:C:721:MET:SD	2.33	0.69
1:C:31:LEU:HB2	1:C:32:PRO:HD2	1.75	0.68
1:C:18:ASP:OD1	1:C:72:GLN:NE2	2.26	0.67
1:B:478:LEU:HD21	1:B:670:LEU:HD22	1.76	0.67
1:C:199:ARG:HA	1:C:229:ARG:HE	1.59	0.66
1:B:388:ILE:HG21	1:B:652:ILE:HD13	1.77	0.66
1:A:23:LEU:HD12	1:A:724:ALA:HB2	1.77	0.65
1:C:22:ALA:HB2	1:C:84:LEU:HD21	1.78	0.64
1:A:29:LEU:HG	1:A:30:GLU:H	1.63	0.64
1:A:478:LEU:HD21	1:A:670:LEU:HD23	1.79	0.64
1:B:332:MET:HE3	1:B:449:PHE:HE2	1.62	0.64
1:C:66:ARG:HD2	1:C:105:THR:HG21	1.80	0.63
1:A:69:LEU:HB3	1:A:136:ASP:HB3	1.81	0.63
1:C:13:VAL:HG21	1:C:289:ILE:HD13	1.82	0.62
1:C:390:TYR:O	1:C:394:ASN:ND2	2.33	0.61
1:A:66:ARG:NH1	1:A:106:ASP:OD1	2.32	0.61
1:C:332:MET:HE1	1:C:448:ASN:HD21	1.66	0.61
1:C:69:LEU:HB3	1:C:136:ASP:HB3	1.83	0.61
1:B:439:VAL:HG21	1:B:460:VAL:HG11	1.82	0.60
1:C:413:VAL:HG13	1:C:660:MET:HE3	1.82	0.60
1:C:29:LEU:HG	1:C:30:GLU:H	1.66	0.60
1:A:72:GLN:HB2	1:A:123:ARG:HG2	1.84	0.60
1:B:379:PHE:HE1	1:B:419:LYS:HD2	1.66	0.60
1:C:7:GLU:HG3	1:C:8:GLU:HG3	1.84	0.59
1:C:592:VAL:HG12	1:C:598:PHE:HA	1.84	0.59
1:A:312:GLU:HG3	1:A:313:ALA:H	1.67	0.59
1:D:388:ILE:HG12	1:D:412:ILE:HG13	1.83	0.58
1:A:161:MET:O	1:A:165:THR:OG1	2.18	0.58
1:A:413:VAL:HG13	1:A:660:MET:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:MET:O	1:C:165:THR:OG1	2.20	0.58
1:B:299:LYS:HB2	1:C:465:ARG:HH22	1.66	0.58
1:C:252:MET:HE1	1:C:274:THR:HB	1.85	0.58
1:A:13:VAL:HG21	1:A:289:ILE:HD13	1.85	0.58
1:B:421:LYS:HG2	1:B:479:ILE:HG21	1.86	0.58
1:C:312:GLU:HG3	1:C:313:ALA:H	1.68	0.58
1:C:396:HIS:CE1	1:C:405:PRO:HD3	2.38	0.58
1:D:332:MET:HE3	1:D:449:PHE:HE2	1.67	0.58
1:D:341:GLU:OE2	1:D:688:ASN:ND2	2.37	0.58
1:A:198:LEU:HD23	1:A:228:ARG:HG3	1.84	0.58
1:C:29:LEU:HA	1:C:31:LEU:HD23	1.86	0.58
1:A:485:TYR:HB2	1:B:676:MET:HG2	1.86	0.57
1:B:653:ARG:NH1	1:B:654:ASN:OD1	2.36	0.57
1:A:552:ASP:OD1	1:A:552:ASP:N	2.37	0.57
1:A:592:VAL:HG12	1:A:598:PHE:HA	1.86	0.57
1:A:341:GLU:OE2	1:A:688:ASN:ND2	2.33	0.57
1:C:341:GLU:OE2	1:C:688:ASN:ND2	2.31	0.57
1:D:325:LYS:HD3	1:D:702:ASN:HA	1.86	0.57
1:A:304:LEU:HD13	1:A:729:LEU:HD12	1.86	0.56
1:B:353:THR:HG22	1:C:391:ALA:HB2	1.87	0.56
1:C:526:ASN:HB2	1:C:600:GLU:H	1.70	0.56
1:B:652:ILE:HD12	1:B:653:ARG:N	2.21	0.56
1:B:377:MET:HG2	1:B:419:LYS:HE2	1.88	0.56
