



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:38 PM UTC

PDB ID : 2J7N / pdb_00002j7n
Title : Structure of the RNAi polymerase from *Neurospora crassa*
Authors : Salgado, P.S.; Koivunen, M.R.L.; Makeyev, E.V.; Bamford, D.H.; Stuart, D.I.; Grimes, J.M.
Deposited on : 2006-10-13
Resolution : 2.30 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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

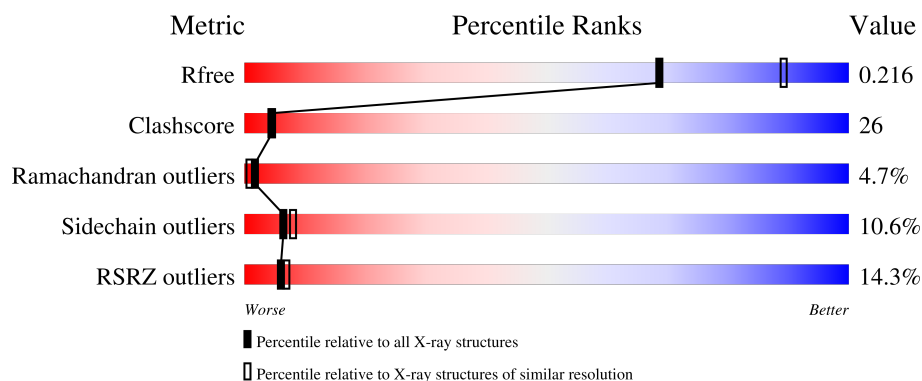
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	1022	9% 60% 23% 6% • 9%
1	B	1022	17% 56% 25% 8% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15945 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 RNA-DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	935	Total	C	N	O	S	0	0	1
			7520	4814	1304	1368	34			
1	B	932	Total	C	N	O	S	0	0	1
			7498	4798	1300	1366	34			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	ALA	GLY	conflict	UNP Q9Y7G6
B	559	ALA	GLY	conflict	UNP Q9Y7G6

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			5	3	2		

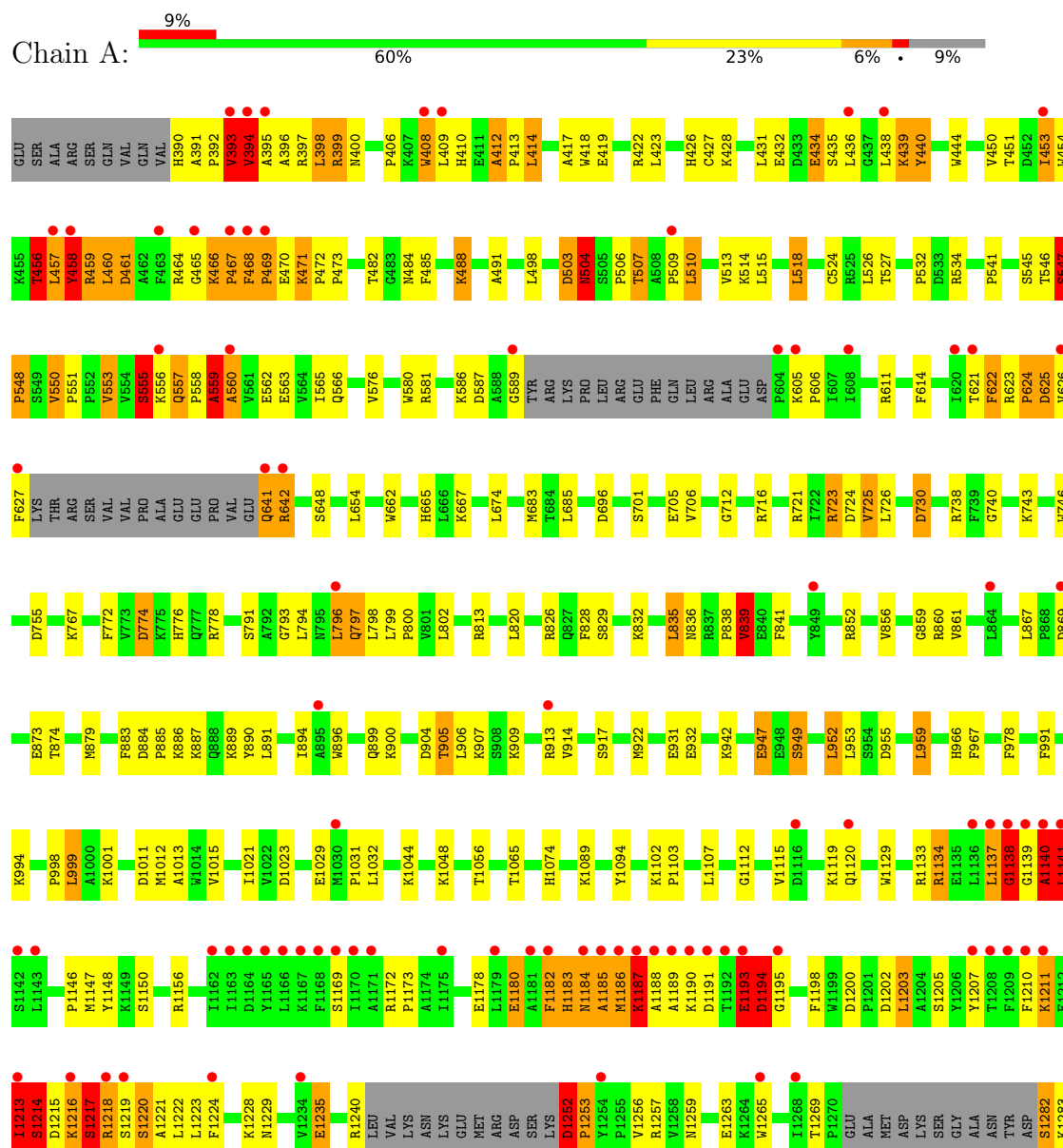
- Molecule 4 is water.

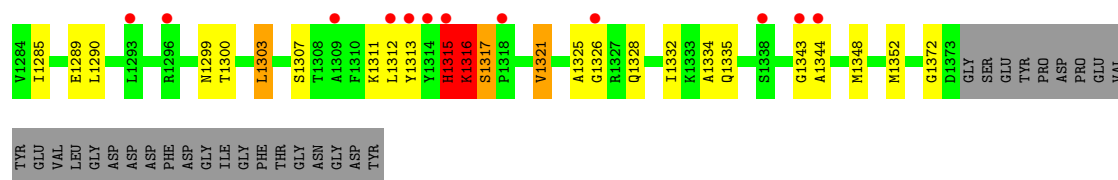
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	499	Total	O	0	0
			499	499		
4	B	421	Total	O	0	0
			421	421		

3 Residue-property plots

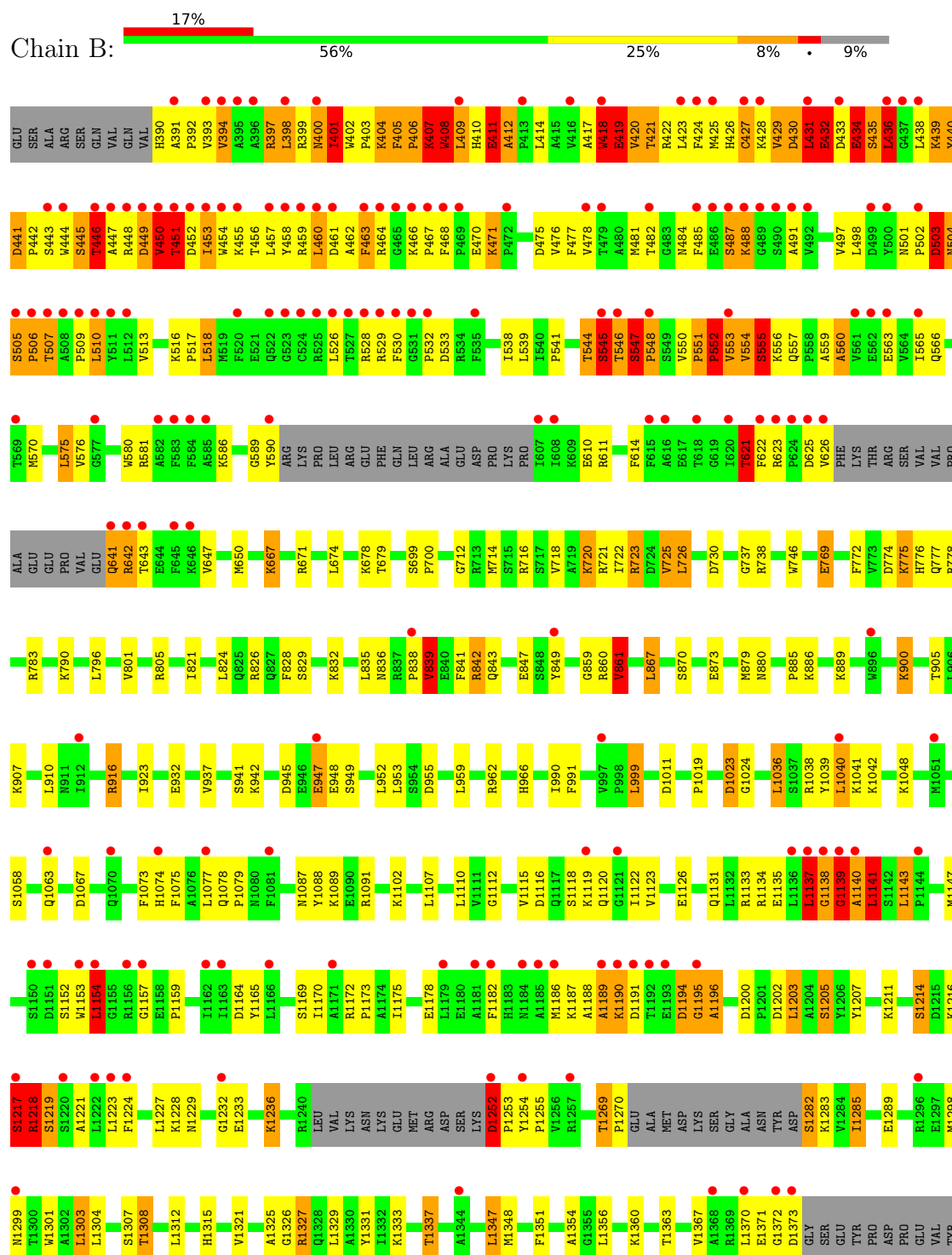
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





• Molecule 1: RNA-DEPENDENT RNA POLYMERASE



GLU
VAL
LEU
GLY
ASP
ASP
ASP
PHE
ASP
GLY
ILE
GLY
PHE
THR
GLY
ASN
GLY
ASP
TYR

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.02Å 122.55Å 114.70Å 90.00° 108.90° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 19.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.98-2.30) 97.5 (19.98-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.264 0.218 , 0.216	Depositor DCC
R_{free} test set	5728 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15945	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1432e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG

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	0.83	14/7713 (0.2%)	1.05	41/10439 (0.4%)
1	B	0.69	12/7689 (0.2%)	1.05	33/10407 (0.3%)
All	All	0.77	26/15402 (0.2%)	1.05	74/20846 (0.4%)

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	16
1	B	0	16
All	All	0	32

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	GLU	CD-OE2	29.13	1.80	1.25
1	A	436	LEU	C-N	19.55	1.62	1.33
1	A	434	GLU	CD-OE1	14.85	1.53	1.25
1	B	436	LEU	C-N	13.76	1.53	1.33
1	A	434	GLU	C-O	13.53	1.42	1.24
1	B	434	GLU	C-N	11.51	1.49	1.33
1	A	432	GLU	CD-OE1	9.82	1.44	1.25
1	B	435	SER	CB-OG	-8.89	1.24	1.42
1	A	436	LEU	C-O	8.82	1.35	1.24
1	A	1257	ARG	CZ-NH1	7.16	1.42	1.32
1	B	1372	GLY	C-N	-7.05	1.23	1.33
1	A	434	GLU	CA-CB	6.95	1.64	1.53
1	B	410	HIS	CG-ND1	-6.72	1.30	1.38
1	A	1372	GLY	C-N	-6.16	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	434	GLU	C-O	6.16	1.35	1.23
1	A	435	SER	CA-CB	-6.07	1.43	1.53
1	B	432	GLU	CD-OE1	5.97	1.36	1.25
1	A	1229	ASN	CG-OD1	5.82	1.34	1.23
1	B	440	TYR	C-N	5.52	1.45	1.33
1	B	411	GLU	CD-OE2	5.50	1.35	1.25
1	A	1257	ARG	CD-NE	5.40	1.53	1.46
1	B	861	VAL	CA-CB	5.23	1.60	1.54
1	B	410	HIS	CE1-NE2	-5.17	1.27	1.32
1	A	1215	ASP	CG-OD1	5.14	1.35	1.25
1	A	436	LEU	CA-CB	5.12	1.62	1.53
1	B	436	LEU	C-O	5.02	1.33	1.23

