



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:52 PM UTC

PDB ID : 3CB4 / pdb_00003cb4
Title : The Crystal Structure of LepA
Authors : Evans, R.N.; Blaha, G.; Bailey, S.; Steitz, T.A.
Deposited on : 2008-02-21
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

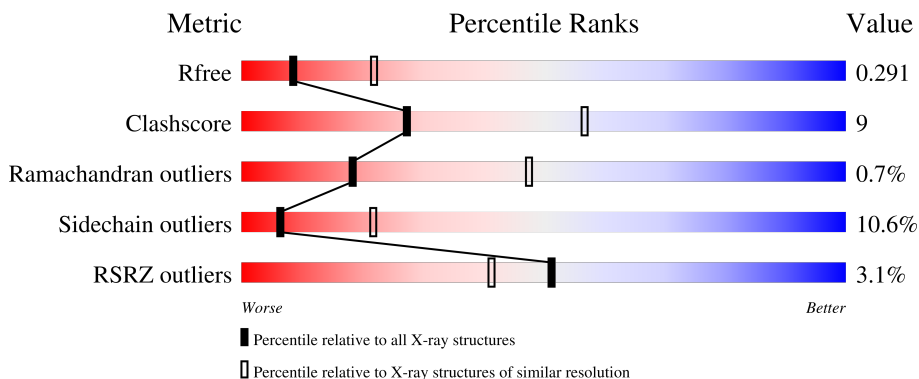
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



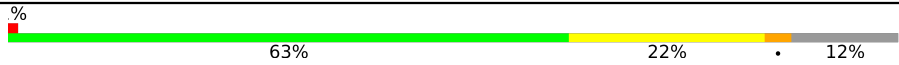
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	599	 2% (poor fit), 67% (0-1 outliers), 17% (2 outliers), 12% (3+ outliers)
1	B	599	 3% (poor fit), 64% (0-1 outliers), 20% (2 outliers), 12% (3+ outliers)
1	C	599	 4% (poor fit), 63% (0-1 outliers), 20% (2 outliers), 12% (3+ outliers)
1	D	599	 2% (poor fit), 66% (0-1 outliers), 18% (2 outliers), 12% (3+ outliers)
1	E	599	 5% (poor fit), 66% (0-1 outliers), 20% (2 outliers), 12% (3+ outliers)

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Mol	Chain	Length	Quality of chain
1	F	599	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a green segment on the left labeled '63%', a yellow segment in the middle labeled '22%', and a grey segment on the right labeled '12%'. A small red square is at the beginning of the bar, and a small black dot is at the end of the grey segment. A '%' symbol is positioned above the start of the bar.</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24495 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 lepA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	525	4082	2579	698	785	20	0	0	0
1	A	525	4082	2579	698	785	20	0	0	0
1	B	525	4082	2579	698	785	20	0	0	0
1	C	525	4082	2579	698	785	20	0	0	0
1	E	525	4082	2579	698	785	20	0	0	0
1	F	525	4082	2579	698	785	20	0	0	0

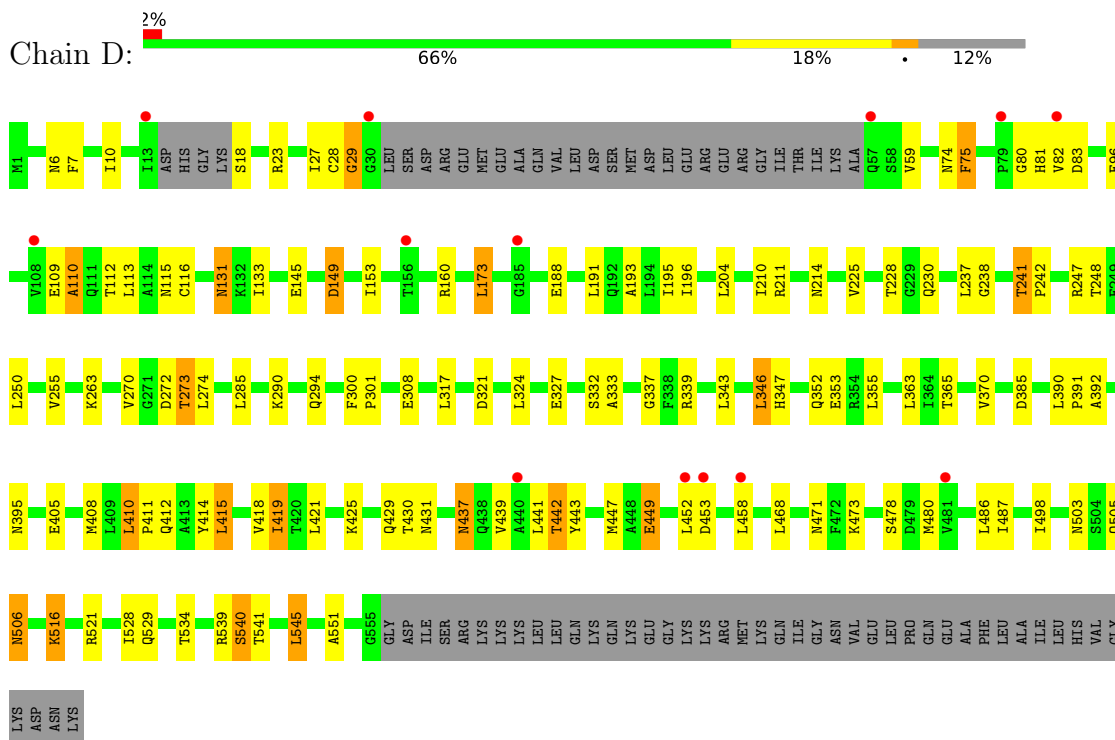
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	3	Total	O	0	0
			3	3		

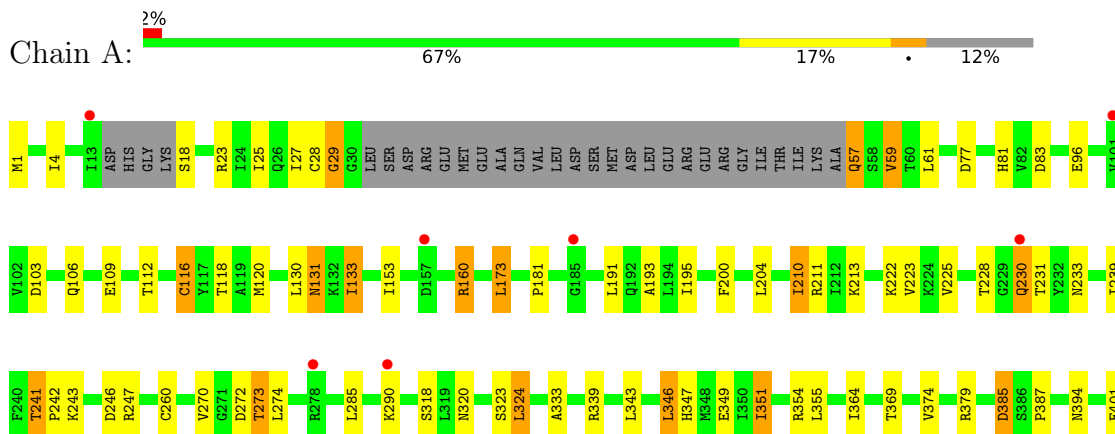
3 Residue-property plots [i](#)

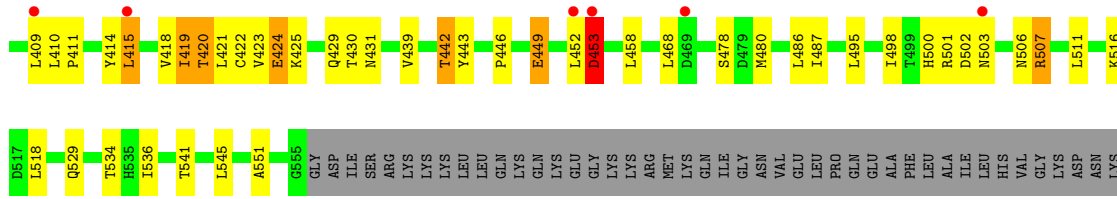
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