1:C:659:TYR:OH	1:D:673:LYS:NZ	2.37	0.56
1:C:366:PHE:HE2	1:C:676:MET:HE2	1.70	0.56
1:A:242:ILE:HD12	1:A:242:ILE:H	1.71	0.56
1:A:465:ARG:NH1	1:D:295:ASN:HB2	2.20	0.56
1:D:421:LYS:HG2	1:D:479:ILE:HG21	1.87	0.56
1:A:616:LEU:HB3	1:A:621:VAL:HG13	1.88	0.55
1:C:420:LEU:HD13	1:C:667:ILE:HD13	1.88	0.55
1:C:317:PHE:CD2	1:C:323:THR:HG21	2.41	0.55
1:C:313:ALA:HB3	1:C:315:LYS:HE2	1.88	0.55
1:A:526:ASN:HB2	1:A:600:GLU:H	1.70	0.55
1:C:23:LEU:O	1:C:25:GLN:N	2.40	0.55
1:C:616:LEU:HB3	1:C:621:VAL:HG13	1.89	0.55
1:D:12:LEU:HD11	1:D:732:ILE:HA	1.87	0.55
1:A:420:LEU:HD13	1:A:667:ILE:HD13	1.88	0.55
1:C:242:ILE:HD12	1:C:242:ILE:H	1.72	0.55
1:A:252:MET:HE1	1:A:274:THR:HB	1.88	0.55
1:A:374:ILE:O	1:A:377:MET:HG2	2.07	0.54
1:D:20:PHE:HD2	1:D:31:LEU:HD11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:HB2	1:A:725:LEU:HD13	1.90	0.54
1:C:20:PHE:HB3	1:C:29:LEU:HD13	1.89	0.54
1:A:471:THR:HG21	1:A:679:MET:HE2	1.88	0.54
1:B:379:PHE:CE1	1:B:419:LYS:HD2	2.42	0.54
1:A:313:ALA:HB3	1:A:315:LYS:HE2	1.88	0.54
1:C:36:VAL:HG22	1:C:172:LEU:HD23	1.89	0.54
1:C:374:ILE:O	1:C:377:MET:HG2	2.08	0.54
1:B:295:ASN:HB2	1:C:465:ARG:NH1	2.22	0.54
1:C:381:GLU:OE2	1:C:653:ARG:NE	2.40	0.54
1:D:648:GLN:O	1:D:651:THR:HG22	2.08	0.54
1:A:673:LYS:HG2	1:B:485:TYR:HD2	1.73	0.53
1:A:394:ASN:ND2	1:D:352:ASP:O	2.41	0.53
1:A:375:VAL:HG21	1:A:617:LEU:HD11	1.90	0.53
1:A:704:LEU:HD23	1:A:705:MET:HG2	1.90	0.53
1:C:321:ASP:HB3	1:C:323:THR:HG22	1.91	0.53
1:D:652:ILE:HD12	1:D:653:ARG:N	2.24	0.53
1:A:194:ASP:OD2	1:A:198:LEU:N	2.42	0.52
1:C:370:PHE:HB3	1:C:371:PRO:HD3	1.90	0.52
1:C:471:THR:HG21	1:C:679:MET:HE2	1.91	0.52
1:C:485:TYR:HB2	1:D:676:MET:HG2	1.91	0.52
1:A:370:PHE:HB3	1:A:371:PRO:HD3	1.92	0.52
1:A:714:ARG:O	1:A:718:MET:HG2	2.09	0.52
1:D:377:MET:SD	1:D:423:PRO:HD3	2.51	0.51
1:C:489:ASN:HD22	1:D:367:HIS:CG	2.29	0.51
1:C:567:LYS:HD3	1:C:624:ASP:HB3	1.91	0.51
1:A:559:TYR:HD1	1:A:560:MET:H	1.59	0.51
1:C:502:ARG:HH11	1:C:502:ARG:HB2	1.74	0.51
1:D:292:THR:HA	1:D:295:ASN:OD1	2.11	0.51
1:D:476:LEU:O	1:D:479:ILE:HG22	2.11	0.51
1:C:486:ILE:HG13	1:C:659:TYR:CZ	2.46	0.51
1:B:292:THR:HA	1:B:295:ASN:ND2	2.26	0.51
1:A:366:PHE:HE2	1:A:676:MET:HE2	1.75	0.50
1:D:471:THR:HG21	1:D:679:MET:HE2	1.93	0.50
