Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 04:55 AM EDT

PDB ID	:	3CB4
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 (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:

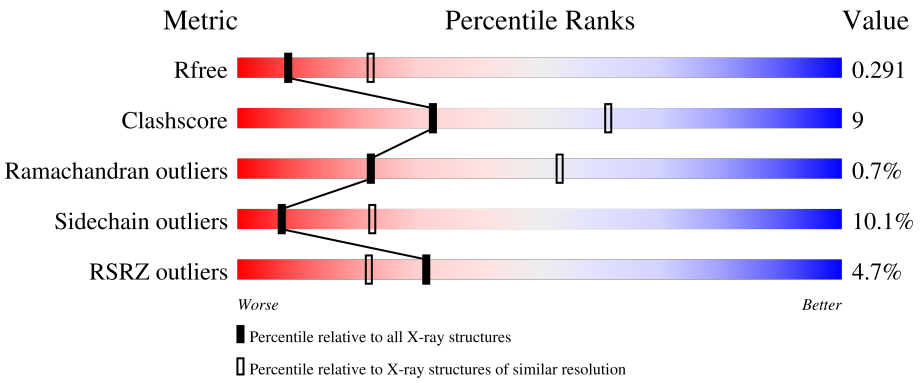
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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% 67% 17% • 12%
1	B	599	3% 65% 19% • 12%
1	C	599	6% 64% 20% • 12%
1	D	599	5% 67% 18% • 12%
1	E	599	7% 67% 19% • 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	599	3% 64% 22% • 12%

2 Entry composition (i)

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.

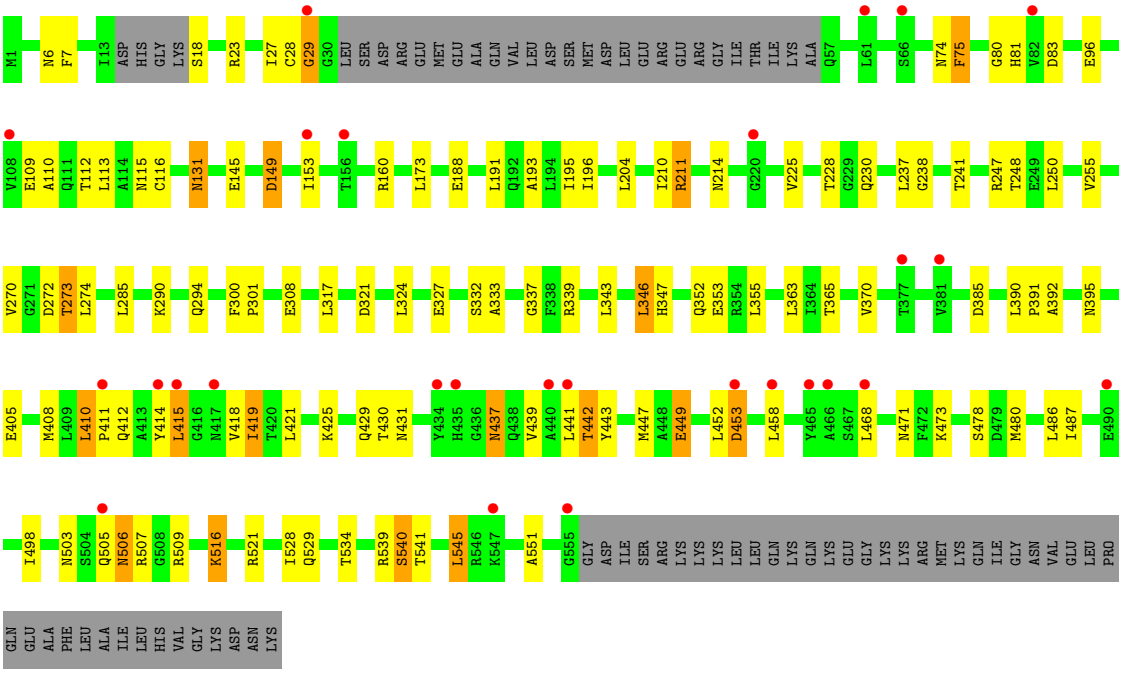
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	D	3	3	3	0	0

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.