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1252	ASP	CA-C-N	18.93	138.38	120.21
1	B	1252	ASP	C-N-CA	18.93	138.38	120.21
1	A	547	SER	CA-C-N	14.06	135.52	120.47
1	A	547	SER	C-N-CA	14.06	135.52	120.47
1	B	547	SER	CA-C-N	12.69	135.71	119.84
1	B	547	SER	C-N-CA	12.69	135.71	119.84
1	A	560	ALA	N-CA-C	10.83	125.06	112.93
1	A	1213	ILE	N-CA-C	10.72	121.85	111.67
1	B	405	PHE	CA-C-N	10.09	132.45	119.84
1	B	405	PHE	C-N-CA	10.09	132.45	119.84
1	A	1252	ASP	CA-C-N	9.15	131.28	119.84
1	A	1252	ASP	C-N-CA	9.15	131.28	119.84
1	A	436	LEU	O-C-N	8.96	135.13	122.41
1	A	556	LYS	N-CA-C	-8.81	99.40	111.56
1	B	839	VAL	CB-CA-C	-8.51	100.66	112.14
1	A	1316	LYS	N-CA-C	-8.23	93.28	110.80
1	B	1253	PRO	N-CA-C	7.41	121.59	111.22
1	A	1215	ASP	N-CA-C	7.33	122.30	111.96
1	A	1183	HIS	N-CA-C	-7.13	102.60	112.30
1	B	560	ALA	N-CA-C	-7.07	103.00	113.61
1	B	551	PRO	CA-C-N	6.96	128.54	119.84
1	B	551	PRO	C-N-CA	6.96	128.54	119.84
1	A	1215	ASP	CA-C-N	6.88	134.09	121.70
1	A	1215	ASP	C-N-CA	6.88	134.09	121.70
1	B	1218	ARG	CA-C-N	6.73	133.81	121.70
1	B	1218	ARG	C-N-CA	6.73	133.81	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	GLU	OE1-CD-OE2	6.67	138.91	122.90
1	A	641	GLN	CA-C-N	6.53	133.45	121.70
1	A	641	GLN	C-N-CA	6.53	133.45	121.70
1	A	393	VAL	N-CA-C	6.31	122.46	109.34
1	A	1283	LYS	N-CA-C	-6.29	93.40	111.00
1	B	488	LYS	N-CA-C	-6.26	103.99	111.69
1	A	1184	ASN	N-CA-C	6.24	121.29	113.43
1	B	1139	GLY	N-CA-C	-6.23	98.41	113.18
1	B	420	VAL	N-CA-C	-6.22	105.77	111.67
1	B	932	GLU	N-CA-C	6.08	117.91	111.28
1	A	548	PRO	N-CA-C	-6.01	104.53	114.75
1	B	1023	ASP	N-CA-C	6.00	117.82	111.28
1	B	407	LYS	CA-C-N	5.95	132.41	121.70
1	B	407	LYS	C-N-CA	5.95	132.41	121.70
1	B	1154	LEU	N-CA-C	5.87	117.94	110.61
1	B	937	VAL	CB-CA-C	-5.71	103.94	110.73
1	A	1315	HIS	CA-C-N	5.71	132.44	121.54
1	A	1315	HIS	C-N-CA	5.71	132.44	121.54
1	A	839	VAL	CB-CA-C	-5.68	104.48	112.14
1	A	932	GLU	N-CA-C	5.66	118.18	111.33
1	B	552	PRO	N-CA-C	5.66	124.12	112.47
1	A	393	VAL	CA-C-N	5.65	131.86	121.70
1	A	393	VAL	C-N-CA	5.65	131.86	121.70
1	B	839	VAL	N-CA-CB	5.63	118.20	110.54
1	B	545	SER	CA-C-N	5.56	131.71	121.70
1	B	545	SER	C-N-CA	5.56	131.71	121.70
1	A	1186	MET	N-CA-C	5.51	120.50	113.55
1	A	458	TYR	CA-C-N	5.44	131.49	121.70
1	A	458	TYR	C-N-CA	5.44	131.49	121.70
1	A	1213	ILE	CA-C-N	5.42	131.89	121.54
1	A	1213	ILE	C-N-CA	5.42	131.89	121.54
1	B	642	ARG	N-CA-C	5.35	115.46	108.07
1	A	1217	SER	N-CA-C	5.35	116.79	111.07
1	B	556	LYS	N-CA-C	5.32	117.36	110.65
1	A	435	SER	CA-CB-OG	5.30	121.71	111.10
1	A	551	PRO	CA-C-N	5.25	124.43	118.97
1	A	551	PRO	C-N-CA	5.25	124.43	118.97
1	A	1217	SER	O-C-N	5.21	127.44	122.07
1	A	1137	LEU	CA-C-N	5.21	131.62	121.41
1	A	1137	LEU	C-N-CA	5.21	131.62	121.41
1	A	1140	ALA	N-CA-C	-5.19	99.74	110.80
1	B	1217	SER	CA-C-N	5.11	130.90	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1217	SER	C-N-CA	5.11	130.90	121.70
1	B	418	TRP	CA-C-N	5.08	130.84	121.70
1	B	418	TRP	C-N-CA	5.08	130.84	121.70
1	A	1138	GLY	N-CA-C	5.06	125.17	113.18
1	A	1023	ASP	N-CA-C	5.01	117.63	111.82
1	B	1217	SER	N-CA-C	5.01	121.47	110.80

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1138	GLY	Peptide
1	A	1139	GLY	Peptide
1	A	1213	ILE	Peptide
1	A	1217	SER	Peptide
1	A	1220	SER	Peptide
1	A	1252	ASP	Peptide
1	A	1282	SER	Peptide
1	A	1315	HIS	Peptide
1	A	456	THR	Peptide
1	A	504	ASN	Peptide
1	A	506	PRO	Peptide
1	A	545	SER	Peptide
1	A	547	SER	Peptide
1	A	555	SER	Peptide
1	A	559	ALA	Peptide
1	A	624	PRO	Peptide
1	B	1137	LEU	Peptide
1	B	1138	GLY	Peptide
1	B	1139	GLY	Peptide
1	B	1154	LEU	Peptide
1	B	1218	ARG	Peptide
1	B	1252	ASP	Peptide
1	B	1282	SER	Peptide
1	B	436	LEU	Mainchain
1	B	487	SER	Peptide
1	B	506	PRO	Peptide
1	B	545	SER	Peptide
1	B	547	SER	Peptide
1	B	552	PRO	Peptide
1	B	555	SER	Peptide
1	B	559	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	641	GLN	Peptide

5.2 Too-close contacts ⓘ

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	7520	0	7468	375	1
1	B	7498	0	7440	416	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	5	0	5	2	0
4	A	499	0	0	21	2
4	B	421	0	0	23	2
All	All	15945	0	14913	781	3

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 26.

