



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 06:21 am GMT

PDB ID : 4BEJ
Title : Nucleotide-free Dynamin 1-like protein (DNM1L, DRP1, DLP1)
Authors : Froehlich, C.; Schwefel, D.; Faelber, K.; Daumke, O.
Deposited on : 2013-03-11
Resolution : 3.48 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

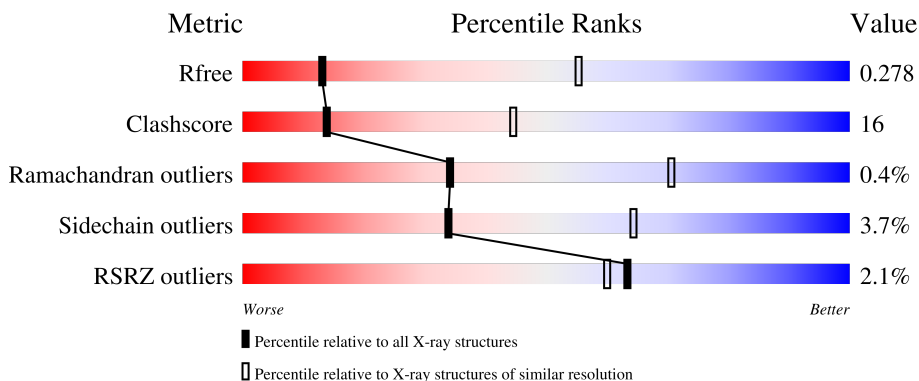
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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}	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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	617	
1	B	617	
1	C	617	
1	D	617	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 17076 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 1-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	540	4263	2701	740	801	21	0	0	0
1	B	547	4313	2728	755	810	20	0	0	0
1	C	534	4218	2678	736	785	19	0	0	0
1	D	540	4282	2717	748	797	20	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP O00429
A	-5	PRO	-	expression tag	UNP O00429
A	-4	HIS	-	expression tag	UNP O00429
A	-3	MET	-	expression tag	UNP O00429
A	-2	GLY	-	expression tag	UNP O00429
A	-1	GLY	-	expression tag	UNP O00429
A	0	SER	-	expression tag	UNP O00429
A	401	ALA	GLY	engineered mutation	UNP O00429
A	402	ALA	PRO	engineered mutation	UNP O00429
A	403	ALA	ARG	engineered mutation	UNP O00429
A	404	ALA	PRO	engineered mutation	UNP O00429
B	-6	GLY	-	expression tag	UNP O00429
B	-5	PRO	-	expression tag	UNP O00429
B	-4	HIS	-	expression tag	UNP O00429
B	-3	MET	-	expression tag	UNP O00429
B	-2	GLY	-	expression tag	UNP O00429
B	-1	GLY	-	expression tag	UNP O00429
B	0	SER	-	expression tag	UNP O00429
B	401	ALA	GLY	engineered mutation	UNP O00429
B	402	ALA	PRO	engineered mutation	UNP O00429
B	403	ALA	ARG	engineered mutation	UNP O00429

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Chain	Residue	Modelled	Actual	Comment	Reference
B	404	ALA	PRO	engineered mutation	UNP O00429
C	-6	GLY	-	expression tag	UNP O00429
C	-5	PRO	-	expression tag	UNP O00429
C	-4	HIS	-	expression tag	UNP O00429
C	-3	MET	-	expression tag	UNP O00429
C	-2	GLY	-	expression tag	UNP O00429
C	-1	GLY	-	expression tag	UNP O00429
C	0	SER	-	expression tag	UNP O00429
C	401	ALA	GLY	engineered mutation	UNP O00429
C	402	ALA	PRO	engineered mutation	UNP O00429
C	403	ALA	ARG	engineered mutation	UNP O00429
C	404	ALA	PRO	engineered mutation	UNP O00429
D	-6	GLY	-	expression tag	UNP O00429
D	-5	PRO	-	expression tag	UNP O00429
D	-4	HIS	-	expression tag	UNP O00429
D	-3	MET	-	expression tag	UNP O00429
D	-2	GLY	-	expression tag	UNP O00429
D	-1	GLY	-	expression tag	UNP O00429
D	0	SER	-	expression tag	UNP O00429
D	401	ALA	GLY	engineered mutation	UNP O00429
D	402	ALA	PRO	engineered mutation	UNP O00429
D	403	ALA	ARG	engineered mutation	UNP O00429
D	404	ALA	PRO	engineered mutation	UNP O00429

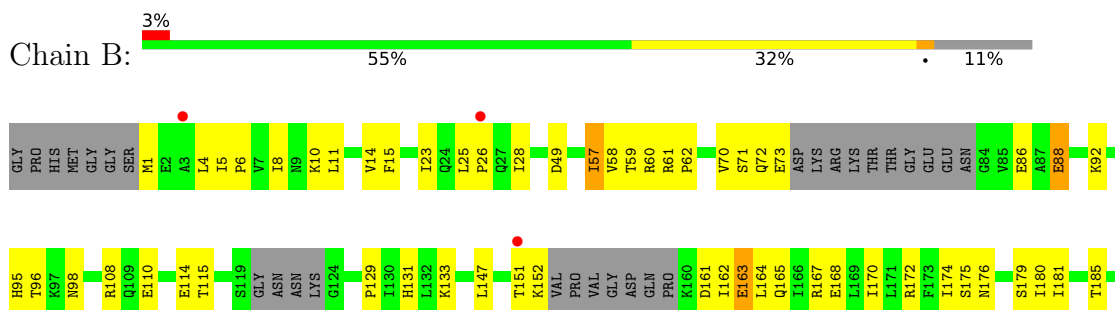
3 Residue-property plots [i](#)

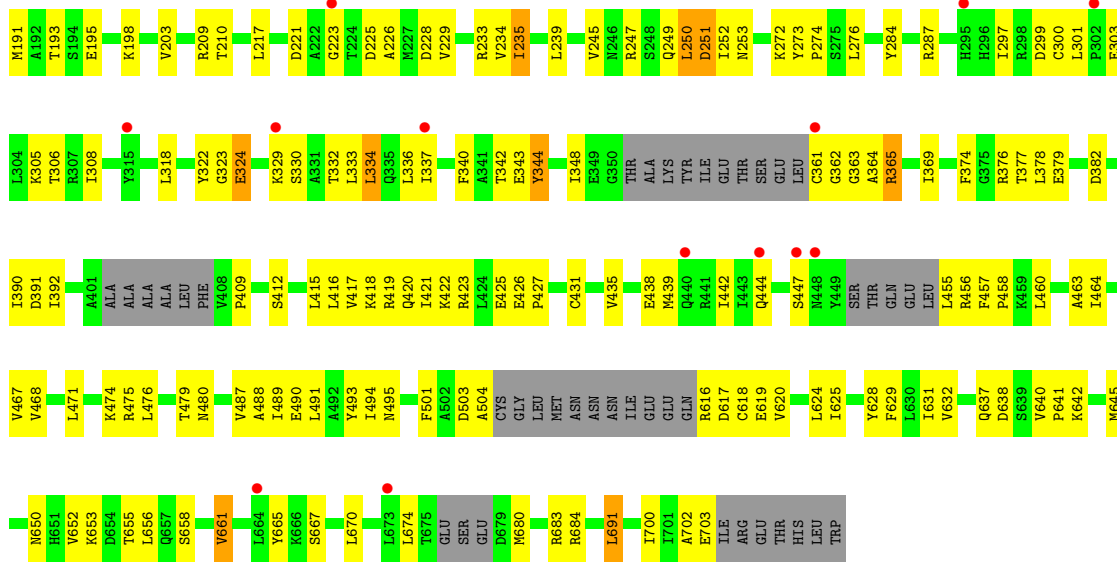
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 1-LIKE PROTEIN

