WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:23 PM GMT

PDB ID	:	5A3F
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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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.
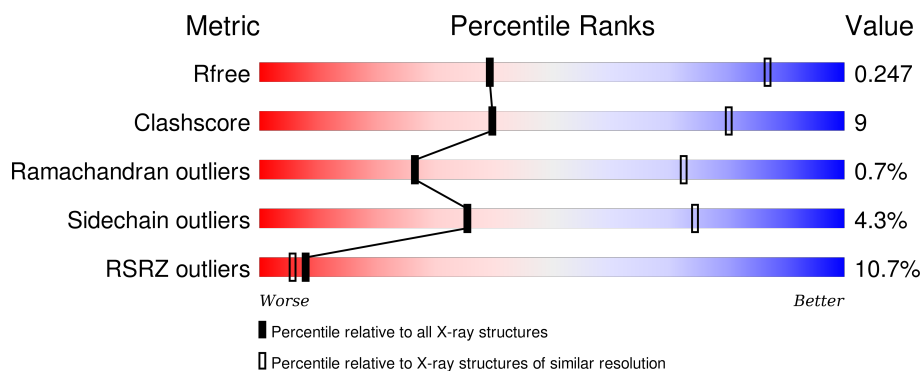
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	754	% 66% 23% • 8%
1	B	754	15% 65% 9% 26%
1	C	754	2% 67% 23% • 7%
1	D	754	17% 64% 8% • 27%

2 Entry composition (i)

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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain C:

