



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2021 – 12:10 PM EDT

PDB ID : 6WPC
Title : Crystal structure of Bacillus thuringiensis Cry1A.2 tryptic core variant
Authors : Rydel, T.J.; Evdokimov, A.
Deposited on : 2020-04-27
Resolution : 2.99 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.1
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) : 2.23.1

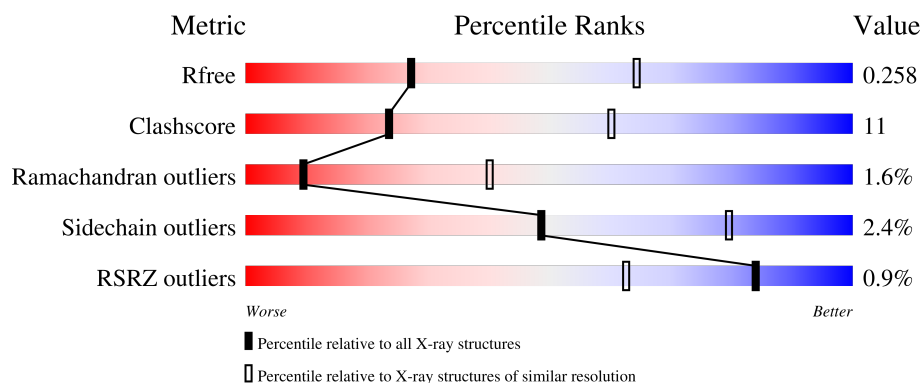
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	591	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>...</div> </div> </div>
1	B	591	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
1	C	591	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div> </div>
1	D	591	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>...</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18743 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 Cry1A.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	1	0
			4668	2970	816	874	8			
1	B	588	Total	C	N	O	S	0	1	0
			4671	2972	817	874	8			
1	C	588	Total	C	N	O	S	0	0	0
			4665	2968	816	873	8			
1	D	588	Total	C	N	O	S	0	1	0
			4673	2973	819	873	8			

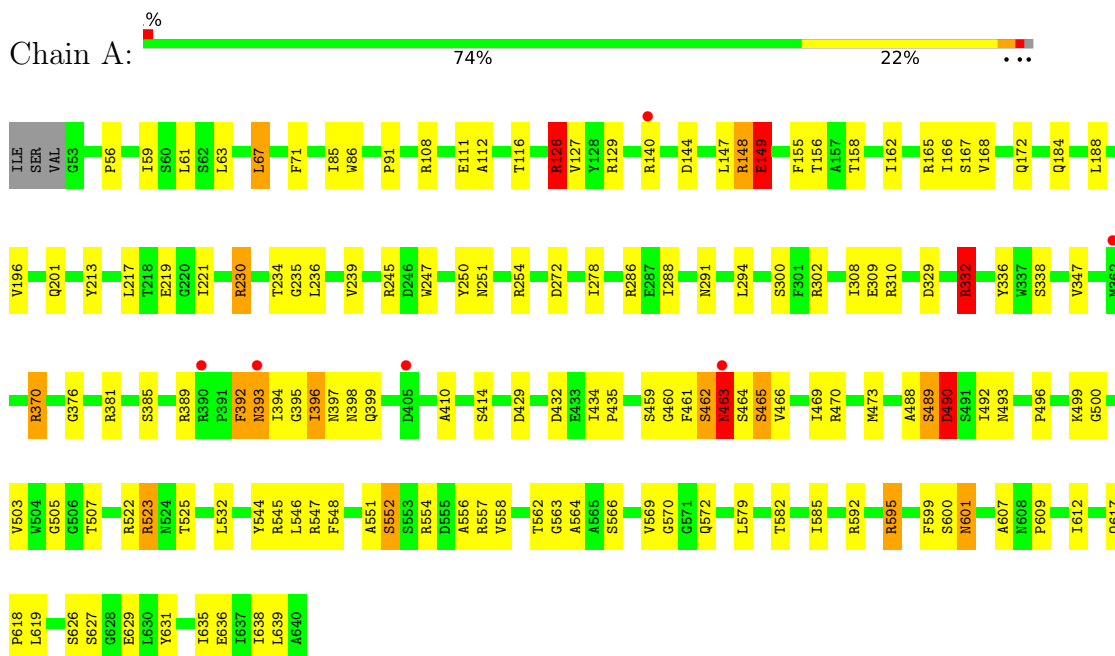
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		
2	B	20	Total	O	0	0
			20	20		
2	C	13	Total	O	0	0
			13	13		
2	D	17	Total	O	0	0
			17	17		