1:A:178:ASN:OD1	1:A:179:THR:N	2.44	0.50
1:C:20:PHE:CE2	1:C:28:LEU:HB2	2.47	0.50
1:C:552:ASP:OD1	1:C:552:ASP:N	2.38	0.50
1:A:489:ASN:HD22	1:B:367:HIS:CG	2.30	0.50
1:B:341:GLU:OE2	1:B:688:ASN:ND2	2.45	0.50
1:C:131:ASN:O	1:C:282:ASN:ND2	2.33	0.50
1:A:567:LYS:HD3	1:A:624:ASP:HB3	1.92	0.50
1:A:66:ARG:HD3	1:A:113:LYS:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:MET:SD	1:A:641:MET:N	2.84	0.50
1:B:312:GLU:CD	1:B:313:ALA:H	2.20	0.50
1:A:570:ASP:OD1	1:A:570:ASP:N	2.45	0.50
1:C:516:VAL:HG11	1:C:519:LYS:HG3	1.94	0.50
1:A:316:ASN:HA	1:A:324:ARG:HG3	1.94	0.49
1:D:333:VAL:HG21	1:D:692:LEU:HD23	1.93	0.49
1:A:53:GLY:HA2	1:A:248:ILE:HD13	1.94	0.49
1:C:502:ARG:O	1:C:504:SER:N	2.41	0.49
1:A:571:VAL:HB	1:A:581:ILE:HB	1.95	0.49
1:C:485:TYR:CD1	1:D:676:MET:HE3	2.48	0.49
1:C:160:ILE:O	1:C:164:ILE:HG13	2.12	0.49
1:C:673:LYS:HG2	1:D:485:TYR:HD2	1.77	0.49
1:A:28:LEU:HD11	1:A:721:MET:SD	2.53	0.49
1:B:370:PHE:HB3	1:B:371:PRO:HD3	1.94	0.49
1:C:241:ASP:HB3	1:C:247:ASP:HB2	1.94	0.49
1:C:641:MET:SD	1:C:641:MET:N	2.86	0.49
1:C:714:ARG:O	1:C:718:MET:HG2	2.12	0.49
1:A:140:ILE:HG23	1:A:157:ARG:HE	1.77	0.49
1:B:476:LEU:O	1:B:479:ILE:HG22	2.12	0.49
1:A:381:GLU:OE2	1:A:653:ARG:NE	2.46	0.48
1:A:729:LEU:HA	1:A:732:ILE:HG22	1.94	0.48
1:C:29:LEU:HD12	1:C:31:LEU:HD21	1.94	0.48
1:C:198:LEU:HD23	1:C:228:ARG:HG3	1.94	0.48
1:B:334:GLN:O	1:B:338:VAL:HG22	2.13	0.48
1:B:388:ILE:HG21	1:B:652:ILE:CD1	2.43	0.48
1:D:645:LEU:O	1:D:649:VAL:HG13	2.14	0.48
1:A:36:VAL:HG22	1:A:172:LEU:HD23	1.95	0.48
1:A:237:ARG:HH21	1:A:254:ALA:HB1	1.77	0.48
1:D:646:GLU:O	1:D:649:VAL:HG22	2.14	0.48
1:B:471:THR:HG21	1:B:679:MET:HE2	1.96	0.48
1:A:164:ILE:O	1:A:199:ARG:NH2	2.45	0.48
1:A:484:SER:OG	1:B:677:HIS:HB2	2.14	0.48
1:A:18:ASP:OD1	1:A:72:GLN:NE2	2.45	0.48
1:A:370:PHE:HE1	1:A:424:SER:HA	1.76	0.48
1:B:20:PHE:CD2	1:B:31:LEU:HD21	2.44	0.48
1:D:303:GLN:O	1:D:307:ILE:HD13	2.15	0.47
1:A:604:ASP:OD1	1:A:604:ASP:N	2.48	0.47
1:A:149:PRO:HD2	1:A:152:ILE:HB	1.96	0.47
1:A:572:GLU:H	1:A:572:GLU:CD	2.23	0.47
1:C:518:ARG:HH12	1:C:611:SER:HB3	1.80	0.47
1:C:570:ASP:OD1	1:C:570:ASP:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:HD11	1:A:476:LEU:HD21	1.97	0.47
1:C:72:GLN:HB2	1:C:123:ARG:HG2	1.96	0.47