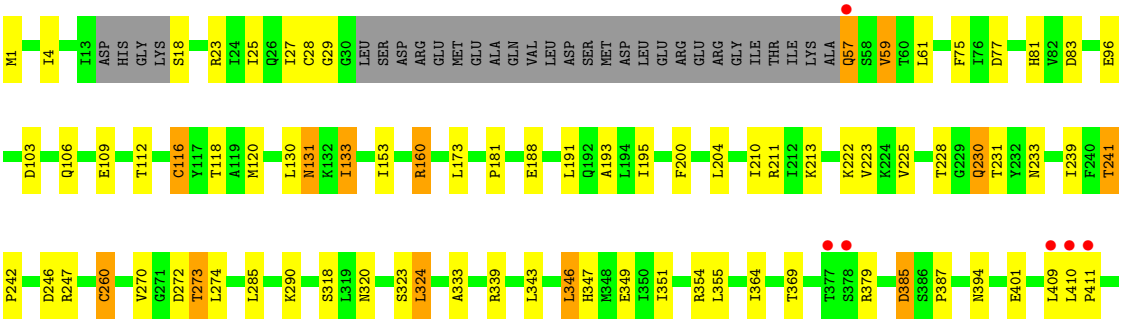
• Molecule 1: GTP-binding protein lepA

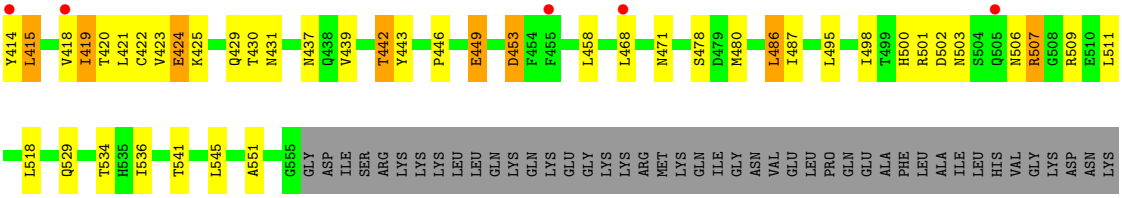
Chain D:



• Molecule 1: GTP-binding protein lepA

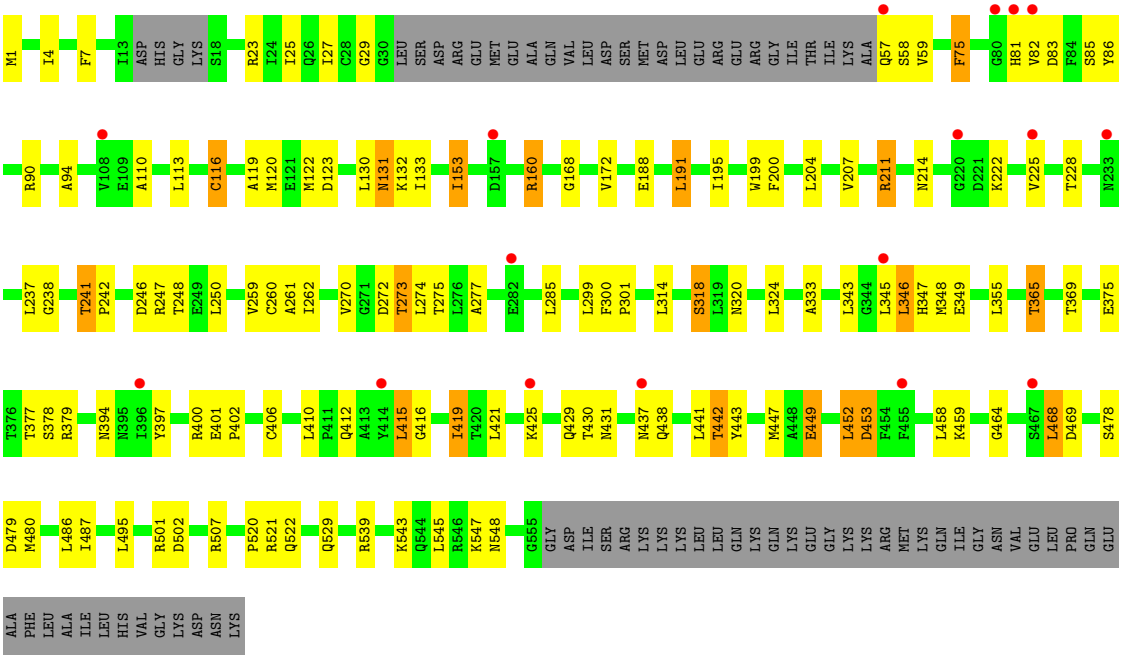
Chain A:





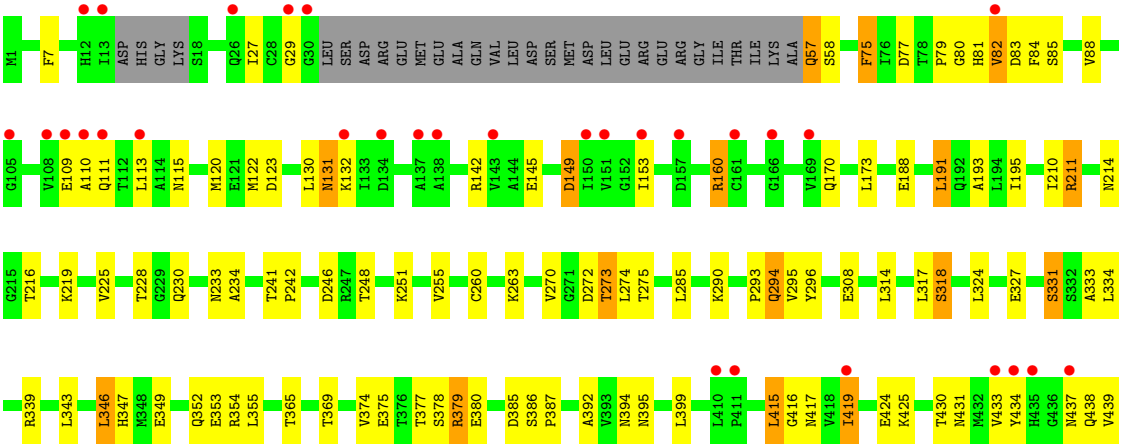
• Molecule 1: GTP-binding protein lepA

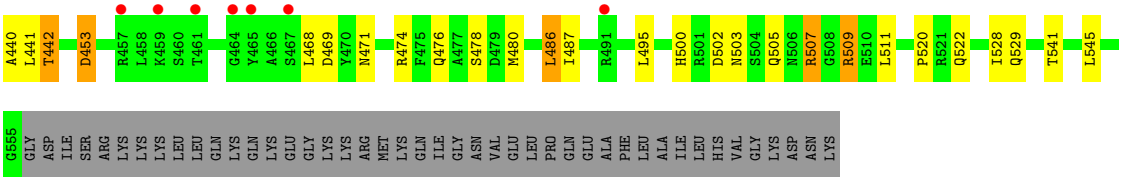
Chain B:



• Molecule 1: GTP-binding protein lepA

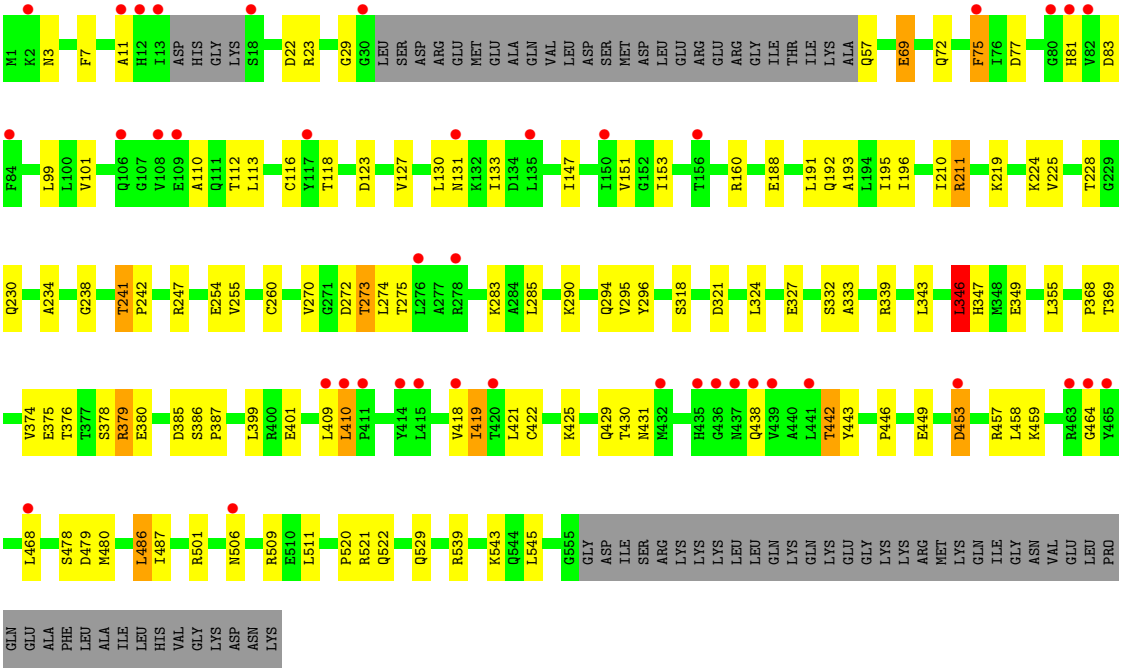
Chain C:





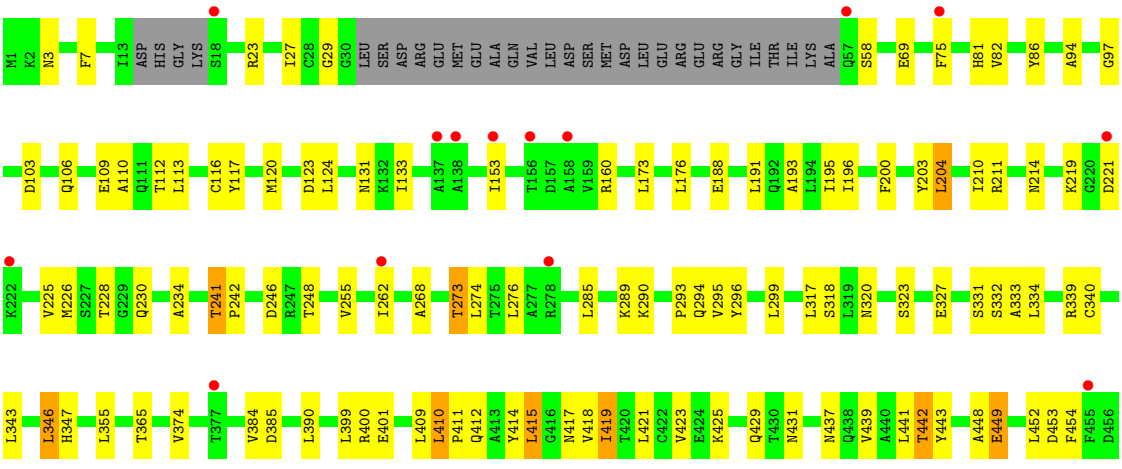
• Molecule 1: GTP-binding protein lepA

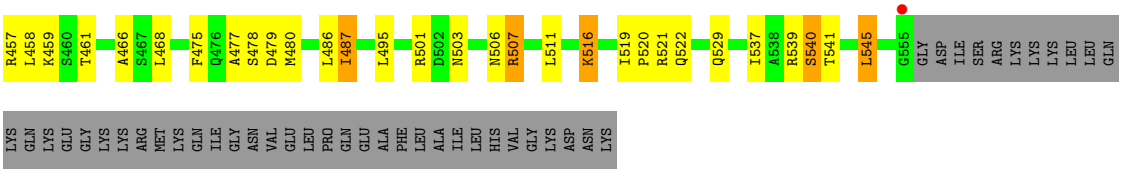
Chain E:



• Molecule 1: GTP-binding protein lepA

Chain F:




R457
L458
K459
S460
T461
A466
S467
L468
F475
Q476
A477
S478
D479
M480
L486
I487
L495
R501
D502
N503
N506
R507
L511
K516
I519
P520
R521
Q522
Q529
I537
A538
R539
S540
T541
L545
G555
LYS
GLN
LYS
GLU
GLY
LYS
LYS
ARG
MET
LYS
GLN
ILE
GLY
ASN
VAL
GLU
LEU
PRO
GLN
GLU
ALA
PHE
LEU
ALA
ILE
LEU
HIS
VAL
GLY
LYS
ASP
ASN
LYS
GLY
ASP
ILE
SER
ARG
LYS
LYS
LYS
LEU
LEU
GLN

4 Data and refinement statistics (i)

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 43.31 – 2.81	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.80) 94.6 (43.31-2.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.81Å)	Xtriage
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 (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	53.0	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	24495	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage'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.*

[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	0.35	0/4150	0.56	0/5626
1	B	0.35	0/4150	0.56	0/5626
1	C	0.38	2/4150 (0.0%)	0.59	2/5626 (0.0%)
1	D	0.34	0/4150	0.56	0/5626
1	E	0.34	0/4150	0.55	1/5626 (0.0%)
1	F	0.35	0/4150	0.55	0/5626
All	All	0.35	2/24900 (0.0%)	0.56	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	6.50	1.41	1.33
1	C	142	ARG	CZ-NH1	5.67	1.40	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	142	ARG	NE-CZ-NH1	12.29	126.44	120.30
1	C	142	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	E	346	LEU	CA-CB-CG	5.31	127.52	115.30

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	75	0
1	B	4082	0	4095	72	0
1	C	4082	0	4095	76	0
1	D	4082	0	4095	68	0
1	E	4082	0	4095	68	0
1	F	4082	0	4095	85	0
2	D	3	0	0	0	0
All	All	24495	0	24570	430	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 (430) 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

Continued on next page...

Continued from previous page...

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: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
1:F:23:ARG:HH22	1:F:131:ASN:ND2	1.85	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:F:241:THR:H	1:F:242:PRO:C	2.06	0.58
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:241:THR:H	1:E:242:PRO:C	2.07	0.56
1:F:478:SER:HB3	1:F:480:MET:CE	2.36	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:HE1	1.88	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:B:241:THR:H	1:B:242:PRO:C	2.10	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: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
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:28:CYS:O	1:D:29:GLY:C	2.51	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: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:F:117:TYR:HA	1:F:120:MET:HE2	1.95	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:A:241:THR:H	1:A:242:PRO:C	2.17	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
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:C:241:THR:H	1:C:242:PRO:C	2.19	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:241:THR:O	1:E:241:THR:CG2	2.63	0.46
1:D:370:VAL:HG11	1:D:447:MET:HG3	1.97	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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:478:SER:HB3	1:C:480:MET:HE2	1.98	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: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: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: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:A:500:HIS:CD2	1:A:502:ASP:H	2.36	0.43
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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: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:F:333:ALA:HB1	1:F:487:ILE:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:478:SER:HB3	1:B:480:MET:HE2	2.02	0.41
1:D:429:GLN:HB2	1:D:443:TYR:CZ	2.56	0.41
1:B:27:ILE:HG22	1:F:537:ILE:C	2.41	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:B:521:ARG:HD2	1:B:543:LYS:O	2.21	0.41
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
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%)	25	56
1	B	519/599 (87%)	494 (95%)	20 (4%)	5 (1%)	15	44
1	C	519/599 (87%)	495 (95%)	20 (4%)	4 (1%)	19	49
1	D	519/599 (87%)	490 (94%)	27 (5%)	2 (0%)	34	66
1	E	519/599 (87%)	492 (95%)	22 (4%)	5 (1%)	15	44
1	F	519/599 (87%)	495 (95%)	21 (4%)	3 (1%)	25	56
All	All	3114/3594 (87%)	2967 (95%)	125 (4%)	22 (1%)	22	53