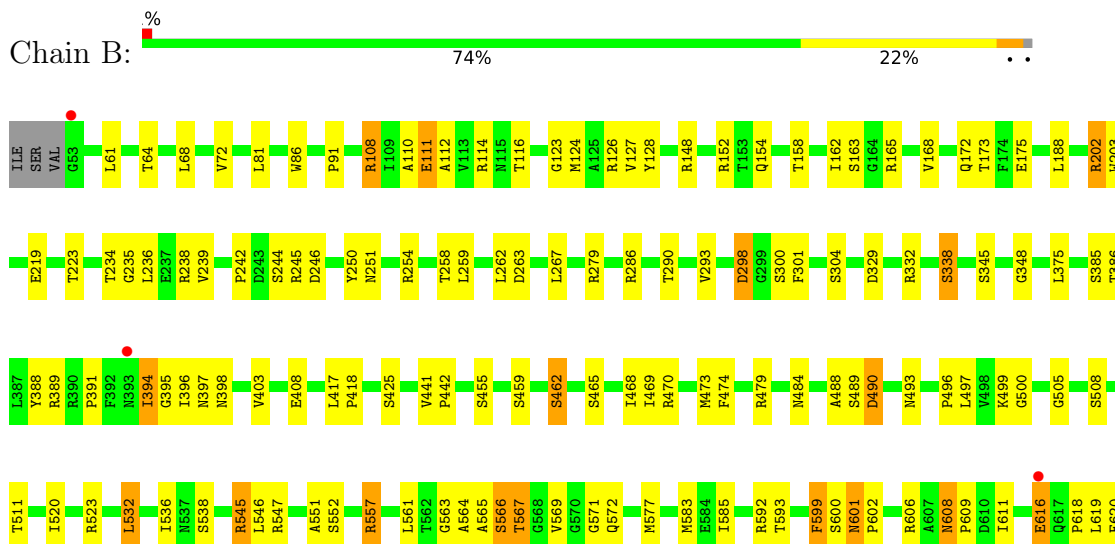
3 Residue-property plots

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: Cry1A.2



• Molecule 1: Cry1A.2





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	120.58Å 225.82Å 239.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.12 – 2.99 46.12 – 2.99	Depositor EDS
% Data completeness (in resolution range)	94.5 (46.12-2.99) 94.8 (46.12-2.99)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.198 , 0.258 0.198 , 0.258	Depositor DCC
R_{free} test set	3189 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 21.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18743	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 41.48 % 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 2.3461e-04. 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

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	0.64	4/4786 (0.1%)	0.96	32/6509 (0.5%)
1	B	0.63	5/4789 (0.1%)	0.86	13/6513 (0.2%)
1	C	0.60	0/4780	0.82	10/6501 (0.2%)
1	D	0.61	1/4791 (0.0%)	0.94	28/6515 (0.4%)
All	All	0.62	10/19146 (0.1%)	0.90	83/26038 (0.3%)

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	6
1	B	0	5
1	C	0	4
1	D	0	5
All	All	0	20

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	616	GLU	CG-CD	8.49	1.64	1.51
1	D	237	GLU	CB-CG	-6.22	1.40	1.52
1	A	332	ARG	CB-CG	-5.69	1.37	1.52
1	B	616	GLU	CD-OE2	5.52	1.31	1.25
1	A	557	ARG	CZ-NH2	-5.43	1.25	1.33
1	B	111	GLU	CG-CD	5.39	1.60	1.51
1	A	149	GLU	CD-OE2	5.32	1.31	1.25
1	B	616	GLU	CD-OE1	5.29	1.31	1.25
1	A	126	ARG	CD-NE	5.21	1.55	1.46
1	B	490	ASP	CB-CG	5.16	1.62	1.51

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ARG	NE-CZ-NH2	-16.84	111.88	120.30
1	B	298	ASP	CB-CG-OD2	-15.64	104.22	118.30
1	D	332	ARG	NE-CZ-NH1	15.24	127.92	120.30
1	B	111	GLU	CA-CB-CG	-15.16	80.04	113.40
1	D	557	ARG	NE-CZ-NH2	-13.49	113.55	120.30
1	D	332	ARG	NE-CZ-NH2	-13.29	113.65	120.30
1	D	557	ARG	NE-CZ-NH1	12.15	126.37	120.30
1	A	557	ARG	CB-CG-CD	11.46	141.41	111.60
1	D	557	ARG	CD-NE-CZ	10.76	138.66	123.60
1	A	126	ARG	CD-NE-CZ	10.31	138.03	123.60
1	A	310	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	C	202	ARG	CG-CD-NE	-9.65	91.53	111.80
1	C	606	ARG	CD-NE-CZ	9.55	136.98	123.60
1	B	298	ASP	CB-CG-OD1	9.48	126.84	118.30
1	A	332	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	D	140	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	A	595	ARG	CB-CG-CD	-8.60	89.25	111.60
1	A	393	ASN	CB-CA-C	-8.42	93.56	110.40
1	A	332	ARG	CG-CD-NE	-8.38	94.19	111.80
1	A	557	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	126	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	310	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	D	310	ARG	CB-CG-CD	8.03	132.49	111.60
1	D	140	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	A	140	ARG	CB-CG-CD	7.76	131.77	111.60
1	C	249	ARG	CB-CG-CD	-7.69	91.59	111.60
1	A	126	ARG	CB-CG-CD	7.68	131.58	111.60
1	C	202	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	C	238	ARG	NE-CZ-NH1	-7.65	116.48	120.30
1	A	490	ASP	CB-CG-OD1	7.63	125.17	118.30
1	A	370	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	C	249	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	B	616	GLU	CA-CB-CG	7.48	129.86	113.40
1	B	616	GLU	CG-CD-OE1	-7.32	103.66	118.30
1	A	463	ASN	CB-CA-C	-7.12	96.16	110.40
1	A	201	GLN	CA-CB-CG	7.00	128.79	113.40
1	D	236	LEU	CB-CG-CD2	-6.97	99.15	111.00
1	C	238	ARG	NE-CZ-NH2	6.95	123.78	120.30
1	A	126	ARG	CG-CD-NE	6.92	126.34	111.80
1	A	149	GLU	CG-CD-OE2	-6.76	104.78	118.30
1	A	566	SER	N-CA-CB	-6.69	100.47	110.50
1	B	490	ASP	CB-CG-OD1	6.66	124.29	118.30
1	D	145	PRO	C-N-CA	-6.62	105.16	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	595	ARG	CG-CD-NE	6.59	125.65	111.80
1	A	557	ARG	CA-CB-CG	-6.56	98.97	113.40
1	D	310	ARG	CG-CD-NE	6.52	125.49	111.80
1	D	310	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	B	532	LEU	CA-CB-CG	6.48	130.21	115.30
1	D	332	ARG	CA-CB-CG	6.46	127.61	113.40
1	D	126	ARG	CB-CG-CD	6.28	127.93	111.60
1	D	310	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	D	140	ARG	CB-CG-CD	6.21	127.76	111.60
1	B	616	GLU	OE1-CD-OE2	6.18	130.72	123.30
1	A	201	GLN	CG-CD-OE1	-6.08	109.43	121.60
1	D	490	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	393	ASN	N-CA-CB	6.07	121.53	110.60
1	A	230	ARG	CG-CD-NE	-6.03	99.14	111.80
1	D	543[A]	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	D	543[B]	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	566	SER	CB-CA-C	5.87	121.25	110.10
1	D	202	ARG	CA-CB-CG	5.86	126.29	113.40
1	D	557	ARG	CB-CA-C	5.83	122.06	110.40
1	D	546	LEU	CA-CB-CG	5.80	128.64	115.30
1	C	302	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	140	ARG	CG-CD-NE	5.77	123.92	111.80
1	B	538	SER	CB-CA-C	5.71	120.96	110.10
1	C	490	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	201	GLN	CB-CA-C	5.48	121.36	110.40
1	B	394	ILE	CG1-CB-CG2	-5.46	99.40	111.40
1	B	110	ALA	C-N-CA	-5.37	108.29	121.70
1	A	370	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	D	332	ARG	CD-NE-CZ	5.34	131.08	123.60
1	B	545	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	D	310	ARG	CA-CB-CG	-5.29	101.77	113.40
1	A	140	ARG	CA-CB-CG	-5.23	101.90	113.40
1	D	126	ARG	CG-CD-NE	5.16	122.64	111.80
1	C	546	LEU	CA-CB-CG	5.13	127.11	115.30
1	D	381	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	607	ALA	C-N-CA	-5.06	109.04	121.70
1	D	473	MET	CA-CB-CG	-5.05	104.72	113.30
1	A	67	LEU	CA-CB-CG	-5.02	103.75	115.30
1	B	616	GLU	CB-CA-C	5.01	120.42	110.40
1	D	149	GLU	CA-CB-CG	-5.00	102.39	113.40