1:A:241:ASP:HB3	1:A:247:ASP:HB2	1.97	0.47
1:A:320:GLU:HB3	1:A:325:LYS:HE2	1.95	0.47
1:A:518:ARG:HH12	1:A:611:SER:HB3	1.80	0.47
1:C:318:LYS:HB2	1:C:321:ASP:OD2	2.14	0.47
1:C:375:VAL:HG21	1:C:617:LEU:HD11	1.97	0.47
1:C:395:ILE:H	1:C:395:ILE:HG12	1.53	0.47
1:D:370:PHE:HB3	1:D:371:PRO:HD3	1.95	0.47
1:B:377:MET:SD	1:B:423:PRO:HD3	2.55	0.47
1:C:47:VAL:HG22	1:C:236:ASN:HD21	1.80	0.47
1:C:248:ILE:O	1:C:252:MET:HG2	2.15	0.46
1:C:420:LEU:HD13	1:C:667:ILE:HG21	1.97	0.46
1:C:516:VAL:HG21	1:C:519:LYS:HE3	1.96	0.46
1:C:53:GLY:HA2	1:C:248:ILE:HD13	1.96	0.46
1:C:304:LEU:HD12	1:C:725:LEU:HD13	1.98	0.46
1:B:727:GLU:O	1:B:731:ILE:HG12	2.15	0.46
1:D:653:ARG:C	1:D:653:ARG:HD3	2.40	0.46
1:A:169:CYS:O	1:A:199:ARG:NH1	2.48	0.46
1:C:316:ASN:HA	1:C:324:ARG:HG3	1.97	0.46
1:A:486:ILE:HG13	1:A:659:TYR:CZ	2.51	0.46
1:C:370:PHE:HE1	1:C:424:SER:HA	1.79	0.46
1:A:402:LEU:HA	1:A:403:PHE:HA	1.65	0.46
1:C:718:MET:HA	1:C:721:MET:HB3	1.98	0.46
1:C:365:ILE:HA	1:C:369:ARG:HB3	1.98	0.46
1:C:559:TYR:HD1	1:C:560:MET:H	1.64	0.46
1:C:425:LEU:HD11	1:C:476:LEU:HD21	1.98	0.45
1:A:396:HIS:CE1	1:A:405:PRO:HD3	2.51	0.45
1:A:448:ASN:H	1:A:448:ASN:HD22	1.64	0.45
1:C:305:LEU:HD12	1:C:309:HIS:NE2	2.32	0.45
1:C:572:GLU:H	1:C:572:GLU:CD	2.24	0.45
1:A:317:PHE:CD2	1:A:323:THR:HG21	2.52	0.45
1:A:485:TYR:CD1	1:B:676:MET:HE3	2.52	0.45
1:B:365:ILE:HA	1:B:369:ARG:HB3	1.97	0.45
1:C:232:VAL:HG11	1:C:277:LEU:HB2	1.98	0.45
1:D:704:LEU:HD12	1:D:705:MET:HG2	1.98	0.45
1:A:659:TYR:OH	1:B:673:LYS:NZ	2.49	0.45
1:C:409:PHE:CE1	1:C:655:LEU:HB3	2.52	0.45
1:C:20:PHE:HE2	1:C:28:LEU:HB2	1.80	0.45
1:A:377:MET:HE1	1:A:419:LYS:O	2.17	0.45
1:C:164:ILE:O	1:C:199:ARG:NH2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:LEU:HA	1:C:403:PHE:HA	1.61	0.45
1:C:548:TRP:CZ2	1:C:559:TYR:HB3	2.52	0.45
1:D:461:ALA:O	1:D:465:ARG:HG2	2.17	0.45
1:A:171:ILE:HD12	1:A:200:THR:HG22	1.99	0.45
1:A:206:LYS:HB3	1:A:209:LEU:HD12	1.98	0.45
1:C:140:ILE:HG23	1:C:157:ARG:HE	1.82	0.45
1:C:366:PHE:HE2	1:C:676:MET:CE	2.30	0.45
1:D:655:LEU:HD12	1:D:655:LEU:HA	1.86	0.45
1:A:488:THR:HG23	1:A:493:PHE:CE2	2.51	0.45
1:C:318:LYS:HB3	1:C:319:PRO:CD	2.48	0.44
1:A:516:VAL:HG11	1:A:519:LYS:HG3	1.99	0.44
1:C:676:MET:HE2	1:C:676:MET:HB2	1.76	0.44