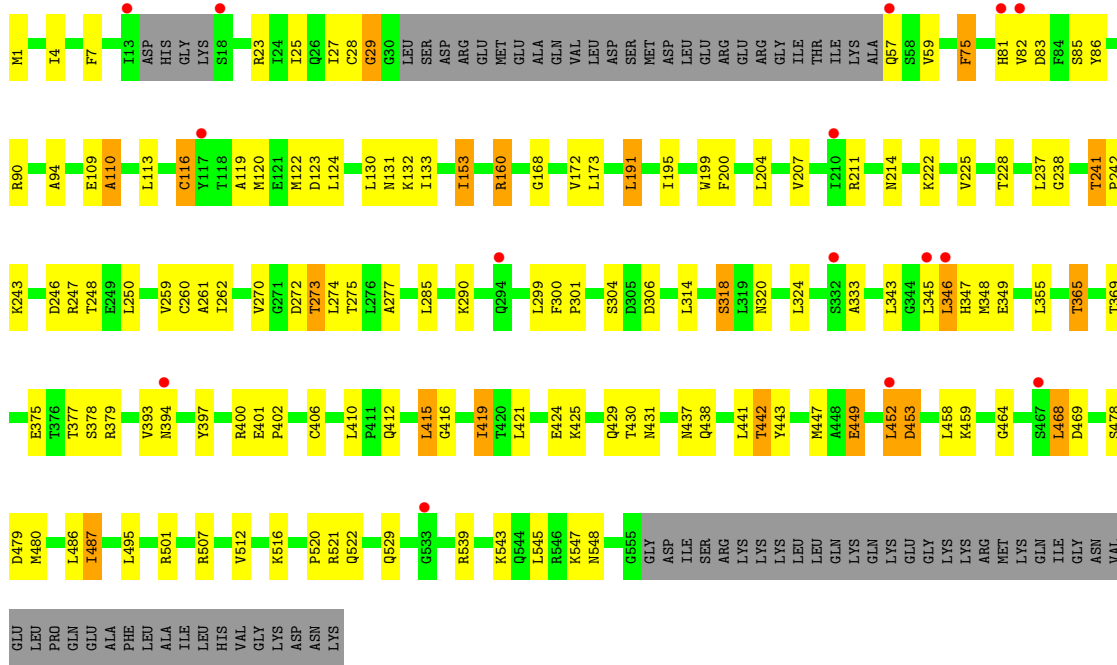


- Molecule 1: GTP-binding protein lepA

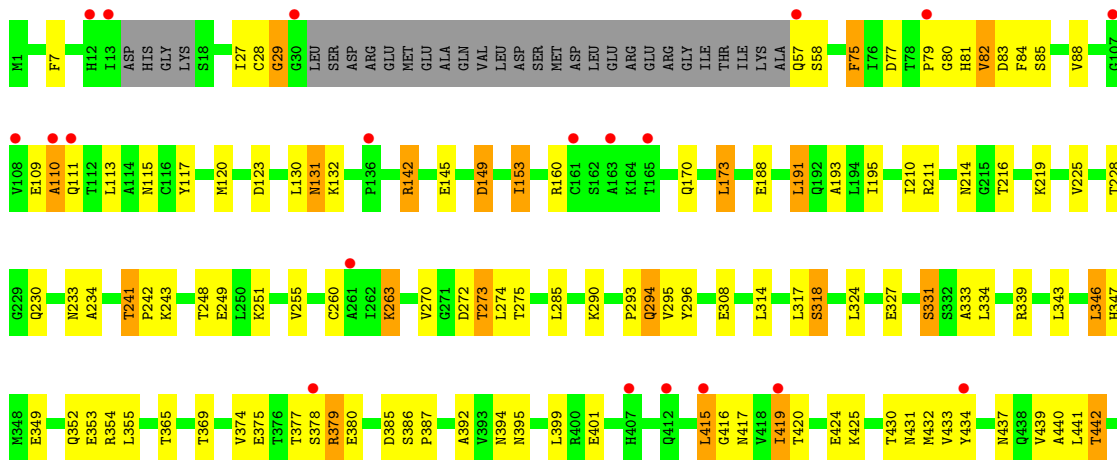




• Molecule 1: GTP-binding protein lepA



• Molecule 1: GTP-binding protein lepA



ILE
GLY
ASN
VAL
GLU
LEU
PRO
GLN
GLU
ALA
PHE
LEU
ALA
ILE
LEU
HIS
VAL
GLY
LYS
ASP
ASN
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.96Å 146.24Å 139.32Å 90.00° 100.60° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.80) 94.6 (50.00-2.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.246 , 0.295 0.242 , 0.291	Depositor DCC
R_{free} test set	4590 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24495	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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	0.45	0/4150	0.81	0/5626
1	B	0.45	0/4150	0.80	1/5626 (0.0%)
1	C	0.47	2/4150 (0.0%)	0.80	1/5626 (0.0%)
1	D	0.45	0/4150	0.82	1/5626 (0.0%)
1	E	0.44	0/4150	0.80	0/5626
1	F	0.45	0/4150	0.81	0/5626
All	All	0.45	2/24900 (0.0%)	0.81	3/33756 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	142	ARG	NE-CZ	7.68	1.41	1.33
1	C	142	ARG	CZ-NH1	5.48	1.40	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	ALA	N-CA-C	5.74	118.27	111.33
1	D	110	ALA	N-CA-C	5.51	118.81	111.75
1	C	110	ALA	N-CA-C	5.13	117.61	111.71

There are no chirality outliers.

There are no planarity outliers.