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	ARG	Sidechain
1	A	149	GLU	Sidechain
1	A	392	PHE	Peptide
1	A	462	SER	Peptide
1	A	488	ALA	Peptide
1	A	599	PHE	Peptide
1	B	298	ASP	Sidechain
1	B	462	SER	Peptide
1	B	488	ALA	Peptide
1	B	599	PHE	Peptide
1	B	608	ASN	Peptide
1	C	249	ARG	Sidechain
1	C	488	ALA	Peptide
1	C	599	PHE	Peptide
1	C	606	ARG	Sidechain
1	D	392	PHE	Peptide
1	D	488	ALA	Peptide
1	D	557	ARG	Sidechain
1	D	599	PHE	Peptide
1	D	608	ASN	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	4668	0	4547	97	1
1	B	4671	0	4552	106	0
1	C	4665	0	4544	105	0
1	D	4673	0	4557	107	1
2	A	16	0	0	2	0
2	B	20	0	0	2	0
2	C	13	0	0	2	0
2	D	17	0	0	3	0
All	All	18743	0	18200	411	1

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 11.

All (411) 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:616:GLU:OE1	1:B:630:LEU:HD23	1.09	1.24
1:B:616:GLU:OE1	1:B:630:LEU:CD2	2.02	1.07
1:B:552:SER:HB2	1:B:630:LEU:HD13	1.39	1.04
1:D:400:GLN:HB2	1:D:467:SER:HB2	1.44	0.99
1:B:547:ARG:NE	1:B:599:PHE:CZ	2.34	0.95
1:B:618:PRO:HB2	1:B:622:ALA:HB2	1.53	0.91
1:B:563:GLY:HA3	1:B:571:GLY:HA2	1.58	0.85
1:D:608:ASN:O	1:D:608:ASN:ND2	2.10	0.83
1:A:376:GLY:HA2	1:C:490:ASP:OD2	1.79	0.82
1:A:609:PRO:HG2	1:C:609:PRO:HG3	1.62	0.81
1:D:390:ARG:NH2	1:D:402:SER:OG	2.13	0.81
1:C:121:LEU:HD11	1:C:181:VAL:HG11	1.62	0.80
1:C:563:GLY:HA3	1:C:571:GLY:HA3	1.62	0.79
1:B:547:ARG:NH2	1:B:599:PHE:CZ	2.50	0.79
1:B:616:GLU:CD	1:B:630:LEU:HD23	2.03	0.79
1:C:565:ALA:HB3	1:C:569:VAL:HG22	1.65	0.79
1:A:394:ILE:HB	1:A:398:ASN:HB3	1.63	0.79
1:D:236:LEU:HD12	1:D:253:PHE:HD1	1.48	0.79
1:A:489:SER:O	1:A:490:ASP:OD1	2.01	0.78
1:D:236:LEU:HD12	1:D:253:PHE:CD1	2.19	0.78
1:A:460:GLY:O	1:A:470:ARG:NH2	2.18	0.77
1:A:394:ILE:O	2:A:701:HOH:O	2.03	0.76
1:A:392:PHE:O	1:A:394:ILE:N	2.20	0.75
1:A:585:ILE:H	1:A:585:ILE:HD12	1.52	0.75
1:B:585:ILE:HD12	1:B:585:ILE:H	1.53	0.74
1:C:608:ASN:O	1:C:608:ASN:ND2	2.20	0.74
1:B:547:ARG:HH21	1:B:599:PHE:HZ	1.34	0.74
1:B:505:GLY:O	1:B:523:ARG:NH2	2.21	0.73
1:A:291:ASN:HD22	1:A:473:MET:CE	2.02	0.72
1:C:459:SER:HB3	1:C:469:ILE:HB	1.72	0.72
1:B:219:GLU:OE1	1:B:592:ARG:NH2	2.22	0.72
1:D:529:PHE:CZ	1:D:630:LEU:HD23	2.24	0.71
1:D:552:SER:HB3	1:D:630:LEU:HD12	1.72	0.71
1:A:332:ARG:HD3	1:A:389:ARG:HH12	1.56	0.71
1:B:557:ARG:HG3	1:B:619:LEU:HD13	1.72	0.70
1:D:212:ASN:OD1	2:D:701:HOH:O	2.09	0.70
1:D:505:GLY:O	1:D:523:ARG:NH2	2.25	0.69
1:B:630:LEU:HD12	1:B:631:TYR:N	2.08	0.69
1:D:557:ARG:HH12	1:D:620:PHE:H	1.42	0.68
1:B:618:PRO:CB	1:B:622:ALA:HB2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:554:ARG:HH22	1:C:616:GLU:CD	1.98	0.67
1:C:582:THR:HG22	1:C:595:ARG:HD3	1.76	0.67
1:D:547:ARG:HD2	1:D:636:GLU:OE1	1.94	0.67
1:B:245:ARG:HB2	1:B:300:SER:HB2	1.75	0.67