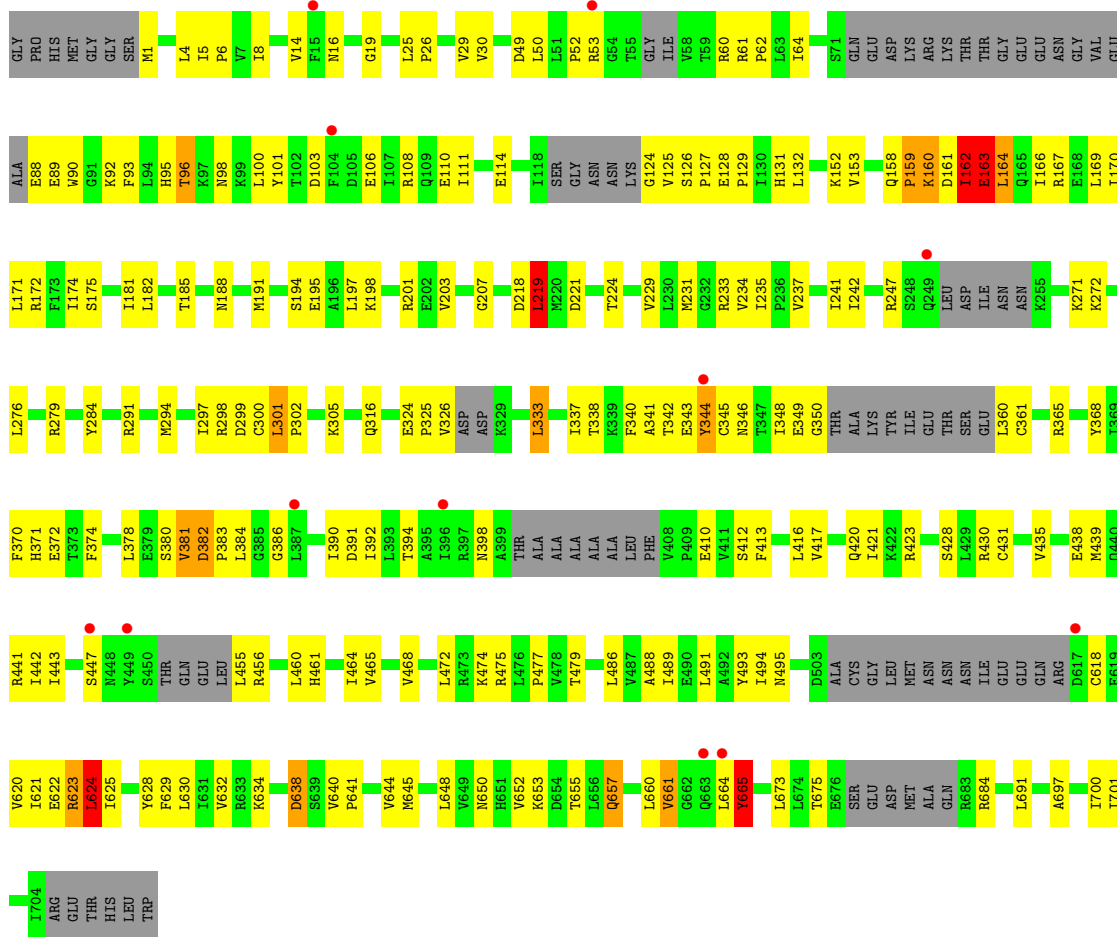


• Molecule 1: DYNAMIN 1-LIKE PROTEIN

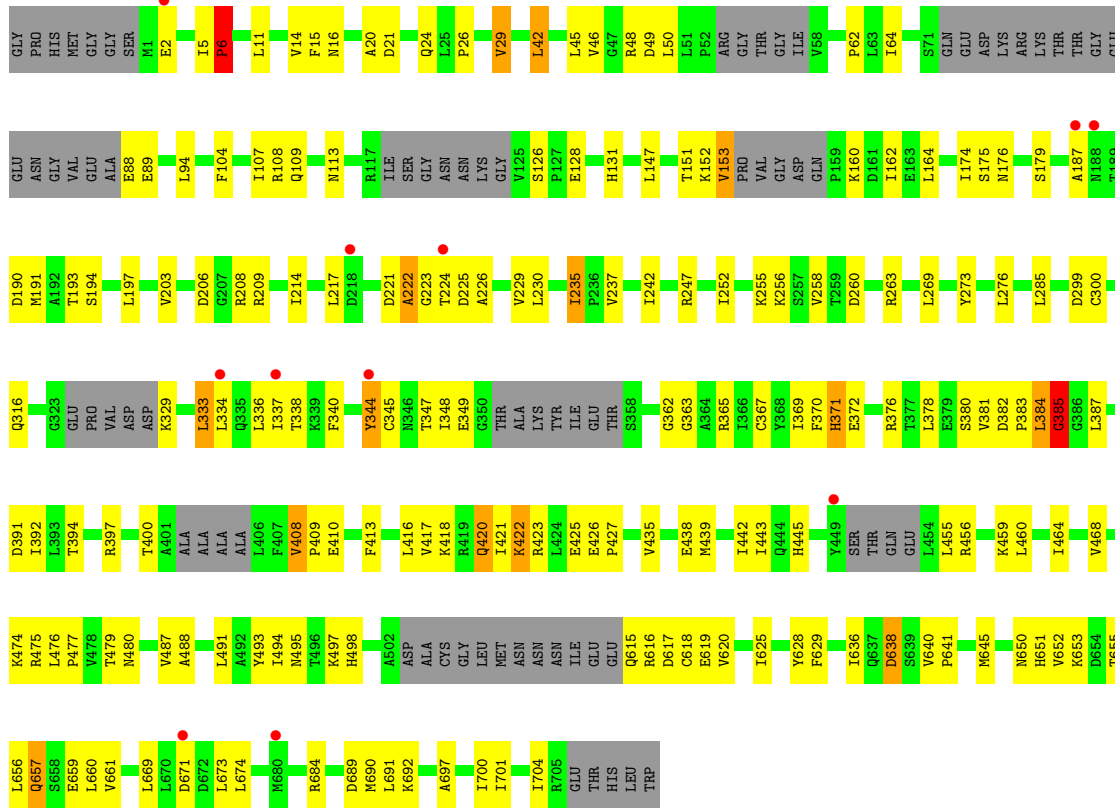




• Molecule 1: DYNAMIN 1-LIKE PROTEIN



• Molecule 1: DYNAMIN 1-LIKE PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.47Å 80.77Å 208.27Å 90.00° 93.45° 90.00°	Depositor
Resolution (Å)	47.57 – 3.48 48.54 – 3.48	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.57-3.48) 97.3 (48.54-3.48)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.48Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.251 , 0.276 0.251 , 0.278	Depositor DCC
R_{free} test set	2124 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtrriage
Anisotropy	0.207	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	17076	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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 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	0.31	0/4314	0.72	1/5830 (0.0%)
1	B	0.32	0/4366	0.76	7/5900 (0.1%)
1	C	0.39	3/4271 (0.1%)	0.81	16/5771 (0.3%)
1	D	0.34	1/4335 (0.0%)	0.77	8/5855 (0.1%)
All	All	0.34	4/17286 (0.0%)	0.76	32/23356 (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	B	0	1
1	C	0	2
1	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	LYS	CD-CE	7.11	1.69	1.51
1	C	160	LYS	CB-CG	7.11	1.71	1.52
1	D	6	PRO	CG-CD	6.52	1.72	1.50
1	C	160	LYS	CA-CB	5.12	1.65	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	LEU	CA-CB-CG	-9.36	93.78	115.30
1	D	387	LEU	CA-CB-CG	9.26	136.61	115.30
1	D	6	PRO	CA-N-CD	-8.55	99.52	111.50
1	B	334	LEU	CA-CB-CG	-8.02	96.86	115.30
1	D	385	GLY	C-N-CA	7.45	137.95	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	LEU	CB-CG-CD2	-7.21	98.75	111.00
1	C	160	LYS	CA-CB-CG	6.81	128.38	113.40
1	B	96	THR	N-CA-C	-6.58	93.25	111.00
1	C	638	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	D	638	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	B	301	LEU	CA-CB-CG	6.26	129.71	115.30
1	D	371	HIS	C-N-CA	-5.98	106.75	121.70
1	A	344	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	C	301	LEU	CA-CB-CG	5.89	128.85	115.30
1	B	15	PHE	CB-CG-CD2	5.85	124.89	120.80
1	C	382	ASP	C-N-CD	-5.82	107.79	120.60
1	C	164	LEU	CB-CG-CD1	5.78	120.82	111.00
1	D	344	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	B	344	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	C	344	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	B	15	PHE	CB-CG-CD1	-5.55	116.92	120.80
1	C	160	LYS	CD-CE-NZ	5.51	124.38	111.70
1	C	163	GLU	CB-CG-CD	-5.46	99.45	114.20
1	C	624	LEU	CA-CB-CG	5.41	127.75	115.30
1	C	160	LYS	CB-CG-CD	5.38	125.58	111.60
1	C	160	LYS	CG-CD-CE	-5.33	95.91	111.90
1	C	162	ILE	CA-CB-CG1	5.32	121.11	111.00
1	C	219	LEU	CA-CB-CG	5.28	127.45	115.30
1	B	691	LEU	CA-CB-CG	5.13	127.10	115.30
1	C	159	PRO	C-N-CA	5.11	134.47	121.70
1	D	370	PHE	C-N-CA	-5.06	109.06	121.70
1	D	384	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250	LEU	Peptide
1	C	361	CYS	Peptide
1	C	381	VAL	Peptide
1	D	385	GLY	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	4263	0	4407	139	0
1	B	4313	0	4462	145	0
1	C	4218	0	4382	157	0
1	D	4282	0	4448	127	0
All	All	17076	0	17699	548	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 16.