All (781) 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:B:431:LEU:CB	1:B:432:GLU:HB2	1.34	1.51
1:B:407:LYS:CB	1:B:408:TRP:HB3	1.41	1.51
1:A:641:GLN:CB	1:A:642:ARG:HB2	1.50	1.41
1:B:407:LYS:HB2	1:B:408:TRP:CB	1.47	1.41
1:B:431:LEU:HB3	1:B:432:GLU:CB	1.48	1.40
1:A:1184:ASN:N	1:A:1185:ALA:HB3	1.49	1.25
1:A:1193:GLU:HA	1:A:1194:ASP:O	1.37	1.25
1:B:462:ALA:HB3	1:B:463:PHE:O	1.29	1.24
1:A:434:GLU:OE2	1:A:434:GLU:CD	1.80	1.23
1:A:399:ARG:CB	1:A:400:ASN:HB3	1.69	1.21
1:A:1315:HIS:HB2	1:A:1316:LYS:CB	1.72	1.18
1:A:438:LEU:HA	1:A:439:LYS:CB	1.71	1.17
1:B:879:MET:HE3	1:B:885:PRO:CD	1.75	1.15
1:A:438:LEU:HA	1:A:439:LYS:HB3	1.18	1.15
1:A:465:GLY:HA2	1:A:466:LYS:HB2	1.29	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:TRP:CB	1:B:419:GLU:HB2	1.76	1.15
1:A:399:ARG:HD2	1:A:507:THR:HG22	1.23	1.14
1:A:641:GLN:HB2	1:A:642:ARG:CB	1.77	1.14
1:B:505:SER:CB	1:B:506:PRO:HD3	1.75	1.14
1:A:503:ASP:O	1:A:504:ASN:HB2	1.38	1.14
1:A:1210:PHE:O	1:A:1214:SER:HB2	1.47	1.14
1:A:393:VAL:HG23	1:A:394:VAL:HG23	1.14	1.13
1:B:461:ASP:N	1:B:462:ALA:HA	1.63	1.12
1:B:879:MET:HE3	1:B:885:PRO:HD3	1.28	1.12
1:A:439:LYS:HG3	1:A:440:TYR:H	1.06	1.11
1:A:1186:MET:H	1:A:1187:LYS:HB3	1.01	1.10
1:B:505:SER:HB2	1:B:506:PRO:CD	1.81	1.10
1:A:1315:HIS:CB	1:A:1316:LYS:HB2	1.81	1.10
1:B:459:ARG:N	1:B:460:LEU:HB2	1.67	1.10
1:A:723:ARG:HH11	1:A:723:ARG:HG2	0.99	1.07
1:A:1184:ASN:H	1:A:1185:ALA:CB	1.68	1.07
1:B:505:SER:HB3	1:B:506:PRO:HD3	1.32	1.06
1:A:412:ALA:HB1	1:A:413:PRO:HA	1.37	1.06
1:A:879:MET:HE3	1:A:885:PRO:HD3	1.28	1.06
1:B:403:PRO:HA	1:B:404:LYS:HB2	1.28	1.06
1:A:438:LEU:CA	1:A:439:LYS:HB3	1.86	1.05
1:B:723:ARG:HH11	1:B:723:ARG:CG	1.70	1.05
1:A:439:LYS:HG3	1:A:440:TYR:N	1.65	1.05
1:A:879:MET:HE3	1:A:885:PRO:CD	1.87	1.05
1:B:829:SER:HA	1:B:832:LYS:HE3	1.05	1.04
1:B:418:TRP:HB3	1:B:419:GLU:HB2	1.04	1.04
1:A:1194:ASP:HB2	1:A:1195:GLY:HA2	1.36	1.02
1:B:1137:LEU:HB3	1:B:1138:GLY:HA3	1.37	1.02
1:B:545:SER:HA	1:B:546:THR:HG22	1.41	1.01
1:A:457:LEU:HB3	1:A:458:TYR:CB	1.90	1.01
1:B:505:SER:CB	1:B:506:PRO:CD	2.34	1.01
1:B:403:PRO:HA	1:B:404:LYS:CB	1.90	1.01
1:B:433:ASP:HB2	1:B:434:GLU:HB3	1.40	1.01
1:A:412:ALA:HB1	1:A:413:PRO:CA	1.90	1.00
1:B:450:VAL:H	1:B:451:THR:HB	1.27	0.99
1:B:723:ARG:HG2	1:B:723:ARG:NH1	1.65	0.99
1:A:399:ARG:HB3	1:A:400:ASN:CB	1.91	0.99
1:A:412:ALA:CB	1:A:413:PRO:HA	1.92	0.99
1:B:723:ARG:HH11	1:B:723:ARG:HG2	0.82	0.98
1:B:1188:ALA:N	1:B:1189:ALA:HB2	1.78	0.98
1:B:397:ARG:CG	1:B:397:ARG:HH21	1.77	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:LEU:N	1:B:461:ASP:HA	1.77	0.96
1:B:829:SER:CA	1:B:832:LYS:HE3	1.96	0.96
1:A:1220:SER:N	1:A:1221:ALA:HB3	1.80	0.96
1:A:399:ARG:HB3	1:A:400:ASN:HB3	0.96	0.96
1:A:624:PRO:HA	1:A:625:ASP:HB2	1.45	0.95
1:A:723:ARG:HG2	1:A:723:ARG:NH1	1.77	0.95
1:B:397:ARG:HH21	1:B:397:ARG:HG2	1.28	0.95
1:A:399:ARG:HE	1:A:399:ARG:HA	1.29	0.95
1:A:457:LEU:HB3	1:A:458:TYR:HB3	1.48	0.95
1:A:1186:MET:N	1:A:1187:LYS:HB3	1.83	0.94
1:B:451:THR:HB	1:B:452:ASP:HB2	1.49	0.94
1:A:1217:SER:CB	1:A:1221:ALA:HB2	1.97	0.94
1:B:452:ASP:O	1:B:454:TRP:N	2.00	0.94
1:A:1193:GLU:CA	1:A:1194:ASP:O	2.14	0.94
1:B:462:ALA:CB	1:B:463:PHE:O	2.15	0.93
1:A:393:VAL:H	1:A:394:VAL:C	1.77	0.93
1:B:418:TRP:HB3	1:B:419:GLU:CB	1.97	0.92
1:A:1194:ASP:CB	1:A:1195:GLY:HA2	1.98	0.92
1:B:403:PRO:CA	1:B:404:LYS:HB2	1.99	0.92
1:A:439:LYS:CG	1:A:440:TYR:N	2.33	0.91
1:A:1217:SER:OG	1:A:1221:ALA:HB2	1.70	0.91
1:B:1232:GLY:O	1:B:1236:LYS:HG3	1.72	0.90
1:B:451:THR:H	1:B:452:ASP:C	1.80	0.90
1:B:1147:MET:HE2	1:B:1147:MET:HA	1.54	0.90
1:A:1210:PHE:O	1:A:1214:SER:CB	2.21	0.89
1:A:395:ALA:HB1	1:A:396:ALA:HA	1.52	0.89
1:A:456:THR:HG22	1:A:457:LEU:HA	1.53	0.89
1:B:450:VAL:O	1:B:453:ILE:HB	1.73	0.88
1:B:714:MET:HE2	1:B:718:VAL:HG12	1.53	0.88
1:A:922:MET:HE2	1:A:1012:MET:C	1.98	0.88
1:B:879:MET:HE3	1:B:885:PRO:CG	2.04	0.88
1:A:399:ARG:CB	1:A:400:ASN:CB	2.48	0.87
1:A:1194:ASP:HB2	1:A:1195:GLY:CA	2.04	0.87
1:A:466:LYS:H	1:A:467:PRO:HA	1.39	0.87
1:B:463:PHE:HA	1:B:464:ARG:C	2.00	0.87
1:B:1139:GLY:O	4:B:2339:HOH:O	1.90	0.87
1:A:1140:ALA:O	1:A:1141:LEU:O	1.94	0.86
1:A:468:PHE:HA	1:A:469:PRO:O	1.76	0.85
1:A:559:ALA:CB	1:A:562:GLU:OE1	2.23	0.85
1:B:576:VAL:HG12	1:B:576:VAL:O	1.75	0.85
1:A:641:GLN:CB	1:A:642:ARG:CB	2.45	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1112:GLY:O	1:B:1115:VAL:HG22	1.77	0.85
1:B:450:VAL:H	1:B:451:THR:CB	1.90	0.84
1:A:641:GLN:HB2	1:A:642:ARG:HB2	0.85	0.84
1:B:1137:LEU:HB3	1:B:1138:GLY:CA	2.08	0.84
1:B:431:LEU:CB	1:B:432:GLU:CB	2.25	0.84
1:A:1217:SER:HB3	1:A:1221:ALA:HB2	1.59	0.84
1:A:723:ARG:HH11	1:A:723:ARG:CG	1.86	0.83
1:A:417:ALA:HB1	1:A:576:VAL:HG13	1.61	0.83
1:A:559:ALA:HB1	1:A:562:GLU:OE1	1.78	0.83
1:B:1134:ARG:O	4:B:2333:HOH:O	1.96	0.83
1:A:454:TRP:O	1:A:458:TYR:HB3	1.77	0.83
1:B:460:LEU:H	1:B:461:ASP:CA	1.92	0.83
1:A:457:LEU:HB3	1:A:458:TYR:HB2	1.60	0.83
1:B:1041:LYS:O	1:B:1123:VAL:HG12	1.80	0.82
1:B:461:ASP:H	1:B:462:ALA:HA	1.43	0.81
1:A:423:LEU:HD11	1:A:458:TYR:CE1	2.16	0.81
1:A:438:LEU:CA	1:A:439:LYS:CB	2.52	0.81
1:B:418:TRP:CA	1:B:419:GLU:HB2	2.11	0.80
1:B:456:THR:N	1:B:457:LEU:O	2.14	0.80
1:A:1315:HIS:HB2	1:A:1316:LYS:HB2	0.85	0.80
1:B:460:LEU:N	1:B:461:ASP:CA	2.43	0.80
1:A:450:VAL:HG11	1:A:472:PRO:HD2	1.64	0.80
1:B:1218:ARG:N	1:B:1219:SER:HB3	1.95	0.80
1:B:1131:GLN:O	1:B:1135:GLU:HG3	1.82	0.80
1:B:829:SER:HA	1:B:832:LYS:CE	2.00	0.80
1:B:723:ARG:HD3	1:B:730:ASP:C	2.08	0.79
1:B:942:LYS:HD2	1:B:949:SER:OG	1.82	0.79
1:B:429:VAL:O	1:B:430:ASP:HB2	1.81	0.79
1:B:400:ASN:CG	1:B:401:ILE:N	2.40	0.78
1:A:1186:MET:H	1:A:1187:LYS:CB	1.90	0.78
1:B:419:GLU:H	1:B:422:ARG:HB2	1.48	0.78
1:B:433:ASP:HA	1:B:434:GLU:HB2	1.64	0.78
1:B:460:LEU:HB3	1:B:462:ALA:HB2	1.64	0.78
1:B:1217:SER:HB3	1:B:1221:ALA:HB2	1.65	0.78
1:B:409:LEU:HD12	1:B:409:LEU:H	1.49	0.78
1:A:503:ASP:O	1:A:504:ASN:CB	2.25	0.78
1:B:460:LEU:H	1:B:461:ASP:HB3	1.49	0.78
1:A:1029:GLU:HB3	4:A:2359:HOH:O	1.82	0.78
1:B:407:LYS:CA	1:B:408:TRP:HB3	2.14	0.78
1:B:505:SER:HB2	1:B:506:PRO:HD2	1.62	0.77
1:A:453:ILE:O	1:A:454:TRP:HD1	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:PHE:CD1	1:A:1178:GLU:HG2	2.19	0.77
1:B:1137:LEU:CB	1:B:1138:GLY:HA3	2.14	0.77
1:A:393:VAL:HG23	1:A:394:VAL:CG2	2.07	0.77
1:A:412:ALA:HB2	4:A:2004:HOH:O	1.83	0.77
1:B:667:LYS:HE2	4:B:2033:HOH:O	1.85	0.77
1:A:1112:GLY:O	1:A:1115:VAL:HG22	1.84	0.77
1:B:431:LEU:HB2	1:B:432:GLU:HB2	1.61	0.77
1:B:459:ARG:CA	1:B:460:LEU:HB2	2.15	0.76
1:A:399:ARG:HB2	1:A:400:ASN:O	1.86	0.76
1:A:438:LEU:HA	1:A:439:LYS:HB2	1.66	0.76
1:B:390:HIS:CD2	1:B:566:GLN:HE22	2.02	0.76
1:B:879:MET:HE3	1:B:885:PRO:HG3	1.67	0.76
1:A:457:LEU:HD12	1:A:457:LEU:O	1.85	0.75
1:B:1269:THR:HG23	1:B:1270:PRO:HD2	1.67	0.75
1:A:829:SER:HA	1:A:832:LYS:HE3	1.68	0.75
1:B:836:ASN:HA	1:B:886:LYS:HD2	1.69	0.75
1:A:488:LYS:HG3	1:B:1373:ASP:N	2.01	0.75
1:A:796:LEU:HA	1:A:799:LEU:HD12	1.68	0.75
1:B:400:ASN:O	1:B:402:TRP:N	2.20	0.75
1:B:867:LEU:HD13	1:B:1326:GLY:HA3	1.66	0.75
1:A:423:LEU:HD21	1:A:458:TYR:HD1	1.52	0.74
1:A:922:MET:HE2	1:A:1013:ALA:N	2.02	0.74
1:B:433:ASP:HB2	1:B:434:GLU:CB	2.17	0.74
1:B:460:LEU:H	1:B:461:ASP:CB	2.00	0.74
1:B:801:VAL:HG23	4:B:2130:HOH:O	1.88	0.74
1:A:1219:SER:C	1:A:1221:ALA:HB3	2.13	0.73
1:A:408:TRP:HZ3	1:A:431:LEU:O	1.71	0.73
1:A:1315:HIS:ND1	4:A:2470:HOH:O	2.21	0.73
1:B:456:THR:H	1:B:457:LEU:CB	2.00	0.73
1:A:576:VAL:O	1:A:576:VAL:HG12	1.86	0.73
1:A:393:VAL:CG2	1:A:394:VAL:HG23	2.08	0.73
1:B:1270:PRO:HG2	1:B:1289:GLU:HG3	1.69	0.73
1:A:1214:SER:HA	1:A:1217:SER:OG	1.89	0.72
1:B:462:ALA:HB3	1:B:463:PHE:C	2.14	0.72
1:B:1188:ALA:HB3	1:B:1189:ALA:HA	1.70	0.72
1:B:433:ASP:CB	1:B:434:GLU:HB3	2.18	0.72
1:A:412:ALA:HB1	1:A:413:PRO:C	2.14	0.72
1:A:470:GLU:O	1:A:471:LYS:HB3	1.89	0.72
1:B:431:LEU:HB3	1:B:432:GLU:CA	2.19	0.72
1:A:705:GLU:OE2	1:A:1001:LYS:NZ	2.15	0.72
1:B:451:THR:CB	1:B:452:ASP:HB2	2.20	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:ARG:NH1	1:A:913:ARG:HH22	1.88	0.72
1:B:391:ALA:HB3	1:B:563:GLU:HG3	1.70	0.72
1:A:457:LEU:H	1:A:459:ARG:HB2	1.55	0.71
1:B:449:ASP:HB3	1:B:451:THR:HB	1.72	0.71
1:B:450:VAL:N	1:B:451:THR:CB	2.53	0.71
1:B:841:PHE:HB3	1:B:879:MET:HE1	1.72	0.71
1:B:879:MET:CE	1:B:885:PRO:HG3	2.20	0.71
1:B:1139:GLY:HA3	1:B:1141:LEU:HB3	1.71	0.71
1:A:1253:PRO:HD2	1:A:1256:VAL:HB	1.72	0.71
1:A:457:LEU:N	1:A:459:ARG:HB2	2.06	0.71
1:B:398:LEU:HD13	1:B:510:LEU:HD23	1.71	0.70
1:B:435:SER:HB2	1:B:436:LEU:HB2	1.72	0.70
1:B:774:ASP:HB3	1:B:777:GLN:HG2	1.73	0.70
1:A:1184:ASN:N	1:A:1185:ALA:CB	2.41	0.70
1:B:576:VAL:O	1:B:576:VAL:CG1	2.40	0.70
1:B:626:VAL:O	1:B:626:VAL:HG13	1.91	0.70
1:B:842:ARG:HD2	4:B:2168:HOH:O	1.92	0.70
1:B:1269:THR:CG2	4:B:2377:HOH:O	2.39	0.70