1:C:535:ASN:OD1	2:C:701:HOH:O	2.12	0.67
1:C:389:ARG:HG2	1:C:391:PRO:HD3	1.75	0.67
1:C:563:GLY:HA3	1:C:571:GLY:CA	2.24	0.67
1:C:563:GLY:CA	1:C:571:GLY:HA3	2.25	0.66
1:C:234:THR:HG22	1:C:238:ARG:HE	1.60	0.66
1:D:524:ASN:O	1:D:554:ARG:NH2	2.29	0.66
1:B:496:PRO:HG2	1:B:499:LYS:HG3	1.78	0.66
1:B:547:ARG:CZ	1:B:599:PHE:CZ	2.79	0.66
1:A:236:LEU:HD22	1:A:250:TYR:CE1	2.31	0.65
1:C:381:ARG:CZ	1:C:431:LEU:HD12	2.26	0.65
1:B:112:ALA:O	1:B:116:THR:HG23	1.97	0.64
1:B:546:LEU:HB3	1:B:637:ILE:HD13	1.79	0.64
1:B:417:LEU:HD23	1:B:418:PRO:HD2	1.78	0.64
1:D:206:SER:HB2	1:D:209:THR:H	1.63	0.64
1:B:609:PRO:HG2	1:D:609:PRO:HG2	1.79	0.64
1:A:61:LEU:HD12	1:A:435:PRO:HG2	1.80	0.64
1:B:547:ARG:NH2	1:B:599:PHE:CE2	2.66	0.64
1:B:565:ALA:O	1:B:567:THR:N	2.31	0.63
1:B:489:SER:O	1:B:490:ASP:OD1	2.17	0.63
1:D:557:ARG:NE	1:D:619:LEU:HD23	2.13	0.63
1:A:86:TRP:CE2	1:A:188:LEU:HD22	2.33	0.63
1:B:391:PRO:HB2	1:B:398:ASN:HD21	1.63	0.63
1:D:395:GLY:O	1:D:397:ASN:N	2.30	0.63
1:C:489:SER:O	1:C:490:ASP:CG	2.38	0.62
1:A:396:ILE:H	1:A:466:VAL:HG23	1.62	0.62
1:B:395:GLY:O	1:B:397:ASN:N	2.32	0.62
1:C:565:ALA:HB3	1:C:569:VAL:CG2	2.28	0.62
1:D:291:ASN:HD22	1:D:473:MET:CE	2.12	0.62
1:A:376:GLY:CA	1:C:490:ASP:OD2	2.47	0.62
1:A:552:SER:OG	1:A:554:ARG:O	2.18	0.62
1:D:245:ARG:HB2	1:D:300:SER:HB2	1.80	0.61
1:A:108:ARG:NH1	1:A:111:GLU:OE1	2.33	0.61
1:D:396:ILE:N	1:D:466:VAL:HG12	2.16	0.61
1:A:556:ALA:HA	1:A:619:LEU:HD11	1.82	0.61
1:A:562:THR:HG22	1:A:612:ILE:HG22	1.82	0.61
1:A:112:ALA:O	1:A:116:THR:HG22	2.01	0.60
1:D:361:THR:HG23	1:D:458:ARG:HH21	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:THR:OG1	1:B:569:VAL:HG22	2.00	0.60
1:C:552:SER:HB2	1:C:630:LEU:HD13	1.83	0.60
1:D:566:SER:O	1:D:567:THR:OG1	2.11	0.60
1:B:547:ARG:NH2	1:B:599:PHE:HZ	1.91	0.60
1:C:194:ARG:NH1	1:C:195:ASP:OD1	2.34	0.60
1:D:552:SER:CB	1:D:630:LEU:HD12	2.32	0.60
1:D:458:ARG:HD2	2:D:711:HOH:O	2.01	0.60
1:A:230:ARG:O	1:A:234:THR:HG23	2.01	0.59
1:A:600:SER:O	1:A:601:ASN:HB2	2.01	0.59
1:C:417:LEU:HD12	1:C:418:PRO:HD2	1.84	0.59
1:C:234:THR:HG22	1:C:238:ARG:NE	2.17	0.59
1:C:489:SER:O	1:C:490:ASP:OD1	2.21	0.59
1:A:155:PHE:CE1	1:A:196:VAL:HG13	2.36	0.59
1:A:396:ILE:HD11	1:A:464:SER:CA	2.32	0.59
1:A:67:LEU:O	1:A:71:PHE:HD2	1.84	0.59
1:A:291:ASN:HD22	1:A:473:MET:HE2	1.67	0.59
1:D:87:GLY:HA2	1:D:129:ARG:HH11	1.67	0.59
1:D:219:GLU:OE2	1:D:592:ARG:NH2	2.36	0.59
1:D:291:ASN:HD22	1:D:473:MET:HE2	1.66	0.59
1:D:400:GLN:HB2	1:D:467:SER:CB	2.27	0.59
1:D:543[A]:ARG:HG3	1:D:543[A]:ARG:HH11	1.67	0.59
1:D:396:ILE:H	1:D:466:VAL:HG12	1.68	0.59
1:B:561:LEU:HB3	1:B:571:GLY:HA3	1.86	0.58
1:D:146:GLU:O	1:D:146:GLU:HG2	2.02	0.58
1:A:582:THR:HG22	1:A:595:ARG:HH11	1.68	0.58
1:B:375:LEU:HD23	1:B:417:LEU:HD11	1.86	0.58
