



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:32 AM UTC

PDB ID : 5OWV / pdb_00005owv
Title : An oligomerised bacterial dynamin pair provides a mechanism for the long-range sensing and tethering of membranes
Authors : Liu, J.W.; Noel, J.K.; Low, H.H.
Deposited on : 2017-09-04
Resolution : 3.72 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

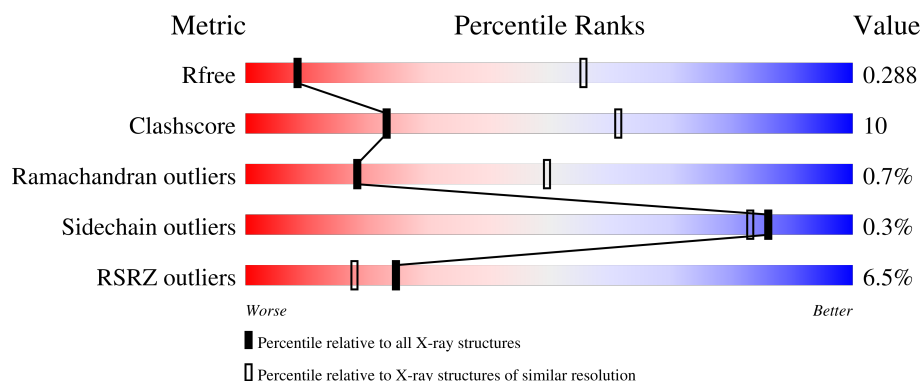
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.72 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	1182 (3.84-3.60)
Clashscore	190562	1222 (3.84-3.60)
Ramachandran outliers	187476	1178 (3.84-3.60)
Sidechain outliers	187428	1174 (3.84-3.60)
RSRZ outliers	180081	1181 (3.84-3.60)

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	732	10% 77% 18% • 5%
1	B	732	5% 64% 15% 20%
2	C	614	4% 75% 22% •
2	D	614	5% 70% 26% ••

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19375 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 GTP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	699	Total	C	N	O	S	0	0	0
			5021	3179	858	970	14			
1	B	587	Total	C	N	O	S	0	0	0
			4436	2828	739	855	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	729	LYS	-	expression tag	UNP A0A1D9BJX7
A	730	LEU	-	expression tag	UNP A0A1D9BJX7
A	731	HIS	-	expression tag	UNP A0A1D9BJX7
A	732	HIS	-	expression tag	UNP A0A1D9BJX7
B	729	LYS	-	expression tag	UNP A0A1D9BJX7
B	730	LEU	-	expression tag	UNP A0A1D9BJX7
B	731	HIS	-	expression tag	UNP A0A1D9BJX7
B	732	HIS	-	expression tag	UNP A0A1D9BJX7

- Molecule 2 is a protein called GTP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	598	Total	C	N	O	S	0	0	0
			4959	3206	799	943	11			
2	D	598	Total	C	N	O	S	0	0	0
			4959	3206	799	943	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0A1D9BKH6
C	-1	SER	-	expression tag	UNP A0A1D9BKH6
C	0	HIS	-	expression tag	UNP A0A1D9BKH6
C	610	HIS	-	expression tag	UNP A0A1D9BKH6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	611	HIS	-	expression tag	UNP A0A1D9BKH6
D	-2	GLY	-	expression tag	UNP A0A1D9BKH6
D	-1	SER	-	expression tag	UNP A0A1D9BKH6
D	0	HIS	-	expression tag	UNP A0A1D9BKH6
D	610	HIS	-	expression tag	UNP A0A1D9BKH6
D	611	HIS	-	expression tag	UNP A0A1D9BKH6

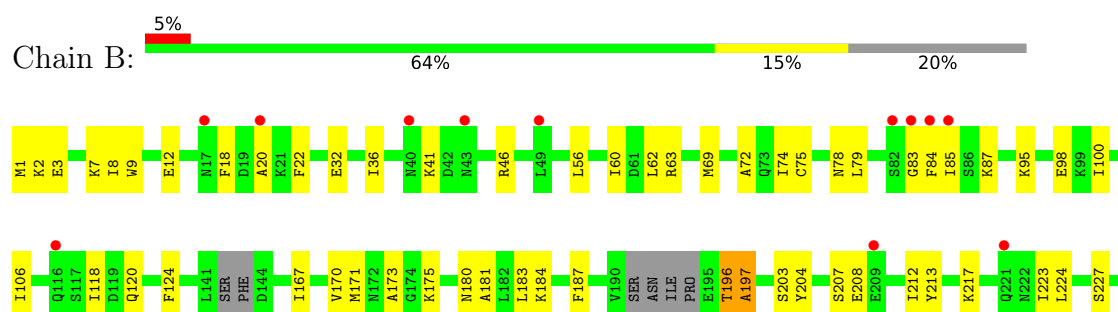
3 Residue-property plots

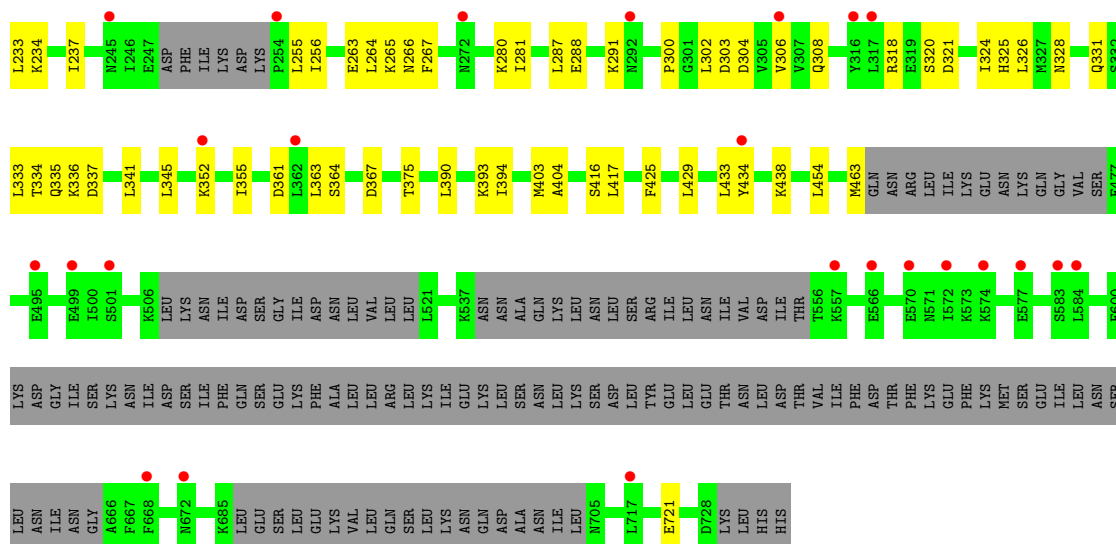
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