1:B:1315:HIS:O	4:B:2386:HOH:O	2.09	0.70
1:B:400:ASN:CG	1:B:401:ILE:H	1.98	0.70
1:A:465:GLY:HA2	1:A:466:LYS:CB	2.15	0.70
1:A:641:GLN:CA	1:A:642:ARG:HB2	2.21	0.69
1:A:395:ALA:HB1	1:A:396:ALA:CA	2.23	0.69
1:B:397:ARG:HG2	1:B:397:ARG:NH2	1.99	0.69
1:B:462:ALA:H	1:B:463:PHE:C	1.99	0.69
1:B:1217:SER:HB2	1:B:1218:ARG:C	2.16	0.69
1:A:459:ARG:O	1:A:461:ASP:N	2.23	0.69
1:A:466:LYS:N	1:A:467:PRO:HA	2.06	0.69
1:A:1184:ASN:CA	1:A:1185:ALA:HB3	2.22	0.69
1:A:1344:ALA:HB1	1:B:1327:ARG:HD3	1.75	0.69
1:B:433:ASP:HA	1:B:434:GLU:CB	2.21	0.69
1:B:456:THR:H	1:B:457:LEU:HB2	1.57	0.69
1:B:459:ARG:HB2	1:B:460:LEU:HD23	1.75	0.69
1:B:1337:THR:HG22	4:B:2395:HOH:O	1.93	0.69
1:A:922:MET:HE3	1:A:1011:ASP:C	2.18	0.68
1:B:491:ALA:HB1	1:B:532:PRO:HB3	1.75	0.68
1:A:408:TRP:CZ3	1:A:431:LEU:O	2.45	0.68
1:B:433:ASP:CA	1:B:434:GLU:CB	2.72	0.68
1:B:1304:LEU:O	1:B:1308:THR:CG2	2.41	0.68
1:B:461:ASP:N	1:B:462:ALA:CA	2.51	0.68
1:B:406:PRO:HB3	1:B:408:TRP:NE1	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:LEU:HD22	1:A:513:VAL:HG22	1.75	0.67
1:A:391:ALA:HB3	1:A:392:PRO:HA	1.75	0.67
1:B:546:THR:HG23	1:B:546:THR:O	1.94	0.67
1:B:424:PHE:HA	1:B:428:LYS:O	1.95	0.67
1:B:843:GLN:HG3	1:B:1363:THR:HG21	1.77	0.67
1:A:399:ARG:HB2	1:A:400:ASN:CB	2.23	0.67
1:B:1188:ALA:H	1:B:1189:ALA:HB2	1.59	0.67
1:B:1304:LEU:O	1:B:1308:THR:HG22	1.95	0.67
1:A:412:ALA:CB	1:A:413:PRO:CA	2.55	0.67
1:B:555:SER:HA	1:B:557:GLN:H	1.60	0.67
1:A:456:THR:O	1:A:459:ARG:HD2	1.95	0.67
1:A:397:ARG:O	1:A:398:LEU:HB2	1.93	0.66
1:B:547:SER:OG	1:B:548:PRO:HD3	1.95	0.66
1:A:453:ILE:O	1:A:454:TRP:CD1	2.48	0.66
1:A:828:PHE:CG	1:A:1178:GLU:HG2	2.29	0.66
1:B:403:PRO:HA	1:B:404:LYS:CG	2.25	0.66
1:A:838:PRO:HA	1:A:879:MET:HE2	1.77	0.66
1:B:456:THR:N	1:B:457:LEU:HB2	2.11	0.66
1:B:1159:PRO:HB3	1:B:1164:ASP:HB3	1.76	0.66
1:B:505:SER:HB2	1:B:506:PRO:HD3	1.55	0.66
1:A:1217:SER:OG	1:A:1221:ALA:CB	2.44	0.66
1:B:408:TRP:HE3	1:B:408:TRP:O	1.78	0.66
1:B:509:PRO:O	1:B:510:LEU:HB3	1.96	0.66
1:A:1044:LYS:HD2	4:A:2207:HOH:O	1.96	0.65
1:A:399:ARG:NH2	4:A:2002:HOH:O	2.29	0.65
1:B:402:TRP:HB3	1:B:575:LEU:HD23	1.78	0.65
1:B:667:LYS:CE	4:B:2033:HOH:O	2.40	0.65
1:A:560:ALA:HB1	1:A:563:GLU:HB3	1.78	0.65
1:A:418:TRP:CD1	1:A:518:LEU:HD13	2.32	0.65
1:A:836:ASN:OD1	1:A:886:LYS:HE3	1.96	0.65
1:B:714:MET:HE1	1:B:722:ILE:HD11	1.77	0.65
1:B:450:VAL:HG12	1:B:451:THR:OG1	1.97	0.65
1:A:399:ARG:HD2	1:A:507:THR:CG2	2.13	0.65
1:B:429:VAL:HG21	1:B:463:PHE:CZ	2.32	0.65
1:B:443:SER:H	1:B:445:SER:N	1.95	0.65
1:B:406:PRO:HB3	1:B:408:TRP:CD1	2.32	0.65
1:A:465:GLY:CA	1:A:466:LYS:HB2	2.16	0.64
1:A:942:LYS:HG3	1:A:949:SER:OG	1.97	0.64
1:B:625:ASP:HB3	1:B:643:THR:CG2	2.27	0.64
1:B:879:MET:CE	1:B:885:PRO:CD	2.66	0.64
1:A:796:LEU:HD12	1:A:797:GLN:N	2.12	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ASP:O	1:B:464:ARG:HG3	1.97	0.64
1:A:1220:SER:N	1:A:1221:ALA:CB	2.58	0.64
1:B:429:VAL:O	1:B:430:ASP:CB	2.44	0.64
1:B:879:MET:CE	1:B:885:PRO:HD3	2.18	0.64
1:B:429:VAL:CG2	1:B:463:PHE:CZ	2.81	0.64
1:A:393:VAL:N	1:A:394:VAL:C	2.54	0.64
1:A:550:VAL:HG22	4:A:2058:HOH:O	1.96	0.63
1:A:922:MET:CE	1:A:1012:MET:C	2.71	0.63
1:B:453:ILE:C	1:B:455:LYS:H	2.05	0.63
1:B:394:VAL:HG21	1:B:560:ALA:HB1	1.80	0.63
1:B:444:TRP:H	1:B:453:ILE:HG13	1.63	0.63
1:A:841:PHE:HB3	1:A:879:MET:HE1	1.80	0.63
1:B:405:PHE:CE2	1:B:409:LEU:HD13	2.33	0.63
1:B:450:VAL:N	1:B:451:THR:OG1	2.31	0.63
1:A:1180:GLU:OE1	1:A:1180:GLU:HA	1.99	0.63
1:A:605:LYS:HD2	1:A:605:LYS:H	1.63	0.62
1:B:671:ARG:HH22	1:B:1119:LYS:HZ2	1.46	0.62
1:B:1041:LYS:HB2	1:B:1123:VAL:HG13	1.80	0.62
1:B:714:MET:HE2	1:B:718:VAL:CG1	2.29	0.62
1:A:423:LEU:HD11	1:A:458:TYR:HE1	1.63	0.62
1:A:565:ILE:HD13	1:A:1074:HIS:HA	1.81	0.62
1:B:836:ASN:OD1	1:B:886:LYS:HE3	1.98	0.62
1:A:1216:LYS:HE3	1:A:1216:LYS:HA	1.81	0.62
1:B:1203:LEU:O	1:B:1307:SER:HB2	2.00	0.62
1:A:626:VAL:N	1:A:627:PHE:HA	2.15	0.61
1:B:393:VAL:HG22	1:B:394:VAL:H	1.64	0.61
1:B:431:LEU:CA	1:B:432:GLU:HB2	2.27	0.61
1:B:431:LEU:CA	1:B:432:GLU:CB	2.79	0.61
1:B:516:LYS:HD3	1:B:517:PRO:HD2	1.83	0.61
1:A:1202:ASP:O	1:A:1205:SER:HB2	2.00	0.61
1:B:418:TRP:CD1	1:B:518:LEU:HD13	2.35	0.61
1:A:390:HIS:CE1	1:A:566:GLN:HE22	2.18	0.61
1:A:838:PRO:HA	1:A:879:MET:CE	2.31	0.61
1:B:838:PRO:HA	1:B:879:MET:HE2	1.83	0.61
1:A:624:PRO:CA	1:A:625:ASP:HB2	2.27	0.61
1:A:408:TRP:CH2	1:A:438:LEU:HD13	2.36	0.60
1:A:457:LEU:O	1:A:460:LEU:HB2	2.01	0.60
1:B:460:LEU:HD12	1:B:462:ALA:HB1	1.82	0.60
1:A:412:ALA:HB3	1:A:413:PRO:HA	1.82	0.60
1:B:941:SER:HB2	4:B:2225:HOH:O	2.01	0.60
1:A:1207:TYR:CD2	1:A:1311:LYS:HG3	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1300:THR:HA	1:A:1303:LEU:HD23	1.83	0.60
1:B:1285:ILE:HD12	1:B:1285:ILE:C	2.27	0.60
1:A:408:TRP:CD1	1:A:408:TRP:C	2.78	0.60
1:A:797:GLN:O	1:A:797:GLN:HG3	1.97	0.60
1:B:451:THR:N	1:B:452:ASP:C	2.55	0.60
1:A:423:LEU:HD21	1:A:458:TYR:CD1	2.35	0.60
1:A:509:PRO:O	1:A:510:LEU:HB3	2.01	0.60
1:B:400:ASN:C	1:B:401:ILE:HG12	2.27	0.60
1:B:503:ASP:O	1:B:504:ASN:ND2	2.29	0.60
1:B:481:MET:HE3	4:B:2003:HOH:O	2.01	0.60
1:B:916:ARG:HH21	1:B:1019:PRO:CD	2.15	0.60
1:A:1186:MET:HB2	1:A:1187:LYS:HB2	1.82	0.60
1:B:393:VAL:O	1:B:394:VAL:HB	2.02	0.60
1:A:820:LEU:HD11	1:A:906:LEU:HD21	1.83	0.60
1:A:1184:ASN:CA	1:A:1185:ALA:CB	2.79	0.60
1:B:641:GLN:HB3	1:B:642:ARG:HG2	1.84	0.60
1:B:1207:TYR:HD1	1:B:1308:THR:HB	1.66	0.60
1:A:460:LEU:O	1:A:461:ASP:CB	2.49	0.60
1:A:399:ARG:HA	1:A:399:ARG:NE	2.11	0.59
1:A:884:ASP:HB3	1:A:887:LYS:HB2	1.84	0.59
1:B:459:ARG:H	1:B:460:LEU:HB2	1.65	0.59
1:B:428:LYS:O	1:B:429:VAL:HG23	2.02	0.59
1:B:408:TRP:CE3	1:B:408:TRP:C	2.80	0.59
1:A:453:ILE:O	1:A:453:ILE:HG22	2.02	0.59
1:A:393:VAL:N	1:A:394:VAL:O	2.25	0.59
1:A:491:ALA:HB1	1:A:532:PRO:HB3	1.84	0.59
1:B:428:LYS:C	1:B:429:VAL:HG23	2.28	0.59
1:A:1141:LEU:HD12	4:A:2421:HOH:O	2.02	0.59
1:A:835:LEU:HD13	1:A:841:PHE:CE1	2.38	0.58
1:A:723:ARG:NH1	1:A:724:ASP:OD1	2.33	0.58
1:B:1194:ASP:O	1:B:1196:ALA:N	2.35	0.58
1:B:1218:ARG:H	1:B:1219:SER:HB3	1.66	0.58
1:A:1285:ILE:O	1:A:1289:GLU:HB2	2.03	0.58
1:B:1042:LYS:HG2	1:B:1122:ILE:HG12	1.85	0.58
1:B:1227:LEU:HD13	1:B:1301:TRP:CZ2	2.38	0.58
1:B:1217:SER:HB2	1:B:1218:ARG:CA	2.34	0.58
1:B:417:ALA:O	1:B:421:THR:OG1	2.20	0.58
1:A:624:PRO:HA	1:A:625:ASP:CB	2.28	0.58
1:B:1333:LYS:O	1:B:1337:THR:HB	2.04	0.58
1:B:528:ARG:NH2	1:B:679:THR:O	2.37	0.57
1:B:723:ARG:CG	1:B:723:ARG:NH1	2.41	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:772:PHE:O	1:B:778:ARG:HD2	2.04	0.57
1:A:674:LEU:CD1	4:A:2095:HOH:O	2.53	0.57
1:A:509:PRO:O	1:A:510:LEU:CB	2.53	0.57
1:A:1259:ASN:O	1:A:1263:GLU:HG3	2.05	0.57
1:B:714:MET:HE1	1:B:722:ILE:CD1	2.33	0.57
1:B:916:ARG:HH21	1:B:1019:PRO:HD3	1.69	0.57
1:A:820:LEU:CD1	1:A:906:LEU:HD21	2.35	0.57
1:A:1235:GLU:HG2	1:A:1313:TYR:CZ	2.39	0.57
1:A:879:MET:HE3	1:A:885:PRO:CG	2.34	0.57
1:B:400:ASN:O	1:B:401:ILE:HG12	2.05	0.57
1:A:439:LYS:HA	4:A:2013:HOH:O	2.04	0.57
1:A:861:VAL:HG13	1:A:873:GLU:HG2	1.86	0.57
1:A:456:THR:O	1:A:459:ARG:NH1	2.38	0.57
1:B:431:LEU:HB3	1:B:432:GLU:HB2	0.60	0.57
1:B:721:ARG:O	1:B:725:VAL:HG13	2.04	0.57
1:B:418:TRP:CA	1:B:419:GLU:CB	2.83	0.56
1:A:622:PHE:HA	1:A:642:ARG:O	2.05	0.56
1:B:397:ARG:CG	1:B:397:ARG:NH2	2.49	0.56
1:B:589:GLY:H	1:B:611:ARG:HH21	1.53	0.56
1:B:419:GLU:H	1:B:422:ARG:CB	2.17	0.56
1:B:441:ASP:HB3	1:B:442:PRO:CA	2.36	0.56
1:B:450:VAL:CG1	1:B:451:THR:HA	2.35	0.56
1:A:454:TRP:O	1:A:458:TYR:CB	2.52	0.56
1:B:1189:ALA:O	1:B:1190:LYS:C	2.48	0.56
1:A:555:SER:O	1:A:555:SER:OG	2.21	0.55
1:B:411:GLU:HG2	1:B:412:ALA:N	2.21	0.55
1:B:445:SER:O	1:B:446:THR:HG23	2.05	0.55
1:B:1194:ASP:C	1:B:1196:ALA:H	2.13	0.55
1:B:441:ASP:HB3	1:B:442:PRO:C	2.31	0.55
1:B:462:ALA:N	1:B:463:PHE:C	2.63	0.55
1:B:419:GLU:OE2	1:B:419:GLU:HA	2.07	0.55
1:A:1217:SER:OG	1:A:1221:ALA:N	2.40	0.55
1:B:879:MET:CE	1:B:885:PRO:CG	2.80	0.55
1:B:1116:ASP:HB3	1:B:1120:GLN:HG2	1.87	0.55
1:B:1172:ARG:HB3	1:B:1173:PRO:HD3	1.88	0.55
1:B:1363:THR:O	1:B:1367:VAL:HG13	2.06	0.55
1:A:1315:HIS:HB2	1:A:1316:LYS:CA	2.36	0.55
1:B:769:GLU:HG3	4:B:2030:HOH:O	2.07	0.55
1:B:397:ARG:HH21	1:B:397:ARG:HG3	1.69	0.55
1:B:533:ASP:OD1	1:B:642:ARG:NH2	2.39	0.55
1:B:1270:PRO:HG3	1:B:1301:TRP:CD2	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:LYS:H	1:B:408:TRP:CD1	2.23	0.55
1:B:443:SER:HA	1:B:444:TRP:C	2.32	0.55
1:B:1327:ARG:HD2	1:B:1331:TYR:OH	2.07	0.55
1:A:547:SER:HB2	1:A:548:PRO:CA	2.35	0.55
1:A:395:ALA:CB	1:A:396:ALA:HA	2.31	0.54
1:A:400:ASN:C	1:A:400:ASN:OD1	2.50	0.54
1:A:813:ARG:HD2	4:A:2227:HOH:O	2.07	0.54
1:B:456:THR:CA	1:B:457:LEU:HB2	2.37	0.54
1:A:558:PRO:O	1:A:559:ALA:C	2.50	0.54
1:A:1193:GLU:N	1:A:1194:ASP:O	2.40	0.54
1:A:399:ARG:CB	1:A:400:ASN:CA	2.85	0.54