• Molecule 1: DYNAMIN 3

Chain D:
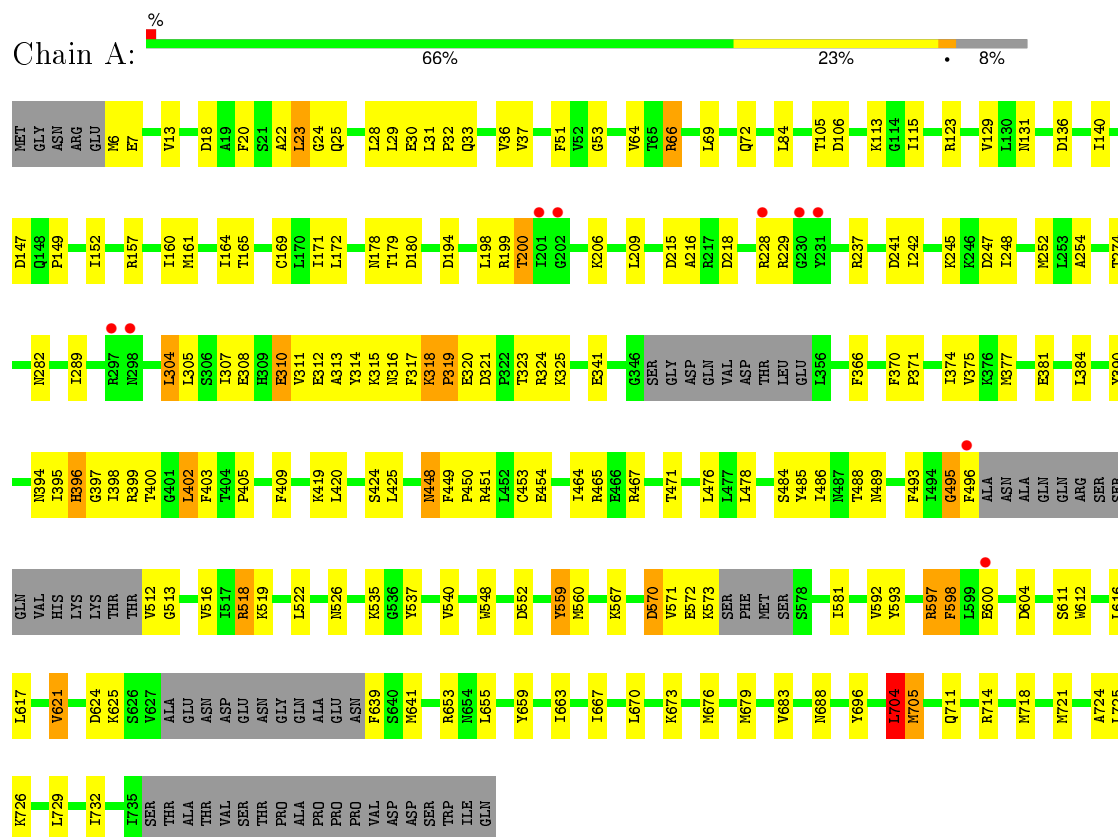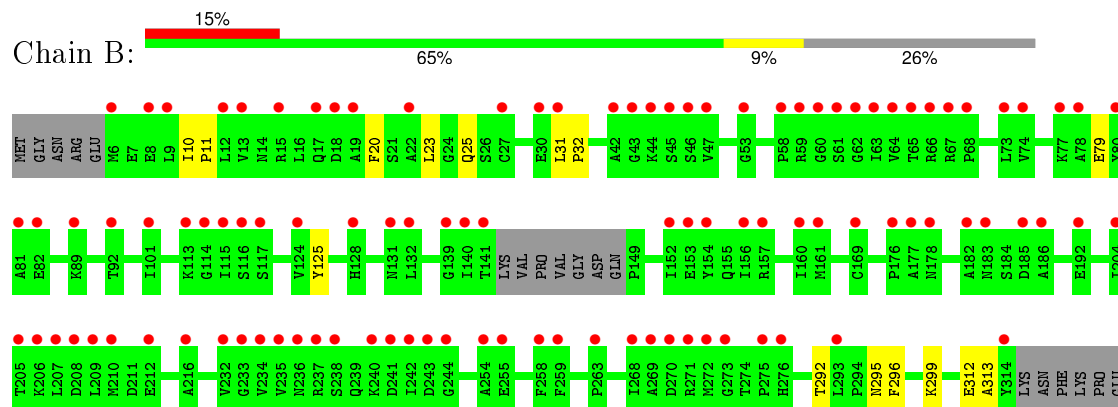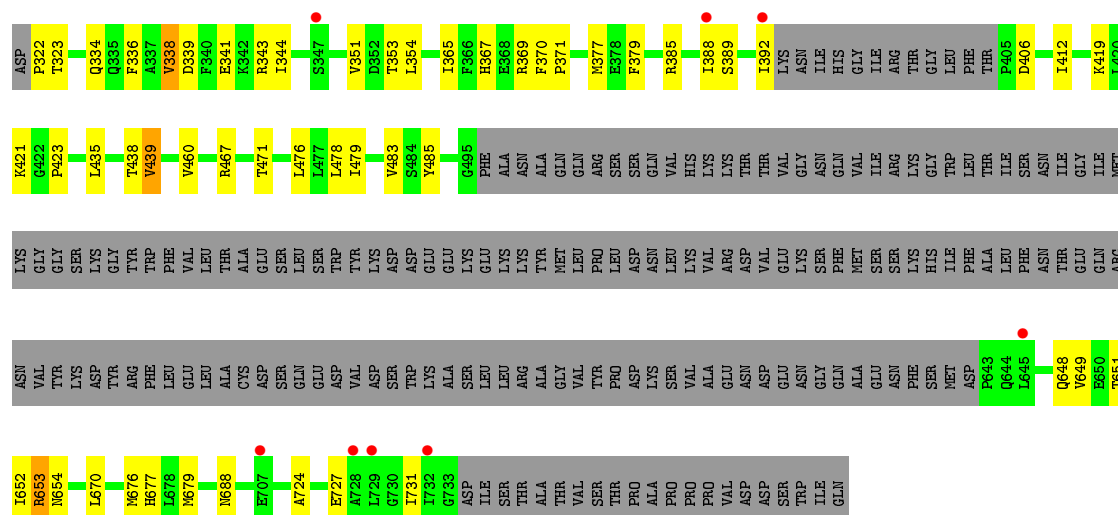