All (548) 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:616:ARG:HB2	1:A:619:GLU:HB2	1.43	0.99
1:B:249:GLN:HA	1:B:252:ILE:HB	1.53	0.90
1:A:214:ILE:HG13	1:A:241:ILE:HD11	1.54	0.89
1:B:175:SER:HA	1:B:203:VAL:HG11	1.62	0.81
1:A:113:ASN:ND2	1:C:231:MET:O	2.13	0.80
1:C:175:SER:HA	1:C:203:VAL:HG11	1.65	0.78
1:A:11:LEU:HD11	1:A:701:ILE:HD11	1.67	0.76
1:A:61:ARG:NH1	1:A:114:GLU:OE2	2.19	0.76
1:B:324:GLU:OE2	1:B:456:ARG:NE	2.18	0.75
1:D:616:ARG:HB3	1:D:619:GLU:HB2	1.67	0.74
1:B:468:VAL:HG22	1:B:656:LEU:HD11	1.70	0.72
1:C:447:SER:HB2	1:C:461:HIS:NE2	2.04	0.72
1:A:494:ILE:HG13	1:A:628:TYR:CE2	2.24	0.72
1:A:422:LYS:HG2	1:A:491:LEU:HD21	1.71	0.72
1:B:251:ASP:OD1	1:B:251:ASP:N	2.21	0.71
1:A:284:TYR:HD1	1:A:287:ARG:HH21	1.36	0.71
1:A:216:LYS:HB3	1:A:219:LEU:HD13	1.73	0.70
1:D:160:LYS:HG3	1:D:162:ILE:H	1.55	0.70
1:D:422:LYS:HG2	1:D:491:LEU:HD21	1.73	0.70
1:A:217:LEU:HB2	1:A:245:VAL:HG13	1.74	0.70
1:A:207:GLY:HA3	1:A:237:VAL:HA	1.73	0.70
1:B:494:ILE:HG13	1:B:628:TYR:CE2	2.27	0.69
1:C:4:LEU:HD22	1:C:297:ILE:HG22	1.74	0.69
1:C:235:ILE:HD11	1:C:241:ILE:HG12	1.74	0.69
1:C:394:THR:O	1:C:398:ASN:ND2	2.26	0.69
1:C:337:ILE:HD11	1:C:661:VAL:HG23	1.75	0.68
1:B:61:ARG:NH1	1:B:114:GLU:OE2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ARG:HD3	1:C:126:SER:HB3	1.74	0.68
1:C:494:ILE:HG13	1:C:628:TYR:CE2	2.29	0.68
1:D:175:SER:HA	1:D:203:VAL:HG11	1.77	0.67
1:C:152:LYS:HE2	1:C:195:GLU:HG2	1.76	0.67
1:A:175:SER:HA	1:A:203:VAL:HG11	1.75	0.66
1:B:174:ILE:HD11	1:B:181:ILE:HD13	1.77	0.66
1:B:382:ASP:O	1:B:423:ARG:NH2	2.28	0.66
1:C:61:ARG:NH2	1:C:114:GLU:O	2.26	0.66
1:B:129:PRO:HG2	1:B:131:HIS:HE1	1.60	0.66
1:D:362:GLY:HA3	1:D:442:ILE:HD11	1.77	0.66
1:A:16:ASN:HD22	1:A:94:LEU:HD23	1.61	0.66
1:C:620:VAL:HG22	1:C:624:LEU:HD11	1.77	0.66
1:C:163:GLU:HA	1:C:166:ILE:HD12	1.77	0.65
1:A:348:ILE:HD11	1:A:653:LYS:HE2	1.79	0.65
1:B:225:ASP:HB2	1:B:226:ALA:HA	1.79	0.65
1:C:1:MET:HG2	1:C:294:MET:HG2	1.79	0.65
1:A:176:ASN:HB3	1:A:179:SER:HB3	1.78	0.65
1:A:231:MET:SD	1:A:276:LEU:HD21	2.37	0.65
1:C:4:LEU:HD11	1:C:298:ARG:HB3	1.79	0.65
1:A:230:LEU:O	1:A:279:ARG:NH2	2.29	0.64
1:C:620:VAL:O	1:C:624:LEU:HD13	1.97	0.64
1:C:378:LEU:HA	1:C:381:VAL:HG23	1.80	0.64
1:A:378:LEU:O	1:A:381:VAL:HG12	1.97	0.64
1:A:468:VAL:HG22	1:A:656:LEU:HD11	1.80	0.64
1:C:49:ASP:OD1	1:C:247:ARG:NH2	2.31	0.64
1:A:456:ARG:HG2	1:A:680:MET:HE1	1.80	0.64
1:B:362:GLY:HA3	1:B:364:ALA:H	1.62	0.63
1:B:1:MET:HA	1:B:4:LEU:HD13	1.78	0.63
1:C:348:ILE:HD11	1:C:653:LYS:HE2	1.81	0.63
1:C:443:ILE:HD11	1:C:465:VAL:HA	1.81	0.63
1:A:361:CYS:HB3	1:A:363:GLY:H	1.64	0.63
1:B:348:ILE:HD11	1:B:653:LYS:HE2	1.80	0.62
1:C:93:PHE:HB3	1:C:95:HIS:CD2	2.34	0.62
1:D:468:VAL:HG22	1:D:656:LEU:HD11	1.80	0.62
1:C:153:VAL:HG11	1:C:159:PRO:HD2	1.79	0.62
1:B:336:LEU:HD21	1:B:455:LEU:HD22	1.81	0.62
1:A:271:LYS:HG3	1:A:272:LYS:H	1.64	0.62
1:A:361:CYS:HB3	1:A:363:GLY:N	2.15	0.62
1:C:620:VAL:HG22	1:C:624:LEU:CD1	2.29	0.62
1:B:337:ILE:HG22	1:B:464:ILE:HD11	1.82	0.62
1:A:642:LYS:NZ	1:B:490:GLU:HA	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ASP:OD1	1:C:162:ILE:N	2.34	0.61
1:B:273:TYR:HB3	1:B:276:LEU:HD12	1.82	0.61
1:A:667:SER:HA	1:A:670:LEU:HD13	1.83	0.61
1:B:420:GLN:OE1	1:B:423:ARG:NH1	2.32	0.61
1:C:129:PRO:HG2	1:C:131:HIS:HE1	1.65	0.61
1:B:365:ARG:NH1	1:B:438:GLU:HB2	2.16	0.61
1:C:207:GLY:HA3	1:C:237:VAL:HA	1.82	0.60
1:C:160:LYS:HA	1:C:164:LEU:HD12	1.83	0.60
1:D:382:ASP:OD2	1:D:423:ARG:NH2	2.35	0.60
1:D:494:ILE:HG13	1:D:628:TYR:CE2	2.37	0.60
1:A:64:ILE:HD12	1:A:131:HIS:CE1	2.37	0.59
1:C:95:HIS:HE1	1:C:110:GLU:OE2	1.85	0.59
1:A:105:ASP:OD1	1:A:108:ARG:NH1	2.36	0.59
1:A:378:LEU:HD23	1:A:637:GLN:HB3	1.85	0.59
1:A:61:ARG:HD2	1:A:118:ILE:HG12	1.86	0.58
1:D:29:VAL:HG21	1:D:174:ILE:HG22	1.85	0.58
1:A:336:LEU:HD21	1:A:455:LEU:HD21	1.86	0.58
1:A:421:ILE:HD12	1:A:632:VAL:HG11	1.86	0.58
1:C:185:THR:HG21	1:C:191:MET:HG2	1.85	0.58
1:C:618:CYS:HA	1:C:621:ILE:HG12	1.86	0.58
1:D:26:PRO:HB3	1:D:300:CYS:SG	2.43	0.58
1:D:697:ALA:HA	1:D:700:ILE:HD12	1.85	0.58
1:D:247:ARG:NH1	1:D:252:ILE:HG12	2.19	0.58
1:A:677:SER:HB3	1:A:680:MET:HG2	1.85	0.58
1:C:163:GLU:O	1:C:166:ILE:HB	2.04	0.58
1:D:16:ASN:HD22	1:D:94:LEU:HD23	1.69	0.57
1:A:501:PHE:O	1:A:505:CYS:HB2	2.03	0.57
1:C:174:ILE:HD11	1:C:181:ILE:HD13	1.86	0.57
1:D:179:SER:O	1:D:209:ARG:NH1	2.35	0.57
1:C:464:ILE:HG23	1:C:660:LEU:HD11	1.86	0.57
1:D:488:ALA:HA	1:D:491:LEU:HD13	1.86	0.57
1:C:621:ILE:HG13	1:C:622:GLU:N	2.20	0.57
1:A:117:ARG:HB2	1:A:117:ARG:NH1	2.20	0.56
1:D:340:PHE:HZ	1:D:443:ILE:HG23	1.70	0.56
1:B:456:ARG:O	1:B:458:PRO:HD3	2.05	0.56
1:A:117:ARG:HB2	1:A:117:ARG:HH11	1.70	0.56
1:B:489:ILE:HG13	1:B:490:GLU:OE1	2.05	0.56
1:D:247:ARG:HE	1:D:258:VAL:HG22	1.69	0.56
1:D:187:ALA:HA	1:D:191:MET:CE	2.36	0.56
1:D:94:LEU:HB2	1:D:131:HIS:HB2	1.87	0.56
