Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 11:49 PM EDT

PDB ID	:	5OWV
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 (i) 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 (1)) were used in the production of this report:

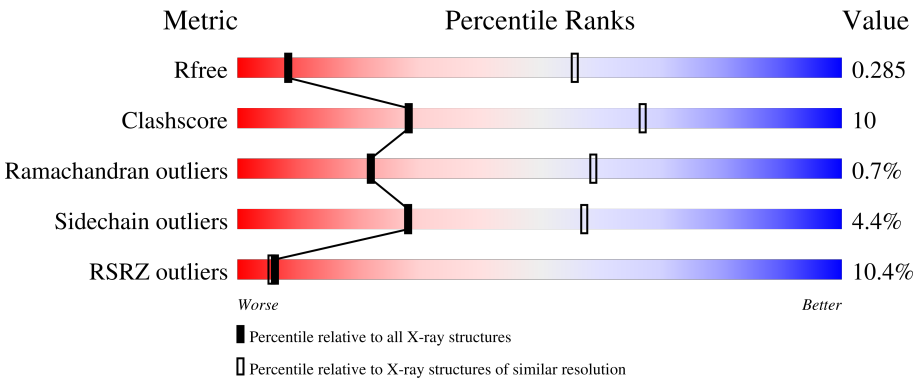
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

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 <=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	9% 65% 14% • 20%
2	C	614	10% 74% 21% • •
2	D	614	9% 68% 25% • •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	699	5021	3179	858	970	14	0	0	0
1	B	587	4436	2828	739	855	14	0	0	0

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
			Total	C	N	O	S			
2	C	598	4959	3206	799	943	11	0	0	0
2	D	598	4959	3206	799	943	11	0	0	0

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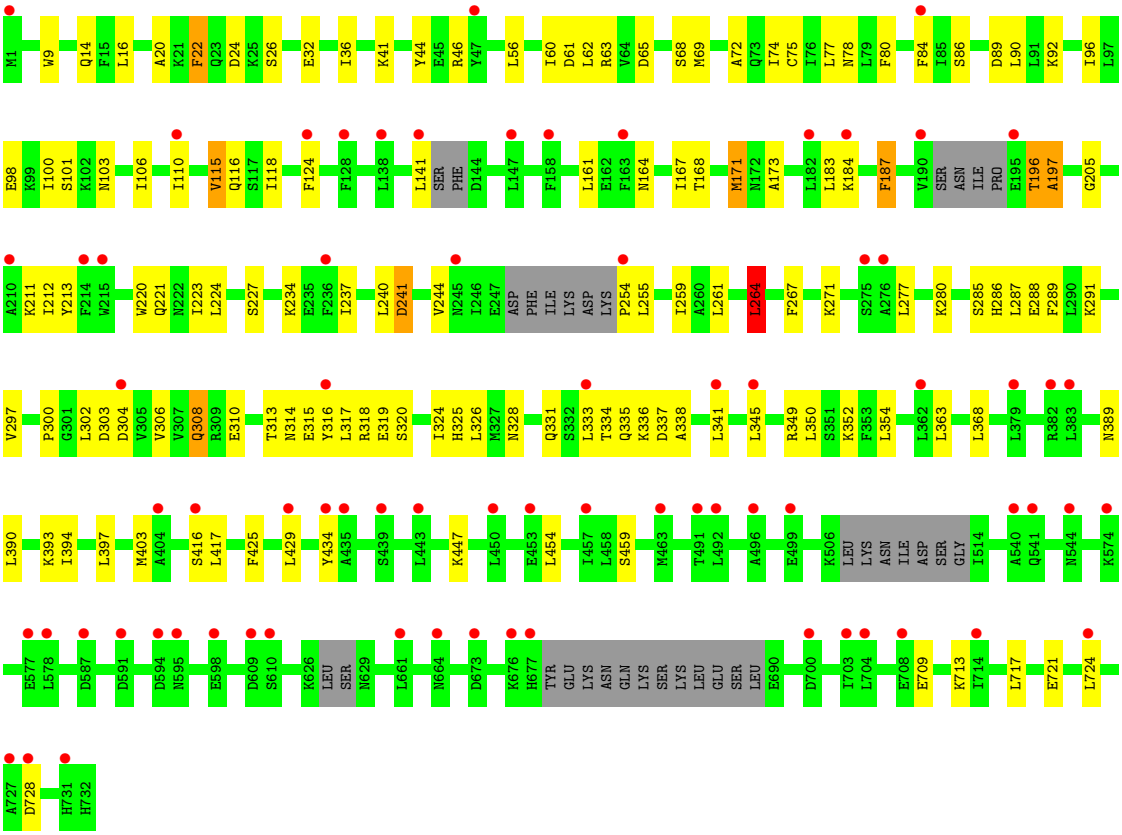
Chain	Residue	Modelled	Actual	Comment	Reference
C	611	HIS	-	expression tag	UNP A0A1D9BKH6
D	-2	GLY	-	expression tag	UNP A0A1D9BKH6
D	-1	SER	-	expression tag	UNP A0A1D9BKH6
D	0	HIS	-	expression tag	UNP A0A1D9BKH6
D	610	HIS	-	expression tag	UNP A0A1D9BKH6
D	611	HIS	-	expression tag	UNP A0A1D9BKH6