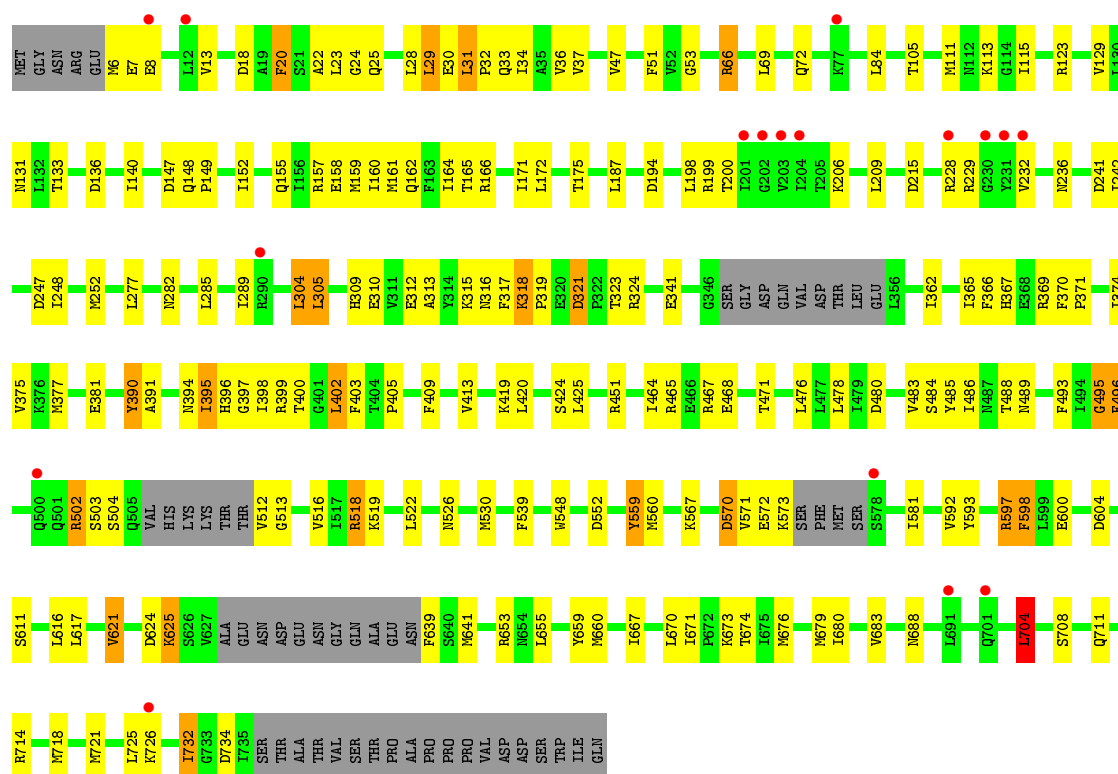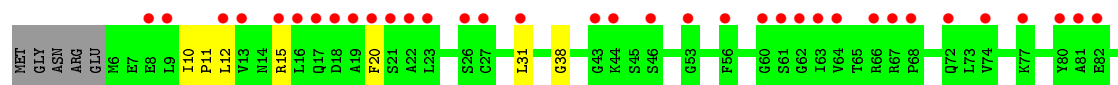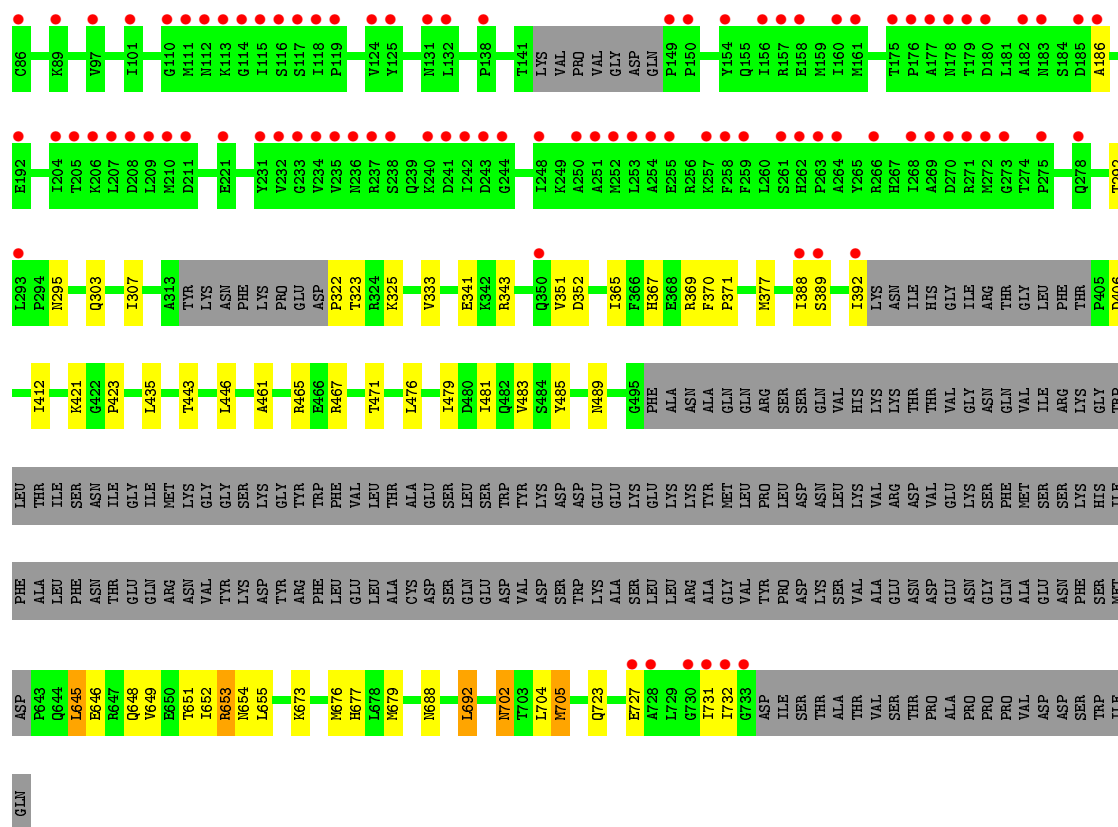
4 Data and refinement statistics (i)