1:A:60:ARG:HB3	1:A:125:VAL:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ASP:HA	1:B:504:ALA:HB3	1.86	0.56
1:A:29:VAL:HG21	1:A:174:ILE:HG22	1.87	0.55
1:A:8:ILE:HG13	1:A:297:ILE:HD13	1.88	0.55
1:B:658:SER:HA	1:B:661:VAL:HG13	1.87	0.55
1:C:103:ASP:O	1:C:106:GLU:HG2	2.07	0.55
1:D:260:ASP:OD1	1:D:263:ARG:NH2	2.39	0.55
1:B:476:LEU:O	1:B:480:ASN:ND2	2.40	0.55
1:A:645:MET:HG3	1:B:493:TYR:CD1	2.41	0.55
1:C:384:LEU:HD21	1:C:622:GLU:HG3	1.89	0.55
1:A:488:ALA:HA	1:A:491:LEU:HD13	1.88	0.55
1:C:382:ASP:OD2	1:C:423:ARG:NH2	2.34	0.55
1:B:503:ASP:HB3	1:B:504:ALA:C	2.26	0.54
1:C:96:THR:HG21	1:C:101:TYR:HE1	1.70	0.54
1:B:163:GLU:OE2	1:B:167:ARG:NH1	2.40	0.54
1:A:340:PHE:HE1	1:A:446:CYS:HB2	1.72	0.54
1:C:383:PRO:HB3	1:C:629:PHE:CD1	2.43	0.54
1:A:63:LEU:HA	1:A:130:ILE:HG23	1.89	0.54
1:B:229:VAL:HG23	1:B:234:VAL:O	2.08	0.54
1:B:423:ARG:HD2	1:C:372:GLU:CD	2.27	0.54
1:B:488:ALA:HA	1:B:491:LEU:HD13	1.90	0.54
1:A:417:VAL:HG11	1:A:628:TYR:HD2	1.72	0.54
1:B:162:ILE:O	1:B:165:GLN:HB2	2.08	0.54
1:D:413:PHE:O	1:D:417:VAL:HG12	2.07	0.54
1:D:247:ARG:HE	1:D:258:VAL:CG2	2.21	0.54
1:B:92:LYS:HE3	1:B:133:LYS:HD2	1.90	0.54
1:D:435:VAL:O	1:D:439:MET:HG3	2.08	0.54
1:A:176:ASN:HD22	1:A:179:SER:N	2.06	0.53
1:A:305:LYS:NZ	1:A:309:ASN:OD1	2.38	0.53
1:B:471:LEU:HA	1:B:474:LYS:HD3	1.89	0.53
1:C:160:LYS:HA	1:C:164:LEU:CD1	2.38	0.53
1:B:377:THR:HG22	1:C:380:SER:HB2	1.90	0.53
1:B:418:LYS:HD2	1:B:491:LEU:HA	1.91	0.53
1:B:418:LYS:NZ	1:B:490:GLU:O	2.42	0.53
1:D:378:LEU:HA	1:D:381:VAL:HG23	1.89	0.53
1:A:645:MET:O	1:A:650:ASN:HB2	2.08	0.53
1:B:26:PRO:HB2	1:B:297:ILE:HG22	1.90	0.53
1:B:250:LEU:HD23	1:B:253:ASN:HD21	1.74	0.53
1:A:85:VAL:N	1:A:86:GLU:HA	2.23	0.53
1:B:170:ILE:O	1:B:174:ILE:HG22	2.09	0.53
1:D:206:ASP:OD2	1:D:208:ARG:NH2	2.42	0.53
1:A:478:VAL:O	1:A:481:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:667:SER:HA	1:B:670:LEU:HD13	1.90	0.53
1:A:95:HIS:CD2	1:A:96:THR:HG23	2.44	0.53
1:B:49:ASP:HB3	1:B:247:ARG:NH2	2.24	0.53
1:A:305:LYS:HD3	1:A:701:ILE:HG21	1.90	0.52
1:A:361:CYS:CB	1:A:363:GLY:H	2.23	0.52
1:B:129:PRO:HG2	1:B:131:HIS:CE1	2.43	0.52
1:B:652:VAL:HA	1:B:655:THR:OG1	2.09	0.52
1:D:221:ASP:OD1	1:D:222:ALA:N	2.42	0.52
1:A:455:LEU:HB3	1:A:457:PHE:H	1.74	0.52
1:C:325:PRO:HB3	1:C:684:ARG:HH21	1.72	0.52
1:A:271:LYS:HG3	1:A:272:LYS:N	2.24	0.52
1:B:435:VAL:O	1:B:439:MET:HG3	2.10	0.52
1:D:426:GLU:HB3	1:D:427:PRO:HD3	1.91	0.52
1:B:362:GLY:HA3	1:B:364:ALA:N	2.24	0.52
1:A:435:VAL:O	1:A:439:MET:HG3	2.10	0.52
1:B:162:ILE:HG13	1:B:163:GLU:N	2.25	0.52
1:B:221:ASP:C	1:B:223:GLY:HA3	2.30	0.52
1:B:415:LEU:HD21	1:B:419:ARG:HH21	1.75	0.52
1:D:252:ILE:O	1:D:255:LYS:HB3	2.10	0.52
1:C:93:PHE:HB3	1:C:95:HIS:HD2	1.75	0.51
1:C:488:ALA:HA	1:C:491:LEU:HD13	1.92	0.51
1:C:630:LEU:HD21	1:C:634:LYS:HE3	1.91	0.51
1:C:421:ILE:HD13	1:C:629:PHE:CD2	2.44	0.51
1:D:347:THR:O	1:D:363:GLY:N	2.43	0.51
1:A:387:LEU:HD12	1:A:391:ASP:HB2	1.93	0.51
1:A:217:LEU:HB2	1:A:245:VAL:CG1	2.40	0.51
1:C:88:GLU:HG2	1:C:89:GLU:HG3	1.93	0.51
1:A:62:PRO:HB3	1:A:147:LEU:HD23	1.93	0.51
1:A:435:VAL:HG21	1:A:644:VAL:HG11	1.92	0.51
1:B:438:GLU:O	1:B:442:ILE:HG13	2.10	0.51
1:C:93:PHE:HB2	1:C:96:THR:HB	1.92	0.51
1:C:129:PRO:HG2	1:C:131:HIS:CE1	2.45	0.51
1:B:161:ASP:OD1	1:B:162:ILE:N	2.43	0.51
1:C:360:LEU:HB2	1:C:365:ARG:HD3	1.92	0.51
1:B:318:LEU:HG	1:B:322:TYR:CE2	2.45	0.51
1:C:645:MET:HG3	1:D:493:TYR:CD1	2.46	0.51
1:C:661:VAL:O	1:C:665:TYR:HB2	2.11	0.51
1:A:4:LEU:HD11	1:A:298:ARG:HB3	1.92	0.51
1:A:348:ILE:HG13	1:A:349:GLU:N	2.26	0.51
1:B:365:ARG:CZ	1:B:369:ILE:HD11	2.41	0.51
1:D:88:GLU:HG2	1:D:89:GLU:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:LEU:O	1:D:480:ASN:ND2	2.44	0.51
1:C:657:GLN:HA	1:C:657:GLN:NE2	2.25	0.50
1:B:228:ASP:HB2	1:B:233:ARG:O	2.10	0.50
1:D:42:LEU:HA	1:D:45:LEU:HD12	1.93	0.50
1:D:689:ASP:HA	1:D:692:LYS:HE3	1.93	0.50
1:D:160:LYS:HG2	1:D:162:ILE:HG22	1.94	0.50
1:D:242:ILE:HG21	1:D:285:LEU:HB2	1.93	0.50
1:B:217:LEU:HB2	1:B:245:VAL:HG13	1.94	0.50
1:A:460:LEU:HD12	1:A:673:LEU:HB3	1.93	0.50
1:C:346:ASN:O	1:C:350:GLY:N	2.43	0.50
1:A:671:ASP:OD1	1:A:672:ASP:N	2.45	0.50
1:B:457:PHE:HB2	1:B:460:LEU:HB3	1.93	0.50
1:C:392:ILE:HG23	1:C:621:ILE:HD11	1.94	0.50
1:C:49:ASP:O	1:C:108:ARG:NH1	2.45	0.50
1:C:53:ARG:HH11	1:C:53:ARG:HG3	1.76	0.50
1:C:127:PRO:HB3	1:C:172:ARG:NH2	2.27	0.50
1:C:645:MET:O	1:C:650:ASN:HB2	2.11	0.50
1:B:57:ILE:HG22	1:B:58:VAL:H	1.76	0.49
1:B:234:VAL:HG22	1:B:235:ILE:H	1.77	0.49
1:D:367:CYS:O	1:D:371:HIS:N	2.36	0.49
1:A:5:ILE:N	1:A:6:PRO:HD2	2.27	0.49
1:B:59:THR:HA	1:B:115:THR:HG21	1.94	0.49
1:B:176:ASN:HB3	1:B:179:SER:HB3	1.93	0.49
1:C:271:LYS:HG3	1:C:272:LYS:H	1.76	0.49
1:D:413:PHE:CE2	1:D:494:ILE:HD11	2.47	0.49
1:B:284:TYR:O	1:B:287:ARG:HG2	2.13	0.49
1:B:409:PRO:O	1:B:412:SER:OG	2.19	0.49
1:D:493:TYR:CE2	1:D:495:ASN:HB3	2.47	0.49
1:A:432:VAL:HG22	1:A:644:VAL:HG22	1.95	0.49
1:B:185:THR:HG21	1:B:191:MET:HG2	1.95	0.49