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	453	ASP
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 15
1	B	447/511 (88%)	402 (90%)	45 (10%)	7 22
1	C	447/511 (88%)	398 (89%)	49 (11%)	6 19
1	D	447/511 (88%)	401 (90%)	46 (10%)	7 21
1	E	447/511 (88%)	413 (92%)	34 (8%)	13 36
1	F	447/511 (88%)	403 (90%)	44 (10%)	8 24
All	All	2682/3066 (88%)	2410 (90%)	272 (10%)	7 22

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	75	PHE
1	D	109	GLU
1	D	131	ASN
1	D	149	ASP
1	D	153	ILE
1	D	160	ARG
1	D	188	GLU
1	D	191	LEU
1	D	204	LEU
1	D	211	ARG
1	D	214	ASN
1	D	241	THR
1	D	248	THR
1	D	270	VAL
1	D	273	THR
1	D	290	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	453	ASP
1	D	458	LEU
1	D	468	LEU
1	D	471	ASN
1	D	486	LEU
1	D	506	ASN
1	D	507	ARG
1	D	509	ARG
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	75	PHE
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	188	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	191	LEU
1	A	204	LEU
1	A	222	LYS
1	A	230	GLN
1	A	241	THR
1	A	246	ASP
1	A	260	CYS
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	354	ARG
1	A	355	LEU
1	A	369	THR
1	A	385	ASP
1	A	394	ASN
1	A	409	LEU
1	A	415	LEU
1	A	419	ILE
1	A	421	LEU
1	A	424	GLU
1	A	430	THR
1	A	437	ASN
1	A	442	THR
1	A	449	GLU
1	A	453	ASP
1	A	458	LEU
1	A	468	LEU
1	A	471	ASN
1	A	486	LEU
1	A	495	LEU
1	A	501	ARG
1	A	506	ASN
1	A	507	ARG
1	A	509	ARG
1	A	511	LEU
1	A	534	THR
1	A	541	THR
1	A	545	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	57	GLN
1	B	58	SER
1	B	75	PHE
1	B	82	VAL
1	B	85	SER
1	B	116	CYS
1	B	123	ASP
1	B	131	ASN
1	B	153	ILE
1	B	160	ARG
1	B	188	GLU
1	B	191	LEU
1	B	204	LEU
1	B	211	ARG
1	B	214	ASN
1	B	246	ASP
1	B	248	THR
1	B	270	VAL
1	B	273	THR
1	B	318	SER
1	B	324	LEU
1	B	346	LEU
1	B	355	LEU
1	B	365	THR
1	B	369	THR
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	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	495	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	502	ASP
1	B	507	ARG
1	B	545	LEU
1	C	57	GLN
1	C	58	SER
1	C	75	PHE
1	C	82	VAL
1	C	109	GLU
1	C	111	GLN
1	C	122	MET
1	C	131	ASN
1	C	149	ASP
1	C	160	ARG
1	C	188	GLU
1	C	191	LEU
1	C	211	ARG
1	C	214	ASN
1	C	246	ASP
1	C	248	THR
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	424	GLU
1	C	430	THR
1	C	434	TYR
1	C	437	ASN
1	C	438	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	442	THR
1	C	453	ASP
1	C	471	ASN