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 49.46 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.47-3.70) 98.8 (49.46-3.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.61 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.232 , 0.278 0.233 , 0.247	Depositor DCC
R_{free} test set	2103 reflections (5.00%)	DCC
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 , 134.0	EDS
Estimated twinning fraction	0.368 for k,h,-l	Xtriage
L-test for twinning [2]	$<|L|> = 0.44, <L^2> = 0.27$	Xtriage
Outliers	0 of 49435 reflections	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.*

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[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.25	0/5635	0.47	2/7588 (0.0%)
1	B	0.25	0/3782	0.46	0/5134
1	C	0.25	0/5703	0.46	2/7679 (0.0%)
1	D	0.25	0/3769	0.46	0/5116
All	All	0.25	0/18889	0.46	4/25517 (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	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	704	LEU	CA-CB-CG	6.24	129.65	115.30
1	C	495	GLY	N-CA-C	-6.00	98.10	113.10
1	A	495	GLY	N-CA-C	-5.39	99.62	113.10
1	C	704	LEU	CA-CB-CG	5.15	127.14	115.30

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5548	0	5670	120	0
1	B	3751	0	3183	43	0
1	C	5616	0	5733	132	0
1	D	3739	0	3174	43	0
All	All	18654	0	17760	322	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 (322) 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
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:C:366:PHE:HE2	1:C:676:MET:HE2	1.57	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:366:PHE:HE2	1:A:676:MET:HE2	1.61	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:69:LEU:HB3	1:C:136:ASP:HB3	1.83	0.61
1:C:471:THR:HG21	1:C:679:MET:HE2	1.81	0.61
1:B:439:VAL:HG21	1:B:460:VAL:HG11	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:471:THR:HG21	1:A:679:MET:HE2	1.84	0.58
1:A:161:MET:O	1:A:165:THR:OG1	2.18	0.58
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:B:421:LYS:HG2	1:B:479:ILE:HG21	1.86	0.58
1:A:13:VAL:HG21	1:A:289:ILE:HD13	1.85	0.58
1:C:396:HIS:CE1	1:C:405:PRO:HD3	2.38	0.58
1:C:312:GLU:HG3	1:C:313:ALA:H	1.68	0.58
1:D:341:GLU:OE2	1:D:688:ASN:ND2	2.37	0.58
1:C:29:LEU:HA	1:C:31:LEU:HD23	1.86	0.58
1:A:198:LEU:HD23	1:A:228:ARG:HG3	1.84	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:592:VAL:HG12	1:A:598:PHE:HA	1.86	0.57
1:A:552:ASP:OD1	1:A:552:ASP:N	2.37	0.57
1:C:341:GLU:OE2	1:C:688:ASN:ND2	2.31	0.57
1:A:341:GLU:OE2	1:A:688:ASN:ND2	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ILE:H	1:A:242:ILE:HD12	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:C:420:LEU:HD13	1:C:667:ILE:HD13	1.88	0.55
1:A:616:LEU:HB3	1:A:621:VAL:HG13	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:B:471:THR:HG21	1:B:679:MET:HE2	1.88	0.55
1:C:616:LEU:HB3	1:C:621:VAL:HG13	1.89	0.55
1:C:23:LEU:O	1:C:25:GLN:N	2.40	0.55
1:D:12:LEU:HD11	1:D:732:ILE:HA	1.87	0.55
1:A:526:ASN:HB2	1:A:600:GLU:H	1.70	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: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
1:C:20:PHE:HB3	1:C:29:LEU:HD13	1.89	0.54
1:A:304:LEU:HB2	1:A:725:LEU:HD13	1.90	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:704:LEU:HD23	1:A:705:MET:HG2	1.90	0.53
1:A:375:VAL:HG21	1:A:617:LEU:HD11	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:413:VAL:HG13	1:C:660:MET:HE3	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:C:502:ARG:HB2	1:C:502:ARG:HH11	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:TYR:HD1	1:A:560:MET:H	1.59	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:C:20:PHE:CE2	1:C:28:LEU:HB2	2.47	0.50
1:A:178:ASN:OD1	1:A:179:THR:N	2.44	0.50
1:C:552:ASP:N	1:C:552:ASP:OD1	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
1:A:641:MET:SD	1:A:641:MET:N	2.84	0.50
1:C:516:VAL:HG11	1:C:519:LYS:HG3	1.94	0.50
1:A:570:ASP:OD1	1:A:570:ASP:N	2.45	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: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:C:714:ARG:O	1:C:718:MET:HG2	2.12	0.49
1:C:241:ASP:HB3	1:C:247:ASP:HB2	1.94	0.49
1:B:370:PHE:HB3	1:B:371:PRO:HD3	1.94	0.49
1:C:641:MET:N	1:C:641:MET:SD	2.86	0.49
1:B:476:LEU:O	1:B:479:ILE:HG22	2.12	0.49
1:A:140:ILE:HG23	1:A:157:ARG:HE	1.77	0.49
1:C:29:LEU:HD12	1:C:31:LEU:HD21	1.94	0.48
1:A:729:LEU:HA	1:A:732:ILE:HG22	1.94	0.48
1:C:115:ILE:HD12	1:C:159:MET:HE3	1.95	0.48
1:A:381:GLU:OE2	1:A:653:ARG:NE	2.46	0.48
1:C:198:LEU:HD23	1:C:228:ARG:HG3	1.94	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:B:334:GLN:O	1:B:338:VAL:HG22	2.13	0.48
1:D:646:GLU:O	1:D:649:VAL:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:20:PHE:CD2	1:B:31:LEU:HD21	2.44	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:D:303:GLN:O	1:D:307:ILE:HD13	2.15	0.47
1:A:604:ASP:N	1:A:604:ASP:OD1	2.48	0.47
1:C:518:ARG:HH12	1:C:611:SER:HB3	1.80	0.47
1:C:570:ASP:N	1:C:570:ASP:OD1	2.45	0.47
1:A:149:PRO:HD2	1:A:152:ILE:HB	1.96	0.47
1:C:72:GLN:HB2	1:C:123:ARG:HG2	1.96	0.47
1:A:425:LEU:HD11	1:A:476:LEU:HD21	1.97	0.47
1:C:318:LYS:HB2	1:C:321:ASP:OD2	2.14	0.47
1:A:320:GLU:HB3	1:A:325:LYS:HE2	1.95	0.47
1:A:241:ASP:HB3	1:A:247:ASP:HB2	1.97	0.47
1:A:518:ARG:HH12	1:A:611:SER:HB3	1.80	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: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:248:ILE:O	1:C:252:MET:HG2	2.15	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: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:C:370:PHE:HE1	1:C:424:SER:HA	1.79	0.46
1:A:486:ILE:HG13	1:A:659:TYR:CZ	2.51	0.46
1:C:718:MET:HA	1:C:721:MET:HB3	1.98	0.46