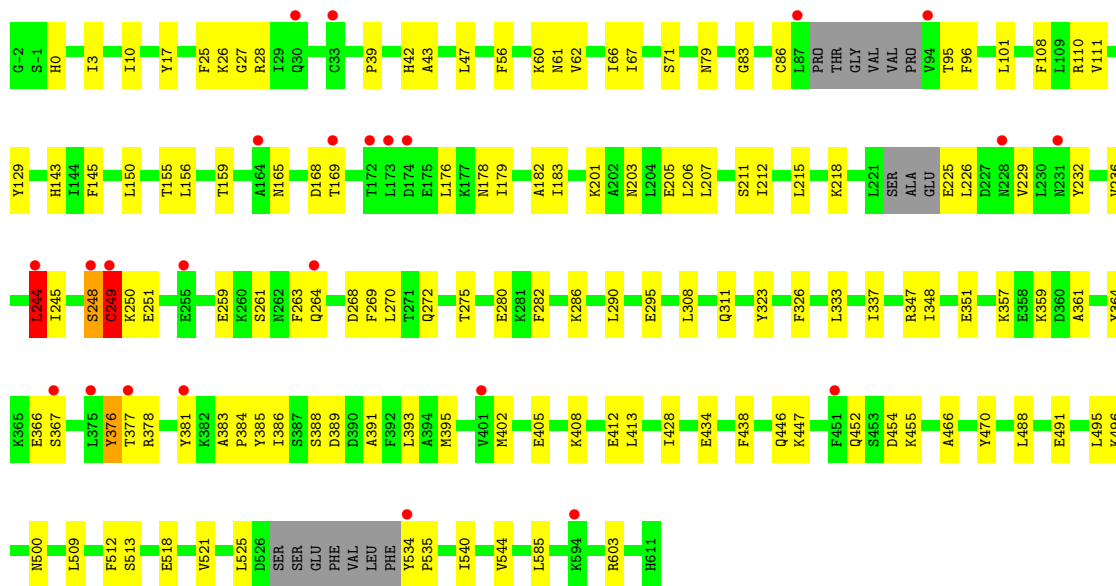
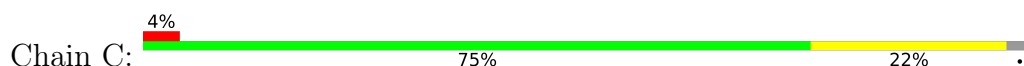


• Molecule 1: GTP-binding protein

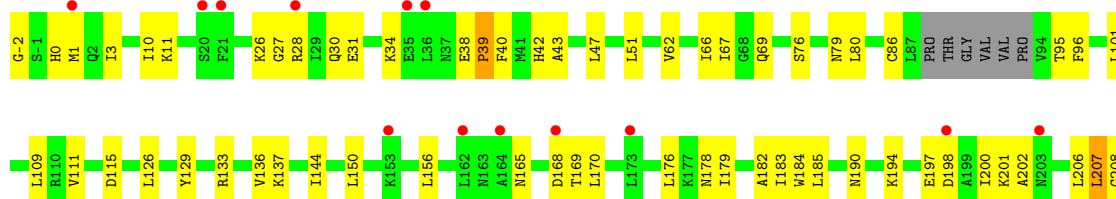


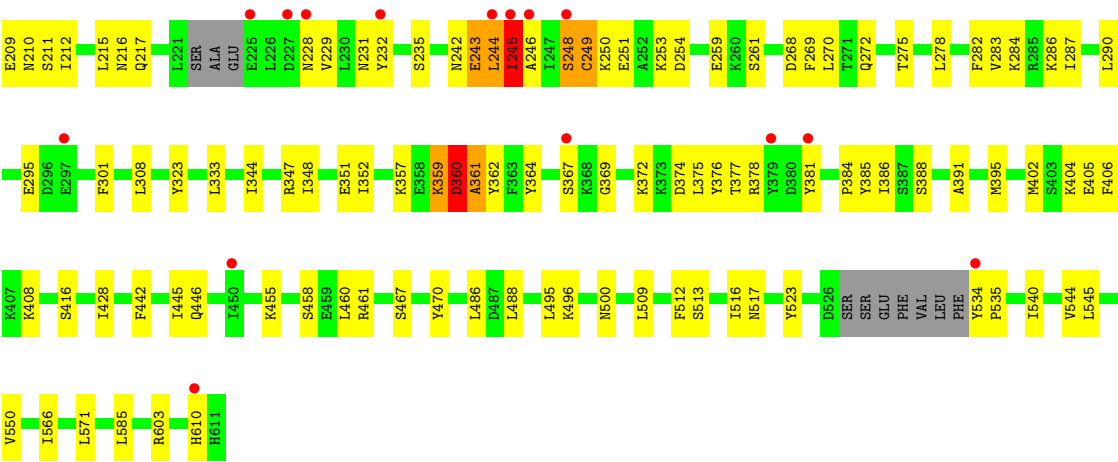


• Molecule 2: GTP-binding protein



• Molecule 2: GTP-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.59Å 226.06Å 317.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.13 – 3.72 106.13 – 3.72	Depositor EDS
% Data completeness (in resolution range)	99.5 (106.13-3.72) 99.5 (106.13-3.72)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.259 , 0.286 0.263 , 0.288	Depositor DCC
R_{free} test set	4195 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	147.9	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 216.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19375	wwPDB-VP
Average B, all atoms (Å ²)	212.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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	0.15	0/5069	0.43	0/6846
1	B	0.15	0/4480	0.43	0/6024
2	C	0.20	0/5044	0.54	1/6771 (0.0%)
2	D	0.20	0/5044	0.57	2/6771 (0.0%)
All	All	0.18	0/19637	0.50	3/26412 (0.0%)

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	3
1	B	0	4
2	C	0	6
2	D	0	5
All	All	0	18

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	245	ILE	N-CA-C	6.80	123.48	109.34
2	C	376	TYR	N-CA-C	6.17	118.14	110.91
2	D	207	LEU	CA-CB-CG	5.47	135.44	116.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	LEU	Peptide
1	A	196	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	255	LEU	Peptide
1	B	196	THR	Peptide
1	B	255	LEU	Peptide
1	B	433	LEU	Peptide
1	B	84	PHE	Peptide
2	C	244	LEU	Peptide
2	C	248	SER	Peptide
2	C	249	CYS	Peptide
2	C	259	GLU	Peptide
2	C	359	LYS	Peptide
2	C	95	THR	Peptide
2	D	248	SER	Peptide
2	D	259	GLU	Peptide
2	D	359	LYS	Peptide
2	D	360	ASP	Peptide
2	D	95	THR	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	5021	0	4509	89	0
1	B	4436	0	4219	77	0
2	C	4959	0	5000	108	0
2	D	4959	0	5000	140	0
All	All	19375	0	18728	392	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 10.