1:D:727:GLU:O	1:D:731:ILE:HG12	2.17	0.44
1:A:488:THR:HG23	1:A:493:PHE:HE2	1.83	0.44
1:C:34:ILE:HG13	1:C:285:LEU:HD13	1.99	0.44
1:D:389:SER:O	1:D:392:ILE:HG12	2.18	0.44
1:A:215:ASP:N	1:A:215:ASP:OD1	2.49	0.44
1:A:310:GLU:HG3	1:A:311:VAL:N	2.32	0.44
1:C:559:TYR:CE2	1:C:593:TYR:HB2	2.53	0.44
1:A:29:LEU:HD12	1:A:31:LEU:HD21	1.99	0.44
1:C:111:MET:O	1:C:113:LYS:HG3	2.18	0.44
1:C:115:ILE:HD11	1:C:155:GLN:HB3	2.00	0.44
1:D:365:ILE:HA	1:D:369:ARG:HB3	1.98	0.44
1:A:597:ARG:H	1:A:597:ARG:HD3	1.83	0.44
1:B:322:PRO:HB2	1:B:323:THR:H	1.62	0.44
1:C:115:ILE:HD12	1:C:159:MET:HE3	1.99	0.44
1:A:663:ILE:HD13	1:A:663:ILE:HA	1.80	0.44
1:C:194:ASP:OD2	1:C:198:LEU:N	2.51	0.44
1:C:465:ARG:NE	1:C:468:GLU:OE1	2.51	0.44
1:D:322:PRO:HB2	1:D:323:THR:H	1.63	0.44
1:A:597:ARG:H	1:A:597:ARG:CD	2.31	0.44
1:A:318:LYS:HB3	1:A:319:PRO:CD	2.47	0.43
1:B:10:ILE:HB	1:B:11:PRO:HD3	2.00	0.43
1:A:307:ILE:HG21	1:A:725:LEU:HD21	2.01	0.43
1:A:409:PHE:CE1	1:A:655:LEU:HB3	2.53	0.43
1:D:653:ARG:HD2	1:D:654:ASN:OD1	2.17	0.43
1:A:131:ASN:O	1:A:282:ASN:ND2	2.35	0.43
1:A:66:ARG:HD2	1:A:105:THR:HG21	2.00	0.43
1:C:484:SER:OG	1:D:677:HIS:HB2	2.17	0.43
1:A:216:ALA:O	1:A:218:ASP:N	2.45	0.43
1:A:241:ASP:OD1	1:A:245:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:TYR:CE2	1:A:593:TYR:HB2	2.54	0.43
1:C:149:PRO:HD2	1:C:152:ILE:HB	2.01	0.43
1:C:215:ASP:OD1	1:C:215:ASP:N	2.49	0.43
1:C:571:VAL:HB	1:C:581:ILE:HB	2.01	0.43
1:A:495:GLY:O	1:A:496:PHE:HB2	2.19	0.43
1:A:304:LEU:HD12	1:A:725:LEU:HD13	2.01	0.43
1:B:388:ILE:HG12	1:B:412:ILE:HG13	2.01	0.43
1:C:377:MET:HE1	1:C:419:LYS:O	2.19	0.43
1:C:413:VAL:HG11	1:C:486:ILE:HD12	2.00	0.43
1:A:512:VAL:HG13	1:A:513:GLY:H	1.84	0.43
1:A:449:PHE:HA	1:A:450:PRO:HD2	1.89	0.42
1:A:725:LEU:HD12	1:A:726:LYS:N	2.34	0.42
1:B:679:MET:HE2	1:B:679:MET:HB2	1.83	0.42
1:C:488:THR:HG23	1:C:493:PHE:CE2	2.54	0.42
1:A:679:MET:HE2	1:A:679:MET:HB2	1.90	0.42
1:C:158:GLU:O	1:C:162:GLN:HG3	2.18	0.42
1:A:512:VAL:HG22	1:A:513:GLY:H	1.84	0.42
1:C:30:GLU:OE2	1:C:166:ARG:HG2	2.19	0.42
1:C:362:ILE:HD13	1:C:680:ILE:HD13	2.00	0.42
1:C:467:ARG:O	1:C:471:THR:HG22	2.19	0.42
1:A:64:VAL:O	1:A:66:ARG:NE	2.51	0.42
1:C:51:PHE:O	1:C:129:VAL:HG12	2.19	0.42
1:C:367:HIS:CD2	1:D:489:ASN:HB2	2.54	0.42