1:B:433:ASP:CA	1:B:434:GLU:HB2	2.35	0.54
1:B:1024:GLY:HA3	4:B:2291:HOH:O	2.07	0.54
1:B:1194:ASP:CG	1:B:1195:GLY:H	2.15	0.54
1:B:1217:SER:CB	1:B:1218:ARG:HA	2.36	0.54
1:A:899:GLN:HA	1:A:899:GLN:OE1	2.07	0.54
1:B:1036:LEU:HB3	1:B:1040:LEU:HD22	1.89	0.54
1:B:1269:THR:HG21	4:B:2377:HOH:O	2.03	0.54
1:A:466:LYS:HB3	1:A:467:PRO:O	2.08	0.54
1:B:433:ASP:CB	1:B:434:GLU:CB	2.83	0.54
1:B:1120:GLN:HA	1:B:1120:GLN:OE1	2.07	0.54
1:B:1147:MET:HA	1:B:1147:MET:CE	2.33	0.54
1:A:470:GLU:HB2	4:A:2020:HOH:O	2.06	0.54
1:A:1186:MET:N	1:A:1187:LYS:CB	2.60	0.54
1:B:1269:THR:HG23	1:B:1270:PRO:CD	2.35	0.54
1:B:1165:TYR:O	1:B:1169:SER:HB2	2.08	0.53
1:A:942:LYS:CG	1:A:949:SER:OG	2.56	0.53
1:B:484:ASN:O	1:B:485:PHE:HB2	2.08	0.53
1:A:767:LYS:NZ	4:A:2183:HOH:O	2.34	0.53
1:A:397:ARG:O	1:A:398:LEU:CB	2.56	0.53
1:A:723:ARG:NH1	1:A:723:ARG:CG	2.53	0.53
1:A:438:LEU:CB	1:A:439:LYS:HB3	2.38	0.53
1:A:641:GLN:HB3	1:A:642:ARG:HB2	1.75	0.53
1:A:1210:PHE:O	1:A:1213:ILE:HG22	2.08	0.53
1:A:457:LEU:CB	1:A:458:TYR:CB	2.78	0.53
1:A:1213:ILE:O	1:A:1216:LYS:HB3	2.08	0.53
1:B:406:PRO:CB	1:B:408:TRP:CD1	2.92	0.53
1:B:453:ILE:C	1:B:455:LYS:N	2.67	0.53
1:B:860:ARG:HA	1:B:1354:ALA:HB2	1.90	0.53
1:A:391:ALA:HB1	1:A:393:VAL:HG22	1.90	0.53
1:A:793:GLY:HA2	1:A:914:VAL:H	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1089:LYS:HA	1:B:1107:LEU:HD13	1.91	0.53
1:A:399:ARG:CD	1:A:507:THR:HG22	2.16	0.53
1:A:1315:HIS:H	1:A:1315:HIS:CD2	2.26	0.53
1:A:1343:GLY:HA3	1:B:860:ARG:HD2	1.91	0.53
1:B:551:PRO:C	1:B:553:VAL:HB	2.34	0.53
1:B:1038:ARG:HG2	1:B:1038:ARG:O	2.09	0.53
1:B:716:ARG:O	1:B:720:LYS:HG2	2.08	0.52
1:A:580:TRP:HB3	1:A:614:PHE:HB3	1.90	0.52
1:A:1146:PRO:HB3	1:A:1148:TYR:CE2	2.44	0.52
1:A:586:LYS:HG2	1:A:587:ASP:N	2.23	0.52
1:B:394:VAL:HG21	1:B:560:ALA:CB	2.39	0.52
1:B:466:LYS:O	1:B:468:PHE:N	2.43	0.52
1:A:458:TYR:N	1:A:459:ARG:C	2.68	0.52
1:A:883:PHE:CE2	1:A:1203:LEU:HD21	2.44	0.52
1:B:546:THR:HA	1:B:547:SER:HB3	1.92	0.52
1:A:417:ALA:CB	1:A:576:VAL:HG13	2.37	0.52
1:B:916:ARG:HD2	1:B:945:ASP:OD2	2.09	0.52
1:A:576:VAL:O	1:A:576:VAL:CG1	2.58	0.52
1:A:605:LYS:HD2	1:A:605:LYS:N	2.25	0.52
1:B:408:TRP:O	1:B:408:TRP:CE3	2.63	0.52
1:B:545:SER:HA	1:B:546:THR:CG2	2.29	0.52
1:A:774:ASP:OD1	1:A:776:HIS:N	2.43	0.52
1:B:452:ASP:HA	1:B:455:LYS:HB2	1.92	0.52
1:A:427:CYS:O	1:A:428:LYS:HB2	2.10	0.52
1:A:456:THR:HG22	1:A:457:LEU:CA	2.33	0.52
1:A:967:PHE:CD2	1:A:1031:PRO:HG3	2.45	0.52
1:B:829:SER:O	1:B:832:LYS:HG2	2.10	0.52
1:A:451:THR:OG1	1:A:471:LYS:HE3	2.09	0.51
1:A:458:TYR:CZ	1:A:465:GLY:O	2.64	0.51
1:A:774:ASP:OD1	1:A:774:ASP:C	2.53	0.51
1:A:1203:LEU:O	1:A:1307:SER:HB2	2.10	0.51
1:B:843:GLN:O	1:B:847:GLU:HG3	2.11	0.51
1:B:1303:LEU:HD13	4:B:2381:HOH:O	2.10	0.51
1:A:439:LYS:O	1:A:440:TYR:HB2	2.11	0.51
1:A:890:TYR:CE2	1:A:894:ILE:HD11	2.45	0.51
1:A:1189:ALA:HB1	1:A:1195:GLY:HA3	1.92	0.51
1:A:1348:MET:HE3	1:B:880:ASN:HB3	1.92	0.51
1:A:828:PHE:CG	1:A:1178:GLU:CG	2.93	0.51
1:A:1219:SER:CA	1:A:1221:ALA:HB3	2.41	0.51
1:B:406:PRO:CB	1:B:408:TRP:NE1	2.74	0.51
1:B:1088:TYR:CE1	1:B:1143:LEU:HD22	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LEU:HD12	1:A:457:LEU:C	2.35	0.51
1:B:468:PHE:HB3	4:B:2007:HOH:O	2.10	0.51
1:B:622:PHE:HA	1:B:642:ARG:O	2.10	0.51
1:A:456:THR:C	1:A:459:ARG:HB2	2.36	0.51
1:A:458:TYR:H	1:A:459:ARG:C	2.19	0.51
1:A:1194:ASP:OD2	1:A:1194:ASP:N	2.43	0.51
1:B:403:PRO:HA	1:B:404:LYS:HG2	1.91	0.51
1:B:450:VAL:HG12	1:B:451:THR:HA	1.92	0.51
1:B:552:PRO:N	1:B:553:VAL:HB	2.26	0.51
1:A:1312:LEU:O	1:A:1315:HIS:CD2	2.64	0.51
1:B:923:ILE:HB	1:B:990:ILE:HD13	1.92	0.51
1:A:534:ARG:HD2	1:A:642:ARG:HD2	1.92	0.51
1:A:839:VAL:HG13	1:B:1351:PHE:CZ	2.45	0.51
1:A:1129:TRP:CZ2	1:A:1133:ARG:HD3	2.46	0.51
1:A:1140:ALA:O	1:A:1141:LEU:C	2.54	0.51
1:B:411:GLU:O	1:B:412:ALA:HB3	2.11	0.51
1:B:449:ASP:O	1:B:477:PHE:CD2	2.63	0.51
1:B:456:THR:H	1:B:457:LEU:CA	2.23	0.51
1:B:1152:SER:O	1:B:1154:LEU:HD13	2.10	0.51
1:A:391:ALA:HB3	1:A:392:PRO:CA	2.40	0.50
1:A:723:ARG:HD3	1:A:730:ASP:C	2.36	0.50
1:A:1335:GLN:HE21	3:B:3375:GOL:H2	1.76	0.50
1:A:1352:MET:O	1:B:842:ARG:NH2	2.43	0.50
1:B:1140:ALA:O	1:B:1141:LEU:O	2.28	0.50
1:B:1348:MET:HE1	1:B:1356:LEU:CD1	2.42	0.50
1:A:450:VAL:HG12	1:A:471:LYS:HE2	1.94	0.50
1:B:1038:ARG:HD2	1:B:1039:TYR:CE2	2.47	0.50
1:B:407:LYS:CB	1:B:408:TRP:CB	2.37	0.50
1:B:1304:LEU:O	1:B:1308:THR:HG23	2.10	0.50
1:A:705:GLU:HG2	1:A:998:PRO:HD2	1.93	0.50
1:B:497:VAL:HG23	1:B:539:LEU:HB2	1.93	0.50
1:B:1252:ASP:O	1:B:1252:ASP:OD2	2.30	0.50
1:A:1328:GLN:O	1:A:1332:ILE:HG13	2.12	0.50
1:B:509:PRO:O	1:B:510:LEU:CB	2.58	0.49
1:A:1186:MET:CA	1:A:1187:LYS:CB	2.90	0.49
1:B:1023:ASP:HB2	4:B:2285:HOH:O	2.11	0.49
1:A:457:LEU:CB	1:A:458:TYR:HB3	2.33	0.49
1:B:460:LEU:HD13	1:B:460:LEU:O	2.12	0.49
1:A:466:LYS:H	1:A:467:PRO:CA	2.18	0.49
1:B:470:GLU:O	1:B:471:LYS:HB3	2.12	0.49
1:A:904:ASP:HA	1:A:907:LYS:HE2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:917:SER:HA	1:A:1015:VAL:O	2.12	0.49
1:A:667:LYS:HE2	1:A:1119:LYS:O	2.13	0.49
1:A:859:GLY:O	1:A:860:ARG:HB3	2.11	0.49
1:B:503:ASP:O	1:B:504:ASN:HB3	2.11	0.49
1:B:678:LYS:H	1:B:783:ARG:NH1	2.11	0.49
1:A:991:PHE:CD2	1:A:999:LEU:HB3	2.48	0.49
1:A:1193:GLU:H	1:A:1194:ASP:C	2.20	0.49
1:B:1200:ASP:OD1	1:B:1202:ASP:HB2	2.13	0.49
1:B:443:SER:CA	1:B:444:TRP:C	2.85	0.49
1:B:1252:ASP:O	1:B:1252:ASP:CG	2.55	0.48
1:A:524:CYS:SG	1:A:527:THR:HG23	2.53	0.48
1:B:554:VAL:O	1:B:555:SER:C	2.55	0.48
1:A:565:ILE:CD1	1:A:1074:HIS:HA	2.43	0.48
1:B:546:THR:HA	1:B:547:SER:CB	2.43	0.48
1:B:570:MET:O	1:B:570:MET:HG3	2.11	0.48
1:B:737:GLY:C	1:B:738:ARG:HD2	2.38	0.48
1:B:861:VAL:HG21	1:B:873:GLU:HG2	1.95	0.48
1:B:1112:GLY:O	1:B:1115:VAL:CG2	2.57	0.48
1:A:464:ARG:HA	1:A:465:GLY:C	2.38	0.48
1:A:498:LEU:O	1:A:541:PRO:HD3	2.13	0.48
1:A:1300:THR:HA	1:A:1303:LEU:CD2	2.43	0.48
1:A:1317:SER:O	1:A:1321:VAL:HG12	2.13	0.48
1:B:1102:LYS:HG3	4:B:2324:HOH:O	2.13	0.48
1:A:399:ARG:HB2	1:A:400:ASN:C	2.38	0.48
1:A:458:TYR:CE2	1:A:465:GLY:O	2.67	0.48
1:B:1195:GLY:O	1:B:1196:ALA:HB3	2.13	0.48
1:B:456:THR:HB	1:B:457:LEU:HB2	1.96	0.47
1:B:459:ARG:N	1:B:460:LEU:CB	2.58	0.47
1:B:1348:MET:HE1	1:B:1356:LEU:HD11	1.96	0.47
1:A:456:THR:O	1:A:459:ARG:CD	2.62	0.47
1:B:454:TRP:HA	1:B:457:LEU:HD23	1.95	0.47
1:B:626:VAL:O	1:B:626:VAL:CG1	2.62	0.47
1:A:457:LEU:CB	1:A:458:TYR:HB2	2.40	0.47
1:A:900:LYS:HB2	1:A:900:LYS:HE3	1.58	0.47
1:A:1211:LYS:O	1:A:1214:SER:HB3	2.14	0.47
1:B:408:TRP:O	1:B:439:LYS:HG3	2.14	0.47
1:B:450:VAL:HG11	1:B:471:LYS:HG2	1.96	0.47
1:A:464:ARG:HA	1:A:464:ARG:HD2	1.70	0.47
1:A:791:SER:HB3	4:A:2214:HOH:O	2.13	0.47
1:B:420:VAL:C	1:B:422:ARG:H	2.22	0.47
1:B:424:PHE:HD2	1:B:430:ASP:H	1.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:ARG:HG2	1:B:478:VAL:HG22	1.97	0.47
1:B:529:ARG:HD3	1:B:776:HIS:CD2	2.49	0.47
1:A:721:ARG:O	1:A:725:VAL:HG13	2.15	0.47
1:A:723:ARG:NH2	1:B:947:GLU:HG2	2.30	0.47
1:A:1186:MET:CB	1:A:1187:LYS:HB2	2.45	0.47
1:B:1119:LYS:HG3	1:B:1120:GLN:NE2	2.30	0.47
1:B:460:LEU:HD12	1:B:462:ALA:CB	2.45	0.47
1:B:1214:SER:HA	1:B:1217:SER:HA	1.96	0.47
1:A:1200:ASP:OD1	1:A:1202:ASP:HB2	2.15	0.47
1:A:464:ARG:HA	1:A:465:GLY:O	2.15	0.47
1:A:589:GLY:H	1:A:611:ARG:HH21	1.63	0.47
1:B:407:LYS:H	1:B:408:TRP:HD1	1.63	0.47
1:B:942:LYS:HD2	1:B:949:SER:CB	2.44	0.47
1:A:1217:SER:OG	1:A:1221:ALA:CA	2.64	0.46
1:A:1224:PHE:CE2	1:A:1228:LYS:HE3	2.50	0.46
1:B:455:LYS:C	1:B:457:LEU:O	2.58	0.46
1:B:1254:TYR:HB3	1:B:1255:PRO:HD3	1.97	0.46
1:A:444:TRP:CE2	1:A:453:ILE:HG23	2.50	0.46
1:A:466:LYS:N	1:A:467:PRO:CA	2.77	0.46
1:B:821:ILE:HG13	1:B:1170:ILE:HG23	1.97	0.46
1:A:395:ALA:HA	1:A:397:ARG:O	2.15	0.46
1:A:406:PRO:HG3	1:A:431:LEU:HB3	1.97	0.46
1:A:622:PHE:CD1	1:A:622:PHE:N	2.84	0.46
1:A:712:GLY:O	1:A:746:TRP:HA	2.16	0.46
1:A:1169:SER:O	1:A:1173:PRO:HG2	2.15	0.46
1:A:1182:PHE:N	1:A:1182:PHE:CD2	2.83	0.46
1:B:501:ASN:HD22	1:B:502:PRO:HD2	1.79	0.46
1:B:859:GLY:O	1:B:860:ARG:HB3	2.15	0.46
1:A:1147:MET:HE2	1:A:1147:MET:HA	1.97	0.46
1:A:1189:ALA:O	1:A:1190:LYS:C	2.59	0.46
1:B:433:ASP:OD2	1:B:438:LEU:HD11	2.16	0.46
1:B:447:ALA:HB3	1:B:453:ILE:HD11	1.98	0.46
1:B:456:THR:H	1:B:457:LEU:C	2.24	0.46
1:B:503:ASP:HB3	1:B:504:ASN:H	1.45	0.46
1:B:459:ARG:HB2	1:B:460:LEU:HB2	1.98	0.46
1:B:1270:PRO:HG3	1:B:1301:TRP:CE3	2.50	0.46
1:A:456:THR:O	1:A:459:ARG:CZ	2.64	0.46
1:A:484:ASN:O	1:A:485:PHE:HB2	2.16	0.46
1:A:966:HIS:ND1	1:A:1089:LYS:HE3	2.31	0.46
1:B:459:ARG:CB	1:B:460:LEU:HB2	2.46	0.46
1:A:434:GLU:OE2	1:A:434:GLU:N	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:ALA:HB2	1:A:562:GLU:OE1	2.13	0.45
1:A:738:ARG:HD3	1:A:743:LYS:HG2	1.98	0.45
1:A:1185:ALA:H	1:A:1188:ALA:HB2	1.81	0.45
1:A:1252:ASP:O	1:A:1252:ASP:CG	2.58	0.45