All (392) 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)
2:C:364:TYR:CE1	2:D:364:TYR:CE2	2.00	1.46
2:C:364:TYR:CE1	2:D:364:TYR:CD2	2.22	1.26
2:C:364:TYR:HE1	2:D:364:TYR:CD2	1.59	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:GLU:OE2	1:B:265:LYS:NZ	1.92	1.00
2:D:202:ALA:HB3	2:D:207:LEU:HD22	1.50	0.94
2:C:364:TYR:OH	2:D:364:TYR:O	1.87	0.92
2:C:364:TYR:CE1	2:D:364:TYR:HE2	1.76	0.88
2:D:364:TYR:HB3	2:D:378:ARG:HA	1.56	0.88
2:C:361:ALA:HB1	2:C:381:TYR:HB3	1.57	0.86
1:A:84:PHE:HE2	1:A:118:ILE:HG23	1.41	0.84
2:C:364:TYR:CZ	2:D:364:TYR:CE2	2.65	0.83
1:B:403:MET:HB3	1:B:416:SER:HB2	1.59	0.82
2:C:364:TYR:CZ	2:D:364:TYR:CD2	2.68	0.82
2:C:364:TYR:HB3	2:C:378:ARG:HA	1.61	0.81
2:D:375:LEU:HD12	2:D:376:TYR:H	1.43	0.81
1:A:16:LEU:HD13	1:A:74:ILE:HD11	1.64	0.80
2:C:364:TYR:CD1	2:D:364:TYR:HE2	2.00	0.80
2:C:366:GLU:H	2:C:376:TYR:HD1	1.30	0.79
2:C:364:TYR:CD1	2:D:364:TYR:CE2	2.69	0.78
1:A:183:LEU:HD22	1:A:287:LEU:HD13	1.67	0.77
2:C:182:ALA:HB3	2:C:207:LEU:HD22	1.68	0.76
1:B:20:ALA:HB2	1:B:78:ASN:HB2	1.67	0.76
2:C:364:TYR:HE1	2:D:364:TYR:HD2	1.26	0.75
2:D:243:GLU:OE2	2:D:243:GLU:HA	1.85	0.75
2:C:364:TYR:CB	2:C:378:ARG:HA	2.17	0.74
1:A:100:ILE:HD11	2:D:10:ILE:HA	1.69	0.74
2:C:377:THR:HG22	2:D:374:ASP:HB3	1.69	0.73
2:D:202:ALA:CB	2:D:207:LEU:HD22	2.19	0.72
2:D:364:TYR:CB	2:D:378:ARG:HA	2.19	0.72
1:B:167:ILE:HD11	1:B:326:LEU:HD11	1.73	0.71
2:C:384:PRO:HB3	2:C:534:TYR:CD2	2.26	0.70
1:A:84:PHE:CE2	1:A:118:ILE:HG23	2.27	0.70
1:A:334:THR:O	1:A:337:ASP:N	2.23	0.70
2:D:133:ARG:HB2	2:D:136:VAL:HG22	1.74	0.70
1:B:266:ASN:O	1:B:266:ASN:ND2	2.24	0.69
2:D:115:ASP:OD2	2:D:137:LYS:NZ	2.24	0.69
1:A:288:GLU:HA	1:A:291:LYS:HB3	1.74	0.69
1:A:184:LYS:HE2	1:A:417:LEU:HD11	1.73	0.69
1:B:217:LYS:HD3	1:B:256:ILE:HG23	1.75	0.69
2:D:34:LYS:HG3	2:D:51:LEU:HB3	1.76	0.68
1:A:167:ILE:HD11	1:A:326:LEU:HD11	1.75	0.68
1:B:63:ARG:NH1	2:D:446:GLN:O	2.26	0.68
1:B:22:PHE:CD2	1:B:75:CYS:HB2	2.28	0.68
2:D:295:GLU:OE1	2:D:603:ARG:NH1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:MET:SD	1:A:196:THR:HG21	2.34	0.67
1:B:183:LEU:HD22	1:B:287:LEU:HD13	1.77	0.67
1:A:334:THR:HB	1:A:337:ASP:HB2	1.76	0.67
1:B:318:ARG:O	1:B:320:SER:N	2.26	0.67
2:C:43:ALA:HB1	2:C:47:LEU:HD23	1.75	0.67
2:D:150:LEU:HD11	2:D:270:LEU:HB3	1.75	0.66
2:D:367:SER:N	2:D:375:LEU:HD13	2.10	0.66
2:D:202:ALA:O	2:D:207:LEU:HD23	1.96	0.65
2:D:126:LEU:HD22	2:D:144:ILE:HD11	1.79	0.65
2:C:295:GLU:OE1	2:C:603:ARG:NH1	2.29	0.65
2:D:216:ASN:HD22	2:D:217:GLN:H	1.45	0.64
2:D:534:TYR:HB2	2:D:535:PRO:HD3	1.78	0.64
2:D:216:ASN:HD21	2:D:250:LYS:HB3	1.63	0.64
1:A:310:GLU:OE2	1:A:314:ASN:ND2	2.30	0.64
2:C:229:VAL:HA	2:C:232:TYR:CD2	2.33	0.64
2:C:229:VAL:HA	2:C:232:TYR:HD2	1.62	0.64
2:D:62:VAL:HG21	2:D:275:THR:HB	1.80	0.64
2:C:150:LEU:HD11	2:C:270:LEU:HB3	1.80	0.63
2:D:229:VAL:HA	2:D:232:TYR:HD2	1.63	0.63
1:A:20:ALA:HB2	1:A:78:ASN:HB2	1.81	0.63
2:D:229:VAL:HA	2:D:232:TYR:CD2	2.33	0.63
2:C:491:GLU:HG3	2:D:488:LEU:HD22	1.81	0.63
1:A:197:ALA:HB3	1:A:308:GLN:OE1	1.99	0.63
1:A:220:TRP:CH2	1:A:237:ILE:HD11	2.34	0.63
1:B:223:ILE:HA	1:B:306:VAL:HG21	1.81	0.63
2:D:228:ASN:HA	2:D:231:ASN:ND2	2.13	0.63
2:C:42:HIS:HB3	2:C:455:LYS:HB3	1.81	0.62
1:B:334:THR:O	1:B:337:ASP:N	2.31	0.62
2:D:101:LEU:HB2	2:D:156:LEU:HB2	1.81	0.62
2:C:347:ARG:HG3	2:C:402:MET:HE3	1.81	0.62
2:D:347:ARG:NH2	2:D:405:GLU:OE1	2.33	0.62
2:D:458:SER:HA	2:D:461:ARG:HH11	1.64	0.62
2:D:284:LYS:HE2	2:D:610:HIS:HB2	1.82	0.62