1:B:563:GLY:CA	1:B:571:GLY:HA2	2.33	0.58
1:B:583:MET:HG2	1:B:593:THR:HB	1.86	0.58
1:B:600:SER:O	1:B:601:ASN:HB2	2.02	0.58
1:C:554:ARG:NH2	1:C:616:GLU:OE2	2.37	0.57
1:C:392:PHE:O	1:C:394:ILE:HG12	2.05	0.57
1:D:239:VAL:HG13	1:D:249:ARG:HD2	1.86	0.57
1:D:553:SER:HB2	1:D:628:GLY:HA3	1.85	0.57
1:D:557:ARG:NH1	1:D:620:PHE:H	2.01	0.57
1:C:206:SER:HB3	1:C:209:THR:HG23	1.86	0.57
1:A:395:GLY:O	1:A:397:ASN:N	2.37	0.57
1:B:536:ILE:HG12	1:B:608:ASN:OD1	2.05	0.57
1:C:137:GLU:OE1	1:C:140:ARG:NH2	2.38	0.57
1:D:584:GLU:O	1:D:586:GLY:N	2.30	0.57
1:A:294:LEU:HD13	1:A:308:ILE:HD13	1.87	0.56
1:C:489:SER:HA	1:C:639:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:563:GLY:H	1:C:572:GLN:H	1.53	0.56
1:C:97:PHE:HB3	1:C:181:VAL:HG23	1.87	0.56
1:C:133:THR:O	1:C:137:GLU:HG2	2.06	0.56
1:D:230:ARG:O	1:D:234:THR:HG23	2.06	0.56
1:A:523:ARG:NH1	1:A:525:THR:HG23	2.20	0.56
1:C:293:VAL:O	1:C:388:TYR:OH	2.21	0.56
1:C:569:VAL:HG23	1:C:570:GLY:O	2.05	0.56
1:D:610:ASP:OD1	1:D:611:ILE:N	2.39	0.56
1:B:128:TYR:CD1	1:B:188:LEU:HD11	2.41	0.56
1:B:172:GLN:O	1:B:173:THR:HB	2.05	0.56
1:D:489:SER:O	1:D:490:ASP:OD1	2.23	0.56
1:B:546:LEU:O	1:B:600:SER:HB3	2.06	0.56
1:B:630:LEU:HD12	1:B:631:TYR:H	1.71	0.56
1:C:113:VAL:HG11	1:C:171:ILE:HG21	1.88	0.56
1:D:144:ASP:OD2	1:D:147:LEU:HG	2.05	0.56
1:B:108:ARG:NH1	1:B:111:GLU:OE2	2.40	0.55
1:B:545:ARG:HH11	1:B:602:PRO:HD3	1.71	0.55
1:D:64:THR:HG22	1:D:68:LEU:HD12	1.88	0.55
1:D:563:GLY:O	1:D:565:ALA:N	2.36	0.55
1:A:563:GLY:H	1:A:572:GLN:H	1.55	0.55
1:A:291:ASN:HD22	1:A:473:MET:HE3	1.71	0.55
1:B:386:THR:HG1	1:B:388:TYR:HE2	1.55	0.55
1:A:251:ASN:OD1	1:A:254:ARG:NH1	2.40	0.54
1:B:545:ARG:CZ	1:B:601:ASN:H	2.21	0.54
1:A:288:ILE:HD11	1:A:434:ILE:CD1	2.37	0.54
1:B:520:ILE:HG22	1:B:633:ASP:HA	1.88	0.54
1:C:206:SER:HB3	1:C:209:THR:H	1.73	0.54
1:D:553:SER:HB3	1:D:585:ILE:HA	1.89	0.54
1:C:67:LEU:O	1:C:71:PHE:HD2	1.91	0.54
1:A:144:ASP:O	1:A:148:ARG:HG3	2.08	0.53
1:D:331:HIS:HB2	2:D:703:HOH:O	2.08	0.53
1:A:155:PHE:CZ	1:A:196:VAL:CG1	2.91	0.53
1:B:606:ARG:HB3	1:B:606:ARG:NH1	2.24	0.53
1:A:219:GLU:OE1	1:A:592:ARG:NH2	2.41	0.53
1:C:441:VAL:HB	1:C:442:PRO:HD2	1.89	0.53
1:D:57:ILE:HD11	1:D:256:GLU:HG2	1.91	0.53
1:D:392:PHE:O	1:D:394:ILE:HG12	2.08	0.53
1:A:544:TYR:CE1	1:A:639:LEU:HD12	2.44	0.53
1:A:464:SER:OG	1:A:465:SER:N	2.41	0.53
1:B:547:ARG:NE	1:B:599:PHE:CE2	2.74	0.53
1:C:116:THR:HG22	1:C:168:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:497:LEU:HB3	1:D:521:LEU:HD12	1.91	0.52
1:A:217:LEU:HD21	1:A:272:ASP:HA	1.91	0.52
1:A:617:GLN:HG3	1:A:618:PRO:HD2	1.90	0.52
1:B:234:THR:O	1:B:238:ARG:HG3	2.09	0.52
1:B:536:ILE:CG1	1:B:608:ASN:OD1	2.58	0.52
1:D:616:GLU:OE1	1:D:630:LEU:HD22	2.10	0.52
1:D:543[A]:ARG:HH11	1:D:543[A]:ARG:CG	2.22	0.52