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	4082	0	4095	78	0
1	B	4082	0	4095	75	0
1	C	4082	0	4095	81	0
1	D	4082	0	4095	69	0
1	E	4082	0	4095	72	0
1	F	4082	0	4095	87	0
2	D	3	0	0	0	0
All	All	24495	0	24570	448	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 (448) 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:419:ILE:HD11	1:F:419:ILE:HD11	1.27	1.16
1:D:23:ARG:HH22	1:D:131:ASN:HD21	1.06	1.00
1:F:23:ARG:HH22	1:F:131:ASN:HD21	1.03	0.99
1:E:273:THR:HG21	1:E:285:LEU:H	1.34	0.93
1:C:273:THR:HG21	1:C:285:LEU:H	1.37	0.89
1:C:81:HIS:NE2	1:C:346:LEU:HD11	1.87	0.88
1:A:210:ILE:HD11	1:A:274:LEU:HD12	1.55	0.87
1:D:23:ARG:NH2	1:D:131:ASN:HD21	1.71	0.86
1:B:131:ASN:HD22	1:B:132:LYS:N	1.72	0.86
1:B:131:ASN:HD22	1:B:132:LYS:H	1.20	0.86
1:D:346:LEU:HD13	1:D:346:LEU:H	1.41	0.86
1:A:503:ASN:CB	1:A:507:ARG:HH21	1.92	0.82
1:F:23:ARG:NH2	1:F:131:ASN:HD21	1.76	0.81
1:D:333:ALA:HB1	1:D:487:ILE:HD11	1.60	0.81
1:A:419:ILE:HD11	1:F:419:ILE:CD1	2.09	0.81
1:B:273:THR:HG21	1:B:285:LEU:H	1.46	0.81
1:A:343:LEU:H	1:A:347:HIS:HD2	1.28	0.80
1:D:419:ILE:HD11	1:C:416:GLY:HA2	1.62	0.80
1:A:23:ARG:NH2	1:A:131:ASN:HD21	1.80	0.80
1:C:333:ALA:HB1	1:C:487:ILE:HD11	1.63	0.80
1:A:273:THR:HG21	1:A:285:LEU:H	1.46	0.79
1:A:23:ARG:HH22	1:A:131:ASN:HD21	1.28	0.78
1:B:346:LEU:HD13	1:B:346:LEU:H	1.50	0.76
1:F:425:LYS:HD2	1:F:449:GLU:HG3	1.66	0.76
1:C:346:LEU:HD13	1:C:346:LEU:H	1.50	0.75
1:A:503:ASN:HB2	1:A:507:ARG:HH21	1.51	0.75
1:D:273:THR:HG21	1:D:285:LEU:H	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LEU:H	1:B:347:HIS:HD2	1.34	0.74
1:C:80:GLY:HA2	1:C:115:ASN:HD21	1.50	0.74
1:A:210:ILE:HD11	1:A:274:LEU:CD1	2.18	0.74
1:F:478:SER:HB3	1:F:480:MET:HE1	1.70	0.74
1:F:503:ASN:HB2	1:F:507:ARG:HH21	1.51	0.74
1:C:343:LEU:H	1:C:347:HIS:HD2	1.37	0.73
1:D:23:ARG:HH22	1:D:131:ASN:ND2	1.83	0.72
1:C:81:HIS:HD2	1:C:83:ASP:H	1.37	0.72
1:F:425:LYS:HD2	1:F:449:GLU:CG	2.19	0.71
1:D:225:VAL:HB	1:D:228:THR:HG22	1.73	0.70
1:D:333:ALA:CB	1:D:487:ILE:HD11	2.20	0.70
1:D:339:ARG:HH12	1:D:385:ASP:HB3	1.56	0.70
1:A:343:LEU:H	1:A:347:HIS:CD2	2.10	0.70
1:B:110:ALA:HA	1:B:113:LEU:HD12	1.74	0.69
1:A:195:ILE:HD11	1:A:274:LEU:HG	1.75	0.69
1:C:81:HIS:CE1	1:C:346:LEU:HD11	2.27	0.69
1:C:503:ASN:HB2	1:C:507:ARG:HH21	1.58	0.68
1:B:23:ARG:HH22	1:B:131:ASN:HD21	1.41	0.68
1:A:23:ARG:HH22	1:A:131:ASN:ND2	1.92	0.67
1:A:273:THR:HG21	1:A:285:LEU:N	2.09	0.67
1:A:503:ASN:HB3	1:A:507:ARG:HH21	1.60	0.67
1:A:423:VAL:HG11	1:F:415:LEU:HD11	1.75	0.67
1:C:293:PRO:HG2	1:C:296:TYR:OH	1.94	0.67
1:E:23:ARG:HH22	1:E:131:ASN:HD21	1.43	0.67
1:F:415:LEU:O	1:F:419:ILE:HD12	1.95	0.67
1:B:81:HIS:HD2	1:B:83:ASP:H	1.43	0.66
1:C:273:THR:HG21	1:C:285:LEU:N	2.07	0.66
1:F:410:LEU:HD13	1:F:418:VAL:HG21	1.76	0.66
1:F:273:THR:HG21	1:F:285:LEU:H	1.59	0.66
1:F:343:LEU:H	1:F:347:HIS:CD2	2.13	0.65
1:E:431:ASN:HB3	1:E:442:THR:HG23	1.76	0.65
1:F:81:HIS:CD2	1:F:82:VAL:H	2.15	0.65
1:F:431:ASN:HB3	1:F:442:THR:HG23	1.78	0.65
1:D:228:THR:HG23	1:D:230:GLN:H	1.62	0.64
1:B:431:ASN:HB3	1:B:442:THR:HG23	1.79	0.64
1:A:425:LYS:HD2	1:A:449:GLU:CG	2.27	0.64
1:C:343:LEU:H	1:C:347:HIS:CD2	2.14	0.64
1:E:3:ASN:HD21	1:E:69:GLU:HG2	1.63	0.64
1:D:273:THR:HG21	1:D:285:LEU:N	2.13	0.64
1:E:343:LEU:H	1:E:347:HIS:CD2	2.16	0.64
1:E:343:LEU:H	1:E:347:HIS:HD2	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:ARG:HH22	1:F:131:ASN:ND2	1.85	0.63
1:F:241:THR:H	1:F:242:PRO:C	2.06	0.63
1:B:431:ASN:HB3	1:B:442:THR:CG2	2.29	0.63
1:C:228:THR:HG23	1:C:230:GLN:H	1.64	0.63
1:A:225:VAL:HB	1:A:228:THR:CG2	2.29	0.62
1:F:200:PHE:H	1:F:320:ASN:ND2	1.96	0.62
1:A:420:THR:O	1:A:424:GLU:HB2	1.99	0.62
1:D:81:HIS:NE2	1:D:346:LEU:HD11	2.13	0.62
1:B:333:ALA:HB1	1:B:487:ILE:HD11	1.81	0.62
1:A:210:ILE:CD1	1:A:274:LEU:HD12	2.28	0.62
1:F:339:ARG:HH12	1:F:385:ASP:HB3	1.63	0.62
1:B:314:LEU:O	1:B:318:SER:HB2	1.99	0.62
1:C:505:GLN:HE21	1:E:23:ARG:HG2	1.63	0.62
1:D:110:ALA:HA	1:D:113:LEU:HD12	1.82	0.62
1:D:343:LEU:H	1:D:347:HIS:CD2	2.18	0.62
1:A:431:ASN:HB3	1:A:442:THR:HG23	1.81	0.61
1:D:529:GLN:HB3	1:D:539:ARG:HG3	1.82	0.61
1:B:81:HIS:NE2	1:B:346:LEU:HD11	2.15	0.61
1:E:241:THR:H	1:E:242:PRO:C	2.07	0.61
1:B:23:ARG:HH22	1:B:131:ASN:ND2	1.98	0.60
1:C:331:SER:HB2	1:C:334:LEU:H	1.66	0.60
1:B:133:ILE:HG21	1:B:160:ARG:HB2	1.82	0.60
1:A:81:HIS:CE1	1:A:346:LEU:HD11	2.35	0.60
1:E:23:ARG:HH22	1:E:131:ASN:ND2	1.99	0.60
1:E:273:THR:HG21	1:E:285:LEU:N	2.14	0.60
1:F:343:LEU:H	1:F:347:HIS:HD2	1.49	0.60
1:A:112:THR:O	1:A:116:CYS:HB2	2.02	0.60
1:B:241:THR:H	1:B:242:PRO:C	2.10	0.59
1:F:117:TYR:HA	1:F:120:MET:HE2	1.85	0.59
1:D:145:GLU:O	1:D:149:ASP:HB2	2.02	0.59
1:B:346:LEU:HA	1:B:349:GLU:HB2	1.84	0.59
1:D:343:LEU:H	1:D:347:HIS:HD2	1.51	0.59
1:D:196:ILE:HD11	1:D:211:ARG:HB2	1.84	0.58
1:B:273:THR:HG21	1:B:285:LEU:N	2.16	0.58
1:A:27:ILE:HD11	1:A:173:LEU:HD22	1.85	0.58
1:B:299:LEU:HD23	1:B:365:THR:HB	1.85	0.58
1:C:225:VAL:HG22	1:C:274:LEU:HD21	1.85	0.58
1:B:23:ARG:NH2	1:B:131:ASN:HD21	2.01	0.58
1:F:346:LEU:HD13	1:F:346:LEU:H	1.68	0.58
1:E:225:VAL:HB	1:E:228:THR:CG2	2.33	0.58