2:D:369:GLY:H	2:D:375:LEU:HD22	1.64	0.62
1:A:454:LEU:HD11	1:A:717:LEU:HB3	1.83	0.61
1:A:62:LEU:HD13	1:A:69:MET:HE1	1.82	0.61
2:D:215:LEU:O	2:D:248:SER:HA	2.00	0.61
1:B:173:ALA:HA	1:B:328:ASN:HB2	1.83	0.60
2:C:178:ASN:HA	2:C:282:PHE:CZ	2.36	0.60
2:C:66:ILE:HD13	2:C:183:ILE:HB	1.83	0.60
1:A:352:LYS:HG2	1:A:393:LYS:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:216:ASN:ND2	2:D:250:LYS:HB3	2.16	0.60
1:B:197:ALA:HB3	1:B:308:GLN:OE1	2.01	0.60
2:C:169:THR:HG21	2:C:201:LYS:HA	1.84	0.60
2:C:67:ILE:HD11	2:C:206:LEU:HD22	1.84	0.60
1:A:223:ILE:HA	1:A:306:VAL:HG21	1.84	0.60
2:C:388:SER:HA	2:C:509:LEU:HG	1.84	0.60
2:C:534:TYR:HB2	2:C:535:PRO:HD3	1.84	0.59
2:C:0:HIS:HA	2:C:3:ILE:HD12	1.85	0.59
2:D:43:ALA:HB1	2:D:47:LEU:HD23	1.84	0.59
2:C:364:TYR:OH	2:D:364:TYR:CD2	2.55	0.59
2:D:375:LEU:CD1	2:D:376:TYR:H	2.16	0.59
2:D:352:ILE:HD12	2:D:509:LEU:HD13	1.85	0.59
2:C:110:ARG:HB3	2:C:143:HIS:HB2	1.86	0.58
2:C:226:LEU:H	2:C:226:LEU:HD23	1.68	0.58
2:C:264:GLN:O	2:C:268:ASP:HB2	2.04	0.58
2:C:218:LYS:HD3	2:C:249:CYS:SG	2.44	0.58
2:D:69:GLN:NE2	2:D:194:LYS:HD2	2.18	0.58
1:B:390:LEU:O	1:B:393:LYS:HB3	2.04	0.57
2:D:202:ALA:CB	2:D:206:LEU:HB3	2.34	0.57
2:D:347:ARG:HG3	2:D:402:MET:HE3	1.86	0.57
1:B:454:LEU:HD21	1:B:721:GLU:HB2	1.86	0.57
1:A:62:LEU:HD21	1:A:72:ALA:HB2	1.85	0.57
2:D:513:SER:O	2:D:517:ASN:ND2	2.35	0.57
2:D:202:ALA:HB2	2:D:206:LEU:HB3	1.87	0.57
2:C:447:LYS:HD2	2:C:452:GLN:HB2	1.85	0.57
1:B:184:LYS:HE2	1:B:417:LEU:HD11	1.87	0.57
2:C:250:LYS:O	2:C:251:GLU:HG3	2.05	0.57
1:A:709:GLU:O	1:A:713:LYS:HG2	2.05	0.57
1:B:100:ILE:HD11	2:C:10:ILE:HA	1.85	0.56
2:D:207:LEU:HD11	2:D:242:ASN:HD21	1.70	0.56
2:C:347:ARG:NH2	2:C:405:GLU:OE1	2.39	0.56
2:C:391:ALA:HB3	2:C:509:LEU:HD21	1.87	0.56
1:A:352:LYS:HA	1:A:393:LYS:HG2	1.86	0.56
1:B:352:LYS:HG2	1:B:393:LYS:O	2.05	0.56
1:A:313:THR:O	1:A:317:LEU:HB3	2.06	0.56
2:D:208:GLY:C	2:D:209:GLU:OE1	2.49	0.56
1:A:16:LEU:HD13	1:A:74:ILE:CD1	2.35	0.56
2:D:361:ALA:CB	2:D:381:TYR:HB3	2.36	0.56
1:B:345:LEU:HD21	1:B:394:ILE:HD11	1.88	0.55
1:B:120:GLN:HB3	1:B:434:TYR:HD2	1.71	0.55
2:D:348:ILE:O	2:D:352:ILE:HG12	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASN:HB3	1:A:331:GLN:HG2	1.86	0.55
2:D:249:CYS:HB2	2:D:261:SER:O	2.06	0.55
1:A:77:LEU:HD21	1:A:106:ILE:HD11	1.87	0.55
2:C:215:LEU:O	2:C:248:SER:HA	2.06	0.55
2:D:0:HIS:HA	2:D:3:ILE:HD12	1.87	0.55
2:C:79:ASN:OD1	2:C:86:CYS:N	2.39	0.55
2:D:244:LEU:HD12	2:D:244:LEU:O	2.07	0.55
1:B:288:GLU:HA	1:B:291:LYS:HB3	1.89	0.54
2:D:386:ILE:HG21	2:D:513:SER:HA	1.89	0.54
2:D:208:GLY:O	2:D:209:GLU:OE1	2.26	0.54
1:A:363:LEU:HD12	1:A:368:LEU:HD13	1.88	0.54
2:D:391:ALA:HB3	2:D:509:LEU:HD21	1.89	0.54
1:A:213:TYR:HB2	1:A:280:LYS:HB3	1.90	0.54
2:C:386:ILE:HG21	2:C:513:SER:HA	1.90	0.53
2:D:333:LEU:HD11	2:D:416:SER:HB3	1.89	0.53
2:D:178:ASN:HA	2:D:282:PHE:CZ	2.43	0.53
2:D:361:ALA:HB3	2:D:381:TYR:HB3	1.89	0.53
1:A:164:ASN:HD22	1:A:320:SER:HA	1.72	0.53
1:B:303:ASP:CG	1:B:304:ASP:H	2.15	0.53
1:B:62:LEU:HD13	1:B:69:MET:HE1	1.89	0.53
1:A:241:ASP:O	1:A:244:VAL:HG22	2.09	0.53
2:D:286:LYS:O	2:D:290:LEU:HG	2.09	0.53
2:C:357:LYS:N	2:C:385:TYR:O	2.42	0.52
1:B:124:PHE:HB2	1:B:434:TYR:CD1	2.44	0.52
2:D:170:LEU:H	2:D:170:LEU:HD23	1.75	0.52
1:A:318:ARG:O	1:A:320:SER:N	2.42	0.52
2:C:495:LEU:O	2:C:500:ASN:ND2	2.41	0.52
1:A:115:VAL:O	1:A:116:GLN:HB2	2.09	0.52
2:C:26:LYS:HD2	2:C:280:GLU:HG2	1.91	0.52
2:C:61:ASN:HB3	2:C:155:THR:HG23	1.91	0.52
1:A:345:LEU:HD21	1:A:394:ILE:HD11	1.92	0.52