1:D:546:LEU:O	1:D:600:SER:HB3	2.10	0.52
1:A:493:ASN:O	1:A:636:GLU:HA	2.10	0.52
1:C:546:LEU:O	1:C:600:SER:HB3	2.10	0.52
1:A:155:PHE:CZ	1:A:196:VAL:HG13	2.45	0.52
1:A:496:PRO:HG2	1:A:499:LYS:HG3	1.92	0.52
1:A:545:ARG:HB2	1:A:638:ILE:HG13	1.92	0.51
1:C:206:SER:CB	1:C:209:THR:HG23	2.41	0.51
1:C:395:GLY:O	1:C:397:ASN:N	2.36	0.51
1:C:561:LEU:HD23	1:C:573:VAL:N	2.25	0.51
1:C:607:ALA:O	1:C:610:ASP:HB2	2.11	0.51
1:B:124:MET:HE3	1:B:162:ILE:HG12	1.92	0.51
1:B:545:ARG:NH1	1:B:602:PRO:HD3	2.25	0.51
1:D:306:GLN:HG2	1:D:310:ARG:HD3	1.92	0.51
1:A:254:ARG:NH2	1:A:309:GLU:OE2	2.42	0.51
1:A:288:ILE:HD11	1:A:434:ILE:HD13	1.92	0.51
1:C:154:GLN:O	1:C:158:THR:HG23	2.10	0.51
1:A:126:ARG:HG3	1:A:129:ARG:NH2	2.25	0.51
1:D:526:PHE:CE1	1:D:618:PRO:HB3	2.45	0.51
1:B:417:LEU:HD23	1:B:418:PRO:CD	2.41	0.51
1:A:523:ARG:HH12	1:A:525:THR:HG23	1.76	0.51
1:C:104:LEU:HD11	1:C:253:PHE:HA	1.93	0.51
1:C:381:ARG:NE	1:C:431:LEU:HD12	2.25	0.51
1:C:554:ARG:NH2	1:C:616:GLU:CD	2.64	0.51
1:C:128:TYR:CD1	1:C:188:LEU:HD11	2.46	0.51
1:A:155:PHE:CE2	1:A:196:VAL:HG11	2.45	0.50
1:C:540:ILE:HD11	1:C:606:ARG:C	2.32	0.50
1:C:558:VAL:HG12	1:C:579:LEU:HD21	1.93	0.50
1:C:104:LEU:O	1:C:104:LEU:HD23	2.11	0.50
1:C:394:ILE:HB	1:C:398:ASN:HB3	1.91	0.50
1:D:522:ARG:HH11	1:D:629:GLU:HG2	1.76	0.50
1:C:489:SER:HA	1:C:639:LEU:CD1	2.41	0.50
1:A:525:THR:HA	1:A:626:SER:OG	2.11	0.50
1:B:293:VAL:O	1:B:388:TYR:OH	2.25	0.50
1:C:608:ASN:HD22	1:C:608:ASN:C	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:VAL:HG12	1:B:470:ARG:HB2	1.94	0.50
1:B:479:ARG:NE	2:B:701:HOH:O	2.03	0.50
1:A:459:SER:HB3	1:A:469:ILE:HB	1.94	0.49
1:B:572:GLN:OE1	1:B:606:ARG:NE	2.45	0.49
1:A:156:THR:HG22	1:A:213:TYR:OH	2.12	0.49
1:A:126:ARG:HG3	1:A:129:ARG:HH21	1.76	0.49
1:A:546:LEU:O	1:A:600:SER:HB3	2.12	0.49
1:B:546:LEU:H	1:B:600:SER:HB3	1.77	0.49
1:B:566:SER:HA	1:B:611:ILE:HD12	1.95	0.49
1:A:551:ALA:HB3	1:A:631:TYR:HB2	1.95	0.49
1:C:577:MET:HE3	1:C:597:THR:CB	2.43	0.49
1:B:493:ASN:O	1:B:636:GLU:HA	2.13	0.49
1:B:123:GLY:HA2	1:B:126:ARG:NH1	2.28	0.49
1:B:622:ALA:CB	1:B:624:SER:H	2.26	0.49
1:D:234:THR:HA	1:D:237:GLU:OE2	2.13	0.49
1:D:391:PRO:HD2	1:D:400:GLN:HG2	1.95	0.49
1:C:292:PRO:HD2	2:C:710:HOH:O	2.13	0.48
1:D:493:ASN:O	1:D:636:GLU:HA	2.12	0.48
1:A:86:TRP:CD2	1:A:188:LEU:HD22	2.48	0.48
1:A:235:GLY:O	1:A:239:VAL:HG23	2.13	0.48
1:B:489:SER:O	1:B:490:ASP:CG	2.51	0.48
1:C:505:GLY:O	1:C:523:ARG:NH2	2.46	0.48
1:A:278:ILE:HG13	1:A:492:ILE:HG13	1.95	0.48
1:C:242:PRO:HD2	1:C:246:ASP:OD2	2.13	0.48
1:D:361:THR:HG23	1:D:458:ARG:NH2	2.29	0.48
1:D:473:MET:HE2	1:D:473:MET:HB2	1.45	0.48
1:D:563:GLY:HA3	1:D:571:GLY:HA2	1.95	0.48
1:D:563:GLY:H	1:D:572:GLN:H	1.61	0.48
1:B:258:THR:HA	1:B:262:LEU:HB2	1.95	0.48
1:B:72:VAL:HG12	1:B:279:ARG:HA	1.94	0.48