1:E:425:LYS:HD2	1:E:449:GLU:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ILE:HD13	1:C:272:ASP:HB3	1.86	0.57
1:B:343:LEU:H	1:B:347:HIS:CD2	2.20	0.57
1:F:3:ASN:HD21	1:F:69:GLU:HG2	1.70	0.57
1:A:81:HIS:NE2	1:A:346:LEU:HD11	2.20	0.56
1:A:195:ILE:HD13	1:A:272:ASP:HB3	1.87	0.56
1:B:478:SER:HB3	1:B:480:MET:CE	2.35	0.56
1:C:294:GLN:HG2	1:C:295:VAL:HG23	1.86	0.56
1:E:333:ALA:CB	1:E:487:ILE:HD11	2.35	0.56
1:E:431:ASN:HB3	1:E:442:THR:CG2	2.36	0.56
1:F:273:THR:HG21	1:F:285:LEU:N	2.21	0.56
1:F:299:LEU:HD23	1:F:365:THR:HB	1.85	0.56
1:E:225:VAL:HB	1:E:228:THR:HG22	1.87	0.56
1:F:529:GLN:HB3	1:F:539:ARG:HG3	1.87	0.56
1:A:233:ASN:O	1:A:260:CYS:HB3	2.06	0.56
1:C:375:GLU:OE1	1:C:379:ARG:HD3	2.06	0.56
1:F:411:PRO:HG2	1:F:414:TYR:HD2	1.70	0.56
1:F:520:PRO:O	1:F:522:GLN:HG3	2.06	0.56
1:F:193:ALA:HB1	1:F:210:ILE:HG23	1.88	0.56
1:A:200:PHE:H	1:A:320:ASN:ND2	2.04	0.55
1:D:480:MET:HG3	1:D:498:ILE:HG22	1.89	0.55
1:C:520:PRO:O	1:C:522:GLN:HG3	2.06	0.55
1:D:195:ILE:HD13	1:D:272:ASP:HB3	1.88	0.55
1:A:225:VAL:HB	1:A:228:THR:HG22	1.89	0.55
1:D:27:ILE:HD11	1:D:173:LEU:HD22	1.88	0.55
1:A:333:ALA:HB1	1:A:487:ILE:HD11	1.89	0.55
1:A:425:LYS:HD2	1:A:449:GLU:HG3	1.87	0.55
1:A:346:LEU:HA	1:A:349:GLU:HB2	1.88	0.55
1:C:339:ARG:HH12	1:C:385:ASP:HB3	1.71	0.55
1:F:478:SER:HB3	1:F:480:MET:CE	2.36	0.55
1:D:225:VAL:HB	1:D:228:THR:CG2	2.35	0.55
1:A:96:GLU:HB3	1:A:181:PRO:HG2	1.89	0.55
1:F:200:PHE:H	1:F:320:ASN:HD21	1.54	0.55
1:A:200:PHE:H	1:A:320:ASN:HD21	1.54	0.54
1:A:81:HIS:HD2	1:A:83:ASP:H	1.56	0.54
1:E:333:ALA:HB1	1:E:487:ILE:HD11	1.90	0.54
1:D:28:CYS:O	1:D:29:GLY:C	2.51	0.54
1:B:81:HIS:CE1	1:B:346:LEU:HD11	2.44	0.53
1:D:346:LEU:H	1:D:346:LEU:CD1	2.17	0.53
1:D:551:ALA:O	1:E:520:PRO:HD2	2.09	0.53
1:A:346:LEU:HD13	1:A:346:LEU:H	1.73	0.53
1:C:81:HIS:CD2	1:C:83:ASP:H	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ALA:HB3	1:C:274:LEU:HB2	1.90	0.53
1:D:18:SER:HB2	1:D:23:ARG:HD2	1.88	0.53
1:E:7:PHE:O	1:E:75:PHE:HA	2.08	0.53
1:C:505:GLN:NE2	1:E:23:ARG:HG2	2.23	0.53
1:B:419:ILE:HG22	1:B:441:LEU:HD11	1.91	0.52
1:C:211:ARG:HG2	1:C:255:VAL:HG22	1.92	0.52
1:A:241:THR:H	1:A:242:PRO:C	2.17	0.52
1:C:191:LEU:HB3	1:C:275:THR:HA	1.90	0.52
1:A:551:ALA:O	1:B:520:PRO:HD2	2.10	0.52
1:B:1:MET:HA	1:B:4:ILE:HD12	1.91	0.52
1:E:376:THR:HG22	1:E:378:SER:H	1.75	0.52
1:E:421:LEU:HD11	1:E:457:ARG:HB3	1.91	0.52
1:F:27:ILE:HD11	1:F:173:LEU:HD22	1.91	0.52
1:A:81:HIS:CD2	1:A:346:LEU:HD11	2.45	0.52
1:A:415:LEU:HD23	1:A:439:VAL:HG21	1.91	0.52
1:E:72:GLN:HE22	1:E:254:GLU:HG2	1.74	0.52
1:F:410:LEU:HD21	1:F:441:LEU:HD12	1.91	0.52
1:B:195:ILE:HD13	1:B:272:ASP:HB3	1.92	0.51
1:C:216:THR:HG23	1:C:251:LYS:HA	1.93	0.51
1:C:241:THR:H	1:C:242:PRO:C	2.19	0.51
1:E:378:SER:O	1:E:380:GLU:N	2.43	0.51
1:E:520:PRO:O	1:E:522:GLN:HG3	2.11	0.51
1:E:81:HIS:HD2	1:E:83:ASP:H	1.58	0.51
1:E:410:LEU:HD13	1:E:418:VAL:HG21	1.91	0.51
1:A:1:MET:HA	1:A:4:ILE:HD12	1.92	0.51
1:E:521:ARG:HD2	1:E:543:LYS:O	2.09	0.51
1:E:346:LEU:HA	1:E:349:GLU:HB2	1.92	0.51
1:F:193:ALA:HB3	1:F:274:LEU:HB2	1.93	0.51
1:F:196:ILE:HD11	1:F:211:ARG:HB2	1.93	0.51
1:A:401:GLU:OE2	1:A:446:PRO:HB3	2.11	0.50
1:B:429:GLN:HB2	1:B:443:TYR:CZ	2.46	0.50
1:F:478:SER:CB	1:F:480:MET:HE1	2.40	0.50
1:C:374:VAL:HG22	1:C:399:LEU:HD13	1.92	0.50
1:B:237:LEU:HD13	1:B:250:LEU:HG	1.93	0.50
1:C:478:SER:HB3	1:C:480:MET:CE	2.41	0.50
1:D:80:GLY:HA2	1:D:115:ASN:HD21	1.76	0.50
1:A:410:LEU:HD13	1:A:418:VAL:HG21	1.93	0.50
1:E:241:THR:N	1:E:242:PRO:CA	2.75	0.50
1:F:294:GLN:HG2	1:F:295:VAL:HG23	1.93	0.50
1:F:7:PHE:CZ	1:F:176:LEU:HD11	2.47	0.50
1:D:411:PRO:HG2	1:D:414:TYR:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:LEU:HD23	1:B:469:ASP:H	1.76	0.50
1:C:225:VAL:HG22	1:C:274:LEU:CD2	2.42	0.50
1:C:314:LEU:O	1:C:318:SER:HB2	2.11	0.49
1:E:23:ARG:NH2	1:E:131:ASN:HD21	2.07	0.49
1:E:195:ILE:HD13	1:E:272:ASP:HB3	1.94	0.49
1:B:260:CYS:O	1:B:262:ILE:N	2.44	0.49
1:A:431:ASN:HB3	1:A:442:THR:CG2	2.43	0.49
1:B:379:ARG:NH2	1:B:397:TYR:CZ	2.80	0.49
1:E:241:THR:O	1:E:241:THR:HG22	2.11	0.49
1:D:431:ASN:HB3	1:D:442:THR:HG23	1.95	0.49
1:D:415:LEU:HD23	1:D:439:VAL:HG21	1.95	0.49
1:B:81:HIS:CD2	1:B:346:LEU:HD21	2.48	0.49
1:B:116:CYS:O	1:B:120:MET:HG3	2.12	0.49
1:B:207:VAL:HG22	1:B:259:VAL:HG22	1.94	0.49
1:B:406:CYS:O	1:B:442:THR:HA	2.13	0.49
1:A:57:GLN:O	1:A:77:ASP:HB2	2.13	0.49
1:C:432:MET:HE2	1:C:439:VAL:HG11	1.94	0.49
1:E:130:LEU:HB2	1:E:160:ARG:HB3	1.94	0.49
1:E:193:ALA:HB1	1:E:210:ILE:CG2	2.43	0.48
1:F:219:LYS:O	1:F:234:ALA:O	2.31	0.48
1:D:516:LYS:HE3	1:D:540:SER:OG	2.13	0.48
1:F:521:ARG:HB2	1:F:545:LEU:HD13	1.94	0.48
1:D:238:GLY:HA2	1:D:247:ARG:HB2	1.96	0.48
1:E:110:ALA:HA	1:E:113:LEU:HD12	1.96	0.48
1:E:374:VAL:HG22	1:E:399:LEU:HD13	1.96	0.48
1:A:536:ILE:HD12	1:C:170:GLN:HE22	1.79	0.48
1:D:301:PRO:HA	1:D:363:LEU:HD23	1.95	0.48
1:A:503:ASN:HB2	1:A:507:ARG:NH2	2.25	0.48
1:F:81:HIS:CD2	1:F:82:VAL:N	2.82	0.48
1:D:405:GLU:HB2	1:D:473:LYS:HD3	1.96	0.47
1:D:505:GLN:HE21	1:F:23:ARG:HG2	1.80	0.47
1:C:195:ILE:HD11	1:C:274:LEU:HG	1.96	0.47
1:E:192:GLN:NE2	1:E:283:LYS:O	2.47	0.47