2:D:26:LYS:HE2	2:D:30:GLN:CD	2.35	0.52
2:D:197:GLU:HA	2:D:200:ILE:HG13	1.92	0.52
1:A:403:MET:HB3	1:A:416:SER:HB2	1.92	0.52
2:C:225:GLU:HG3	2:C:226:LEU:HD23	1.92	0.52
2:D:86:CYS:HB3	2:D:126:LEU:HD23	1.92	0.52
1:B:22:PHE:HD2	1:B:75:CYS:HB2	1.71	0.51
1:B:170:VAL:HG21	1:B:334:THR:HG21	1.92	0.51
1:B:233:LEU:O	1:B:237:ILE:HG12	2.09	0.51
2:D:202:ALA:O	2:D:207:LEU:CD2	2.58	0.51
2:D:388:SER:HA	2:D:509:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LYS:O	1:B:98:GLU:HB2	2.11	0.51
1:B:46:ARG:O	2:C:17:TYR:OH	2.19	0.51
1:B:72:ALA:HA	1:B:75:CYS:SG	2.50	0.51
2:D:404:LYS:O	2:D:408:LYS:HG2	2.11	0.51
1:B:1:MET:HE3	1:B:18:PHE:HD1	1.75	0.51
1:A:96:ILE:HG23	1:A:389:ASN:HD22	1.76	0.51
1:A:303:ASP:CG	1:A:304:ASP:H	2.19	0.51
2:D:384:PRO:HG3	2:D:534:TYR:CE2	2.46	0.50
1:A:63:ARG:NH1	2:C:446:GLN:O	2.44	0.50
2:D:245:ILE:HG23	2:D:246:ALA:O	2.11	0.50
1:A:187:PHE:CE1	1:A:287:LEU:HD11	2.46	0.50
1:A:22:PHE:CD2	1:A:75:CYS:HB3	2.47	0.50
2:D:183:ILE:HD11	2:D:270:LEU:HD11	1.94	0.50
1:B:213:TYR:HB2	1:B:280:LYS:HB2	1.93	0.50
1:B:324:ILE:HD11	1:B:429:LEU:HD21	1.93	0.50
1:A:205:GLY:O	1:A:286:HIS:NE2	2.45	0.50
1:A:264:LEU:HD13	1:A:267:PHE:CD1	2.47	0.50
1:B:124:PHE:HB2	1:B:434:TYR:HB2	1.92	0.50
2:C:111:VAL:HG21	2:C:129:TYR:CD2	2.47	0.50
1:A:86:SER:HB3	1:A:90:LEU:HB2	1.94	0.50
1:A:224:LEU:O	1:A:227:SER:OG	2.25	0.50
1:B:171:MET:SD	1:B:196:THR:HG21	2.51	0.50
2:D:202:ALA:HB1	2:D:207:LEU:N	2.27	0.50
2:D:169:THR:OG1	2:D:201:LYS:HA	2.12	0.50
2:D:301:PHE:CE1	2:D:460:LEU:HD22	2.47	0.50
1:B:197:ALA:HB1	1:B:300:PRO:HB3	1.94	0.49
2:C:203:ASN:C	2:C:205:GLU:H	2.21	0.49
2:C:108:PHE:HB2	2:C:145:PHE:HB2	1.94	0.49
2:C:367:SER:OG	2:C:377:THR:N	2.44	0.49
2:D:216:ASN:HD22	2:D:217:GLN:N	2.10	0.49
2:D:369:GLY:H	2:D:375:LEU:CD2	2.25	0.49
1:B:8:ILE:O	1:B:41:LYS:HB3	2.13	0.49
2:C:182:ALA:O	2:C:211:SER:OG	2.21	0.49
2:D:357:LYS:N	2:D:385:TYR:O	2.46	0.49
2:C:165:ASN:HB3	2:C:168:ASP:HB2	1.95	0.49
2:D:442:PHE:HA	2:D:445:ILE:HG12	1.94	0.49
2:D:367:SER:OG	2:D:377:THR:N	2.45	0.49
2:C:212:ILE:HD11	2:C:269:PHE:CG	2.48	0.48
1:B:224:LEU:O	1:B:227:SER:OG	2.25	0.48
1:B:227:SER:O	1:B:234:LYS:HB2	2.14	0.48
2:C:251:GLU:O	2:C:261:SER:OG	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:HD11	1:A:277:LEU:HD21	1.95	0.48
1:B:18:PHE:HA	1:B:74:ILE:HG21	1.96	0.48
2:D:28:ARG:N	2:D:28:ARG:HD2	2.27	0.48
1:A:447:LYS:HD3	1:A:728:ASP:HB2	1.95	0.48
2:C:357:LYS:HB2	2:C:385:TYR:CD2	2.49	0.48
2:D:27:GLY:C	2:D:28:ARG:HD2	2.38	0.48
2:C:215:LEU:HB3	2:C:248:SER:HB3	1.96	0.48
2:C:364:TYR:HB2	2:C:378:ARG:HA	1.94	0.48
1:A:227:SER:O	1:A:234:LYS:HB2	2.14	0.48
2:C:27:GLY:C	2:C:28:ARG:HD2	2.39	0.48
2:C:496:LYS:HE3	2:D:495:LEU:HD22	1.96	0.48
1:A:141:LEU:HD22	1:A:713:LYS:HD2	1.95	0.47
1:B:341:LEU:O	1:B:345:LEU:HG	2.15	0.47
2:C:169:THR:OG1	2:C:201:LYS:HG2	2.13	0.47
1:B:62:LEU:HD21	1:B:72:ALA:HB2	1.96	0.47
1:A:447:LYS:CD	1:A:728:ASP:HB2	2.44	0.47
1:A:324:ILE:HD13	1:A:425:PHE:HZ	1.80	0.47
1:A:390:LEU:O	1:A:393:LYS:HB3	2.14	0.47
1:A:341:LEU:O	1:A:345:LEU:HG	2.14	0.47
1:B:217:LYS:HB2	1:B:256:ILE:HA	1.96	0.47
2:C:466:ALA:HB3	2:C:470:TYR:HE2	1.80	0.47
2:D:66:ILE:HD11	2:D:156:LEU:HD22	1.96	0.47
2:C:308:LEU:HB2	2:C:438:PHE:CE2	2.49	0.47
1:A:90:LEU:HD12	1:A:110:ILE:HG21	1.97	0.47
1:B:321:ASP:OD2	1:B:438:LYS:NZ	2.33	0.47
2:C:101:LEU:HB2	2:C:156:LEU:HB2	1.97	0.47
2:C:308:LEU:HD23	2:C:585:LEU:HD21	1.96	0.47
2:C:268:ASP:O	2:C:272:GLN:HG2	2.15	0.47
2:C:389:ASP:O	2:C:393:LEU:HD13	2.14	0.47
2:D:250:LYS:HD2	2:D:251:GLU:N	2.29	0.47