1:A:402:LEU:HA	1:A:403:PHE:HA	1.65	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:C:604:ASP:N	1:C:604:ASP:OD1	2.47	0.45
1:A:396:HIS:CE1	1:A:405:PRO:HD3	2.51	0.45
1:A:448:ASN:HD22	1:A:448:ASN:H	1.64	0.45
1:C:305:LEU:HD12	1:C:309:HIS:NE2	2.32	0.45
1:B:365:ILE:HA	1:B:369:ARG:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:704:LEU:HD12	1:D:705:MET:HG2	1.98	0.45
1:C:232:VAL:HG11	1:C:277:LEU:HB2	1.98	0.45
1:A:317:PHE:CD2	1:A:323:THR:HG21	2.52	0.45
1:C:409:PHE:CE1	1:C:655:LEU:HB3	2.52	0.45
1:B:312:GLU:CD	1:B:313:ALA:H	2.20	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
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:C:402:LEU:HA	1:C:403:PHE:HA	1.61	0.45
1:C:140:ILE:HG23	1:C:157:ARG:HE	1.82	0.45
1:A:206:LYS:HB3	1:A:209:LEU:HD12	1.98	0.45
1:D:655:LEU:HD12	1:D:655:LEU:HA	1.86	0.45
1:A:171:ILE:HD12	1:A:200:THR:HG22	1.99	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:D:727:GLU:O	1:D:731:ILE:HG12	2.17	0.44
1:A:516:VAL:HG11	1:A:519:LYS:HG3	1.99	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:C:559:TYR:CE2	1:C:593:TYR:HB2	2.53	0.44
1:A:215:ASP:OD1	1:A:215:ASP:N	2.49	0.44
1:A:310:GLU:HG3	1:A:311:VAL:N	2.32	0.44
1:C:111:MET:O	1:C:113:LYS:HG3	2.18	0.44
1:A:29:LEU:HD12	1:A:31:LEU:HD21	1.99	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:HD3	1:A:597:ARG:H	1.83	0.44
1:B:322:PRO:HB2	1:B:323:THR:H	1.62	0.44
1:C:465:ARG:NE	1:C:468:GLU:OE1	2.51	0.44
1:C:194:ASP:OD2	1:C:198:LEU:N	2.51	0.44
1:D:322:PRO:HB2	1:D:323:THR:H	1.63	0.44
1:A:663:ILE:HA	1:A:663:ILE:HD13	1.80	0.44
1:A:597:ARG:H	1:A:597:ARG:CD	2.31	0.44
1:B:10:ILE:HB	1:B:11:PRO:HD3	2.00	0.43
1:A:318:LYS:HB3	1:A:319:PRO:CD	2.47	0.43
1:D:653:ARG:HD2	1:D:654:ASN:OD1	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:377:MET:HE1	1:C:419:LYS:O	2.18	0.43
1:A:559:TYR:CE2	1:A:593:TYR:HB2	2.54	0.43
1:A:241:ASP:OD1	1:A:245:LYS:N	2.51	0.43
1:C:149:PRO:HD2	1:C:152:ILE:HB	2.01	0.43
1:C:215:ASP:N	1:C:215:ASP:OD1	2.49	0.43
1:C:571:VAL:HB	1:C:581:ILE:HB	2.01	0.43
1:A:216:ALA:O	1:A:218:ASP:N	2.45	0.43
1:A:495:GLY:O	1:A:496:PHE:HB2	2.19	0.43
1:B:388:ILE:HG12	1:B:412:ILE:HG13	2.01	0.43
1:A:304:LEU:HD12	1:A:725:LEU:HD13	2.01	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:725:LEU:HD12	1:A:726:LYS:N	2.34	0.42
1:C:488:THR:HG23	1:C:493:PHE:CE2	2.54	0.42
1:A:449:PHE:HA	1:A:450:PRO:HD2	1.89	0.42
1:C:158:GLU:O	1:C:162:GLN:HG3	2.18	0.42
1:C:30:GLU:OE2	1:C:166:ARG:HG2	2.19	0.42
1:C:467:ARG:O	1:C:471:THR:HG22	2.19	0.42
1:A:512:VAL:HG22	1:A:513:GLY:H	1.84	0.42
1:C:362:ILE:HD13	1:C:680:ILE:HD13	2.00	0.42
1:A:64:VAL:O	1:A:66:ARG:NE	2.51	0.42
1:D:443:THR:HA	1:D:446:LEU:HD13	2.01	0.42
1:C:367:HIS:CD2	1:D:489:ASN:HB2	2.54	0.42
1:C:51:PHE:O	1:C:129:VAL:HG12	2.19	0.42
1:B:295:ASN:OD1	1:B:296:PHE:N	2.52	0.42
1:A:718:MET:HA	1:A:721:MET:HB3	2.01	0.42
1:A:248:ILE:O	1:A:252:MET:HG2	2.18	0.42
1:C:512:VAL:HG13	1:C:513:GLY:H	1.85	0.42
1:A:573:LYS:H	1:A:573:LYS:HG2	1.63	0.42
1:A:37:VAL:HG21	1:A:164:ILE:HD11	2.01	0.42
1:C:512:VAL:HG22	1:C:513:GLY:H	1.85	0.42
1:A:453:CYS:SG	1:A:454:GLU:N	2.93	0.42
1:A:572:GLU:CD	1:A:572:GLU:H	2.23	0.42
1:A:51:PHE:HE1	1:A:274:THR:HG23	1.83	0.42
1:A:20:PHE:CE2	1:A:28:LEU:HB2	2.42	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:51:PHE:CE1	1:A:274:THR:HG23	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:480:ASP:O	1:C:483:VAL:HG22	2.19	0.42
1:A:535:LYS:HB3	1:A:537:TYR:CE1	2.55	0.42
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:D:653:ARG:C	1:D:653:ARG:HD3	2.40	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:C:72:GLN:HG2	1:C:133:THR:HG23	2.02	0.41
1:B:648:GLN:O	1:B:651:THR:HG22	2.20	0.41
1:D:471:THR:HG21	1:D:679:MET:HE2	2.02	0.41
1:C:493:PHE:CE1	1:C:659:TYR:HB2	2.56	0.41
1:A:548:TRP:CZ2	1:A:559:TYR:HB3	2.55	0.41
1:D:723:GLN:O	1:D:727:GLU:HG2	2.20	0.41
1:C:671:ILE:HD13	1:C:671:ILE:HA	1.86	0.41
1:A:522:LEU:HD21	1:A:612:TRP:NE1	2.36	0.41
1:A:51:PHE:O	1:A:129:VAL:HG12	2.21	0.41
1:D:471:THR:HG21	1:D:679:MET:CE	2.51	0.41
1:D:467:ARG:HA	1:D:467:ARG:HD2	1.86	0.41
1:B:79:GLU:HA	1:B:125:TYR:O	2.21	0.41
1:C:18:ASP:OD2	1:C:123:ARG:HD2	2.21	0.41
1:B:478:LEU:CD2	1:B:670:LEU:HD22	2.47	0.41
1:B:679:MET:HE2	1:B:679:MET:HB2	1.94	0.41
1:C:305:LEU:HA	1:C:305:LEU:HD13	1.89	0.41
1:D:10:ILE:HB	1:D:11:PRO:HD3	2.03	0.41
1:C:573:LYS:H	1:C:573:LYS:HG2	1.64	0.41
1:C:573:LYS:HB3	1:C:573:LYS:HE3	1.80	0.41
1:A:180:ASP:OD1	1:A:180:ASP:N	2.54	0.41
1:C:674:THR:HA	1:D:481:ILE:HD13	2.02	0.41
1:C:725:LEU:HD12	1:C:726:LYS:N	2.35	0.41
1:C:402:LEU:HB2	1:C:403:PHE:CD1	2.55	0.41
1:A:519:LYS:HG2	1:A:540:VAL:HG22	2.02	0.41
1:C:488:THR:HG23	1:C:493:PHE:HE2	1.86	0.41
1:C:317:PHE:CD1	1:C:317:PHE:N	2.88	0.41
1:B:467:ARG:O	1:B:471:THR:HG22	2.21	0.41
1:C:370:PHE:CE1	1:C:424:SER:HA	2.55	0.41
1:A:402:LEU:HB2	1:A:403:PHE:CD1	2.56	0.41
1:C:175:THR:HG21	1:C:187:LEU:HD23	2.02	0.41
1:D:38:GLY:HA2	1:D:186:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:572:GLU:H	1:C:572:GLU:CD	2.24	0.41
1:C:597:ARG:H	1:C:597:ARG:HD3	1.85	0.41
1:B:389:SER:O	1:B:392:ILE:HG12	2.21	0.41
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:B:344:ILE:HD11	1:B:438:THR:HG21	2.02	0.40
1:C:522:LEU:HB2	1:C:539:PHE:CD1	2.56	0.40
1:C:171:ILE:HD12	1:C:200:THR:OG1	2.20	0.40
1:C:148:GLN:HG3	1:C:149:PRO:HA	2.03	0.40
1:B:23:LEU:HD13	1:B:724:ALA:HB1	2.04	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%)	21	68
1	B	545/754 (72%)	528 (97%)	15 (3%)	2 (0%)	39	80
1	C	690/754 (92%)	660 (96%)	22 (3%)	8 (1%)	16	63
1	D	544/754 (72%)	530 (97%)	13 (2%)	1 (0%)	52	87
All	All	2460/3016 (82%)	2372 (96%)	71 (3%)	17 (1%)	26	72