3 Residue-property plots (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.

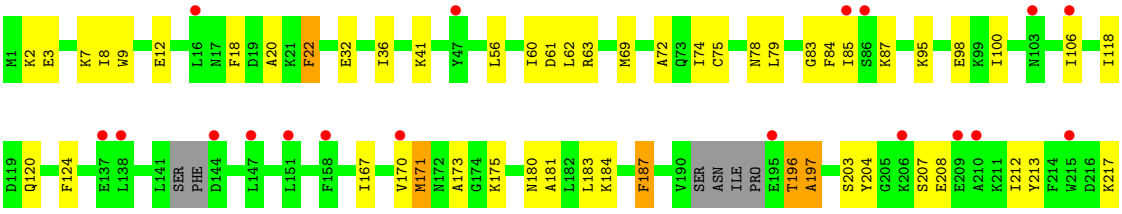
• Molecule 1: GTP-binding protein

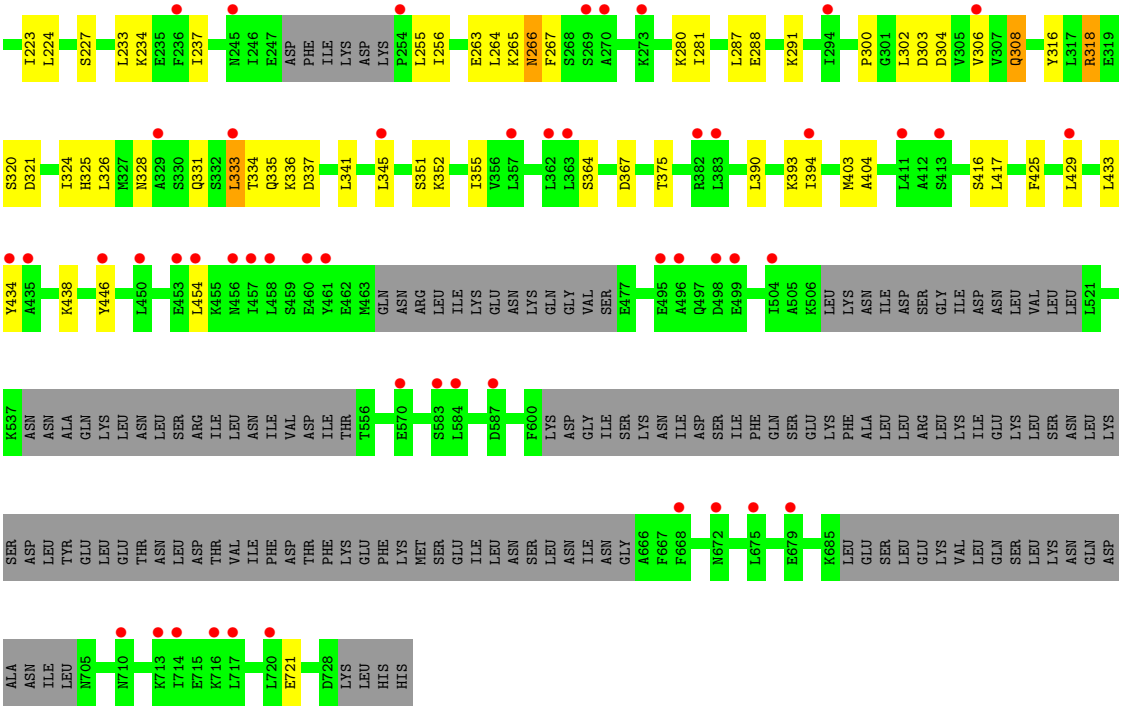
Chain A:



• Molecule 1: GTP-binding protein

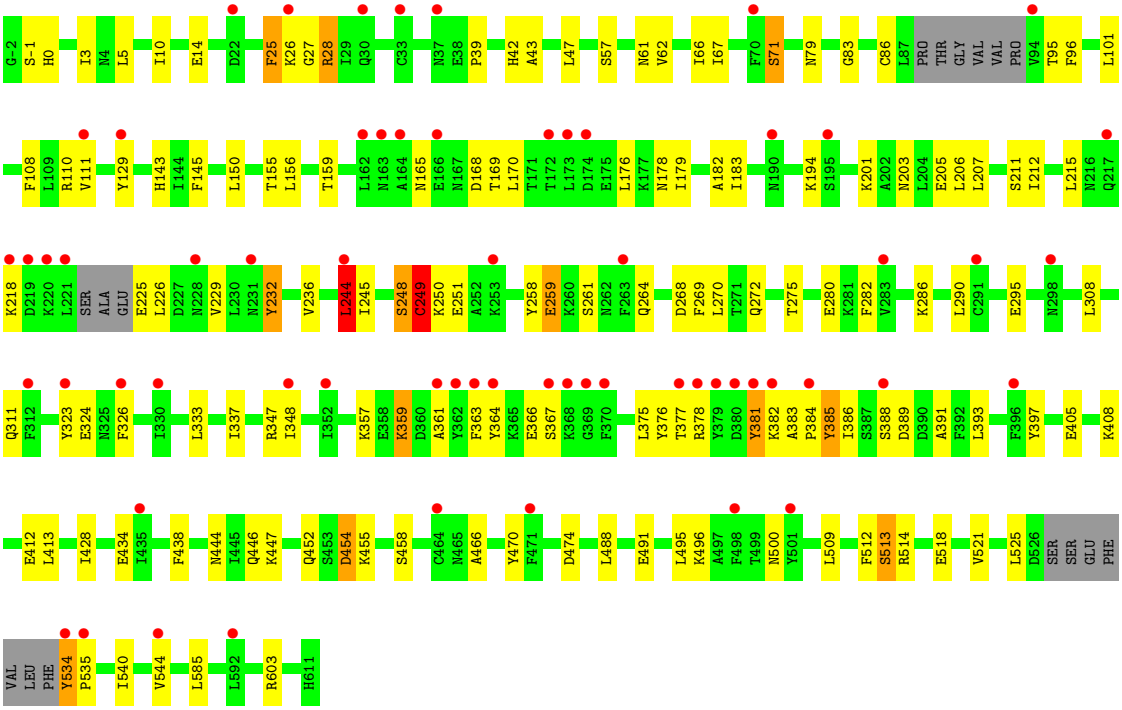
Chain B:





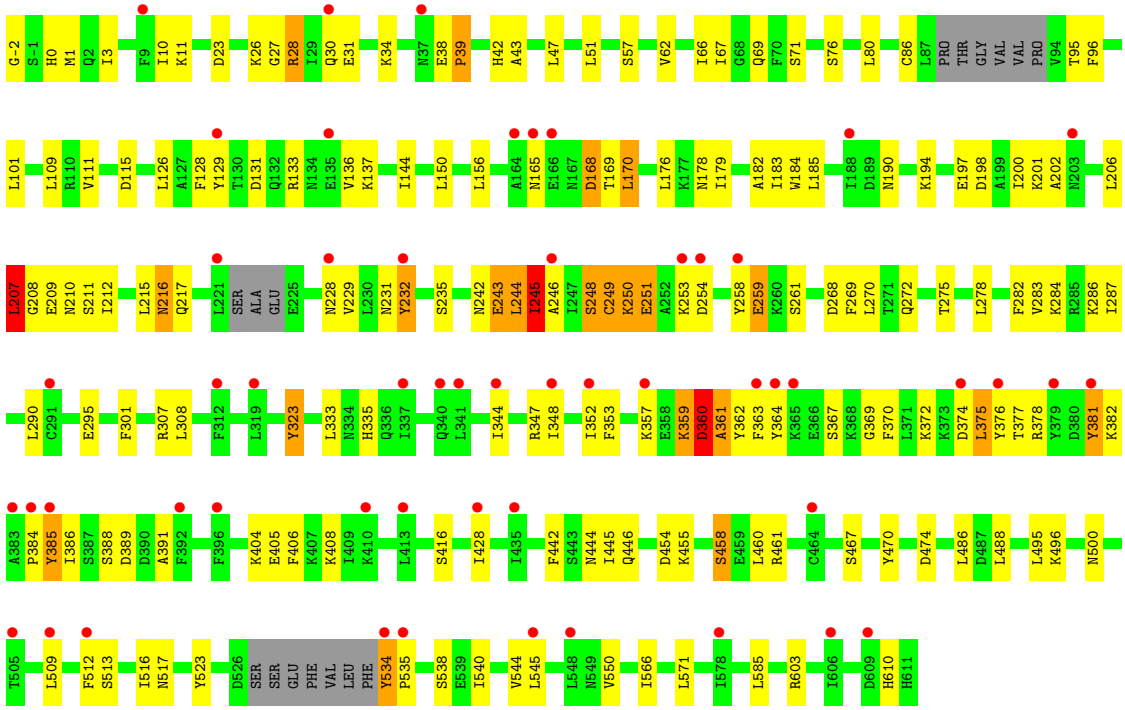
- Molecule 2: GTP-binding protein

Chain C:



- Molecule 2: GTP-binding protein

Chain D:


G-2 S-1 H0 M1 Q2 I3 F9 I10 K11 D23 K26 G27 R28 I29 Q30 E31 K34 N37 E38 P39 H42 A43 L47 L51 S57 V62 I66 I67 G68 Q69 F70 S71 S76 L80 C86 L87 PRO THR GLY VAL VAL PRO V94 T95 F96
L101 L109 R110 V111 D115 L126 A127 F128 Y129 T130 D131 Q132 R133 N134 E135 V136 K137 I144 L150 L156 A164 N165 E166 N167 D168 T169 L170 L176 K177 N178 I179 A182 I183 W184 L185 I188 D189 N190 K194 E197 D198 A199 I200 K201 A202 N203 L206
L207 G208 E209 N210 S211 I212 L215 N216 Q217 L221 SER ALA GLU E225 N228 V229 L230 N231 Y232 S235 N242 E243 L244 I245 A246 I247 S248 C249 K250 E251 A252 K253 D254 Y258 E259 K260 S261 D268 F269 L270 T271 Q272 T275 L278 F282 V283 K284 R285 K286 I287
L290 C291 E295 F301 R307 L308 F312 L319 Y323 L333 N334 H335 Q336 I337 Q340 L341 I344 R347 I348 I352 F353 K357 E358 K359 D360 A361 Y362 F363 Y364 K365 E366 S367 K368 G369 F370 L371 K372 K373 D374 L375 Y376 T377 R378 Y379 D380 Y381 K382
A383 P384 Y385 I386 S387 S388 D389 D390 A391 F392 F396 K404 E405 F406 K407 K408 I409 K410 L413 S416 I428 I435 F442 S443 N444 I445 Q446 D454 K455 S458 E459 L460 R461 C464 S467 Y470 D474 L486 D487 L488 L495 K496 N500
T505 L509 F512 S513 I516 N517 Y523 D526 SER SER GLU PHE VAL LEU PHE Y534 P535 S538 E539 I540 V544 L545 L548 N549 V550 I566 L571 I578 L585 R603 I606 D609 H610 H611