2:C:361:ALA:HB2	2:C:383:ALA:CB	2.45	0.46
2:D:-2:GLY:O	2:D:1:MET:HG2	2.16	0.46
1:B:180:ASN:OD1	1:B:187:PHE:N	2.44	0.46
1:B:41:LYS:O	1:B:41:LYS:HG2	2.13	0.46
1:A:713:LYS:O	1:A:717:LEU:HG	2.16	0.46
1:A:24:ASP:C	1:A:26:SER:H	2.24	0.45
1:A:80:PHE:CZ	1:A:110:ILE:HG23	2.51	0.45
1:A:173:ALA:HA	1:A:328:ASN:HB2	1.98	0.45
1:A:334:THR:O	1:A:336:LYS:N	2.49	0.45
1:B:264:LEU:HD13	1:B:267:PHE:HD1	1.80	0.45
2:C:351:GLU:HB2	2:C:395:MET:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:323:TYR:CE2	2:D:571:LEU:HB2	2.50	0.45
2:C:337:ILE:HG12	2:C:413:LEU:HD13	1.97	0.45
2:D:182:ALA:O	2:D:211:SER:HB3	2.17	0.45
1:A:32:GLU:O	1:A:36:ILE:HG12	2.16	0.45
1:B:264:LEU:HD13	1:B:267:PHE:CD1	2.51	0.45
1:A:197:ALA:HB1	1:A:300:PRO:HB3	1.98	0.45
1:B:324:ILE:HD13	1:B:425:PHE:HZ	1.81	0.45
2:C:525:LEU:HD12	2:C:525:LEU:HA	1.78	0.45
1:B:32:GLU:O	1:B:36:ILE:HG12	2.16	0.45
2:C:67:ILE:HD11	2:C:206:LEU:CD2	2.46	0.45
2:D:190:ASN:ND2	2:D:235:SER:OG	2.50	0.45
1:B:83:GLY:HA2	1:B:118:ILE:HG21	1.99	0.45
1:B:212:ILE:HD13	1:B:281:ILE:HG12	1.99	0.45
1:B:334:THR:O	1:B:336:LYS:N	2.50	0.45
2:C:286:LYS:O	2:C:290:LEU:HG	2.17	0.45
2:D:384:PRO:HB2	2:D:516:ILE:HG23	1.99	0.45
2:C:232:TYR:O	2:C:236:VAL:HG23	2.16	0.45
2:D:165:ASN:OD1	2:D:168:ASP:N	2.49	0.44
1:A:212:ILE:HB	1:A:261:LEU:HB2	1.99	0.44
2:D:283:VAL:O	2:D:287:ILE:HG13	2.17	0.44
1:A:124:PHE:HB2	1:A:434:TYR:HB2	1.98	0.44
1:B:263:GLU:HG3	1:B:264:LEU:N	2.33	0.44
2:C:311:GLN:NE2	2:C:434:GLU:HB3	2.32	0.44
1:A:167:ILE:HA	1:A:324:ILE:O	2.18	0.44
1:A:271:LYS:HE2	1:A:271:LYS:HB3	1.79	0.44
1:A:288:GLU:HG3	1:A:289:PHE:N	2.32	0.44
1:B:56:LEU:O	1:B:60:ILE:HG13	2.17	0.44
2:D:301:PHE:HE1	2:D:460:LEU:HD22	1.82	0.44
2:D:458:SER:HA	2:D:461:ARG:NH1	2.31	0.44
1:A:9:TRP:HA	1:A:41:LYS:HB3	2.00	0.44
1:A:324:ILE:HD11	1:A:429:LEU:HD21	1.99	0.44
1:B:167:ILE:HA	1:B:324:ILE:O	2.16	0.44
2:D:176:LEU:HD12	2:D:179:ILE:HD11	1.98	0.44
2:D:245:ILE:HG23	2:D:246:ALA:N	2.31	0.44
2:D:216:ASN:ND2	2:D:249:CYS:O	2.51	0.44
1:A:354:LEU:HD11	1:A:397:LEU:HG	2.00	0.44
2:D:210:ASN:HB2	2:D:278:LEU:HD21	1.99	0.44
2:D:359:LYS:HG2	2:D:360:ASP:H	1.82	0.44
2:D:361:ALA:O	2:D:362:TYR:HD1	2.01	0.44
2:D:495:LEU:O	2:D:500:ASN:ND2	2.51	0.44
1:A:124:PHE:HB2	1:A:434:TYR:CD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:25:PHE:CE2	2:C:27:GLY:HA3	2.53	0.43
2:C:249:CYS:O	2:C:250:LYS:HB2	2.18	0.43
2:C:364:TYR:OH	2:D:364:TYR:CG	2.71	0.43
2:D:212:ILE:HD11	2:D:269:PHE:CG	2.52	0.43
1:A:297:VAL:HG11	1:A:315:GLU:HG2	1.99	0.43
2:C:495:LEU:HD22	2:D:496:LYS:HE3	2.00	0.43
2:C:518:GLU:O	2:C:521:VAL:HG12	2.18	0.43
1:A:87:LYS:HB2	1:A:89:ASP:CG	2.43	0.43
2:C:367:SER:OG	2:C:377:THR:HG23	2.18	0.43
1:B:12:GLU:HG3	1:B:41:LYS:HG3	2.01	0.43
2:C:244:LEU:HD22	2:C:269:PHE:HD1	1.84	0.43
2:D:351:GLU:HB2	2:D:395:MET:HE3	1.98	0.43
2:D:512:PHE:CE2	2:D:540:ILE:HA	2.53	0.43
1:B:3:GLU:O	1:B:7:LYS:HG3	2.18	0.43
1:B:328:ASN:HB3	1:B:331:GLN:HG2	2.01	0.43
2:D:34:LYS:O	2:D:38:GLU:HG3	2.17	0.43
1:A:168:THR:HG23	1:A:325:HIS:CD2	2.54	0.43
2:D:253:LYS:O	2:D:254:ASP:HB2	2.19	0.43
1:A:90:LEU:CD1	1:A:110:ILE:HD13	2.49	0.43
1:A:721:GLU:HA	1:A:724:LEU:HD12	2.01	0.43
1:B:333:LEU:HD13	1:B:375:THR:HA	2.00	0.43
2:C:28:ARG:HD2	2:C:28:ARG:N	2.34	0.43
2:C:488:LEU:HD23	2:D:488:LEU:HD23	2.01	0.43
1:B:463:MET:HE3	1:B:463:MET:HB3	1.81	0.42
2:D:207:LEU:O	2:D:211:SER:OG	2.33	0.42
2:D:344:ILE:HG12	2:D:406:PHE:CD1	2.53	0.42
2:D:359:LYS:HG2	2:D:360:ASP:N	2.34	0.42
1:A:56:LEU:O	1:A:60:ILE:HG13	2.19	0.42