1	C	486	LEU
1	C	495	LEU
1	C	507	ARG
1	C	509	ARG
1	C	511	LEU
1	C	541	THR
1	C	545	LEU
1	E	22	ASP
1	E	69	GLU
1	E	75	PHE
1	E	118	THR
1	E	123	ASP
1	E	153	ILE
1	E	188	GLU
1	E	191	LEU
1	E	211	ARG
1	E	260	CYS
1	E	270	VAL
1	E	273	THR
1	E	290	LYS
1	E	318	SER
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	410	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	509	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	511	LEU
1	E	545	LEU
1	F	58	SER
1	F	75	PHE
1	F	109	GLU
1	F	123	ASP
1	F	153	ILE
1	F	160	ARG
1	F	188	GLU
1	F	191	LEU
1	F	204	LEU
1	F	214	ASN
1	F	230	GLN
1	F	246	ASP
1	F	248	THR
1	F	273	THR
1	F	290	LYS
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	401	GLU
1	F	410	LEU
1	F	415	LEU
1	F	419	ILE
1	F	421	LEU
1	F	437	ASN
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	81	HIS
1	D	131	ASN
1	D	320	ASN
1	D	347	HIS
1	D	352	GLN
1	D	407	HIS
1	D	438	GLN
1	D	471	ASN
1	D	503	ASN
1	D	505	GLN
1	D	506	ASN
1	D	523	GLN
1	A	81	HIS
1	A	131	ASN
1	A	294	GLN
1	A	320	ASN
1	A	347	HIS
1	A	395	ASN
1	A	429	GLN
1	A	500	HIS
1	A	522	GLN
1	A	523	GLN
1	B	81	HIS
1	B	131	ASN
1	B	320	ASN
1	B	347	HIS
1	B	352	GLN
1	B	429	GLN
1	B	438	GLN
1	B	500	HIS
1	C	81	HIS
1	C	115	ASN
1	C	131	ASN
1	C	170	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	266	HIS
1	C	320	ASN
1	C	347	HIS
1	C	352	GLN
1	C	437	ASN
1	C	500	HIS
1	C	505	GLN
1	C	523	GLN
1	E	3	ASN
1	E	72	GLN
1	E	81	HIS
1	E	131	ASN
1	E	266	HIS
1	E	347	HIS
1	E	352	GLN
1	E	435	HIS
1	E	505	GLN
1	E	523	GLN
1	E	544	GLN
1	F	57	GLN
1	F	81	HIS
1	F	131	ASN
1	F	320	ASN
1	F	347	HIS
1	F	395	ASN
1	F	429	GLN
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 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	525/599 (87%)	0.31	11 (2%)	63	54	46, 53, 59, 62	0
1	B	525/599 (87%)	0.36	17 (3%)	47	37	46, 53, 60, 66	0
1	C	525/599 (87%)	0.51	38 (7%)	15	8	48, 54, 61, 65	0
1	D	525/599 (87%)	0.45	27 (5%)	28	19	47, 54, 59, 63	0
1	E	525/599 (87%)	0.53	41 (7%)	13	7	46, 54, 60, 63	0
1	F	525/599 (87%)	0.38	15 (2%)	51	41	46, 54, 59, 61	0
All	All	3150/3594 (87%)	0.42	149 (4%)	31	22	46, 54, 60, 66	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	411	PRO	6.2
1	E	463	ARG	5.2
1	D	440	ALA	5.0
1	E	409	LEU	4.9
1	D	414	TYR	4.8
1	C	434	TYR	4.7
1	E	436	GLY	4.4
1	E	410	LEU	4.4
1	A	378	SER	4.3
1	C	105	GLY	4.3
1	C	410	LEU	4.3
1	E	278	ARG	4.2
1	E	439	VAL	4.0
1	A	468	LEU	4.0
1	C	419	ILE	4.0
1	C	108	VAL	3.9