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.62 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.259 , 0.286 0.258 , 0.285	Depositor DCC
R_{free} test set	4195 reflections (4.90%)	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)	0.33 , 202.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.26	0/5069	0.47	1/6846 (0.0%)
1	B	0.26	0/4480	0.46	0/6024
2	C	0.29	0/5044	0.53	2/6771 (0.0%)
2	D	0.29	0/5044	0.55	1/6771 (0.0%)
All	All	0.27	0/19637	0.51	4/26412 (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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	207	LEU	CA-CB-CG	8.76	135.44	115.30
2	C	244	LEU	CA-CB-CG	-6.75	99.78	115.30
1	A	264	LEU	CB-CG-CD2	-5.71	101.29	111.00
2	C	5	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	196	THR	Peptide
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 (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	5021	0	4509	86	0
1	B	4436	0	4219	73	0
2	C	4959	0	5000	103	0
2	D	4959	0	5000	134	0
All	All	19375	0	18728	375	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 (375) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:364:TYR:HE1	2:D:364:TYR:CD2	1.59	1.14
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:GLU:OE1	2:D:603:ARG:NH1	2.27	0.68
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: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
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
2:D:216:ASN:ND2	2:D:250:LYS:HB3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:208:GLY:C	2:D:209:GLU:OE1	2.49	0.51
2:D:388:SER:HA	2:D:509:LEU:HG	1.93	0.51
1:B:95:LYS:O	1:B:98:GLU:HB2	2.11	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:A:62:LEU:HD13	1:A:69:MET:HE1	1.93	0.51
1:A:96:ILE:HG23	1:A:389:ASN:HD22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
1:B:303:ASP:CG	1:B:304:ASP:H	2.15	0.48
2:C:357:LYS:HB2	2:C:385:TYR:CD2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:26:LYS:HE2	2:D:30:GLN:CD	2.35	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
1:B:62:LEU:HD13	1:B:69:MET:HE1	1.97	0.46
1:A:303:ASP:CG	1:A:304:ASP:H	2.19	0.46
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:67:ILE:HD11	2:C:206:LEU:CD2	2.46	0.45
2:C:182:ALA:O	2:C:211:SER:OG	2.21	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
2:C:203:ASN:C	2:C:205:GLU:H	2.21	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
1:A:288:GLU:HG3	1:A:289:PHE:N	2.32	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:367:SER:OG	2:C:377:THR:HG23	2.18	0.43
2:D:27:GLY:C	2:D:28:ARG:HD2	2.38	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: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:C:27:GLY:C	2:C:28:ARG:HD2	2.39	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:187:PHE:HZ	1:A:285:SER:HG	1.67	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
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: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
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:B:2:LYS:HB2	1:B:18:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D:428:ILE:HD13	2:D:428:ILE:HA	1.85	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
1:A:24:ASP:C	1:A:26:SER:H	2.24	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
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: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:C:79:ASN:O	2:C:83:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	25	61
1	B	569/732 (78%)	514 (90%)	53 (9%)	2 (0%)	34	69
2	C	590/614 (96%)	526 (89%)	59 (10%)	5 (1%)	19	56
2	D	590/614 (96%)	533 (90%)	50 (8%)	7 (1%)	13	48
All	All	2434/2692 (90%)	2200 (90%)	216 (9%)	18 (1%)	22	59