1:A:96:ILE:HG23	1:A:389:ASN:ND2	2.34	0.42
1:A:98:GLU:HA	1:A:101:SER:O	2.19	0.42
2:D:244:LEU:C	2:D:244:LEU:CD1	2.91	0.42
2:D:308:LEU:HD23	2:D:585:LEU:HD21	2.01	0.42
1:B:325:HIS:HB3	1:B:355:ILE:HD13	2.01	0.42
2:D:357:LYS:HB2	2:D:385:TYR:CD2	2.54	0.42
1:A:90:LEU:HD11	1:A:110:ILE:HD13	2.00	0.42
1:A:89:ASP:O	1:A:92:LYS:HB2	2.19	0.42
1:B:79:LEU:HD23	1:B:85:ILE:HG22	2.02	0.42
1:A:333:LEU:HG	1:A:338:ALA:HB2	2.01	0.42
2:D:111:VAL:HG21	2:D:129:TYR:CD2	2.55	0.42
2:C:428:ILE:HD13	2:C:428:ILE:HA	1.84	0.42
1:A:65:ASP:OD1	1:A:68:SER:N	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LYS:HA	1:A:261:LEU:O	2.20	0.42
1:B:9:TRP:CE3	1:B:41:LYS:HB2	2.55	0.42
1:B:203:SER:OG	1:B:204:TYR:N	2.53	0.42
2:C:333:LEU:HD12	2:C:333:LEU:HA	1.92	0.42
2:D:76:SER:O	2:D:80:LEU:HG	2.20	0.42
1:B:170:VAL:HG23	1:B:302:LEU:HD11	2.02	0.42
2:C:67:ILE:HA	2:C:159:THR:OG1	2.20	0.42
2:C:348:ILE:HB	2:C:544:VAL:HG11	2.02	0.42
1:A:178:LEU:HD12	1:A:422:MET:HE1	2.02	0.42
1:B:2:LYS:HB2	1:B:18:PHE:CE2	2.55	0.42
1:B:207:SER:OG	1:B:208:GLU:N	2.52	0.42
2:D:348:ILE:HB	2:D:544:VAL:HG11	2.02	0.42
2:D:545:LEU:HG	2:D:550:VAL:HB	2.01	0.42
1:B:361:ASP:C	1:B:363:LEU:H	2.27	0.41
2:C:71:SER:O	2:C:71:SER:OG	2.35	0.41
2:D:202:ALA:HB1	2:D:207:LEU:H	1.83	0.41
2:D:250:LYS:O	2:D:251:GLU:HB3	2.21	0.41
2:D:372:LYS:HD3	2:D:372:LYS:N	2.36	0.41
1:B:287:LEU:O	1:B:291:LYS:N	2.44	0.41
1:A:324:ILE:HD13	1:A:425:PHE:CZ	2.55	0.41
1:A:14:GLN:O	1:A:16:LEU:HG	2.21	0.41
1:A:118:ILE:HG22	1:A:120:GLN:CD	2.45	0.41
2:D:428:ILE:HD13	2:D:428:ILE:HA	1.85	0.41
2:C:261:SER:C	2:C:263:PHE:N	2.79	0.41
2:C:364:TYR:HB2	2:C:377:THR:O	2.21	0.41
2:C:512:PHE:CE2	2:C:540:ILE:HA	2.55	0.41
1:A:254:PRO:N	1:A:259:ILE:HG12	2.35	0.41
2:D:442:PHE:HD1	2:D:445:ILE:HG13	1.85	0.41
1:B:87:LYS:HE2	1:B:87:LYS:HB3	1.94	0.41
1:B:95:LYS:O	1:B:98:GLU:CB	2.69	0.41
1:B:181:ALA:HB1	1:B:404:ALA:HB3	2.03	0.41
2:C:176:LEU:HD12	2:C:179:ILE:HD11	2.03	0.41
2:C:454:ASP:OD1	2:C:454:ASP:N	2.51	0.41
2:D:67:ILE:HD11	2:D:206:LEU:HD12	2.03	0.41
2:D:79:ASN:CG	2:D:86:CYS:H	2.27	0.41
1:A:319:GLU:O	1:A:320:SER:C	2.63	0.41
2:C:466:ALA:HB3	2:C:470:TYR:CE2	2.55	0.41
2:D:11:LYS:HD2	2:D:11:LYS:HA	1.82	0.41
2:D:42:HIS:HB3	2:D:455:LYS:HB3	2.02	0.41
2:D:486:LEU:HD23	2:D:566:ILE:HD12	2.02	0.41
2:C:323:TYR:HA	2:C:326:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:408:LYS:O	2:C:412:GLU:HG2	2.21	0.41
2:D:28:ARG:NE	2:D:31:GLU:OE2	2.54	0.41
1:A:171:MET:HG3	1:A:302:LEU:HB2	2.02	0.40
2:C:56:PHE:C	2:C:60:LYS:HE2	2.46	0.40
2:D:184:TRP:CH2	2:D:198:ASP:HA	2.56	0.40
2:D:268:ASP:O	2:D:272:GLN:HG2	2.21	0.40
2:D:445:ILE:HD13	2:D:445:ILE:HA	1.94	0.40
1:B:106:ILE:H	1:B:106:ILE:HG13	1.73	0.40
1:B:364:SER:O	1:B:367:ASP:HB2	2.21	0.40
2:D:109:LEU:HD22	2:D:126:LEU:HA	2.04	0.40
2:D:467:SER:HA	2:D:470:TYR:HB2	2.03	0.40
1:B:175:LYS:H	1:B:175:LYS:HG2	1.78	0.40
2:C:42:HIS:ND1	2:C:455:LYS:HD3	2.36	0.40
2:C:62:VAL:HG21	2:C:275:THR:HB	2.03	0.40
2:D:40:PHE:CD1	2:D:40:PHE:C	3.00	0.40
2:C:79:ASN:O	2:C:83:GLY:N	2.54	0.40
2:C:384:PRO:HB3	2:C:534:TYR:CE2	2.55	0.40
1:A:221:GLN:O	1:A:224:LEU:HG	2.22	0.40
2:C:61:ASN:OD1	2:C:61:ASN:N	2.54	0.40
2:D:38:GLU:N	2:D:39:PRO:HD3	2.37	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	685/732 (94%)	627 (92%)	54 (8%)	4 (1%)	21	52
1	B	569/732 (78%)	514 (90%)	53 (9%)	2 (0%)	30	60
2	C	590/614 (96%)	526 (89%)	59 (10%)	5 (1%)	16	47
2	D	590/614 (96%)	533 (90%)	50 (8%)	7 (1%)	10	39
All	All	2434/2692 (90%)	2200 (90%)	216 (9%)	18 (1%)	18	49