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	A	397	GLY
1	A	398	ILE

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Mol	Chain	Res	Type
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%)	588 (95%)	29 (5%)	32	72
1	B	293/671 (44%)	282 (96%)	11 (4%)	40	77
1	C	624/671 (93%)	595 (95%)	29 (5%)	33	73
1	D	292/671 (44%)	283 (97%)	9 (3%)	47	81
All	All	1826/2684 (68%)	1748 (96%)	78 (4%)	35	74

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	33	GLN
1	A	66	ARG
1	A	115	ILE
1	A	147	ASP
1	A	200	THR
1	A	304	LEU

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Mol	Chain	Res	Type
1	A	305	LEU
1	A	308	GLU
1	A	310	GLU
1	A	314	TYR
1	A	321	ASP
1	A	390	TYR
1	A	395	ILE
1	A	399	ARG
1	A	400	THR
1	A	402	LEU
1	A	448	ASN
1	A	518	ARG
1	A	559	TYR
1	A	570	ASP
1	A	597	ARG
1	A	598	PHE
1	A	621	VAL
1	A	639	PHE
1	A	696	TYR
1	A	704	LEU
1	A	705	MET
1	A	711	GLN
1	B	25	GLN
1	B	338	VAL
1	B	339	ASP
1	B	343	ARG
1	B	354	LEU
1	B	406	ASP
1	B	435	LEU
1	B	439	VAL
1	B	483	VAL
1	B	649	VAL
1	B	653	ARG
1	C	20	PHE
1	C	31	LEU
1	C	33	GLN
1	C	66	ARG
1	C	147	ASP
1	C	304	LEU
1	C	305	LEU
1	C	310	GLU
1	C	321	ASP