1:C:417:VAL:HG22	1:C:625:ILE:HG23	1.94	0.49
1:D:345:CYS:O	1:D:349:GLU:HG2	2.13	0.49
1:D:391:ASP:O	1:D:394:THR:HG22	2.12	0.49
1:D:417:VAL:HG22	1:D:421:ILE:HG13	1.93	0.49
1:A:362:GLY:HA2	1:A:442:ILE:HD11	1.93	0.49
1:C:345:CYS:O	1:C:349:GLU:HG2	2.12	0.49
1:C:439:MET:O	1:C:442:ILE:HG22	2.12	0.49
1:C:493:TYR:CD1	1:D:645:MET:HG3	2.47	0.49
1:C:621:ILE:HG13	1:C:622:GLU:H	1.78	0.49
1:D:62:PRO:HB3	1:D:147:LEU:HD23	1.94	0.49
1:D:230:LEU:HD22	1:D:276:LEU:HD13	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:GLU:OE1	1:C:324:GLU:N	2.45	0.49
1:C:421:ILE:HD13	1:C:629:PHE:HD2	1.78	0.49
1:A:48:ARG:NH1	1:A:89:GLU:OE1	2.41	0.49
1:A:426:GLU:HB3	1:A:427:PRO:HD3	1.94	0.49
1:C:276:LEU:HD23	1:C:279:ARG:NH2	2.28	0.49
1:D:337:ILE:HD11	1:D:661:VAL:HG22	1.95	0.49
1:A:230:LEU:HA	1:A:241:ILE:HG21	1.94	0.48
1:A:438:GLU:O	1:A:442:ILE:HG13	2.13	0.48
1:B:72:GLN:NE2	1:B:73:GLU:OE2	2.44	0.48
1:B:365:ARG:CZ	1:C:386:GLY:H	2.26	0.48
1:C:435:VAL:O	1:C:439:MET:HG3	2.13	0.48
1:A:408:VAL:O	1:A:411:VAL:HG12	2.12	0.48
1:B:300:CYS:O	1:B:303:GLU:HG2	2.12	0.48
1:D:460:LEU:HD23	1:D:673:LEU:HB3	1.95	0.48
1:A:442:ILE:O	1:A:445:HIS:HB3	2.13	0.48
1:B:702:ALA:O	1:B:703:GLU:HG2	2.13	0.48
1:C:101:TYR:HD2	1:C:106:GLU:HG3	1.78	0.48
1:D:372:GLU:OE2	1:D:376:ARG:NH2	2.40	0.48
1:A:436:HIS:CE1	1:A:476:LEU:HD11	2.48	0.48
1:C:198:LYS:O	1:C:201:ARG:HG2	2.13	0.48
1:D:15:PHE:O	1:D:20:ALA:HB2	2.14	0.48
1:D:126:SER:OG	1:D:128:GLU:OE1	2.30	0.48
1:A:4:LEU:CD1	1:A:298:ARG:HB3	2.43	0.48
1:C:161:ASP:OD1	1:C:162:ILE:HG22	2.14	0.48
1:D:48:ARG:NE	1:D:89:GLU:OE1	2.36	0.48
1:A:333:LEU:O	1:A:337:ILE:HB	2.13	0.48
1:D:333:LEU:O	1:D:337:ILE:HG12	2.13	0.48
1:A:307:ARG:O	1:A:311:LEU:HD13	2.14	0.48
1:B:297:ILE:HA	1:B:300:CYS:SG	2.54	0.48
1:B:329:LYS:O	1:B:332:THR:HG22	2.14	0.48
1:B:426:GLU:HB3	1:B:427:PRO:HD3	1.95	0.48
1:C:170:ILE:O	1:C:174:ILE:HG22	2.14	0.48
1:D:336:LEU:HD21	1:D:455:LEU:HG	1.96	0.48
1:B:323:GLY:HA2	1:B:324:GLU:HB3	1.95	0.48
1:B:378:LEU:HD23	1:B:637:GLN:HB2	1.96	0.48
1:B:417:VAL:HG22	1:B:625:ILE:HG23	1.95	0.48
1:C:348:ILE:HG13	1:C:349:GLU:N	2.29	0.48
1:D:217:LEU:HD21	1:D:273:TYR:CE1	2.49	0.48
1:D:438:GLU:O	1:D:442:ILE:HG13	2.14	0.48
1:C:61:ARG:CD	1:C:126:SER:HB3	2.42	0.47
1:C:98:ASN:O	1:C:100:LEU:HD12	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:TYR:CE2	1:A:495:ASN:HB3	2.49	0.47
1:D:381:VAL:HG11	1:D:629:PHE:HZ	1.78	0.47
1:D:615:GLN:OE1	1:D:615:GLN:HA	2.14	0.47
1:A:21:ASP:OD1	1:A:21:ASP:N	2.48	0.47
1:A:106:GLU:CD	1:C:279:ARG:HD3	2.34	0.47
1:B:493:TYR:CE2	1:B:495:ASN:HB3	2.49	0.47
1:C:421:ILE:HD12	1:C:632:VAL:HG11	1.96	0.47
1:D:222:ALA:HB3	1:D:224:THR:HG23	1.95	0.47
1:D:659:GLU:O	1:D:659:GLU:HG2	2.13	0.47
1:C:368:TYR:O	1:C:372:GLU:N	2.38	0.47
1:C:472:LEU:HD23	1:C:652:VAL:HG21	1.97	0.47
1:D:475:ARG:HD3	1:D:651:HIS:CE1	2.50	0.47
1:A:657:GLN:HA	1:A:657:GLN:NE2	2.30	0.47
1:B:226:ALA:HB1	1:B:229:VAL:CG1	2.44	0.47
1:C:455:LEU:HG	1:C:456:ARG:H	1.79	0.47
1:D:49:ASP:HB3	1:D:247:ARG:NH2	2.29	0.47
1:D:384:LEU:HB2	1:D:385:GLY:HA2	1.96	0.47
1:B:340:PHE:CD2	1:B:464:ILE:HG21	2.49	0.47
1:D:333:LEU:HG	1:D:674:LEU:HD21	1.97	0.47
1:D:348:ILE:HD11	1:D:653:LYS:HG3	1.97	0.47
1:D:392:ILE:HG21	1:D:618:CYS:HB2	1.97	0.47
1:B:421:ILE:HD12	1:B:632:VAL:HG11	1.96	0.47
1:D:417:VAL:HA	1:D:420:GLN:HB2	1.97	0.47
1:C:305:LYS:HD3	1:C:701:ILE:HG21	1.97	0.47
1:C:430:ARG:HG3	1:C:430:ARG:HH11	1.80	0.47
1:D:2:GLU:O	1:D:6:PRO:HD2	2.15	0.47
1:B:421:ILE:HD13	1:B:629:PHE:HD1	1.80	0.47
1:C:16:ASN:HB3	1:C:131:HIS:CE1	2.50	0.47
1:C:26:PRO:HB3	1:C:300:CYS:SG	2.55	0.47
1:C:158:GLN:N	1:C:159:PRO:HD3	2.30	0.47
1:C:493:TYR:CE2	1:C:495:ASN:HB3	2.50	0.47
1:C:475:ARG:O	1:C:479:THR:HG22	2.15	0.46
1:A:93:PHE:CE2	1:A:132:LEU:HD13	2.50	0.46
1:B:463:ALA:O	1:B:467:VAL:HG23	2.15	0.46
1:B:330:SER:HA	1:B:670:LEU:HD21	1.97	0.46
1:D:365:ARG:HG2	1:D:438:GLU:CD	2.36	0.46
1:A:333:LEU:CD2	1:A:460:LEU:HD11	2.46	0.46
1:B:334:LEU:HA	1:B:334:LEU:HD12	1.33	0.46
1:C:171:LEU:HA	1:C:174:ILE:HG22	1.95	0.46
1:C:235:ILE:CD1	1:C:241:ILE:HG12	2.42	0.46
1:D:5:ILE:HB	1:D:6:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:PHE:CE2	1:A:637:GLN:HA	2.50	0.46
1:B:151:THR:O	1:B:151:THR:HG22	2.16	0.46
1:B:225:ASP:CB	1:B:226:ALA:HA	2.42	0.46
1:B:193:THR:O	1:B:198:LYS:NZ	2.48	0.46
1:B:416:LEU:HD23	1:B:416:LEU:HA	1.76	0.46
1:C:340:PHE:CD2	1:C:464:ILE:HG21	2.51	0.46
1:C:697:ALA:HA	1:C:700:ILE:HD12	1.96	0.46
1:D:475:ARG:O	1:D:479:THR:HG22	2.15	0.46
1:A:493:TYR:CD1	1:B:645:MET:HG3	2.50	0.46
1:A:679:ASP:OD1	1:A:680:MET:N	2.49	0.46
1:C:438:GLU:HA	1:C:441:ARG:HD2	1.98	0.46
1:D:408:VAL:H	1:D:409:PRO:HD2	1.81	0.46
1:D:701:ILE:O	1:D:704:ILE:HG22	2.16	0.46
1:D:617:ASP:O	1:D:620:VAL:HG12	2.15	0.46
1:C:374:PHE:CE1	1:C:428:SER:HA	2.51	0.46
1:D:235:ILE:HG23	1:D:237:VAL:HG22	1.97	0.46
1:B:348:ILE:O	1:B:363:GLY:HA2	2.16	0.46