1	E	415	LEU	3.9
1	E	435	HIS	3.8
1	A	411	PRO	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	467	SER	3.7
1	E	80	GLY	3.7
1	E	11	ALA	3.7
1	F	156	THR	3.7
1	E	437	ASN	3.6
1	C	464	GLY	3.6
1	D	435	HIS	3.5
1	E	464	GLY	3.4
1	E	276	LEU	3.4
1	A	410	LEU	3.4
1	B	282	GLU	3.3
1	E	418	VAL	3.3
1	C	143	VAL	3.2
1	D	458	LEU	3.2
1	E	441	LEU	3.2
1	B	220	GLY	3.1
1	E	156	THR	3.1
1	F	153	ILE	3.1
1	E	432	MET	3.1
1	F	158	ALA	3.1
1	D	441	LEU	3.1
1	E	12	HIS	3.0
1	B	80	GLY	3.0
1	C	12	HIS	3.0
1	E	13	ILE	3.0
1	F	18	SER	2.9
1	A	409	LEU	2.9
1	D	434	TYR	2.9
1	A	414	TYR	2.9
1	F	138	ALA	2.9
1	E	453	ASP	2.9
1	C	437	ASN	2.8
1	E	30	GLY	2.8
1	E	465	TYR	2.8
1	C	26	GLN	2.8
1	D	381	VAL	2.8
1	C	157	ASP	2.8
1	D	466	ALA	2.8
1	C	110	ALA	2.8
1	E	2	LYS	2.7
1	D	555	GLY	2.7
1	E	81	HIS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	414	TYR	2.7
1	B	81	HIS	2.7
1	E	82	VAL	2.6
1	D	377	THR	2.6
1	A	57	GLN	2.6
1	D	82	VAL	2.6
1	C	132	LYS	2.6
1	D	453	ASP	2.6
1	F	221	ASP	2.5
1	A	505	GLN	2.5
1	E	468	LEU	2.5
1	D	411	PRO	2.5
1	C	137	ALA	2.5
1	B	57	GLN	2.5
1	C	457	ARG	2.5
1	E	117	TYR	2.5
1	E	150	ILE	2.5
1	D	61	LEU	2.4
1	D	66	SER	2.4
1	A	455	PHE	2.4
1	C	29	GLY	2.4
1	B	437	ASN	2.4
1	C	465	TYR	2.4
1	C	30	GLY	2.4
1	A	377	THR	2.4
1	C	150	ILE	2.4
1	D	220	GLY	2.3
1	F	75	PHE	2.3
1	F	555	GLY	2.3
1	D	505	GLN	2.3
1	C	111	GLN	2.3
1	D	465	TYR	2.3
1	F	137	ALA	2.3
1	D	153	ILE	2.3
1	B	233	ASN	2.3
1	E	109	GLU	2.3
1	E	414	TYR	2.3
1	B	345	LEU	2.3
1	E	84	PHE	2.3
1	F	455	PHE	2.3
1	E	18	SER	2.3
1	A	418	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	57	GLN	2.3
1	E	75	PHE	2.3
1	D	108	VAL	2.2
1	C	82	VAL	2.2
1	C	169	VAL	2.2
1	F	278	ARG	2.2
1	C	411	PRO	2.2
1	C	433	VAL	2.2
1	D	417	ASN	2.2
1	C	491	ARG	2.2
1	E	506	ASN	2.2
1	F	262	ILE	2.2
1	E	106	GLN	2.2
1	E	438	GLN	2.2
1	D	29	GLY	2.2
1	E	420	THR	2.2
1	C	153	ILE	2.2
1	B	225	VAL	2.2
1	C	461	THR	2.2
1	C	13	ILE	2.1
1	C	435	HIS	2.1
1	D	156	THR	2.1
1	B	157	ASP	2.1
1	F	377	THR	2.1
1	B	425	LYS	2.1
1	E	108	VAL	2.1
1	D	415	LEU	2.1
1	C	113	LEU	2.1
1	F	222	LYS	2.1
1	B	82	VAL	2.1
1	C	138	ALA	2.1
1	C	166	GLY	2.1
1	E	131	ASN	2.1
1	D	468	LEU	2.0
1	C	467	SER	2.0
1	D	490	GLU	2.0
1	C	109	GLU	2.0
1	C	459	LYS	2.0
1	C	151	VAL	2.0
1	C	161	CYS	2.0
1	D	547	LYS	2.0
1	B	396	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	134	ASP	2.0
1	B	108	VAL	2.0
1	B	455	PHE	2.0
1	E	135	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.