1:B:426:HIS:HA	1:B:427:CYS:HA	1.57	0.45
1:B:546:THR:O	1:B:546:THR:CG2	2.63	0.45
1:B:589:GLY:O	1:B:590:TYR:HB2	2.15	0.45
1:B:462:ALA:H	1:B:464:ARG:N	2.15	0.45
1:B:503:ASP:O	1:B:504:ASN:CB	2.64	0.45
1:B:1041:LYS:HB2	1:B:1123:VAL:CG1	2.45	0.45
1:B:403:PRO:CB	1:B:404:LYS:HB2	2.45	0.45
1:B:457:LEU:HA	1:B:458:TYR:HA	1.58	0.45
1:B:839:VAL:HG22	4:B:2167:HOH:O	2.16	0.45
1:A:456:THR:O	1:A:459:ARG:HB2	2.16	0.45
1:A:1102:LYS:N	1:A:1103:PRO:HD2	2.32	0.45
1:B:557:GLN:HG3	1:B:557:GLN:O	2.17	0.45
1:B:610:GLU:HG3	1:B:1077:LEU:HD22	1.99	0.45
1:B:621:THR:HG22	1:B:622:PHE:CD2	2.52	0.45
1:A:399:ARG:HB2	1:A:400:ASN:CA	2.46	0.45
1:B:828:PHE:CD2	1:B:1178:GLU:HG2	2.51	0.45
1:B:826:ARG:NH1	1:B:826:ARG:HB3	2.32	0.45
1:B:966:HIS:ND1	1:B:1089:LYS:HE2	2.32	0.45
1:A:674:LEU:HD11	4:A:2095:HOH:O	2.17	0.45
1:A:952:LEU:HG	1:A:978:PHE:CD1	2.52	0.45
1:B:441:ASP:CB	1:B:442:PRO:HA	2.46	0.45
1:A:391:ALA:CB	1:A:393:VAL:HG22	2.47	0.44
1:A:394:VAL:HA	1:A:395:ALA:HA	1.76	0.44
1:A:396:ALA:HB1	1:A:399:ARG:CZ	2.48	0.44
1:B:447:ALA:CB	1:B:453:ILE:HD11	2.47	0.44
1:A:414:LEU:HD13	1:A:485:PHE:CZ	2.53	0.44
1:A:867:LEU:HD22	1:A:874:THR:HG23	1.99	0.44
1:A:1182:PHE:HA	1:A:1185:ALA:CB	2.47	0.44
1:B:551:PRO:HB2	1:B:553:VAL:HG11	1.99	0.44
1:B:861:VAL:CG2	1:B:873:GLU:HG2	2.48	0.44
1:B:407:LYS:HB2	1:B:408:TRP:HB3	0.56	0.44
1:B:451:THR:H	1:B:452:ASP:CA	2.31	0.44
1:B:1298:MET:HE3	3:B:3375:GOL:C3	2.47	0.44
1:A:883:PHE:CZ	1:A:1203:LEU:HD21	2.53	0.44
1:A:959:LEU:HD22	1:A:1021:ILE:HG22	2.00	0.44
1:B:475:ASP:OD1	1:B:476:VAL:N	2.51	0.44
1:B:1063:GLN:CB	4:B:2306:HOH:O	2.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:PRO:O	1:A:410:HIS:CD2	2.71	0.44
1:A:1134:ARG:HG3	4:A:2232:HOH:O	2.16	0.44
1:B:407:LYS:N	1:B:408:TRP:CD1	2.85	0.44
1:B:861:VAL:HG21	1:B:873:GLU:CG	2.47	0.44
1:A:839:VAL:HG22	4:A:2246:HOH:O	2.18	0.44
1:A:1190:LYS:HG3	1:A:1191:ASP:H	1.81	0.44
1:A:468:PHE:CA	1:A:469:PRO:O	2.56	0.44
1:A:1184:ASN:H	1:A:1185:ALA:HB3	0.71	0.44
1:B:1194:ASP:C	1:B:1196:ALA:N	2.76	0.44
1:A:624:PRO:CA	1:A:625:ASP:CB	2.93	0.44
1:A:931:GLU:OE2	1:A:994:LYS:NZ	2.51	0.44
1:B:1217:SER:CB	1:B:1218:ARG:CA	2.94	0.43
1:A:947:GLU:H	1:A:947:GLU:HG2	1.65	0.43
1:A:1094:TYR:CE2	1:A:1146:PRO:HA	2.53	0.43
1:B:429:VAL:HG22	1:B:463:PHE:CE2	2.53	0.43
1:A:467:PRO:HB2	1:A:468:PHE:H	1.53	0.43
1:B:544:THR:HG21	1:B:1079:PRO:HD3	1.99	0.43
1:B:551:PRO:HA	1:B:552:PRO:HD3	1.67	0.43
1:B:916:ARG:HD3	4:B:2284:HOH:O	2.17	0.43
1:B:962:ARG:HD3	1:B:1011:ASP:HB3	2.00	0.43
1:B:1289:GLU:O	1:B:1299:ASN:ND2	2.51	0.43
1:B:772:PHE:O	1:B:778:ARG:CD	2.67	0.43
1:A:665:HIS:HE1	4:A:2366:HOH:O	2.00	0.43
1:A:905:THR:HG23	1:A:909:LYS:HD2	2.01	0.43
1:A:1299:ASN:O	1:A:1303:LEU:HD22	2.19	0.43
1:B:432:GLU:O	1:B:433:ASP:HB3	2.18	0.43
1:B:456:THR:O	1:B:456:THR:CG2	2.67	0.43
1:B:1073:PHE:O	1:B:1077:LEU:HG	2.18	0.43
1:B:1138:GLY:C	4:B:2338:HOH:O	2.60	0.43
1:A:444:TRP:HZ2	1:A:456:THR:HG21	1.84	0.43
1:A:835:LEU:HD13	1:A:841:PHE:CZ	2.54	0.43
1:B:428:LYS:O	1:B:429:VAL:CB	2.66	0.43
1:B:451:THR:N	1:B:452:ASP:CA	2.81	0.43
1:B:451:THR:CA	1:B:452:ASP:HB2	2.49	0.43
1:B:498:LEU:O	1:B:541:PRO:HD3	2.19	0.43
1:B:900:LYS:HE3	1:B:900:LYS:HB2	1.64	0.43
1:B:1211:LYS:HE2	1:B:1211:LYS:HB3	1.86	0.43
1:B:1325:ALA:O	1:B:1326:GLY:C	2.62	0.43
1:A:852:ARG:O	1:A:856:VAL:HG23	2.19	0.43
1:A:1193:GLU:CA	1:A:1194:ASP:C	2.84	0.43
1:B:1075:PHE:O	1:B:1078:GLN:HG2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:TRP:CD1	1:A:453:ILE:HG23	2.53	0.43
1:A:547:SER:CB	1:A:548:PRO:CA	2.96	0.43
1:A:740:GLY:HA3	1:A:772:PHE:CE2	2.54	0.43
1:A:1344:ALA:HB1	1:B:1327:ARG:CD	2.48	0.43
1:B:462:ALA:CA	1:B:463:PHE:C	2.92	0.43
1:B:1143:LEU:HD12	1:B:1143:LEU:HA	1.81	0.43
1:A:408:TRP:CH2	1:A:431:LEU:HD23	2.54	0.42
1:A:683:MET:HE2	1:A:685:LEU:CD2	2.49	0.42
1:B:423:LEU:HD21	1:B:458:TYR:HE2	1.84	0.42
1:B:1139:GLY:HA2	1:B:1140:ALA:HB3	2.01	0.42
1:A:460:LEU:O	1:A:461:ASP:HB3	2.19	0.42
1:A:654:LEU:HD12	4:A:2200:HOH:O	2.19	0.42
1:A:1222:LEU:HD12	1:A:1222:LEU:HA	1.86	0.42
1:A:1348:MET:HE2	1:A:1348:MET:HB3	1.79	0.42
1:B:459:ARG:HB2	1:B:460:LEU:CB	2.49	0.42
1:B:1229:ASN:O	1:B:1233:GLU:HG3	2.19	0.42
1:A:683:MET:HE2	1:A:685:LEU:HD21	2.02	0.42
1:B:429:VAL:HG12	1:B:430:ASP:H	1.83	0.42
1:B:530:PHE:CE2	1:B:650:MET:HG2	2.55	0.42
1:B:580:TRP:HB3	1:B:614:PHE:HB3	1.99	0.42
1:B:991:PHE:CD2	1:B:999:LEU:HB3	2.54	0.42
1:A:419:GLU:OE1	1:A:422:ARG:HD3	2.20	0.42
1:A:467:PRO:HG2	1:A:468:PHE:HD2	1.85	0.42
1:A:1190:LYS:HG3	1:A:1191:ASP:N	2.34	0.42
1:A:1325:ALA:O	1:A:1326:GLY:C	2.63	0.42
1:B:404:LYS:HA	1:B:404:LYS:HD3	1.76	0.42
1:B:879:MET:HE1	1:B:885:PRO:HG3	1.98	0.42
1:B:1187:LYS:HE2	1:B:1187:LYS:HB3	1.89	0.42
1:A:454:TRP:HA	1:A:457:LEU:HD23	2.01	0.42
1:A:547:SER:CB	1:A:548:PRO:HA	2.50	0.42
1:B:667:LYS:HE2	1:B:667:LYS:HB2	1.56	0.42
1:A:454:TRP:O	1:A:458:TYR:CG	2.72	0.42
1:A:772:PHE:O	1:A:778:ARG:CD	2.67	0.42
1:B:441:ASP:HB2	1:B:444:TRP:CG	2.54	0.42
1:B:1224:PHE:CE2	1:B:1228:LYS:HE3	2.55	0.42
1:A:426:HIS:HB3	1:A:469:PRO:HD3	2.02	0.42
1:A:444:TRP:CD2	1:A:453:ILE:HG23	2.54	0.42
1:B:1182:PHE:O	1:B:1186:MET:HG2	2.19	0.42
1:A:472:PRO:HA	1:A:473:PRO:HD3	1.90	0.42
1:A:796:LEU:HA	1:A:799:LEU:CD1	2.46	0.42
1:B:429:VAL:HG12	1:B:430:ASP:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:THR:HG22	1:A:457:LEU:HD13	2.01	0.42
1:A:705:GLU:HG2	1:A:998:PRO:CD	2.50	0.42
1:B:441:ASP:CB	1:B:442:PRO:CA	2.96	0.42
1:B:555:SER:CA	1:B:557:GLN:H	2.32	0.42
1:B:712:GLY:O	1:B:746:TRP:HA	2.20	0.42
1:A:889:LYS:HG2	1:A:1198:PHE:CZ	2.55	0.41
1:A:966:HIS:ND1	1:A:1089:LYS:CE	2.83	0.41
1:B:1131:GLN:HG2	1:B:1135:GLU:CD	2.45	0.41
1:A:662:TRP:CD1	1:A:662:TRP:H	2.36	0.41
1:A:1220:SER:H	1:A:1221:ALA:HB3	1.73	0.41
1:B:459:ARG:HB2	1:B:460:LEU:CD2	2.48	0.41
1:B:551:PRO:HB2	1:B:553:VAL:CG1	2.50	0.41
1:B:1075:PHE:HE2	1:B:1118:SER:HA	1.84	0.41
1:B:449:ASP:HB3	1:B:450:VAL:H	1.65	0.41
1:B:907:LYS:HG3	1:B:1175:ILE:HD13	2.02	0.41
1:B:1153:TRP:NE1	1:B:1157:GLY:O	2.52	0.41
1:A:423:LEU:HD11	1:A:458:TYR:CD1	2.54	0.41
1:A:696:ASP:HB3	1:A:706:VAL:HG13	2.02	0.41
1:A:1182:PHE:HA	1:A:1185:ALA:HB1	2.01	0.41
1:A:1183:HIS:HA	1:A:1186:MET:HG3	2.03	0.41
1:A:1334:ALA:HB3	1:B:1347:LEU:HD13	2.01	0.41
1:B:407:LYS:CA	1:B:408:TRP:CB	2.92	0.41
1:B:565:ILE:HD13	1:B:1074:HIS:HA	2.03	0.41
1:B:722:ILE:O	1:B:726:LEU:HB2	2.20	0.41
1:A:514:LYS:HB3	1:A:514:LYS:HE3	1.88	0.41
1:A:581:ARG:NH1	4:A:2068:HOH:O	2.54	0.41
1:A:605:LYS:HA	1:A:606:PRO:HD3	1.88	0.41
1:B:393:VAL:O	1:B:394:VAL:CB	2.64	0.41
1:B:400:ASN:OD1	1:B:509:PRO:HB3	2.20	0.41
1:A:794:LEU:HD11	1:A:802:LEU:HD11	2.03	0.41
1:A:799:LEU:HB2	1:A:800:PRO:HD3	2.02	0.41
1:A:869:ASP:HB3	4:A:2264:HOH:O	2.21	0.41
1:A:1141:LEU:HD13	1:A:1141:LEU:HA	1.89	0.41
1:A:1146:PRO:CB	1:A:1148:TYR:CE2	3.04	0.41
1:A:1289:GLU:O	1:A:1290:LEU:C	2.64	0.41
1:B:428:LYS:O	1:B:429:VAL:CG2	2.68	0.41
1:B:458:TYR:HB3	1:B:463:PHE:O	2.21	0.41
1:B:462:ALA:HB1	1:B:463:PHE:CD2	2.56	0.41
1:B:1203:LEU:HG	1:B:1329:LEU:HD22	2.03	0.41
1:B:1218:ARG:N	1:B:1219:SER:CB	2.77	0.41
1:B:400:ASN:HD22	1:B:404:LYS:NZ	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:VAL:HG22	1:B:463:PHE:CZ	2.55	0.41
1:A:922:MET:HE1	1:A:1011:ASP:HB3	2.03	0.40
1:A:1089:LYS:HB2	1:A:1107:LEU:HB3	2.03	0.40
1:B:457:LEU:H	1:B:459:ARG:HG2	1.86	0.40
1:B:775:LYS:HG2	4:B:2109:HOH:O	2.20	0.40
1:A:410:HIS:C	1:A:412:ALA:H	2.30	0.40
1:A:488:LYS:HE3	1:B:1371:GLU:O	2.22	0.40
1:A:1150:SER:HB2	4:A:2426:HOH:O	2.20	0.40
1:B:419:GLU:N	1:B:422:ARG:HB2	2.26	0.40
1:B:456:THR:O	1:B:459:ARG:HG2	2.21	0.40
1:B:460:LEU:C	1:B:462:ALA:HA	2.38	0.40
1:B:1087:ASN:O	1:B:1091:ARG:HG3	2.21	0.40
1:A:454:TRP:O	1:A:458:TYR:CD1	2.75	0.40
1:A:648:SER:HA	1:A:1065:THR:HG21	2.03	0.40
1:A:879:MET:HE3	1:A:885:PRO:HG3	2.02	0.40
1:B:391:ALA:HB3	1:B:563:GLU:CG	2.45	0.40
1:B:431:LEU:HD13	1:B:432:GLU:OE1	2.21	0.40
1:A:485:PHE:HB3	1:A:532:PRO:HB2	2.02	0.40
1:A:557:GLN:HE21	1:A:557:GLN:HB3	1.68	0.40
1:A:1265:TRP:CZ2	1:A:1325:ALA:HB2	2.56	0.40
1:B:449:ASP:O	1:B:450:VAL:HB	2.22	0.40
1:A:459:ARG:HB3	1:A:460:LEU:H	1.52	0.40
1:A:626:VAL:HG13	1:A:626:VAL:O	2.22	0.40
1:A:1207:TYR:CE2	1:A:1311:LYS:HG3	2.55	0.40
1:A:1220:SER:H	1:A:1221:ALA:CB	2.29	0.40
1:B:441:ASP:HB3	1:B:442:PRO:O	2.20	0.40
1:B:547:SER:CB	1:B:548:PRO:CD	2.99	0.40
1:B:699:SER:HA	1:B:700:PRO:HD3	1.98	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2389:HOH:O	4:B:2333:HOH:O[1_455]	1.90	0.30
1:A:1156:ARG:NH1	1:B:1126:GLU:OE2[1_455]	2.07	0.13
4:A:2109:HOH:O	4:B:2384:HOH:O[2_746]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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	925/1022 (90%)	836 (90%)	51 (6%)	38 (4%)	2	1
1	B	922/1022 (90%)	811 (88%)	63 (7%)	48 (5%)	1	1
All	All	1847/2044 (90%)	1647 (89%)	114 (6%)	86 (5%)	2	1