1:A:94:LEU:HB2	1:A:131:HIS:HB2	1.98	0.45
1:C:474:LYS:O	1:C:477:PRO:HD2	2.15	0.45
1:B:250:LEU:HD23	1:B:253:ASN:ND2	2.32	0.45
1:B:616:ARG:NH1	1:B:617:ASP:OD1	2.41	0.45
1:A:490:GLU:HA	1:B:642:LYS:NZ	2.30	0.45
1:C:242:ILE:HD12	1:C:284:TYR:HE2	1.82	0.45
1:D:464:ILE:O	1:D:468:VAL:HG23	2.17	0.45
1:A:418:LYS:O	1:A:422:LYS:HG3	2.16	0.45
1:A:642:LYS:HZ3	1:B:490:GLU:HA	1.82	0.45
1:B:28:ILE:HG12	1:B:180:ILE:HB	1.98	0.45
1:B:361:CYS:SG	1:B:362:GLY:N	2.89	0.45
1:C:435:VAL:HG21	1:C:644:VAL:HG11	1.97	0.45
1:A:642:LYS:HZ2	1:B:490:GLU:HA	1.80	0.45
1:D:651:HIS:CE1	1:D:655:THR:HG21	2.52	0.45
1:A:225:ASP:O	1:A:229:VAL:HG23	2.17	0.45
1:A:333:LEU:HD22	1:A:333:LEU:HA	1.61	0.45
1:A:378:LEU:O	1:A:633:ARG:HD2	2.17	0.45
1:C:460:LEU:HD12	1:C:673:LEU:HB3	1.99	0.45
1:D:348:ILE:HG13	1:D:349:GLU:N	2.31	0.45
1:A:370:PHE:CD2	1:A:641:PRO:HB3	2.51	0.45
1:C:101:TYR:CD2	1:C:106:GLU:HG3	2.51	0.45
1:C:316:GLN:N	1:C:691:LEU:HD21	2.32	0.45
1:C:333:LEU:HA	1:C:333:LEU:HD22	1.59	0.45
1:B:95:HIS:NE2	1:B:110:GLU:OE2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:THR:CG2	1:C:380:SER:HB2	2.47	0.45
1:D:24:GLN:HA	1:D:176:ASN:HD21	1.82	0.45
1:C:413:PHE:CZ	1:C:417:VAL:HG21	2.52	0.44
1:A:46:VAL:HG11	1:A:50:LEU:HD21	1.98	0.44
1:A:493:TYR:HB3	1:B:642:LYS:HG2	1.98	0.44
1:B:8:ILE:HG13	1:B:297:ILE:HG21	1.98	0.44
1:B:8:ILE:HD13	1:B:11:LEU:HD12	1.99	0.44
1:B:620:VAL:O	1:B:624:LEU:HG	2.17	0.44
1:C:64:ILE:HD12	1:C:131:HIS:NE2	2.31	0.44
1:C:126:SER:HA	1:C:127:PRO:HD3	1.78	0.44
1:A:100:LEU:HD13	1:C:291:ARG:NH2	2.33	0.44
1:B:5:ILE:HB	1:B:6:PRO:HD3	1.99	0.44
1:B:25:LEU:HA	1:B:26:PRO:HD3	1.78	0.44
1:D:194:SER:HB3	1:D:197:LEU:HD13	1.98	0.44
1:D:225:ASP:OD1	1:D:226:ALA:N	2.51	0.44
1:A:15:PHE:O	1:A:20:ALA:HB2	2.18	0.44
1:C:233:ARG:HA	1:C:234:VAL:HA	1.57	0.44
1:D:190:ASP:HB3	1:D:193:THR:HG22	1.98	0.44
1:A:231:MET:HA	1:A:279:ARG:HH22	1.83	0.44
1:B:62:PRO:HB3	1:B:147:LEU:HD23	2.00	0.44
1:B:340:PHE:HA	1:B:343:GLU:HG2	2.00	0.44
1:B:645:MET:O	1:B:650:ASN:HB2	2.17	0.44
1:C:162:ILE:HG23	1:C:163:GLU:N	2.33	0.44
1:A:104:PHE:CD2	1:A:107:ILE:HD12	2.53	0.44
1:A:463:ALA:O	1:A:467:VAL:HG23	2.18	0.44
1:B:168:GLU:O	1:B:172:ARG:HG3	2.17	0.44
1:B:209:ARG:HA	1:B:239:LEU:HD11	1.98	0.44
1:C:365:ARG:HG3	1:C:438:GLU:HG3	1.98	0.44
1:C:443:ILE:HD12	1:C:468:VAL:HB	2.00	0.44
1:D:235:ILE:CG2	1:D:237:VAL:HG22	2.47	0.44
1:A:148:PRO:HB2	1:A:166:ILE:HG23	1.99	0.44
1:B:226:ALA:O	1:B:229:VAL:HG12	2.18	0.44
1:C:374:PHE:CD1	1:C:431:CYS:HB2	2.53	0.44
1:D:256:LYS:HE3	1:D:256:LYS:HB2	1.83	0.44
1:A:242:ILE:HD12	1:A:284:TYR:HE2	1.82	0.43
1:A:365:ARG:HA	1:A:365:ARG:HD2	1.78	0.43
1:A:417:VAL:HG22	1:A:625:ILE:HG23	1.99	0.43
1:A:640:VAL:HB	1:A:641:PRO:HD3	1.99	0.43
1:C:486:LEU:O	1:C:489:ILE:HG12	2.17	0.43
1:B:10:LYS:HG3	1:B:700:ILE:HD13	2.00	0.43
1:C:301:LEU:N	1:C:302:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:GLN:NE2	1:D:113:ASN:OD1	2.48	0.43
1:D:657:GLN:OE1	1:D:657:GLN:HA	2.17	0.43
1:C:52:PRO:HD3	1:C:111:ILE:HG21	1.99	0.43
1:C:374:PHE:CZ	1:C:378:LEU:HD11	2.54	0.43
1:D:191:MET:HE1	1:D:214:ILE:HG23	2.00	0.43
1:A:297:ILE:HA	1:A:300:CYS:SG	2.59	0.43
1:B:305:LYS:O	1:B:308:ILE:HG13	2.19	0.43
1:B:322:TYR:HB3	1:B:684:ARG:HG2	2.00	0.43
1:A:336:LEU:HD21	1:A:455:LEU:HD11	2.00	0.43
1:A:381:VAL:HG22	1:A:423:ARG:NH2	2.34	0.43
1:B:152:LYS:HG2	1:B:195:GLU:HG3	1.99	0.43
1:D:316:GLN:NE2	1:D:691:LEU:HD21	2.32	0.43
1:B:71:SER:HA	1:B:72:GLN:HA	1.52	0.43
1:B:390:ILE:HG13	1:B:391:ASP:N	2.33	0.43
1:D:333:LEU:HD23	1:D:333:LEU:HA	1.76	0.43
1:D:365:ARG:O	1:D:369:ILE:HG13	2.19	0.43
1:A:106:GLU:OE1	1:C:279:ARG:HD3	2.18	0.43
1:B:303:GLU:O	1:B:306:THR:OG1	2.30	0.43
1:C:8:ILE:HD11	1:C:26:PRO:HD2	2.01	0.43
1:C:221:ASP:O	1:C:224:THR:HG22	2.19	0.43
1:C:390:ILE:HD12	1:C:390:ILE:H	1.84	0.43
1:C:62:PRO:HG3	1:C:169:LEU:HD21	2.00	0.43
1:C:188:ASN:OD1	1:C:219:LEU:HB2	2.18	0.43
1:D:413:PHE:HE1	1:D:625:ILE:N	2.16	0.43
1:A:114:GLU:HA	1:A:117:ARG:NH1	2.33	0.43
1:A:636:ILE:HG23	1:A:640:VAL:CG2	2.49	0.43
1:A:475:ARG:HD3	1:A:651:HIS:CE1	2.54	0.43
1:B:628:TYR:O	1:B:631:ILE:HG13	2.19	0.43
1:C:93:PHE:CZ	1:C:132:LEU:HD13	2.54	0.43
1:C:417:VAL:O	1:C:420:GLN:N	2.52	0.43
1:D:348:ILE:HD11	1:D:653:LYS:HE2	2.00	0.43
1:A:185:THR:O	1:A:214:ILE:HA	2.20	0.42
1:C:163:GLU:O	1:C:167:ARG:HG2	2.19	0.42
1:C:371:HIS:NE2	1:D:497:LYS:HB2	2.34	0.42
1:D:474:LYS:O	1:D:477:PRO:HD2	2.19	0.42
1:A:305:LYS:HD3	1:A:701:ILE:CG2	2.49	0.42
1:B:181:ILE:HD12	1:B:210:THR:OG1	2.19	0.42
1:C:164:LEU:HD23	1:C:167:ARG:HG3	2.00	0.42
1:A:11:LEU:HA	1:A:11:LEU:HD23	1.84	0.42
1:A:341:ALA:O	1:A:344:TYR:HB3	2.20	0.42
1:B:60:ARG:H	1:B:115:THR:HG23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ILE:HD11	1:D:653:LYS:CG	2.49	0.42
1:A:8:ILE:HD13	1:A:11:LEU:HD12	2.01	0.42
1:A:176:ASN:HB3	1:A:179:SER:CB	2.46	0.42
1:A:327:ASP:OD1	1:A:327:ASP:N	2.53	0.42
1:B:225:ASP:HB2	1:B:228:ASP:OD1	2.18	0.42