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

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Mol	Chain	Res	Type
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 (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	448/683 (66%)	434 (97%)	14 (3%)	40	65
1	B	440/683 (64%)	429 (98%)	11 (2%)	47	70
2	C	555/569 (98%)	529 (95%)	26 (5%)	26	56
2	D	555/569 (98%)	519 (94%)	36 (6%)	17	48
All	All	1998/2504 (80%)	1911 (96%)	87 (4%)	28	57

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	44	TYR
1	A	46	ARG
1	A	61	ASP
1	A	103	ASN
1	A	171	MET
1	A	187	PHE
1	A	241	ASP
1	A	264	LEU
1	A	308	GLN
1	A	316	TYR
1	A	349	ARG
1	A	350	LEU
1	A	459	SER

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Mol	Chain	Res	Type
1	B	22	PHE
1	B	61	ASP
1	B	171	MET
1	B	187	PHE
1	B	266	ASN
1	B	308	GLN
1	B	316	TYR
1	B	318	ARG
1	B	333	LEU
1	B	351	SER
1	B	446	TYR
2	C	-1	SER
2	C	14	GLU
2	C	25	PHE
2	C	28	ARG
2	C	57	SER
2	C	71	SER
2	C	170	LEU
2	C	194	LYS
2	C	232	TYR
2	C	258	TYR
2	C	259	GLU
2	C	324	GLU
2	C	359	LYS
2	C	363	PHE
2	C	375	LEU
2	C	381	TYR
2	C	382	LYS
2	C	385	TYR
2	C	397	TYR
2	C	444	ASN
2	C	454	ASP
2	C	458	SER
2	C	474	ASP
2	C	513	SER
2	C	514	ARG
2	C	534	TYR
2	D	23	ASP
2	D	28	ARG
2	D	57	SER
2	D	71	SER
2	D	128	PHE

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Mol	Chain	Res	Type
2	D	131	ASP
2	D	168	ASP
2	D	170	LEU
2	D	185	LEU
2	D	207	LEU
2	D	216	ASN
2	D	232	TYR
2	D	243	GLU
2	D	244	LEU
2	D	245	ILE
2	D	250	LYS
2	D	251	GLU
2	D	258	TYR
2	D	259	GLU
2	D	307	ARG
2	D	323	TYR
2	D	335	HIS
2	D	353	PHE
2	D	363	PHE
2	D	370	PHE
2	D	375	LEU
2	D	381	TYR
2	D	382	LYS
2	D	385	TYR
2	D	389	ASP
2	D	444	ASN
2	D	454	ASP
2	D	458	SER
2	D	474	ASP
2	D	534	TYR
2	D	538	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
2	C	311	GLN
2	D	69	GLN
2	D	216	ASN