1:B:462:SER:HA	1:B:468:ILE:HD11	1.95	0.48
1:C:564:ALA:HA	1:C:611:ILE:HB	1.96	0.48
1:D:529:PHE:HZ	1:D:630:LEU:HD23	1.76	0.48
1:A:503:VAL:HG12	1:A:507:THR:HB	1.95	0.48
1:D:87:GLY:O	1:D:129:ARG:NH1	2.47	0.48
1:D:206:SER:HB3	1:D:208:THR:HG22	1.96	0.48
1:A:547:ARG:NH1	1:A:636:GLU:OE1	2.36	0.47
1:B:165:ARG:O	1:B:168:VAL:HG22	2.14	0.47
1:C:600:SER:O	1:C:601:ASN:HB2	2.14	0.47
1:D:600:SER:O	1:D:601:ASN:HB2	2.14	0.47
1:C:236:LEU:O	1:C:239:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:GLY:C	1:D:129:ARG:HH12	2.18	0.47
1:D:394:ILE:HG21	1:D:398:ASN:HB3	1.96	0.47
1:B:408:GLU:HB2	1:B:425:SER:HB2	1.97	0.47
1:A:63:LEU:HD22	1:A:85:ILE:CD1	2.44	0.47
1:A:85:ILE:HD13	1:A:184:GLN:OE1	2.15	0.47
1:D:156:THR:HG22	1:D:213:TYR:OH	2.15	0.47
1:B:263:ASP:O	1:B:267:LEU:HD12	2.15	0.47
1:D:86:TRP:CE2	1:D:188:LEU:HD22	2.49	0.47
1:B:172:GLN:HA	1:B:175:GLU:OE2	2.15	0.47
1:D:87:GLY:HA2	1:D:129:ARG:NH1	2.28	0.47
1:D:396:ILE:H	1:D:466:VAL:HA	1.80	0.47
1:A:554:ARG:HD3	1:A:627:SER:O	2.15	0.47
1:D:557:ARG:HE	1:D:619:LEU:CD2	2.28	0.47
1:C:493:ASN:O	1:C:636:GLU:HA	2.15	0.46
1:D:66:PHE:CZ	1:D:80:GLY:HA3	2.50	0.46
1:D:557:ARG:CZ	1:D:619:LEU:HD23	2.44	0.46
1:C:569:VAL:HG23	1:C:570:GLY:N	2.31	0.46
1:D:391:PRO:HG3	1:D:398:ASN:OD1	2.16	0.46
1:B:127:VAL:O	1:B:158:THR:HG21	2.14	0.46
1:D:243:ASP:HB3	1:D:300:SER:OG	2.14	0.46
1:B:459:SER:HB3	1:B:469:ILE:HB	1.96	0.46
1:C:152:ARG:NH1	1:C:203:TRP:O	2.46	0.46
1:D:86:TRP:O	1:D:129:ARG:NH1	2.48	0.46
1:A:461:PHE:O	1:A:465:SER:HB2	2.15	0.46
1:C:142:PRO:HB2	1:C:202:ARG:NH2	2.31	0.46
1:C:430:SER:O	1:C:434:ILE:HG13	2.16	0.46
1:D:123:GLY:O	1:D:127:VAL:HG22	2.16	0.46
1:A:155:PHE:CZ	1:A:196:VAL:HG11	2.51	0.46
1:C:559:ILE:HG23	1:C:573:VAL:HG13	1.98	0.46
1:C:244:SER:O	1:C:248:VAL:HG23	2.16	0.46
1:D:236:LEU:CD1	1:D:253:PHE:HD1	2.23	0.46
1:D:544:TYR:CE1	1:D:639:LEU:HD12	2.50	0.46
1:B:441:VAL:HB	1:B:442:PRO:HD2	1.98	0.46
1:C:256:GLU:O	1:C:260:THR:HG23	2.15	0.46
1:D:87:GLY:C	1:D:129:ARG:NH1	2.69	0.46
1:B:585:ILE:H	1:B:585:ILE:CD1	2.25	0.46
1:A:162:ILE:O	1:A:166:ILE:HG12	2.16	0.45
1:C:497:LEU:HD21	1:C:635:ILE:HG23	1.98	0.45
1:B:242:PRO:HD2	1:B:246:ASP:OD2	2.16	0.45
1:D:120:GLU:OE1	1:D:165:ARG:HD2	2.16	0.45
1:A:127:VAL:HG23	1:A:158:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ILE:HD11	1:A:464:SER:HA	1.98	0.45
1:B:154:GLN:O	1:B:158:THR:HG23	2.17	0.45
1:C:79:LEU:HD23	1:C:79:LEU:HA	1.81	0.45
1:B:497:LEU:HD23	1:B:497:LEU:HA	1.58	0.45
1:C:492:ILE:HG12	1:C:638:ILE:CG2	2.46	0.45
1:C:583:MET:HB3	1:C:593:THR:HG22	1.98	0.45
1:B:223:THR:HG22	1:B:592:ARG:HH12	1.81	0.45
1:B:329:ASP:HB2	1:B:338:SER:HB3	1.97	0.45
1:C:559:ILE:CG2	1:C:573:VAL:HG13	2.46	0.45
1:A:245:ARG:HB2	1:A:300:SER:HB2	1.99	0.45
1:B:219:GLU:O	1:B:223:THR:HG23	2.17	0.45