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Mol	Chain	Res	Type
1	C	390	TYR
1	C	395	ILE
1	C	399	ARG
1	C	400	THR
1	C	402	LEU
1	C	502	ARG
1	C	518	ARG
1	C	530	MET
1	C	559	TYR
1	C	570	ASP
1	C	597	ARG
1	C	598	PHE
1	C	621	VAL
1	C	625	LYS
1	C	639	PHE
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	406	ASP
1	D	435	LEU
1	D	483	VAL
1	D	645	LEU
1	D	653	ARG
1	D	692	LEU
1	D	702	ASN
1	D	705	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	691/754 (91%)	-0.28	9 (1%)	79	66	86, 200, 339, 531	0
1	B	555/754 (73%)	1.07	113 (20%)	1	1	92, 227, 356, 545	253 (45%)
1	C	700/754 (92%)	-0.25	17 (2%)	62	46	87, 201, 333, 458	0
1	D	554/754 (73%)	1.13	129 (23%)	1	1	93, 225, 352, 464	253 (45%)
All	All	2500/3016 (82%)	0.34	268 (10%)	8	6	86, 211, 346, 545	506 (20%)

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	241	ASP	22.7
1	D	116	SER	22.3
1	B	60	GLY	21.7
1	B	61	SER	16.3
1	D	233	GLY	15.9
1	B	208	ASP	15.7
1	B	116	SER	14.9
1	D	117	SER	14.8
1	B	232	VAL	13.0
1	B	63	ILE	12.6
1	B	114	GLY	12.3
1	B	62	GLY	11.9
1	B	207	LEU	11.9
1	B	233	GLY	11.5
1	D	234	VAL	11.3
1	B	209	LEU	10.9
1	D	114	GLY	10.7
1	D	242	ILE	10.6
1	B	153	GLU	10.4
1	D	243	ASP	10.4
1	B	234	VAL	10.1

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Mol	Chain	Res	Type	RSRZ
1	B	44	LYS	10.1
1	D	263	PRO	9.9
1	B	18	ASP	9.9
1	D	254	ALA	9.4
1	D	232	VAL	9.4
1	D	115	ILE	9.3
1	B	27	CYS	9.3
1	D	60	GLY	9.1
1	D	207	LEU	9.1
1	D	61	SER	8.9
1	B	64	VAL	8.9
1	B	124	VAL	8.7
1	B	157	ARG	8.7
1	D	22	ALA	8.6
1	B	81	ALA	8.4
1	B	43	GLY	8.3
1	D	27	CYS	8.2
1	D	210	MET	8.1
1	D	18	ASP	8.0
1	D	237	ARG	7.9
1	B	242	ILE	7.8
1	D	81	ALA	7.7
1	D	270	ASP	7.7
1	B	176	PRO	7.7
1	B	259	PHE	7.7
1	B	205	THR	7.4
1	B	273	GLY	7.3
1	B	156	ILE	7.2
1	B	117	SER	7.2
1	B	115	ILE	7.2
1	B	732	ILE	7.1
1	B	59	ARG	6.9
1	B	185	ASP	6.8
1	D	82	GLU	6.8
1	D	206	LYS	6.8
1	B	177	ALA	6.6
1	B	243	ASP	6.6
1	D	119	PRO	6.5
1	D	204	ILE	6.5
1	D	118	ILE	6.3
1	B	31	LEU	6.3
1	D	66	ARG	6.3