1:C:82:VAL:HA	1:C:85:SER:HB2	1.96	0.47
1:B:225:VAL:HB	1:B:228:THR:CG2	2.44	0.47
1:F:94:ALA:HB1	1:F:211:ARG:HG3	1.95	0.47
1:B:25:ILE:HD11	1:B:59:VAL:HG21	1.95	0.47
1:C:241:THR:N	1:C:242:PRO:CA	2.77	0.47
1:C:433:VAL:HB	1:C:440:ALA:HB3	1.96	0.47
1:C:377:THR:HG23	1:C:378:SER:H	1.79	0.47
1:C:486:LEU:HG	1:C:529:GLN:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ASN:O	1:C:260:CYS:HB3	2.15	0.47
1:B:241:THR:N	1:B:242:PRO:CA	2.78	0.47
1:A:425:LYS:HD2	1:A:449:GLU:HG2	1.96	0.47
1:C:130:LEU:HB2	1:C:160:ARG:HB3	1.96	0.47
1:A:364:ILE:HD12	1:A:518:LEU:HD22	1.97	0.46
1:C:503:ASN:HB2	1:C:507:ARG:NH2	2.27	0.46
1:F:241:THR:N	1:F:242:PRO:CA	2.77	0.46
1:F:503:ASN:HB2	1:F:507:ARG:NH2	2.23	0.46
1:F:195:ILE:HD11	1:F:274:LEU:HG	1.96	0.46
1:D:370:VAL:HG11	1:D:447:MET:HG3	1.97	0.46
1:E:241:THR:O	1:E:241:THR:CG2	2.63	0.46
1:E:296:TYR:O	1:E:368:PRO:HA	2.16	0.46
1:E:375:GLU:OE1	1:E:379:ARG:HD3	2.15	0.46
1:F:81:HIS:CD2	1:F:346:LEU:HD11	2.51	0.46
1:F:112:THR:O	1:F:116:CYS:HB2	2.16	0.46
1:F:431:ASN:HB3	1:F:442:THR:CG2	2.43	0.46
1:A:103:ASP:HB3	1:A:106:GLN:HB2	1.97	0.46
1:B:27:ILE:HG22	1:F:537:ILE:C	2.41	0.46
1:C:145:GLU:O	1:C:149:ASP:HB2	2.15	0.46
1:F:193:ALA:HB1	1:F:210:ILE:CG2	2.45	0.46
1:D:96:GLU:OE2	1:D:211:ARG:NH2	2.48	0.46
1:E:193:ALA:HB1	1:E:210:ILE:HG23	1.97	0.46
1:D:352:GLN:HE22	1:D:365:THR:HG21	1.79	0.46
1:D:390:LEU:HD12	1:D:391:PRO:HD2	1.97	0.46
1:D:193:ALA:HB3	1:D:274:LEU:HB2	1.98	0.46
1:E:321:ASP:OD1	1:E:347:HIS:HE1	1.98	0.46
1:E:419:ILE:HB	1:E:443:TYR:OH	2.15	0.46
1:E:99:LEU:HD23	1:E:127:VAL:HB	1.97	0.46
1:B:529:GLN:HB3	1:B:539:ARG:HG3	1.98	0.45
1:C:27:ILE:HD11	1:C:173:LEU:HD22	1.98	0.45
1:D:487:ILE:HG22	1:D:528:ILE:HA	1.98	0.45
1:A:419:ILE:HA	1:A:422:CYS:HB2	1.98	0.45
1:C:415:LEU:HD23	1:C:439:VAL:HG21	1.98	0.45
1:D:6:ASN:HA	1:D:74:ASN:O	2.16	0.45
1:F:412:GLN:HG2	1:F:439:VAL:HG23	1.97	0.45
1:A:429:GLN:HE22	1:F:429:GLN:HE22	1.63	0.45
1:E:195:ILE:HD11	1:E:274:LEU:HG	1.99	0.45
1:A:429:GLN:HB2	1:A:443:TYR:CZ	2.52	0.45
1:C:392:ALA:HB3	1:C:395:ASN:HD22	1.81	0.45
1:C:415:LEU:O	1:C:419:ILE:HG23	2.17	0.45
1:E:112:THR:O	1:E:116:CYS:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:CYS:HB2	1:A:61:LEU:HD22	1.99	0.45
1:C:193:ALA:HA	1:C:211:ARG:O	2.16	0.45
1:A:130:LEU:HB2	1:A:160:ARG:HB3	1.99	0.45
1:C:79:PRO:O	1:C:88:VAL:HG22	2.17	0.45
1:C:346:LEU:HD13	1:C:346:LEU:N	2.27	0.45
1:A:339:ARG:HH12	1:A:385:ASP:HB2	1.80	0.45
1:B:547:LYS:O	1:B:548:ASN:HB2	2.17	0.45
1:C:57:GLN:O	1:C:77:ASP:HB2	2.17	0.45
1:C:352:GLN:NE2	1:C:365:THR:HG21	2.32	0.45
1:E:419:ILE:HA	1:E:422:CYS:HB2	1.99	0.45
1:A:415:LEU:CD1	1:F:423:VAL:HG11	2.46	0.45
1:B:225:VAL:HB	1:B:228:THR:HG22	1.99	0.45
1:C:110:ALA:HA	1:C:113:LEU:HD12	1.99	0.45
1:A:228:THR:HG23	1:A:230:GLN:H	1.82	0.44
1:B:345:LEU:O	1:B:348:MET:HB3	2.17	0.44
1:E:339:ARG:HH12	1:E:385:ASP:HB3	1.81	0.44
1:F:262:ILE:HD13	1:F:268:ALA:HB2	2.00	0.44
1:A:193:ALA:HB3	1:A:274:LEU:HB2	2.00	0.44
1:C:401:GLU:HB2	1:C:480:MET:HE3	2.00	0.44
1:E:196:ILE:HD11	1:E:211:ARG:HB2	1.98	0.44
1:E:294:GLN:HG2	1:E:295:VAL:HG23	1.98	0.44
1:F:110:ALA:HA	1:F:113:LEU:HD12	2.00	0.44
1:F:211:ARG:HG2	1:F:255:VAL:HG22	2.00	0.44
1:C:28:CYS:O	1:C:29:GLY:C	2.60	0.44
1:C:500:HIS:CD2	1:C:502:ASP:H	2.35	0.44
1:D:392:ALA:HB3	1:D:395:ASN:HD22	1.81	0.44
1:B:238:GLY:HA2	1:B:247:ARG:HB2	1.99	0.44
1:F:86:TYR:CE1	1:F:289:LYS:HG2	2.53	0.44
1:F:417:ASN:HB3	1:F:461:THR:OG1	2.18	0.44
1:C:509:ARG:CZ	1:C:509:ARG:HB3	2.46	0.44
1:E:459:LYS:O	1:E:464:GLY:N	2.45	0.44
1:F:400:ARG:HG2	1:F:477:ALA:N	2.33	0.44
1:A:28:CYS:O	1:A:29:GLY:C	2.60	0.44
1:A:133:ILE:H	1:A:133:ILE:HG13	1.55	0.44
1:B:415:LEU:HD12	1:B:416:GLY:H	1.83	0.44
1:D:211:ARG:HG2	1:D:255:VAL:HG22	2.00	0.44
1:D:410:LEU:HD21	1:D:441:LEU:HD12	2.00	0.44
1:A:486:LEU:HG	1:A:529:GLN:HG3	2.00	0.44
1:B:479:ASP:OD1	1:B:501:ARG:HD2	2.18	0.44
1:C:452:LEU:O	1:C:453:ASP:C	2.61	0.44
1:A:500:HIS:CD2	1:A:502:ASP:H	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:425:LYS:HD2	1:F:449:GLU:HG2	1.96	0.43
1:D:521:ARG:HB2	1:D:545:LEU:HD13	2.00	0.43
1:A:387:PRO:HG3	1:A:498:ILE:HG13	1.98	0.43
1:B:28:CYS:O	1:B:29:GLY:C	2.61	0.43
1:B:191:LEU:HB3	1:B:275:THR:HA	1.99	0.43
1:F:516:LYS:HE3	1:F:540:SER:OG	2.18	0.43
1:E:486:LEU:HG	1:E:529:GLN:HG3	2.00	0.43
1:F:409:LEU:O	1:F:466:ALA:HA	2.17	0.43
1:E:294:GLN:HB3	1:E:343:LEU:O	2.19	0.43
1:C:241:THR:N	1:C:242:PRO:HA	2.34	0.43
1:C:349:GLU:O	1:C:353:GLU:HB2	2.18	0.43
1:C:487:ILE:HG22	1:C:528:ILE:HG23	2.01	0.43
1:F:103:ASP:HB3	1:F:106:GLN:HB2	2.01	0.43
1:F:226:MET:HG3	1:F:273:THR:O	2.19	0.43
1:B:377:THR:HG23	1:B:378:SER:H	1.83	0.43
1:B:402:PRO:HG2	1:B:447:MET:HB3	1.99	0.43
1:B:425:LYS:HD2	1:B:449:GLU:HG3	2.00	0.43
1:E:241:THR:N	1:E:242:PRO:HA	2.33	0.43
1:E:529:GLN:HB3	1:E:539:ARG:HG3	2.00	0.43
1:E:28:CYS:O	1:E:29:GLY:C	2.61	0.43
1:A:415:LEU:HD11	1:F:423:VAL:HG11	2.00	0.43
1:E:224:LYS:N	1:E:275:THR:O	2.51	0.43
1:D:81:HIS:HD2	1:D:83:ASP:H	1.65	0.43
1:B:299:LEU:CD2	1:B:365:THR:HB	2.48	0.43
1:A:411:PRO:HG2	1:A:414:TYR:HD2	1.84	0.42
1:A:419:ILE:HD13	1:A:420:THR:N	2.33	0.42
1:A:452:LEU:O	1:A:453:ASP:C	2.62	0.42