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 (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(Å^2)	Q<0.9
1	A	699/732 (95%)	0.57	74 (10%)	6	5	101, 234, 464, 550	0
1	B	587/732 (80%)	0.67	68 (11%)	4	4	100, 213, 427, 486	0
2	C	598/614 (97%)	0.76	63 (10%)	6	5	101, 165, 310, 428	0
2	D	598/614 (97%)	0.72	54 (9%)	9	7	101, 170, 307, 448	0
All	All	2482/2692 (92%)	0.67	259 (10%)	6	5	100, 191, 424, 550	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	221	LEU	9.7
2	C	368	LYS	7.4
2	C	367	SER	7.2
2	C	377	THR	6.6
1	A	591	ASP	6.4
1	A	664	ASN	6.4
1	A	677	HIS	6.3
2	C	220	LYS	6.2
1	B	717	LEU	5.7
1	A	195	GLU	5.7
2	C	164	ALA	5.7
1	B	195	GLU	5.7
1	A	434	TYR	5.6
1	B	583	SER	5.6
1	A	577	GLU	5.5
1	B	713	LYS	5.4
2	C	381	TYR	5.3
1	B	434	TYR	5.3
2	D	228	ASN	5.3
1	A	435	ALA	5.3
1	A	578	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	731	HIS	5.2
1	A	574	LYS	5.2
2	D	166	GLU	5.2
2	D	203	ASN	5.2
1	A	724	LEU	5.1
2	C	380	ASP	5.1
1	A	676	LYS	5.0
2	C	369	GLY	5.0
1	B	714	ILE	4.9
1	B	245	ASN	4.9
1	B	254	PRO	4.7
1	A	245	ASN	4.6
1	A	700	ASP	4.6
2	D	384	PRO	4.5
2	C	30	GLN	4.4
1	B	679	GLU	4.4
1	A	673	ASP	4.4
1	A	541	GLN	4.4
1	A	595	ASN	4.3
1	A	275	SER	4.2
2	D	253	LYS	4.2
2	D	363	PHE	4.2
1	A	210	ALA	4.2
1	A	610	SER	4.1
1	A	492	LEU	4.0
2	D	535	PRO	4.0
1	A	540	ALA	4.0
1	B	210	ALA	4.0
2	C	352	ILE	3.9
1	B	587	ASP	3.9
2	D	164	ALA	3.9
2	D	221	LEU	3.9
1	A	496	ALA	3.9
2	C	219	ASP	3.8
1	B	499	GLU	3.8
2	C	172	THR	3.8
2	C	363	PHE	3.8
1	B	411	LEU	3.7
1	B	85	ILE	3.7
2	D	396	PHE	3.6
1	A	439	SER	3.6
2	D	258	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
2	C	174	ASP	3.5
1	A	141	LEU	3.5
1	A	609	ASP	3.5
2	C	37	ASN	3.5
1	B	306	VAL	3.5
1	A	158	PHE	3.5
2	D	135	GLU	3.5
1	B	495	GLU	3.4
2	C	231	ASN	3.4
1	B	504	ILE	3.4
1	B	672	ASN	3.4
1	A	727	ALA	3.4
2	C	163	ASN	3.3
2	C	348	ILE	3.3
1	A	544	ASN	3.3
2	C	26	LYS	3.3
1	B	496	ALA	3.3
2	D	505	THR	3.3
2	C	22	ASP	3.3
2	D	534	TYR	3.2
1	A	491	THR	3.2
1	A	728	ASP	3.2
2	C	129	TYR	3.2
2	C	173	LEU	3.2
1	B	16	LEU	3.1
1	B	147	LEU	3.1
2	D	509	LEU	3.1
2	C	94	VAL	3.1
2	D	37	ASN	3.1
1	A	276	ALA	3.0
1	B	362	LEU	3.0
1	B	457	ILE	3.0
2	C	370	PHE	3.0
1	A	598	GLU	3.0
1	A	450	LEU	3.0
1	A	138	LEU	3.0
1	B	446	TYR	3.0
2	C	190	ASN	3.0
1	A	443	LEU	3.0
2	D	348	ILE	3.0
2	C	382	LYS	2.9
1	B	86	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	312	PHE	2.9
2	C	228	ASN	2.9
2	D	165	ASN	2.9
1	A	703	ILE	2.9
1	A	184	LYS	2.8
1	A	499	GLU	2.8
1	B	329	ALA	2.8
2	D	337	ILE	2.8
2	C	162	LEU	2.8
1	B	106	ILE	2.8
1	B	460	GLU	2.8
1	B	215	TRP	2.8