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	245	ILE
2	D	245	ILE
2	D	360	ASP
2	D	361	ALA
1	A	319	GLU
1	B	335	GLN
1	A	197	ALA
1	A	335	GLN
1	B	197	ALA
2	C	244	LEU
2	C	96	PHE
2	D	39	PRO
2	C	39	PRO
2	C	249	CYS
2	D	96	PHE
2	D	249	CYS
2	D	523	TYR
1	A	115	VAL

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	448/683 (66%)	447 (100%)	1 (0%)	87	86
1	B	440/683 (64%)	440 (100%)	0	100	100
2	C	555/569 (98%)	555 (100%)	0	100	100
2	D	555/569 (98%)	551 (99%)	4 (1%)	76	77
All	All	1998/2504 (80%)	1993 (100%)	5 (0%)	86	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	411	LEU
2	D	185	LEU

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Mol	Chain	Res	Type
2	D	243	GLU
2	D	244	LEU
2	D	245	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	258	ASN
1	B	257	GLN
1	B	331	GLN
2	C	69	GLN
2	C	163	ASN
2	C	190	ASN
2	C	311	GLN
2	C	500	ASN
2	C	503	ASN
2	D	190	ASN
2	D	216	ASN
2	D	340	GLN
2	D	500	ASN
2	D	503	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 [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	699/732 (95%)	0.67	74 (10%)	11 12	101, 234, 464, 550	0
1	B	587/732 (80%)	0.45	36 (6%)	27 19	100, 213, 427, 486	0
2	C	598/614 (97%)	0.28	24 (4%)	42 27	101, 165, 310, 428	0
2	D	598/614 (97%)	0.27	28 (4%)	36 23	101, 170, 307, 448	0
All	All	2482/2692 (92%)	0.43	162 (6%)	25 18	100, 191, 424, 550	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	ASN	9.0
1	B	245	ASN	8.3
1	B	672	ASN	7.6
1	B	499	GLU	7.3
2	D	203	ASN	6.8
1	B	577	GLU	6.4
1	A	595	ASN	5.9
2	D	228	ASN	5.3
1	A	545	LEU	5.0
1	A	577	GLU	5.0
1	A	242	LYS	4.8
1	B	254	PRO	4.8
1	A	532	GLU	4.8
2	C	367	SER	4.7
1	B	583	SER	4.7
1	A	496	ALA	4.6
2	C	248	SER	4.6
1	A	676	LYS	4.6
1	A	275	SER	4.5
1	A	673	ASP	4.4
1	A	384	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	570	GLU	4.0
1	A	617	PHE	3.9
2	C	534	TYR	3.9
2	D	534	TYR	3.9
1	A	574	LYS	3.9
1	A	499	GLU	3.7
1	B	83	GLY	3.7
1	A	274	ILE	3.6
2	C	30	GLN	3.6
1	B	82	SER	3.5
1	A	362	LEU	3.5
2	D	1	MET	3.4
2	D	367	SER	3.4
1	A	591	ASP	3.4
1	A	340	PHE	3.4
1	A	337	ASP	3.4
1	B	49	LEU	3.3
1	B	85	ILE	3.3
1	B	668	PHE	3.3
1	A	195	GLU	3.3
1	B	116	GLN	3.3
2	C	231	ASN	3.2
1	A	442	ALA	3.2
2	D	232	TYR	3.2
2	D	381	TYR	3.2
1	A	610	SER	3.1
1	A	672	ASN	3.1
1	A	348	SER	3.1
2	D	21	PHE	3.1
1	B	317	LEU	3.0
2	D	162	LEU	3.0
2	D	450	ILE	3.0
1	B	362	LEU	3.0
2	C	375	LEU	3.0
2	D	245	ILE	3.0
1	A	558	ASP	3.0
1	A	373	VAL	2.9
1	A	445	ALA	2.9
2	D	246	ALA	2.9
2	C	94	VAL	2.9
1	A	111	LEU	2.9
1	A	555	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	17	ASN	2.9
2	C	174	ASP	2.8
2	C	451	PHE	2.8
1	B	717	LEU	2.8
1	A	310	GLU	2.8
1	A	541	GLN	2.8
2	D	164	ALA	2.8
1	A	220	TRP	2.7
1	B	495	GLU	2.7
2	C	164	ALA	2.7
2	C	377	THR	2.7
1	A	385	ASP	2.7
2	C	244	LEU	2.7
1	A	49	LEU	2.7
1	A	435	ALA	2.7
1	A	188	LEU	2.7
2	D	173	LEU	2.7
2	C	228	ASN	2.7
1	B	352	LYS	2.7
2	C	594	LYS	2.6
1	A	730	LEU	2.6
1	B	40	ASN	2.6
1	B	306	VAL	2.6
1	B	316	TYR	2.6
2	C	381	TYR	2.6
1	A	303	ASP	2.6
1	A	210	ALA	2.6
1	A	84	PHE	2.6
1	B	209	GLU	2.5
1	A	304	ASP	2.5
1	A	2	LYS	2.5
2	D	198	ASP	2.5
1	A	528	ARG	2.5
1	B	84	PHE	2.5
2	D	227	ASP	2.5
1	A	552	VAL	2.5
1	A	434	TYR	2.5
1	A	588	PHE	2.4
1	A	352	LYS	2.4
1	A	544	ASN	2.4
1	A	196	THR	2.4
1	A	632	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	557	LYS	2.4
2	D	248	SER	2.4
1	A	63	ARG	2.4
2	D	35	GLU	2.4
2	C	33	CYS	2.4
1	B	501	SER	2.4
1	A	365	LYS	2.4
2	C	264	GLN	2.3
1	B	272	ASN	2.3
1	A	316	TYR	2.3
1	A	18	PHE	2.3
1	A	661	LEU	2.3
2	D	36	LEU	2.3
1	A	485	GLU	2.3
1	A	300	PRO	2.3
2	D	20	SER	2.3
1	B	584	LEU	2.3
1	A	614	SER	2.3
1	B	566	GLU	2.3
1	A	11	ASN	2.2
1	A	449	GLU	2.2
2	D	244	LEU	2.2
2	D	379	TYR	2.2
2	D	297	GLU	2.2
2	D	168	ASP	2.2
1	B	20	ALA	2.2
1	B	434	TYR	2.2
2	C	172	THR	2.2
1	A	238	ASP	2.1
2	C	249	CYS	2.1
2	C	255	GLU	2.1
2	D	225	GLU	2.1
2	C	87	LEU	2.1
1	B	17	ASN	2.1
1	A	163	PHE	2.1
1	B	292	ASN	2.1
1	B	221	GLN	2.1
1	A	158	PHE	2.1
1	A	677	HIS	2.1
2	C	173	LEU	2.1
2	D	28	ARG	2.1
1	A	271	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	153	LYS	2.1
1	B	43	ASN	2.1
1	A	190	VAL	2.1
1	A	482	LEU	2.1
1	A	621	ARG	2.1
1	A	182	LEU	2.1
2	D	610	HIS	2.0
1	A	168	THR	2.0
2	C	401	VAL	2.0
1	B	572	ILE	2.0
1	B	574	LYS	2.0
1	A	559	GLY	2.0
1	A	554	ILE	2.0
2	C	169	THR	2.0
1	A	728	ASP	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.