1:C:219:LYS:O	1:C:234:ALA:O	2.37	0.42
1:E:147:ILE:O	1:E:151:VAL:HB	2.18	0.42
1:E:228:THR:HG23	1:E:230:GLN:H	1.84	0.42
1:F:225:VAL:HB	1:F:228:THR:CG2	2.49	0.42
1:D:503:ASN:HD22	1:D:506:ASN:HB2	1.84	0.42
1:F:374:VAL:HG22	1:F:399:LEU:HD13	2.01	0.42
1:F:452:LEU:O	1:F:453:ASP:C	2.62	0.42
1:D:478:SER:HB3	1:D:480:MET:CE	2.49	0.42
1:A:96:GLU:OE2	1:A:211:ARG:NH2	2.52	0.42
1:A:211:ARG:HH11	1:A:213:LYS:HA	1.84	0.42
1:B:222:LYS:HG3	1:B:277:ALA:HB3	2.01	0.42
1:D:193:ALA:HB1	1:D:210:ILE:HG23	2.01	0.42
1:B:153:ILE:HD12	1:B:153:ILE:HA	1.79	0.42
1:F:133:ILE:H	1:F:133:ILE:HG13	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:THR:H	1:F:242:PRO:CA	2.33	0.42
1:D:425:LYS:HD2	1:D:449:GLU:HG3	2.02	0.42
1:A:223:VAL:O	1:A:231:THR:HA	2.20	0.42
1:E:401:GLU:OE2	1:E:446:PRO:HB3	2.19	0.42
1:D:241:THR:H	1:D:242:PRO:C	2.28	0.42
1:D:410:LEU:HD13	1:D:418:VAL:HG21	2.00	0.42
1:C:468:LEU:HD23	1:C:469:ASP:N	2.35	0.42
1:E:11:ALA:HB2	1:E:101:VAL:HB	2.02	0.42
1:D:237:LEU:HD13	1:D:250:LEU:HG	2.01	0.42
1:B:520:PRO:O	1:B:522:GLN:HG3	2.20	0.42
1:C:117:TYR:HA	1:C:120:MET:HE2	2.01	0.42
1:F:333:ALA:HB1	1:F:487:ILE:HD11	2.02	0.42
1:E:219:LYS:O	1:E:234:ALA:O	2.38	0.42
1:E:238:GLY:HA2	1:E:247:ARG:HB2	2.02	0.42
1:E:478:SER:HB3	1:E:480:MET:CE	2.50	0.42
1:F:293:PRO:HG2	1:F:296:TYR:OH	2.20	0.42
1:F:296:TYR:HA	1:F:340:CYS:O	2.19	0.42
1:B:225:VAL:HG22	1:B:274:LEU:HD21	2.02	0.41
1:B:300:PHE:HA	1:B:301:PRO:HD3	1.94	0.41
1:B:375:GLU:OE2	1:B:400:ARG:NH2	2.53	0.41
1:C:386:SER:HA	1:C:387:PRO:HD3	1.96	0.41
1:F:448:ALA:O	1:F:452:LEU:HD23	2.20	0.41
1:A:239:ILE:HD11	1:A:247:ARG:HH21	1.84	0.41
1:B:130:LEU:HB2	1:B:160:ARG:HB3	2.02	0.41
1:B:199:TRP:HB2	1:B:320:ASN:HD22	1.86	0.41
1:C:210:ILE:HD11	1:C:274:LEU:HD12	2.02	0.41
1:C:419:ILE:HG22	1:C:441:LEU:HD11	2.02	0.41
1:E:135:LEU:C	1:E:137:ALA:H	2.28	0.41
1:F:519:ILE:HG23	1:F:522:GLN:NE2	2.36	0.41
1:D:411:PRO:HG2	1:D:414:TYR:CD2	2.55	0.41
1:F:241:THR:N	1:F:242:PRO:HA	2.34	0.41
1:D:7:PHE:O	1:D:75:PHE:HA	2.20	0.41
1:D:308:GLU:H	1:D:308:GLU:HG2	1.69	0.41
1:A:478:SER:HB3	1:A:480:MET:CE	2.50	0.41
1:B:480:MET:HE2	1:B:480:MET:HB2	1.74	0.41
1:D:429:GLN:HB2	1:D:443:TYR:CZ	2.56	0.41
1:F:457:ARG:HG2	1:F:457:ARG:HH11	1.85	0.41
1:D:6:ASN:OD1	1:D:74:ASN:HB2	2.21	0.41
1:D:195:ILE:HD11	1:D:274:LEU:HG	2.02	0.41
1:A:23:ARG:HH22	1:A:131:ASN:CG	2.29	0.41
1:B:521:ARG:HD2	1:B:543:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ASN:HD22	1:C:132:LYS:H	1.67	0.41
1:C:425:LYS:HD2	1:C:425:LYS:HA	1.85	0.41
1:C:474:ARG:NH1	1:C:476:GLN:OE1	2.53	0.41
1:E:57:GLN:O	1:E:77:ASP:HB2	2.20	0.41
1:F:400:ARG:HB3	1:F:475:PHE:HB3	2.02	0.41
1:F:479:ASP:OD1	1:F:501:ARG:HD2	2.20	0.41
1:A:324:LEU:HG	1:A:351:ILE:HD13	2.02	0.41
1:C:7:PHE:O	1:C:75:PHE:HA	2.19	0.41
1:C:377:THR:HG23	1:C:378:SER:N	2.36	0.41
1:B:23:ARG:HH22	1:B:131:ASN:CG	2.29	0.41
1:B:200:PHE:H	1:B:320:ASN:ND2	2.19	0.41
1:B:412:GLN:O	1:B:415:LEU:HG	2.20	0.41
1:C:263:LYS:H	1:C:263:LYS:HG2	1.67	0.41
1:D:321:ASP:OD1	1:D:347:HIS:HE1	2.04	0.41
1:D:521:ARG:HB2	1:D:545:LEU:CD1	2.51	0.41
1:B:86:TYR:O	1:B:90:ARG:HG2	2.20	0.41
1:C:84:PHE:O	1:C:88:VAL:HG23	2.20	0.41
1:C:120:MET:SD	1:C:153:ILE:HD11	2.59	0.41
1:C:480:MET:HE2	1:C:480:MET:HB2	1.84	0.41
1:E:386:SER:HA	1:E:387:PRO:HD3	1.94	0.41
1:F:203:TYR:CD2	1:F:204:LEU:HD13	2.56	0.41
1:F:221:ASP:HB3	1:F:276:LEU:CD2	2.51	0.41
1:F:384:VAL:HG21	1:F:390:LEU:HD12	2.02	0.41
1:A:419:ILE:HD13	1:A:420:THR:H	1.86	0.41
1:B:168:GLY:O	1:B:172:VAL:HG23	2.21	0.41
1:D:300:PHE:CD2	1:D:337:GLY:HA3	2.56	0.40
1:C:378:SER:O	1:C:380:GLU:N	2.54	0.40
1:D:81:HIS:CD2	1:D:346:LEU:HD21	2.56	0.40
1:D:431:ASN:HB3	1:D:442:THR:CG2	2.51	0.40
1:B:7:PHE:O	1:B:75:PHE:HA	2.20	0.40
1:B:304:SER:C	1:B:306:ASP:H	2.28	0.40
1:C:431:ASN:HB3	1:C:442:THR:CG2	2.50	0.40
1:E:211:ARG:HG2	1:E:255:VAL:HG22	2.03	0.40
1:E:429:GLN:HB2	1:E:443:TYR:CZ	2.57	0.40
1:E:452:LEU:O	1:E:453:ASP:C	2.64	0.40
1:F:429:GLN:HB2	1:F:443:TYR:CZ	2.56	0.40
1:A:25:ILE:HD11	1:A:59:VAL:HG21	2.03	0.40
1:C:500:HIS:HD2	1:C:502:ASP:H	1.68	0.40
1:E:93:ALA:HA	1:E:122:MET:HE1	2.04	0.40
1:E:479:ASP:OD1	1:E:501:ARG:HD2	2.22	0.40
1:F:81:HIS:NE2	1:F:346:LEU:HD11	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:GLY:HA2	1:F:124:LEU:HB3	2.04	0.40
1:D:112:THR:O	1:D:116:CYS:HB2	2.21	0.40
1:D:412:GLN:NE2	1:D:437:ASN:HA	2.37	0.40
1:B:425:LYS:HD2	1:B:449:GLU:CG	2.51	0.40
1:D:294:GLN:HB3	1:D:343:LEU:O	2.21	0.40
1:A:116:CYS:O	1:A:120:MET:HG3	2.21	0.40
1:B:94:ALA:HB1	1:B:211:ARG:HG3	2.02	0.40
1:B:119:ALA:O	1:B:122:MET:O	2.40	0.40
1:B:459:LYS:CG	1:B:464:GLY:HA2	2.51	0.40
1:B:459:LYS:HG2	1:B:464:GLY:HA2	2.04	0.40
1:F:331:SER:HB2	1:F:334:LEU:HB2	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	519/599 (87%)	501 (96%)	15 (3%)	3 (1%)	21	51
1	B	519/599 (87%)	494 (95%)	20 (4%)	5 (1%)	12	38
1	C	519/599 (87%)	495 (95%)	20 (4%)	4 (1%)	16	44
1	D	519/599 (87%)	490 (94%)	27 (5%)	2 (0%)	30	60
1	E	519/599 (87%)	492 (95%)	22 (4%)	5 (1%)	12	38
1	F	519/599 (87%)	495 (95%)	21 (4%)	3 (1%)	21	51
All	All	3114/3594 (87%)	2967 (95%)	125 (4%)	22 (1%)	18	47