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	ARG
1	A	412	ALA
1	A	439	LYS
1	A	440	TYR
1	A	459	ARG
1	A	460	LEU
1	A	466	LYS
1	A	467	PRO
1	A	504	ASN
1	A	510	LEU
1	A	547	SER
1	A	553	VAL
1	A	621	THR
1	A	625	ASP
1	A	642	ARG
1	A	1140	ALA
1	A	1141	LEU
1	A	1193	GLU
1	A	1194	ASP
1	B	401	ILE
1	B	406	PRO
1	B	411	GLU
1	B	419	GLU
1	B	429	VAL
1	B	430	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	432	GLU
1	B	434	GLU
1	B	446	THR
1	B	453	ILE
1	B	460	LEU
1	B	463	PHE
1	B	467	PRO
1	B	504	ASN
1	B	505	SER
1	B	547	SER
1	B	548	PRO
1	B	1141	LEU
1	B	1190	LYS
1	B	1217	SER
1	B	1219	SER
1	A	394	VAL
1	A	398	LEU
1	A	461	ASP
1	A	503	ASP
1	A	1138	GLY
1	A	1185	ALA
1	A	1187	LYS
1	A	1214	SER
1	A	1316	LYS
1	B	407	LYS
1	B	408	TRP
1	B	431	LEU
1	B	450	VAL
1	B	451	THR
1	B	503	ASP
1	B	510	LEU
1	B	555	SER
1	B	621	THR
1	B	1196	ALA
1	B	1214	SER
1	A	559	ALA
1	A	1218	ARG
1	A	1315	HIS
1	B	404	LYS
1	B	441	ASP
1	B	1189	ALA
1	B	1194	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	458	TYR
1	A	469	PRO
1	A	471	LYS
1	A	488	LYS
1	B	471	LYS
1	B	553	VAL
1	B	1195	GLY
1	B	1205	SER
1	B	412	ALA
1	B	418	TRP
1	B	445	SER
1	B	507	THR
1	B	1140	ALA
1	A	468	PHE
1	B	392	PRO
1	B	394	VAL
1	A	453	ILE
1	A	1253	PRO
1	B	552	PRO