1:D:344:TYR:CZ	1:D:348:ILE:HG21	2.55	0.42
1:A:71:SER:HB2	1:A:137:PRO:HB3	2.02	0.42
1:A:242:ILE:HD12	1:A:284:TYR:CE2	2.55	0.42
1:A:377:THR:OG1	1:A:378:LEU:N	2.52	0.42
1:B:475:ARG:O	1:B:479:THR:HG22	2.19	0.42
1:C:652:VAL:HA	1:C:655:THR:OG1	2.20	0.42
1:D:152:LYS:HG3	1:D:153:VAL:HB	2.01	0.42
1:C:271:LYS:HG3	1:C:272:LYS:N	2.34	0.42
1:D:221:ASP:O	1:D:223:GLY:N	2.53	0.42
1:D:329:LYS:NZ	1:D:671:ASP:OD1	2.52	0.42
1:D:378:LEU:HD21	1:D:636:ILE:HG22	2.02	0.42
1:D:416:LEU:HD23	1:D:416:LEU:HA	1.81	0.42
1:D:495:ASN:OD1	1:D:498:HIS:HB2	2.20	0.42
1:A:241:ILE:O	1:A:242:ILE:HD13	2.20	0.42
1:A:438:GLU:OE1	1:A:441:ARG:NH1	2.53	0.42
1:D:226:ALA:HB1	1:D:229:VAL:HG12	2.02	0.42
1:D:260:ASP:CG	1:D:263:ARG:HH21	2.22	0.42
1:D:456:ARG:HH12	1:D:684:ARG:HH22	1.66	0.42
1:B:392:ILE:HG21	1:B:618:CYS:SG	2.59	0.42
1:B:640:VAL:HB	1:B:641:PRO:HD3	2.00	0.42
1:D:442:ILE:O	1:D:445:HIS:HB3	2.20	0.42
1:B:272:LYS:HE2	1:B:272:LYS:HB3	1.91	0.42
1:D:64:ILE:HD12	1:D:131:HIS:NE2	2.35	0.42
1:D:334:LEU:O	1:D:338:THR:OG1	2.28	0.42
1:B:191:MET:HB2	1:B:226:ALA:HB2	2.01	0.42
1:A:64:ILE:HG12	1:A:145:VAL:HG22	2.02	0.41
1:A:417:VAL:O	1:A:421:ILE:HG12	2.20	0.41
1:D:376:ARG:O	1:D:380:SER:HB3	2.19	0.41
1:A:4:LEU:HD21	1:A:301:LEU:HD22	2.02	0.41
1:A:620:VAL:HG23	1:A:621:ILE:N	2.35	0.41
1:D:176:ASN:HB3	1:D:179:SER:OG	2.19	0.41
1:D:645:MET:O	1:D:650:ASN:HB2	2.20	0.41
1:B:181:ILE:HB	1:B:210:THR:HA	2.01	0.41
1:C:229:VAL:HA	1:C:233:ARG:O	2.20	0.41
1:D:640:VAL:HB	1:D:641:PRO:HD3	2.01	0.41
1:B:616:ARG:N	1:B:619:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:N	1:C:6:PRO:HD2	2.36	0.41
1:C:60:ARG:HD3	1:C:125:VAL:HG12	2.02	0.41
1:C:128:GLU:H	1:C:128:GLU:HG2	1.60	0.41
1:C:242:ILE:HD12	1:C:284:TYR:CE2	2.56	0.41
1:D:187:ALA:HA	1:D:191:MET:HE2	2.02	0.41
1:B:342:THR:C	1:B:344:TYR:H	2.23	0.41
1:C:338:THR:O	1:C:341:ALA:HB3	2.19	0.41
1:A:180:ILE:HD13	1:A:292:LEU:HD23	2.02	0.41
1:A:475:ARG:O	1:A:479:THR:HG22	2.20	0.41
1:B:60:ARG:H	1:B:115:THR:CG2	2.33	0.41
1:B:226:ALA:HB1	1:B:229:VAL:HG12	2.02	0.41
1:C:90:TRP:HZ3	1:C:92:LYS:HE3	1.86	0.41
1:C:124:GLY:HA3	1:C:162:ILE:CD1	2.51	0.41
1:C:185:THR:CG2	1:C:191:MET:HG2	2.50	0.41
1:D:46:VAL:HG21	1:D:50:LEU:HD21	2.03	0.41
1:D:413:PHE:HE2	1:D:494:ILE:HD11	1.84	0.41
1:D:417:VAL:HG13	1:D:418:LYS:N	2.35	0.41
1:D:652:VAL:HA	1:D:655:THR:OG1	2.20	0.41
1:D:656:LEU:O	1:D:660:LEU:HB3	2.21	0.41
1:C:61:ARG:HA	1:C:62:PRO:HD3	1.93	0.41
1:C:218:ASP:OD1	1:C:218:ASP:N	2.52	0.41
1:D:225:ASP:OD1	1:D:273:TYR:OH	2.25	0.41
1:A:333:LEU:HD21	1:A:460:LEU:HD11	2.03	0.41
1:A:455:LEU:HA	1:A:456:ARG:HB2	2.02	0.41
1:B:322:TYR:O	1:B:324:GLU:HB2	2.21	0.41
1:B:333:LEU:O	1:B:337:ILE:HG12	2.21	0.41
1:B:365:ARG:NE	1:C:386:GLY:H	2.19	0.41
1:C:660:LEU:O	1:C:664:LEU:HB2	2.20	0.41
1:D:459:LYS:HD2	1:D:459:LYS:HA	1.75	0.41
1:D:669:LEU:H	1:D:669:LEU:HD23	1.86	0.41
1:A:340:PHE:HZ	1:A:443:ILE:HG23	1.85	0.41
1:B:4:LEU:HB3	1:B:297:ILE:CD1	2.51	0.41
1:B:365:ARG:NH2	1:C:386:GLY:H	2.18	0.41
1:B:444:GLN:HA	1:B:447:SER:HB2	2.02	0.41
1:B:680:MET:HE3	1:B:683:ARG:HD2	2.03	0.41
1:C:340:PHE:HA	1:C:343:GLU:CD	2.40	0.41
1:C:374:PHE:HE1	1:C:428:SER:HA	1.86	0.41
1:C:640:VAL:HB	1:C:641:PRO:HD3	2.01	0.41
1:A:300:CYS:O	1:A:303:GLU:HG2	2.21	0.41
1:A:457:PHE:N	1:A:458:PRO:HD3	2.36	0.41
1:B:417:VAL:HG11	1:B:628:TYR:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:LEU:HA	1:C:416:LEU:HD23	1.77	0.41
1:B:233:ARG:HA	1:B:234:VAL:HA	1.92	0.40
1:B:273:TYR:N	1:B:274:PRO:HD3	2.37	0.40
1:B:376:ARG:O	1:B:379:GLU:HG2	2.22	0.40
1:B:425:GLU:HA	1:B:487:VAL:HG21	2.02	0.40
1:B:491:LEU:H	1:B:491:LEU:HD12	1.86	0.40
1:C:194:SER:HB3	1:C:197:LEU:HD13	2.03	0.40
1:C:333:LEU:O	1:C:337:ILE:HG12	2.21	0.40
1:C:370:PHE:CD2	1:C:641:PRO:HB3	2.56	0.40
1:D:104:PHE:CD2	1:D:107:ILE:HD12	2.56	0.40
1:D:383:PRO:HB3	1:D:629:PHE:CD1	2.56	0.40
1:D:397:ARG:HB2	1:D:397:ARG:NH1	2.36	0.40
1:D:425:GLU:HA	1:D:487:VAL:HG21	2.03	0.40
1:A:129:PRO:HG2	1:A:131:HIS:HE1	1.87	0.40
1:C:341:ALA:O	1:C:344:TYR:HB3	2.20	0.40
1:C:623:ARG:HD2	1:C:623:ARG:HA	1.80	0.40
1:A:471:LEU:HD11	1:A:655:THR:HG22	2.02	0.40
1:B:88:GLU:H	1:B:88:GLU:CD	2.25	0.40
1:A:230:LEU:O	1:A:230:LEU:HD23	2.22	0.40
1:B:377:THR:OG1	1:B:378:LEU:N	2.53	0.40
1:C:410:GLU:HA	1:C:413:PHE:HB3	2.02	0.40
1:D:21:ASP:OD1	1:D:21:ASP:N	2.48	0.40
1:A:425:GLU:HA	1:A:487:VAL:HG21	2.03	0.40
1:B:374:PHE:CD1	1:B:431:CYS:HB2	2.56	0.40
1:C:25:LEU:HA	1:C:26:PRO:HD3	1.81	0.40
1:C:30:VAL:HG22	1:C:182:LEU:HD23	2.03	0.40
1:C:50:LEU:C	1:C:108:ARG:HG2	2.42	0.40
1:D:11:LEU:HD23	1:D:11:LEU:HA	1.90	0.40
1:D:160:LYS:CG	1:D:162:ILE:HG22	2.51	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	518/617 (84%)	487 (94%)	28 (5%)	3 (1%)	25	63
1	B	529/617 (86%)	497 (94%)	31 (6%)	1 (0%)	47	80
1	C	512/617 (83%)	479 (94%)	30 (6%)	3 (1%)	25	63
1	D	520/617 (84%)	498 (96%)	20 (4%)	2 (0%)	34	70
All	All	2079/2468 (84%)	1961 (94%)	109 (5%)	9 (0%)	34	70