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	453	ASP

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Mol	Chain	Res	Type
1	C	379	ARG
1	E	379	ARG
1	D	29	GLY
1	D	453	ASP
1	A	379	ARG
1	B	29	GLY
1	B	453	ASP
1	C	29	GLY
1	C	453	ASP
1	E	29	GLY
1	E	453	ASP
1	B	261	ALA
1	C	123	ASP
1	F	29	GLY
1	A	29	GLY
1	B	452	LEU
1	E	241	THR
1	F	453	ASP
1	F	241	THR
1	B	241	THR
1	E	133	ILE

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	447/511 (88%)	393 (88%)	54 (12%)	5 16
1	B	447/511 (88%)	397 (89%)	50 (11%)	6 19
1	C	447/511 (88%)	397 (89%)	50 (11%)	6 19
1	D	447/511 (88%)	399 (89%)	48 (11%)	6 21
1	E	447/511 (88%)	413 (92%)	34 (8%)	12 36
1	F	447/511 (88%)	400 (90%)	47 (10%)	6 22
All	All	2682/3066 (88%)	2399 (89%)	283 (11%)	6 22

All (283) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	10	ILE
1	D	59	VAL
1	D	75	PHE
1	D	82	VAL
1	D	109	GLU
1	D	131	ASN
1	D	133	ILE
1	D	149	ASP
1	D	153	ILE
1	D	160	ARG
1	D	173	LEU
1	D	188	GLU
1	D	191	LEU
1	D	204	LEU
1	D	214	ASN
1	D	241	THR
1	D	248	THR
1	D	263	LYS
1	D	270	VAL
1	D	273	THR
1	D	290	LYS
1	D	317	LEU
1	D	324	LEU
1	D	327	GLU
1	D	332	SER
1	D	346	LEU
1	D	353	GLU
1	D	355	LEU
1	D	408	MET
1	D	410	LEU
1	D	415	LEU
1	D	419	ILE
1	D	421	LEU
1	D	430	THR
1	D	437	ASN
1	D	442	THR
1	D	449	GLU
1	D	452	LEU
1	D	458	LEU
1	D	468	LEU
1	D	471	ASN
1	D	486	LEU

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Mol	Chain	Res	Type
1	D	506	ASN
1	D	516	LYS
1	D	534	THR
1	D	540	SER
1	D	541	THR
1	D	545	LEU
1	A	18	SER
1	A	57	GLN
1	A	59	VAL
1	A	109	GLU
1	A	116	CYS
1	A	118	THR
1	A	131	ASN
1	A	133	ILE
1	A	153	ILE
1	A	160	ARG
1	A	173	LEU
1	A	191	LEU
1	A	204	LEU
1	A	210	ILE
1	A	222	LYS
1	A	230	GLN
1	A	241	THR
1	A	243	LYS
1	A	246	ASP
1	A	270	VAL
1	A	273	THR
1	A	290	LYS
1	A	318	SER
1	A	323	SER
1	A	324	LEU
1	A	346	LEU
1	A	351	ILE
1	A	354	ARG
1	A	355	LEU
1	A	369	THR
1	A	374	VAL
1	A	385	ASP
1	A	394	ASN
1	A	409	LEU
1	A	415	LEU
1	A	419	ILE

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Mol	Chain	Res	Type
1	A	420	THR
1	A	421	LEU
1	A	424	GLU
1	A	430	THR
1	A	442	THR
1	A	449	GLU
1	A	453	ASP
1	A	458	LEU
1	A	468	LEU
1	A	495	LEU
1	A	501	ARG
1	A	506	ASN
1	A	507	ARG
1	A	511	LEU
1	A	516	LYS
1	A	534	THR
1	A	541	THR
1	A	545	LEU
1	B	57	GLN
1	B	75	PHE
1	B	82	VAL
1	B	85	SER
1	B	109	GLU
1	B	116	CYS
1	B	123	ASP
1	B	124	LEU
1	B	153	ILE
1	B	160	ARG
1	B	173	LEU
1	B	191	LEU
1	B	204	LEU
1	B	214	ASN
1	B	243	LYS
1	B	246	ASP
1	B	248	THR
1	B	270	VAL
1	B	273	THR
1	B	290	LYS
1	B	318	SER
1	B	324	LEU
1	B	346	LEU
1	B	355	LEU

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Mol	Chain	Res	Type
1	B	365	THR
1	B	369	THR
1	B	393	VAL
1	B	394	ASN
1	B	401	GLU
1	B	410	LEU
1	B	415	LEU
1	B	419	ILE
1	B	421	LEU
1	B	424	GLU
1	B	430	THR
1	B	437	ASN
1	B	438	GLN
1	B	442	THR
1	B	449	GLU
1	B	452	LEU
1	B	453	ASP
1	B	458	LEU
1	B	468	LEU
1	B	486	LEU
1	B	487	ILE
1	B	495	LEU
1	B	507	ARG
1	B	512	VAL
1	B	516	LYS
1	B	545	LEU
1	C	58	SER
1	C	75	PHE
1	C	82	VAL
1	C	109	GLU
1	C	111	GLN
1	C	131	ASN
1	C	142	ARG
1	C	149	ASP
1	C	153	ILE
1	C	173	LEU
1	C	188	GLU
1	C	191	LEU
1	C	214	ASN
1	C	241	THR
1	C	243	LYS
1	C	248	THR

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Mol	Chain	Res	Type
1	C	249	GLU
1	C	263	LYS
1	C	270	VAL
1	C	273	THR
1	C	290	LYS
1	C	294	GLN
1	C	308	GLU
1	C	317	LEU
1	C	318	SER
1	C	324	LEU
1	C	327	GLU
1	C	331	SER
1	C	346	LEU
1	C	354	ARG
1	C	355	LEU
1	C	369	THR
1	C	394	ASN
1	C	415	LEU
1	C	417	ASN
1	C	419	ILE
1	C	420	THR
1	C	424	GLU
1	C	430	THR
1	C	434	TYR
1	C	437	ASN
1	C	442	THR
1	C	471	ASN
1	C	486	LEU
1	C	495	LEU
1	C	509	ARG
1	C	511	LEU
1	C	516	LYS
1	C	541	THR
1	C	545	LEU
1	E	69	GLU
1	E	109	GLU
1	E	118	THR
1	E	133	ILE
1	E	153	ILE
1	E	188	GLU
1	E	191	LEU
1	E	204	LEU