1:D:443:THR:HA	1:D:446:LEU:HD13	2.01	0.42
1:B:295:ASN:OD1	1:B:296:PHE:N	2.52	0.42
1:A:248:ILE:O	1:A:252:MET:HG2	2.18	0.42
1:A:573:LYS:H	1:A:573:LYS:HG2	1.63	0.42
1:A:718:MET:HA	1:A:721:MET:HB3	2.01	0.42
1:C:512:VAL:HG13	1:C:513:GLY:H	1.85	0.42
1:A:37:VAL:HG21	1:A:164:ILE:HD11	2.01	0.42
1:A:51:PHE:HE1	1:A:274:THR:HG23	1.83	0.42
1:C:512:VAL:HG22	1:C:513:GLY:H	1.85	0.42
1:A:20:PHE:CE2	1:A:28:LEU:HB2	2.42	0.42
1:A:51:PHE:CE1	1:A:274:THR:HG23	2.55	0.42
1:A:160:ILE:O	1:A:164:ILE:HG13	2.19	0.42
1:A:467:ARG:O	1:A:471:THR:HG22	2.19	0.42
1:A:317:PHE:N	1:A:317:PHE:CD1	2.88	0.42
1:A:512:VAL:HG22	1:A:513:GLY:N	2.35	0.42
1:A:535:LYS:HB3	1:A:537:TYR:CE1	2.55	0.42
1:C:480:ASP:O	1:C:483:VAL:HG22	2.19	0.42
1:D:332:MET:HE3	1:D:449:PHE:CE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:GLU:HA	1:A:384:LEU:HB3	2.02	0.42
1:C:464:ILE:HD13	1:C:683:VAL:HG21	2.01	0.42
1:B:385:ARG:HH21	1:B:653:ARG:NH2	2.18	0.41
1:A:464:ILE:HD13	1:A:683:VAL:HG21	2.02	0.41
1:C:495:GLY:O	1:C:496:PHE:HB2	2.19	0.41
1:A:660:MET:HE2	1:A:660:MET:HA	2.02	0.41
1:B:648:GLN:O	1:B:651:THR:HG22	2.20	0.41
1:C:72:GLN:HG2	1:C:133:THR:HG23	2.02	0.41
1:A:522:LEU:HD21	1:A:612:TRP:NE1	2.36	0.41
1:A:548:TRP:CZ2	1:A:559:TYR:HB3	2.55	0.41
1:C:23:LEU:C	1:C:25:GLN:H	2.28	0.41
1:C:493:PHE:CE1	1:C:659:TYR:HB2	2.56	0.41
1:C:604:ASP:OD1	1:C:604:ASP:N	2.47	0.41
1:C:659:TYR:HH	1:D:673:LYS:HZ1	1.62	0.41
1:C:671:ILE:HD13	1:C:671:ILE:HA	1.86	0.41
1:D:723:GLN:O	1:D:727:GLU:HG2	2.20	0.41
1:A:51:PHE:O	1:A:129:VAL:HG12	2.21	0.41
1:B:79:GLU:HA	1:B:125:TYR:O	2.21	0.41
1:D:467:ARG:HD2	1:D:467:ARG:HA	1.86	0.41
1:B:332:MET:HE3	1:B:449:PHE:CE2	2.50	0.41
1:B:478:LEU:CD2	1:B:670:LEU:HD22	2.47	0.41
1:C:18:ASP:OD2	1:C:123:ARG:HD2	2.21	0.41
1:C:305:LEU:HD13	1:C:305:LEU:HA	1.89	0.41
1:C:417:ILE:CG1	1:C:660:MET:HE1	2.50	0.41
1:A:453:CYS:SG	1:A:454:GLU:N	2.93	0.41
1:C:573:LYS:H	1:C:573:LYS:HG2	1.64	0.41
1:D:10:ILE:HB	1:D:11:PRO:HD3	2.03	0.41
1:A:180:ASP:OD1	1:A:180:ASP:N	2.54	0.41
1:C:573:LYS:HB3	1:C:573:LYS:HE3	1.80	0.41
1:C:674:THR:HA	1:D:481:ILE:HD13	2.02	0.41
1:D:471:THR:HG21	1:D:679:MET:CE	2.51	0.41
1:A:519:LYS:HG2	1:A:540:VAL:HG22	2.02	0.41
1:B:676:MET:HE2	1:B:676:MET:HB2	1.88	0.41