1	B	584	LEU	2.8
1	B	363	LEU	2.7
1	B	209	GLU	2.7
1	A	316	TYR	2.7
2	C	379	TYR	2.7
2	C	396	PHE	2.7
2	D	381	TYR	2.7
2	C	70	PHE	2.7
2	D	383	ALA	2.7
2	D	344	ILE	2.7
1	A	1	MET	2.7
2	D	246	ALA	2.7
2	C	33	CYS	2.6
1	B	453	GLU	2.6
1	B	382	ARG	2.6
2	C	362	TYR	2.6
1	A	341	LEU	2.6
1	B	103	ASN	2.6
1	A	429	LEU	2.6
1	B	710	ASN	2.6
2	C	498	PHE	2.6
1	A	661	LEU	2.6
1	A	163	PHE	2.6
1	A	453	GLU	2.5
2	C	378	ARG	2.5
2	D	379	TYR	2.5
1	A	215	TRP	2.5
1	A	704	LEU	2.5
1	B	413	SER	2.5
2	C	384	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	498	ASP	2.5
1	B	158	PHE	2.5
2	D	340	GLN	2.5
1	A	182	LEU	2.5
2	D	548	LEU	2.5
2	C	544	VAL	2.5
1	B	269	SER	2.5
2	D	392	PHE	2.5
2	D	352	ILE	2.5
1	A	594	ASP	2.5
1	B	461	TYR	2.5
1	A	345	LEU	2.5
1	B	450	LEU	2.5
2	C	218	LYS	2.4
1	B	345	LEU	2.4
2	C	592	LEU	2.4
1	B	716	LYS	2.4
1	B	273	LYS	2.4
1	A	254	PRO	2.4
1	B	294	ILE	2.4
1	A	47	TYR	2.4
1	B	454	LEU	2.4
2	D	30	GLN	2.4
2	C	501	TYR	2.4
1	B	236	PHE	2.4
2	D	357	LYS	2.4
2	D	319	LEU	2.4
2	D	254	ASP	2.4
1	A	382	ARG	2.4
2	C	330	ILE	2.4
2	D	188	ILE	2.4
2	D	365	LYS	2.4
2	D	232	TYR	2.4
1	A	379	LEU	2.3
1	A	190	VAL	2.3
1	A	214	PHE	2.3
2	D	578	ILE	2.3
1	A	128	PHE	2.3
2	C	263	PHE	2.3
1	A	457	ILE	2.3
1	B	206	LYS	2.3
2	D	606	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	144	ASP	2.3
1	A	708	GLU	2.3
1	B	435	ALA	2.3
1	A	714	ILE	2.3
1	B	357	LEU	2.3
2	D	413	LEU	2.3
2	D	9	PHE	2.3
1	A	383	LEU	2.3
2	D	512	PHE	2.3
1	B	270	ALA	2.2
2	C	244	LEU	2.2
2	C	361	ALA	2.2
1	B	151	LEU	2.2
2	D	428	ILE	2.2
1	B	138	LEU	2.2
1	B	394	ILE	2.2
2	C	253	LYS	2.2
2	D	435	ILE	2.2
2	D	341	LEU	2.2
1	A	463	MET	2.2
2	C	283	VAL	2.2
2	C	388	SER	2.2
2	D	291	CYS	2.2
1	A	362	LEU	2.2
1	A	110	ILE	2.2
1	B	456	ASN	2.2
2	C	217	GLN	2.2
2	D	410	LYS	2.2
2	C	364	TYR	2.2
1	A	236	PHE	2.2
1	A	404	ALA	2.2
2	C	435	ILE	2.2
2	C	535	PRO	2.1
2	C	312	PHE	2.1
2	C	291	CYS	2.1
2	D	545	LEU	2.1
1	B	137	GLU	2.1
1	A	587	ASP	2.1
2	C	166	GLU	2.1
1	B	675	LEU	2.1
2	C	323	TYR	2.1
1	A	84	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	570	GLU	2.1
1	B	668	PHE	2.1
1	B	720	LEU	2.1
2	C	471	PHE	2.1
2	D	376	TYR	2.1
1	A	416	SER	2.1
2	C	195	SER	2.1
1	A	147	LEU	2.1
2	C	298	ASN	2.1
2	C	534	TYR	2.1
1	A	124	PHE	2.1
2	D	609	ASP	2.1
1	B	170	VAL	2.1
2	D	129	TYR	2.1
2	D	385	TYR	2.1
2	D	464	CYS	2.0
1	B	458	LEU	2.0
2	C	111	VAL	2.0
2	C	464	CYS	2.0
1	B	333	LEU	2.0
1	B	383	LEU	2.0
2	C	326	PHE	2.0
1	B	429	LEU	2.0
1	A	304	ASP	2.0
1	B	47	TYR	2.0
2	D	364	TYR	2.0
2	D	374	ASP	2.0
1	A	333	LEU	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.