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Mol	Chain	Res	Type
1	E	243	LYS
1	E	260	CYS
1	E	270	VAL
1	E	273	THR
1	E	290	LYS
1	E	317	LEU
1	E	324	LEU
1	E	327	GLU
1	E	332	SER
1	E	346	LEU
1	E	355	LEU
1	E	369	THR
1	E	409	LEU
1	E	419	ILE
1	E	430	THR
1	E	438	GLN
1	E	442	THR
1	E	453	ASP
1	E	458	LEU
1	E	468	LEU
1	E	486	LEU
1	E	506	ASN
1	E	511	LEU
1	E	516	LYS
1	E	534	THR
1	E	545	LEU
1	F	75	PHE
1	F	109	GLU
1	F	133	ILE
1	F	153	ILE
1	F	160	ARG
1	F	191	LEU
1	F	204	LEU
1	F	212	ILE
1	F	214	ASN
1	F	230	GLN
1	F	243	LYS
1	F	245	VAL
1	F	248	THR
1	F	270	VAL
1	F	273	THR
1	F	290	LYS

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Mol	Chain	Res	Type
1	F	294	GLN
1	F	317	LEU
1	F	318	SER
1	F	323	SER
1	F	327	GLU
1	F	332	SER
1	F	346	LEU
1	F	355	LEU
1	F	381	VAL
1	F	401	GLU
1	F	410	LEU
1	F	419	ILE
1	F	421	LEU
1	F	424	GLU
1	F	430	THR
1	F	442	THR
1	F	449	GLU
1	F	454	PHE
1	F	458	LEU
1	F	459	LYS
1	F	468	LEU
1	F	486	LEU
1	F	487	ILE
1	F	495	LEU
1	F	506	ASN
1	F	507	ARG
1	F	511	LEU
1	F	516	LYS
1	F	540	SER
1	F	541	THR
1	F	545	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	57	GLN
1	D	81	HIS
1	D	131	ASN
1	D	214	ASN
1	D	320	ASN
1	D	347	HIS
1	D	352	GLN

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Mol	Chain	Res	Type
1	D	395	ASN
1	D	407	HIS
1	D	438	GLN
1	D	471	ASN
1	D	503	ASN
1	D	505	GLN
1	D	523	GLN
1	A	72	GLN
1	A	81	HIS
1	A	131	ASN
1	A	192	GLN
1	A	244	GLN
1	A	320	ASN
1	A	347	HIS
1	A	352	GLN
1	A	395	ASN
1	A	500	HIS
1	A	505	GLN
1	A	523	GLN
1	B	81	HIS
1	B	131	ASN
1	B	192	GLN
1	B	214	ASN
1	B	320	ASN
1	B	347	HIS
1	B	352	GLN
1	B	395	ASN
1	B	407	HIS
1	B	429	GLN
1	B	438	GLN
1	B	500	HIS
1	C	81	HIS
1	C	111	GLN
1	C	115	ASN
1	C	131	ASN
1	C	170	GLN
1	C	214	ASN
1	C	233	ASN
1	C	320	ASN
1	C	347	HIS
1	C	352	GLN
1	C	412	GLN

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Mol	Chain	Res	Type
1	C	437	ASN
1	C	500	HIS
1	C	505	GLN
1	C	523	GLN
1	C	529	GLN
1	E	3	ASN
1	E	72	GLN
1	E	81	HIS
1	E	131	ASN
1	E	170	GLN
1	E	192	GLN
1	E	347	HIS
1	E	435	HIS
1	F	3	ASN
1	F	12	HIS
1	F	26	GLN
1	F	57	GLN
1	F	81	HIS
1	F	131	ASN
1	F	170	GLN
1	F	320	ASN
1	F	347	HIS
1	F	352	GLN
1	F	429	GLN
1	F	437	ASN
1	F	471	ASN
1	F	500	HIS
1	F	505	GLN
1	F	523	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	525/599 (87%)	0.38	13 (2%) 58 48	46, 53, 59, 62	0
1	B	525/599 (87%)	0.45	15 (2%) 53 43	46, 53, 60, 66	0
1	C	525/599 (87%)	0.58	24 (4%) 37 29	48, 54, 61, 65	0
1	D	525/599 (87%)	0.43	13 (2%) 58 48	47, 54, 59, 63	0
1	E	525/599 (87%)	0.72	27 (5%) 33 25	46, 54, 60, 63	0
1	F	525/599 (87%)	0.46	7 (1%) 75 66	46, 54, 59, 61	0
All	All	3150/3594 (87%)	0.50	99 (3%) 51 41	46, 54, 60, 66	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	434	TYR	4.4
1	E	453	ASP	4.1
1	C	13	ILE	4.1
1	F	13	ILE	3.9
1	E	13	ILE	3.7
1	E	75	PHE	3.4
1	D	453	ASP	3.2
1	C	30	GLY	3.1
1	B	57	GLN	3.1
1	E	409	LEU	3.1
1	E	278	ARG	3.0
1	C	415	LEU	3.0
1	D	82	VAL	2.9
1	A	13	ILE	2.9
1	B	13	ILE	2.8
1	C	553	CYS	2.8
1	E	411	PRO	2.8
1	D	13	ILE	2.7
1	A	452	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	135	LEU	2.7
1	A	453	ASP	2.7
1	C	412	GLN	2.7
1	B	82	VAL	2.7
1	A	185	GLY	2.6
1	C	452	LEU	2.6
1	E	110	ALA	2.6
1	B	345	LEU	2.6
1	C	111	GLN	2.6
1	D	30	GLY	2.6
1	D	185	GLY	2.6
1	C	136	PRO	2.5
1	E	463	ARG	2.5
1	E	378	SER	2.5
1	E	437	ASN	2.5
1	B	346	LEU	2.4
1	D	79	PRO	2.4
1	A	278	ARG	2.4
1	B	394	ASN	2.4
1	E	30	GLY	2.4
1	C	550	LEU	2.4
1	E	415	LEU	2.4
1	D	108	VAL	2.4
1	E	468	LEU	2.4
1	E	150	ILE	2.4
1	F	75	PHE	2.4
1	E	439	VAL	2.3
1	C	107	GLY	2.3
1	E	168	GLY	2.3
1	C	163	ALA	2.3
1	B	210	ILE	2.3
1	C	79	PRO	2.3
1	D	57	GLN	2.3
1	D	440	ALA	2.2
1	C	261	ALA	2.2
1	C	378	SER	2.2
1	E	414	TYR	2.2
1	D	156	THR	2.2
1	C	108	VAL	2.2
1	C	161	CYS	2.2
1	D	458	LEU	2.2
1	A	503	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	12	HIS	2.2
1	C	453	ASP	2.2
1	E	79	PRO	2.2
1	E	156	THR	2.2
1	B	467	SER	2.2
1	D	452	LEU	2.2
1	A	415	LEU	2.2
1	C	57	GLN	2.2
1	B	81	HIS	2.2
1	F	158	ALA	2.2
1	A	157	ASP	2.1
1	E	377	THR	2.1
1	A	409	LEU	2.1
1	C	110	ALA	2.1
1	E	294	GLN	2.1
1	F	82	VAL	2.1
1	E	80	GLY	2.1
1	E	410	LEU	2.1
1	B	18	SER	2.1
1	A	230	GLN	2.1
1	C	407	HIS	2.1
1	B	452	LEU	2.1
1	F	110	ALA	2.1
1	B	332	SER	2.1
1	E	553	CYS	2.1
1	F	294	GLN	2.1
1	C	419	ILE	2.1
1	A	290	LYS	2.0
1	B	294	GLN	2.0
1	D	481	VAL	2.0
1	E	82	VAL	2.0
1	B	533	GLY	2.0
1	C	165	THR	2.0
1	E	11	ALA	2.0
1	B	117	TYR	2.0
1	F	27	ILE	2.0
1	A	469	ASP	2.0
1	A	101	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.