1:C:402:LEU:HB2	1:C:403:PHE:CD1	2.55	0.41
1:C:679:MET:HE2	1:C:679:MET:HB2	1.89	0.41
1:C:725:LEU:HD12	1:C:726:LYS:N	2.35	0.41
1:A:402:LEU:HB2	1:A:403:PHE:CD1	2.56	0.41
1:B:389:SER:O	1:B:392:ILE:HG12	2.21	0.41
1:B:467:ARG:O	1:B:471:THR:HG22	2.21	0.41
1:C:175:THR:HG21	1:C:187:LEU:HD23	2.02	0.41
1:C:317:PHE:CD1	1:C:317:PHE:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:PHE:CE1	1:C:424:SER:HA	2.55	0.41
1:C:488:THR:HG23	1:C:493:PHE:HE2	1.86	0.41
1:C:597:ARG:H	1:C:597:ARG:HD3	1.85	0.41
1:D:38:GLY:HA2	1:D:186:ALA:HB2	2.03	0.41
1:C:660:MET:HA	1:C:660:MET:HE2	2.03	0.40
1:A:676:MET:HE2	1:A:676:MET:HB2	1.76	0.40
1:B:344:ILE:HD11	1:B:438:THR:HG21	2.02	0.40
1:C:37:VAL:HG21	1:C:164:ILE:HD11	2.04	0.40
1:D:12:LEU:HA	1:D:15:ARG:HE	1.86	0.40
1:C:171:ILE:HD12	1:C:200:THR:OG1	2.20	0.40
1:C:522:LEU:HB2	1:C:539:PHE:CD1	2.56	0.40
1:B:23:LEU:HD13	1:B:724:ALA:HB1	2.04	0.40
1:C:148:GLN:HG3	1:C:149:PRO:HA	2.03	0.40
1:B:336:PHE:HZ	1:B:439:VAL:HG22	1.86	0.40
1:C:206:LYS:HB3	1:C:209:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	681/754 (90%)	654 (96%)	21 (3%)	6 (1%)	14	45
1	B	545/754 (72%)	528 (97%)	15 (3%)	2 (0%)	30	60
1	C	690/754 (92%)	660 (96%)	22 (3%)	8 (1%)	10	40
1	D	544/754 (72%)	530 (97%)	13 (2%)	1 (0%)	43	72
All	All	2460/3016 (82%)	2372 (96%)	71 (3%)	17 (1%)	18	50

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	A	397	GLY
1	A	398	ILE
1	C	24	GLY
1	C	398	ILE
1	C	496	PHE
1	A	318	LYS
1	B	351	VAL
1	C	29	LEU
1	C	318	LYS
1	D	351	VAL
1	C	732	ILE
1	A	396	HIS
1	C	503	SER
1	C	397	GLY
1	A	319	PRO
1	B	32	PRO

5.3.2 Protein sidechains [i](#)

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	617/671 (92%)	583 (94%)	34 (6%)	19	46
1	B	293/671 (44%)	282 (96%)	11 (4%)	29	53
1	C	624/671 (93%)	593 (95%)	31 (5%)	22	48
1	D	292/671 (44%)	282 (97%)	10 (3%)	32	55
All	All	1826/2684 (68%)	1740 (95%)	86 (5%)	23	48

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	31	LEU
1	A	33	GLN
1	A	64	VAL
1	A	66	ARG

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Mol	Chain	Res	Type
1	A	115	ILE
1	A	129	VAL
1	A	147	ASP
1	A	171	ILE
1	A	200	THR
1	A	304	LEU
1	A	305	LEU
1	A	308	GLU
1	A	310	GLU
1	A	314	TYR
1	A	321	ASP
1	A	395	ILE
1	A	399	ARG
1	A	400	THR
1	A	402	LEU
1	A	435	LEU