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	222	ALA
1	A	323	GLY
1	B	665	TYR
1	A	387	LEU
1	C	19	GLY
1	C	665	TYR
1	C	162	ILE
1	A	236	PRO
1	D	408	VAL

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	484/546 (89%)	471 (97%)	13 (3%)	44	72
1	B	488/546 (89%)	467 (96%)	21 (4%)	29	61
1	C	480/546 (88%)	461 (96%)	19 (4%)	31	62
1	D	487/546 (89%)	468 (96%)	19 (4%)	32	63
All	All	1939/2184 (89%)	1867 (96%)	72 (4%)	34	64

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	108	ARG

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Mol	Chain	Res	Type
1	A	130	ILE
1	A	163	GLU
1	A	164	LEU
1	A	299	ASP
1	A	306	THR
1	A	333	LEU
1	A	420	GLN
1	A	505	CYS
1	A	638	ASP
1	A	657	GLN
1	A	668	SER
1	B	14	VAL
1	B	23	ILE
1	B	57	ILE
1	B	70	VAL
1	B	86	GLU
1	B	88	GLU
1	B	98	ASN
1	B	108	ARG
1	B	163	GLU
1	B	164	LEU
1	B	235	ILE
1	B	251	ASP
1	B	299	ASP
1	B	324	GLU
1	B	365	ARG
1	B	422	LYS
1	B	501	PHE
1	B	638	ASP
1	B	661	VAL
1	B	674	LEU
1	B	691	LEU
1	C	14	VAL
1	C	29	VAL
1	C	96	THR
1	C	163	GLU
1	C	219	LEU
1	C	299	ASP
1	C	326	VAL
1	C	333	LEU
1	C	342	THR
1	C	391	ASP

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Mol	Chain	Res	Type
1	C	412	SER
1	C	623	ARG
1	C	624	LEU
1	C	638	ASP
1	C	648	LEU
1	C	657	GLN
1	C	661	VAL
1	C	665	TYR
1	C	675	THR
1	D	6	PRO
1	D	14	VAL
1	D	29	VAL
1	D	42	LEU
1	D	108	ARG
1	D	151	THR
1	D	153	VAL
1	D	164	LEU
1	D	235	ILE
1	D	269	LEU
1	D	299	ASP
1	D	333	LEU
1	D	400	THR
1	D	410	GLU
1	D	420	GLN
1	D	422	LYS
1	D	638	ASP
1	D	657	GLN
1	D	690	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	B	131	HIS
1	B	253	ASN
1	B	651	HIS
1	C	95	HIS
1	C	113	ASN
1	C	131	HIS
1	D	16	ASN
1	D	141	ASN
1	D	420	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 monosaccharides 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	540/617 (87%)	0.06	6 (1%) 80 76	4, 48, 90, 140	0
1	B	547/617 (88%)	0.20	16 (2%) 51 48	8, 58, 105, 141	0
1	C	534/617 (86%)	0.10	12 (2%) 62 58	8, 59, 104, 128	0
1	D	540/617 (87%)	0.11	11 (2%) 65 61	9, 54, 97, 126	0
All	All	2161/2468 (87%)	0.12	45 (2%) 63 60	4, 54, 102, 141	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	617	ASP	4.3
1	A	679	ASP	4.2
1	C	249	GLN	4.2
1	D	671	ASP	4.1
1	B	151	THR	3.6
1	D	449	TYR	3.4
1	C	664	LEU	3.4
1	B	315	TYR	3.4
1	B	361	CYS	3.1
1	C	447	SER	3.1
1	D	344	TYR	3.0
1	B	444	GLN	3.0
1	B	3	ALA	3.0
1	D	224	THR	3.0
1	D	2	GLU	3.0
1	A	361	CYS	2.9
1	B	337	ILE	2.8
1	B	673	LEU	2.8
1	B	447	SER	2.8
1	C	53	ARG	2.7
1	D	218	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	448	ASN	2.7
1	D	337	ILE	2.7
1	B	329	LYS	2.6
1	B	295	HIS	2.6
1	D	188	ASN	2.6
1	C	449	TYR	2.6
1	B	664	LEU	2.5
1	B	302	PRO	2.4
1	D	334	LEU	2.4
1	C	15	PHE	2.4
1	D	187	ALA	2.4
1	A	677	SER	2.3
1	B	440	GLN	2.3
1	C	387	LEU	2.3
1	A	344	TYR	2.3
1	B	223	GLY	2.2
1	D	680	MET	2.2
1	C	344	TYR	2.2
1	A	333	LEU	2.2
1	C	663	GLN	2.2
1	B	26	PRO	2.1
1	C	396	ILE	2.0
1	A	53	ARG	2.0
1	C	104	PHE	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 monosaccharides 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.