5.3.2 Protein sidechains ⓘ

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	815/891 (92%)	744 (91%)	71 (9%)	9	12
1	B	812/891 (91%)	710 (87%)	102 (13%)	4	5
All	All	1627/1782 (91%)	1454 (89%)	173 (11%)	6	8

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	393	VAL
1	A	394	VAL
1	A	408	TRP
1	A	409	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	414	LEU
1	A	456	THR
1	A	457	LEU
1	A	458	TYR
1	A	482	THR
1	A	507	THR
1	A	515	LEU
1	A	518	LEU
1	A	526	LEU
1	A	546	THR
1	A	547	SER
1	A	550	VAL
1	A	553	VAL
1	A	555	SER
1	A	557	GLN
1	A	622	PHE
1	A	623	ARG
1	A	701	SER
1	A	716	ARG
1	A	723	ARG
1	A	725	VAL
1	A	726	LEU
1	A	730	ASP
1	A	755	ASP
1	A	774	ASP
1	A	796	LEU
1	A	797	GLN
1	A	798	LEU
1	A	835	LEU
1	A	839	VAL
1	A	891	LEU
1	A	896	TRP
1	A	905	THR
1	A	947	GLU
1	A	949	SER
1	A	952	LEU
1	A	953	LEU
1	A	955	ASP
1	A	959	LEU
1	A	999	LEU
1	A	1032	LEU
1	A	1048	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1056	THR
1	A	1120	GLN
1	A	1134	ARG
1	A	1137	LEU
1	A	1141	LEU
1	A	1172	ARG
1	A	1180	GLU
1	A	1182	PHE
1	A	1187	LYS
1	A	1193	GLU
1	A	1194	ASP
1	A	1203	LEU
1	A	1211	LYS
1	A	1214	SER
1	A	1216	LYS
1	A	1217	SER
1	A	1218	ARG
1	A	1223	LEU
1	A	1235	GLU
1	A	1240	ARG
1	A	1269	THR
1	A	1282	SER
1	A	1303	LEU
1	A	1317	SER
1	A	1321	VAL
1	B	397	ARG
1	B	398	LEU
1	B	399	ARG
1	B	400	ASN
1	B	401	ILE
1	B	408	TRP
1	B	409	LEU
1	B	411	GLU
1	B	414	LEU
1	B	419	GLU
1	B	421	THR
1	B	425	MET
1	B	427	CYS
1	B	431	LEU
1	B	439	LYS
1	B	440	TYR
1	B	446	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	449	ASP
1	B	450	VAL
1	B	451	THR
1	B	482	THR
1	B	487	SER
1	B	488	LYS
1	B	503	ASP
1	B	507	THR
1	B	513	VAL
1	B	518	LEU
1	B	526	LEU
1	B	538	ILE
1	B	544	THR
1	B	546	THR
1	B	547	SER
1	B	550	VAL
1	B	554	VAL
1	B	575	LEU
1	B	581	ARG
1	B	586	LYS
1	B	621	THR
1	B	623	ARG
1	B	647	VAL
1	B	667	LYS
1	B	674	LEU
1	B	720	LYS
1	B	723	ARG
1	B	725	VAL
1	B	726	LEU
1	B	769	GLU
1	B	775	LYS
1	B	790	LYS
1	B	796	LEU
1	B	805	ARG
1	B	824	LEU
1	B	835	LEU
1	B	839	VAL
1	B	842	ARG
1	B	849	TYR
1	B	861	VAL
1	B	867	LEU
1	B	870	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	889	LYS
1	B	900	LYS
1	B	905	THR
1	B	910	LEU
1	B	916	ARG
1	B	947	GLU
1	B	948	GLU
1	B	952	LEU
1	B	953	LEU
1	B	955	ASP
1	B	959	LEU
1	B	999	LEU
1	B	1036	LEU
1	B	1040	LEU
1	B	1048	LYS
1	B	1058	SER
1	B	1067	ASP
1	B	1110	LEU
1	B	1133	ARG
1	B	1137	LEU
1	B	1141	LEU
1	B	1143	LEU
1	B	1154	LEU
1	B	1191	ASP
1	B	1203	LEU
1	B	1205	SER
1	B	1216	LYS
1	B	1217	SER
1	B	1223	LEU
1	B	1236	LYS
1	B	1269	THR
1	B	1282	SER
1	B	1283	LYS
1	B	1285	ILE
1	B	1303	LEU
1	B	1308	THR
1	B	1312	LEU
1	B	1321	VAL
1	B	1327	ARG
1	B	1337	THR
1	B	1347	LEU
1	B	1360	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1370	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	HIS
1	A	484	ASN
1	A	557	GLN
1	A	566	GLN
1	A	579	GLN
1	A	613	HIS
1	A	673	GLN
1	A	843	GLN
1	B	390	HIS
1	B	501	ASN
1	B	566	GLN
1	B	665	HIS
1	B	688	HIS
1	B	776	HIS
1	B	777	GLN
1	B	822	ASN
1	B	833	HIS
1	B	1054	HIS
1	B	1101	ASN
1	B	1197	HIS
1	B	1299	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	3375	-	4,4,5	0.67	0	4,4,5	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	3375	-	-	0/2/2/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3375	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	436:LEU	C	437:GLY	N	1.62

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	935/1022 (91%)	0.80	96 (10%) 12 13	39, 50, 65, 78	0
1	B	932/1022 (91%)	1.14	171 (18%) 3 4	38, 51, 64, 77	0
All	All	1867/2044 (91%)	0.97	267 (14%) 6 7	38, 51, 64, 78	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	525	ARG	8.4
1	A	1138	GLY	7.8
1	A	1162	ILE	7.0
1	A	1163	ILE	5.8
1	A	1141	LEU	5.7
1	A	1166	LEU	5.7
1	B	526	LEU	5.4
1	B	584	PHE	4.9
1	B	645	PHE	4.9
1	B	508	ALA	4.9
1	A	1139	GLY	4.8
1	B	454	TRP	4.8
1	B	530	PHE	4.7
1	B	1185	ALA	4.6
1	B	512	LEU	4.6
1	A	469	PRO	4.5
1	B	1140	ALA	4.5
1	A	796	LEU	4.4
1	B	507	THR	4.4
1	A	1164	ASP	4.4
1	B	524	CYS	4.4
1	B	1191	ASP	4.4
1	A	1254	TYR	4.3
1	B	528	ARG	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1192	THR	4.3
1	B	1189	ALA	4.2
1	B	527	THR	4.2
1	A	1140	ALA	4.2
1	B	443	SER	4.2
1	A	1344	ALA	4.2
1	B	585	ALA	4.1
1	A	1182	PHE	4.1
1	B	590	TYR	4.0
1	B	553	VAL	4.0
1	B	1182	PHE	3.9
1	B	425	MET	3.9
1	A	1191	ASP	3.9
1	B	583	PHE	3.9
1	A	409	LEU	3.9
1	B	469	PRO	3.9
1	B	626	VAL	3.9
1	B	448	ARG	3.8
1	B	1195	GLY	3.8
1	B	396	ALA	3.7
1	B	522	GLN	3.7
1	B	535	PHE	3.7
1	B	463	PHE	3.7
1	B	468	PHE	3.6
1	B	1138	GLY	3.6
1	B	607	ILE	3.6
1	B	509	PRO	3.6
1	A	849	TYR	3.6
1	A	1165	TYR	3.6
1	B	1121	GLY	3.6
1	A	457	LEU	3.6
1	B	466	LYS	3.5
1	B	458	TYR	3.5
1	B	531	GLY	3.5
1	A	1210	PHE	3.5
1	B	1139	GLY	3.4
1	B	565	ILE	3.4
1	B	523	GLY	3.4
1	B	529	ARG	3.4
1	A	869	ASP	3.4
1	A	1186	MET	3.4
1	B	491	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1370	LEU	3.3
1	A	626	VAL	3.3
1	A	1193	GLU	3.3
1	B	1220	SER	3.3
1	B	502	PRO	3.3
1	A	1315	HIS	3.3
1	B	490	SER	3.3
1	B	489	GLY	3.2
1	A	1179	LEU	3.2
1	A	393	VAL	3.2
1	A	1189	ALA	3.2
1	B	1074	HIS	3.2
1	B	436	LEU	3.2
1	A	1170	ILE	3.2
1	A	395	ALA	3.1
1	B	460	LEU	3.1
1	A	1175	ILE	3.1
1	A	1142	SER	3.1
1	B	624	PRO	3.1
1	B	623	ARG	3.1
1	B	1163	ILE	3.1
1	B	464	ARG	3.0
1	B	488	LYS	3.0
1	B	438	LEU	3.0
1	A	1208	THR	3.0
1	B	546	THR	3.0
1	A	604	PRO	3.0
1	B	1254	TYR	3.0
1	B	394	VAL	2.9
1	A	1216	LYS	2.9
1	A	895	ALA	2.9
1	A	1185	ALA	2.9
1	A	458	TYR	2.9
1	B	1151	ASP	2.9
1	A	438	LEU	2.9
1	B	453	ILE	2.9
1	B	1373	ASP	2.9
1	B	467	PRO	2.8
1	B	418	TRP	2.8
1	B	1157	GLY	2.8
1	A	467	PRO	2.8
1	A	394	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	560	ALA	2.8
1	B	582	ALA	2.8
1	A	1168	PHE	2.8
1	B	482	THR	2.7
1	A	627	PHE	2.7
1	B	393	VAL	2.7
1	B	452	ASP	2.7
1	B	465	GLY	2.7
1	A	1030	MET	2.7
1	B	1344	ALA	2.7
1	B	1184	ASN	2.7
1	B	1252	ASP	2.7
1	A	620	ILE	2.7
1	B	1162	ILE	2.7
1	B	1137	LEU	2.7
1	B	1179	LEU	2.7
1	B	620	ILE	2.7
1	B	492	VAL	2.6
1	A	642	ARG	2.6
1	A	1218	ARG	2.6
1	B	1186	MET	2.6
1	B	1232	GLY	2.6
1	B	641	GLN	2.6
1	A	1167	LYS	2.6
1	B	646	LYS	2.6
1	A	1318	PRO	2.6
1	B	409	LEU	2.6
1	B	642	ARG	2.6
1	B	1181	ALA	2.6
1	B	1368	ALA	2.6
1	B	532	PRO	2.6
1	B	622	PHE	2.6
1	B	511	TYR	2.6
1	B	461	ASP	2.5
1	B	896	TRP	2.5
1	A	465	GLY	2.5
1	A	621	THR	2.5
1	B	1372	GLY	2.5
1	B	562	GLU	2.5
1	B	1156	ARG	2.5
1	B	520	PHE	2.5
1	B	849	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1137	LEU	2.5
1	B	433	ASP	2.5
1	B	1192	THR	2.5
1	B	485	PHE	2.5
1	B	616	ALA	2.5
1	A	1343	GLY	2.5
1	B	416	VAL	2.4
1	B	561	VAL	2.4
1	A	1313	TYR	2.4
1	B	1190	LYS	2.4
1	B	437	GLY	2.4
1	B	643	THR	2.4
1	B	450	VAL	2.4
1	B	608	ILE	2.4
1	B	444	TRP	2.4
1	B	431	LEU	2.4
1	A	1181	ALA	2.4
1	B	472	PRO	2.4
1	B	1150	SER	2.4
1	A	1293	LEU	2.4
1	A	1184	ASN	2.4
1	B	457	LEU	2.4
1	A	1234	VAL	2.3
1	B	615	PHE	2.3
1	B	459	ARG	2.3
1	A	1312	LEU	2.3
1	A	605	LYS	2.3
1	B	447	ALA	2.3
1	B	1171	ALA	2.3
1	A	1219	SER	2.3
1	B	1136	LEU	2.3
1	B	1166	LEU	2.3
1	A	1265	TRP	2.3
1	B	500	TYR	2.3
1	A	1188	ALA	2.3
1	B	479	THR	2.3
1	A	1136	LEU	2.3
1	B	449	ASP	2.3
1	B	1299	ASN	2.3
1	A	1195	GLY	2.3
1	B	618	THR	2.3
1	B	478	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	997	VAL	2.3
1	A	1116	ASP	2.2
1	B	427	CYS	2.2
1	A	1207	TYR	2.2
1	B	487	SER	2.2
1	B	1070	GLN	2.2
1	A	453	ILE	2.2
1	B	1222	LEU	2.2
1	A	463	PHE	2.2
1	A	1224	PHE	2.2
1	A	913	ARG	2.2
1	B	1257	ARG	2.2
1	B	428	LYS	2.2
1	A	1213	ILE	2.2
1	A	1268	ILE	2.2
1	B	912	ILE	2.2
1	B	398	LEU	2.2
1	B	424	PHE	2.2
1	B	395	ALA	2.2
1	A	1169	SER	2.2
1	B	1217	SER	2.2
1	B	510	LEU	2.2
1	B	1296	ARG	2.2
1	B	400	ASN	2.2
1	B	838	PRO	2.2
1	B	625	ASP	2.1
1	A	1209	PHE	2.1
1	A	641	GLN	2.1
1	A	1171	ALA	2.1
1	B	391	ALA	2.1
1	B	446	THR	2.1
1	B	569	THR	2.1
1	A	436	LEU	2.1
1	A	608	ILE	2.1
1	B	423	LEU	2.1
1	B	1040	LEU	2.1
1	B	1119	LYS	2.1
1	A	1120	GLN	2.1
1	B	413	PRO	2.1
1	B	1153	TRP	2.1
1	A	589	GLY	2.1
1	A	1338	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	505	SER	2.1
1	B	455	LYS	2.1
1	A	864	LEU	2.1
1	B	486	GLU	2.1
1	B	1223	LEU	2.1
1	B	499	ASP	2.1
1	B	506	PRO	2.1
1	B	1224	PHE	2.1
1	A	1187	LYS	2.1
1	B	563	GLU	2.1
1	B	1193	GLU	2.1
1	B	1154	LEU	2.1
1	A	1314	TYR	2.1
1	B	548	PRO	2.1
1	B	1144	PRO	2.1
1	A	468	PHE	2.1
1	A	1326	GLY	2.1
1	B	1081	PHE	2.1
1	A	1309	ALA	2.0
1	B	947	GLU	2.0
1	A	1143	LEU	2.0
1	A	509	PRO	2.0
1	B	577	GLY	2.0
1	A	1211	LYS	2.0
1	A	408	TRP	2.0
1	B	1051	MET	2.0
1	B	451	THR	2.0
1	B	545	SER	2.0
1	B	1063	GLN	2.0
1	B	1077	LEU	2.0
1	A	1296	ARG	2.0
1	A	556	LYS	2.0
1	A	1190	LYS	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	3375	5/6	0.84	0.17	66,67,67,67	0
2	MG	A	3374	1/1	0.93	0.05	50,50,50,50	0
2	MG	B	3374	1/1	0.99	0.06	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.