1	A	483	VAL
1	A	518	ARG
1	A	530	MET
1	A	570	ASP
1	A	597	ARG
1	A	598	PHE
1	A	621	VAL
1	A	625	LYS
1	A	696	TYR
1	A	704	LEU
1	A	705	MET
1	A	711	GLN
1	A	732	ILE
1	B	25	GLN
1	B	338	VAL
1	B	343	ARG
1	B	354	LEU
1	B	420	LEU
1	B	435	LEU
1	B	439	VAL
1	B	482	GLN
1	B	483	VAL
1	B	649	VAL
1	B	653	ARG
1	C	20	PHE
1	C	31	LEU

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Mol	Chain	Res	Type
1	C	33	GLN
1	C	66	ARG
1	C	129	VAL
1	C	147	ASP
1	C	171	ILE
1	C	304	LEU
1	C	305	LEU
1	C	310	GLU
1	C	321	ASP
1	C	395	ILE
1	C	399	ARG
1	C	400	THR
1	C	402	LEU
1	C	435	LEU
1	C	483	VAL
1	C	486	ILE
1	C	502	ARG
1	C	518	ARG
1	C	530	MET
1	C	570	ASP
1	C	597	ARG
1	C	598	PHE
1	C	621	VAL
1	C	625	LYS
1	C	704	LEU
1	C	708	SER
1	C	711	GLN
1	C	732	ILE
1	C	734	ASP
1	D	343	ARG
1	D	435	LEU
1	D	482	GLN
1	D	483	VAL
1	D	645	LEU
1	D	653	ARG
1	D	655	LEU
1	D	692	LEU
1	D	702	ASN
1	D	705	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	HIS
1	A	474	GLN
1	A	482	GLN
1	A	489	ASN
1	A	591	ASN
1	A	682	ASN
1	B	463	HIS
1	B	474	GLN
1	B	489	ASN
1	B	677	HIS
1	C	40	GLN
1	C	298	ASN
1	C	367	HIS
1	C	416	GLN
1	C	448	ASN
1	C	474	GLN
1	C	489	ASN
1	C	682	ASN
1	C	711	GLN
1	D	298	ASN
1	D	474	GLN
1	D	711	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	691/754 (91%)	-0.59	6 (0%)	81 58	86, 200, 339, 530	0
1	B	555/754 (73%)	-0.53	8 (1%)	73 48	92, 192, 353, 545	253 (45%)
1	C	700/754 (92%)	-0.61	6 (0%)	81 58	87, 201, 333, 458	0
1	D	554/754 (73%)	-0.54	13 (2%)	61 38	93, 189, 327, 464	253 (45%)
All	All	2500/3016 (82%)	-0.57	33 (1%)	75 50	86, 196, 336, 545	506 (20%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	GLY	7.2
1	B	19	ALA	5.6
1	B	60	GLY	5.4
1	A	230	GLY	5.3
1	D	209	LEU	4.9
1	D	19	ALA	4.8
1	D	16	LEU	4.1
1	D	11	PRO	3.8
1	D	22	ALA	3.6
1	C	230	GLY	3.6
1	C	202	GLY	3.5
1	B	232	VAL	3.4
1	D	495	GLY	3.4
1	A	202	GLY	2.9
1	D	261	SER	2.7
1	B	15	ARG	2.6
1	D	12	LEU	2.5
1	C	283	GLN	2.4
1	B	22	ALA	2.4
1	A	730	GLY	2.4
1	C	728	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	341	GLU	2.3
1	A	536	GLY	2.3
1	C	270	ASP	2.3
1	A	231	TYR	2.2
1	D	233	GLY	2.2
1	D	262	HIS	2.2
1	C	604	ASP	2.1
1	D	263	PRO	2.1
1	B	347	SER	2.1
1	A	564	ASP	2.1
1	D	7	GLU	2.1
1	B	348	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.