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Mol	Chain	Res	Type	RSRZ
1	B	255	GLU	6.3
1	D	209	LEU	6.2
1	B	269	ALA	6.2
1	D	733	GLY	6.1
1	D	16	LEU	6.1
1	B	66	ARG	6.1
1	B	206	LYS	6.0
1	D	269	ALA	5.9
1	B	204	ILE	5.8
1	B	9	LEU	5.8
1	D	132	LEU	5.7
1	B	58	PRO	5.7
1	D	21	SER	5.7
1	D	258	PHE	5.6
1	B	47	VAL	5.6
1	D	236	ASN	5.6
1	D	240	LYS	5.5
1	B	186	ALA	5.5
1	D	68	PRO	5.5
1	D	149	PRO	5.5
1	D	63	ILE	5.5
1	D	113	LYS	5.4
1	D	157	ARG	5.4
1	D	231	TYR	5.4
1	D	238	SER	5.3
1	D	388	ILE	5.3
1	D	53	GLY	5.3
1	D	235	VAL	5.2
1	D	208	ASP	5.2
1	B	22	ALA	5.2
1	D	273	GLY	5.2
1	D	178	ASN	5.1
1	D	161	MET	5.1
1	B	19	ALA	5.1
1	D	15	ARG	5.0
1	D	176	PRO	5.0
1	B	270	ASP	5.0
1	B	241	ASP	5.0
1	D	244	GLY	5.0
1	D	150	PRO	5.0
1	D	177	ALA	4.9
1	D	180	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	64	VAL	4.8
1	B	30	GLU	4.7
1	D	392	ILE	4.6
1	D	154	TYR	4.6
1	D	262	HIS	4.6
1	D	205	THR	4.6
1	B	272	MET	4.6
1	A	231	TYR	4.6
1	D	19	ALA	4.5
1	C	202	GLY	4.5
1	B	212	GLU	4.5
1	D	26	SER	4.4
1	B	67	ARG	4.4
1	B	263	PRO	4.4
1	D	251	ALA	4.4
1	D	730	GLY	4.4
1	D	272	MET	4.3
1	B	141	THR	4.3
1	D	275	PRO	4.3
1	C	232	VAL	4.2
1	B	154	TYR	4.2
1	B	82	GLU	4.2
1	D	182	ALA	4.1
1	B	46	SER	4.0
1	D	264	ALA	4.0
1	A	201	ILE	4.0
1	B	140	ILE	4.0
1	D	12	LEU	4.0
1	A	600	GLU	4.0
1	D	8	GLU	4.0
1	D	125	TYR	3.9
1	D	124	VAL	3.9
1	D	17	GLN	3.9
1	B	12	LEU	3.9
1	D	257	LYS	3.8
1	D	731	ILE	3.8
1	C	578	SER	3.8
1	D	112	ASN	3.7
1	D	211	ASP	3.7
1	D	183	ASN	3.7
1	D	192	GLU	3.7
1	D	67	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	101	ILE	3.7
1	C	77	LYS	3.7
1	B	132	LEU	3.7
1	D	131	ASN	3.6
1	D	89	LYS	3.6
1	A	230	GLY	3.6
1	B	244	GLY	3.6
1	B	65	THR	3.6
1	B	276	HIS	3.6
1	B	183	ASN	3.5
1	D	253	LEU	3.4
1	C	228	ARG	3.4
1	A	202	GLY	3.4
1	B	258	PHE	3.3
1	B	13	VAL	3.3
1	B	101	ILE	3.3
1	B	178	ASN	3.3
1	C	230	GLY	3.3
1	B	77	LYS	3.3
1	D	86	CYS	3.2
1	D	252	MET	3.2
1	B	240	LYS	3.2
1	D	72	GLN	3.2
1	B	237	ARG	3.2
1	D	268	ILE	3.2
1	B	268	ILE	3.2
1	D	20	PHE	3.1
1	D	259	PHE	3.1
1	B	17	GLN	3.1
1	D	9	LEU	3.1
1	C	231	TYR	3.1
1	B	169	CYS	3.1
1	B	235	VAL	3.0
1	B	89	LYS	3.0
1	D	138	PRO	2.9
1	B	113	LYS	2.9
1	D	271	ARG	2.9
1	B	80	TYR	2.9
1	D	179	THR	2.9
1	D	44	LYS	2.9
1	D	43	GLY	2.8
1	C	201	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	496	PHE	2.8
1	D	62	GLY	2.8
1	B	707	GLU	2.8
1	B	6	MET	2.7
1	D	31	LEU	2.7
1	B	68	PRO	2.7
1	D	727	GLU	2.7
1	B	392	ILE	2.7
1	D	350	GLN	2.7
1	D	255	GLU	2.7
1	B	275	PRO	2.7
1	B	216	ALA	2.7
1	D	160	ILE	2.7
1	C	203	VAL	2.7
1	D	80	TYR	2.7
1	D	13	VAL	2.7
1	B	74	VAL	2.6
1	B	92	THR	2.6
1	B	45	SER	2.6
1	D	110	GLY	2.6
1	D	23	LEU	2.6
1	B	42	ALA	2.6
1	B	238	SER	2.6
1	D	732	ILE	2.6
1	C	290	ARG	2.6
1	B	161	MET	2.6
1	D	728	ALA	2.5
1	D	248	ILE	2.5
1	D	261	SER	2.5
1	B	160	ILE	2.5
1	D	186	ALA	2.5
1	D	74	VAL	2.4
1	A	228	ARG	2.4
1	C	12	LEU	2.4
1	B	388	ILE	2.4
1	C	726	LYS	2.4
1	B	254	ALA	2.4
1	B	78	ALA	2.4
1	D	185	ASP	2.3
1	D	97	VAL	2.3
1	D	250	ALA	2.3
1	D	158	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	210	MET	2.3
1	B	15	ARG	2.3
1	D	175	THR	2.3
1	C	701	GLN	2.3
1	C	500	GLN	2.3
1	B	128	HIS	2.3
1	B	182	ALA	2.3
1	C	204	ILE	2.3
1	B	53	GLY	2.2
1	D	221	GLU	2.2
1	B	271	ARG	2.2
1	B	729	LEU	2.2
1	D	278	GLN	2.2
1	A	297	ARG	2.2
1	D	56	PHE	2.2
1	B	73	LEU	2.2
1	B	236	ASN	2.2
1	B	347	SER	2.2
1	B	728	ALA	2.2
1	B	293	LEU	2.1
1	D	46	SER	2.1
1	C	691	LEU	2.1
1	D	293	LEU	2.1
1	B	152	ILE	2.1
1	B	192	GLU	2.1
1	B	139	GLY	2.1
1	D	156	ILE	2.1
1	B	131	ASN	2.1
1	B	8	GLU	2.1
1	B	314	TYR	2.0
1	B	645	LEU	2.0
1	A	298	ASN	2.0
1	C	8	GLU	2.0
1	D	77	LYS	2.0
1	D	111	MET	2.0
1	D	266	ARG	2.0
1	D	389	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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.