1:C:81:LEU:HD23	1:C:81:LEU:HA	1.79	0.45
1:D:624:SER:O	1:D:624:SER:OG	2.33	0.44
1:A:247:TRP:HE1	1:A:309:GLU:HB2	1.83	0.44
1:A:434:ILE:HG22	1:A:434:ILE:O	2.17	0.44
1:B:552:SER:HB2	1:B:630:LEU:CD1	2.28	0.44
1:B:500:GLY:HA2	1:B:532:LEU:HB3	2.00	0.44
1:C:73:PRO:HG2	1:C:198:PHE:CE2	2.51	0.44
1:C:431:LEU:HD23	1:C:435:PRO:HA	2.00	0.44
1:C:562:THR:C	1:C:564:ALA:H	2.20	0.44
1:A:302:ARG:HE	1:A:302:ARG:HB3	1.62	0.44
1:A:394:ILE:HB	1:A:398:ASN:CB	2.42	0.44
1:C:155:PHE:CZ	1:C:196:VAL:HG13	2.52	0.44
1:D:124:MET:HE2	1:D:162:ILE:HA	1.98	0.44
1:D:317:LEU:HD11	1:D:503:VAL:HG13	1.98	0.44
1:B:348:GLY:HA2	1:B:484:ASN:OD1	2.17	0.44
1:C:393:ASN:C	1:C:394:ILE:HD13	2.38	0.44
1:A:399:GLN:HE22	1:A:462:SER:HA	1.83	0.44
1:C:577:MET:CE	1:C:597:THR:OG1	2.66	0.44
1:D:61:LEU:HD12	1:D:435:PRO:HG2	1.99	0.44
1:A:392:PHE:O	1:A:394:ILE:HG13	2.18	0.44
1:D:108:ARG:NH1	1:D:111:GLU:OE2	2.43	0.44
1:B:108:ARG:NH1	1:B:114:ARG:HD3	2.33	0.43
1:C:396:ILE:HD12	1:C:464:SER:HA	2.00	0.43
1:D:585:ILE:HD12	1:D:585:ILE:H	1.82	0.43
1:B:606:ARG:HB3	1:B:606:ARG:HH11	1.82	0.43
1:C:455:SER:HB2	1:C:473:MET:HB3	2.00	0.43
1:A:217:LEU:O	1:A:221:ILE:HG13	2.19	0.43
1:B:572:GLN:OE1	1:B:606:ARG:HD2	2.18	0.43
1:A:236:LEU:HD22	1:A:250:TYR:CZ	2.52	0.43
1:D:79:LEU:HA	1:D:79:LEU:HD23	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:GLY:O	1:B:239:VAL:HG23	2.19	0.43
1:C:619:LEU:HD23	1:C:619:LEU:O	2.18	0.43
1:D:145:PRO:O	1:D:149:GLU:HB2	2.19	0.43
1:D:334:TYR:CE2	1:D:389:ARG:HD2	2.53	0.43
1:D:394:ILE:CG2	1:D:398:ASN:HB3	2.48	0.43
1:C:179:LEU:HD12	1:C:179:LEU:HA	1.77	0.43
1:D:236:LEU:HD11	1:D:254:ARG:HB2	2.01	0.43
1:B:634:LYS:HE3	1:B:636:GLU:OE1	2.19	0.43
1:C:55:THR:HB	1:C:58:ASP:H	1.83	0.43
1:C:561:LEU:HA	1:C:572:GLN:O	2.18	0.43
1:D:577:MET:HG3	1:D:578:PRO:HD2	2.00	0.43
1:B:148:ARG:HD2	1:B:202:ARG:O	2.18	0.43
1:B:394:ILE:HG22	1:B:395:GLY:N	2.33	0.43
1:D:403:VAL:HG12	1:D:470:ARG:HB2	2.00	0.43
1:A:71:PHE:O	1:A:71:PHE:CD1	2.72	0.43
1:A:165:ARG:O	1:A:168:VAL:HG22	2.19	0.43
1:A:329:ASP:HB3	1:A:336:TYR:CE1	2.54	0.43
1:B:64:THR:HG22	1:B:68:LEU:HD12	2.01	0.43
1:B:236:LEU:HG	1:B:250:TYR:CE1	2.54	0.43
1:B:564:ALA:HA	1:B:611:ILE:HB	2.01	0.43
1:D:522:ARG:HD3	1:D:631:TYR:CE1	2.54	0.43
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.92	0.42
1:C:558:VAL:CG1	1:C:579:LEU:HD21	2.49	0.42
1:D:384:SER:C	1:D:426:GLY:HA3	2.39	0.42
1:B:251:ASN:OD1	1:B:254:ARG:NH1	2.52	0.42
1:D:330:ALA:HB2	1:D:335:TYR:CD1	2.55	0.42
1:C:456:MET:HG3	1:C:457:PHE:N	2.35	0.42
1:D:400:GLN:CB	1:D:467:SER:HB2	2.32	0.42
1:A:144:ASP:OD2	1:A:147:LEU:HG	2.19	0.42
1:D:149:GLU:O	1:D:153:THR:HG22	2.18	0.42
1:A:396:ILE:HD11	1:A:464:SER:HB2	2.01	0.42
1:B:124:MET:HE3	1:B:162:ILE:HG23	2.00	0.42
1:B:127:VAL:HB	1:B:158:THR:HG22	2.01	0.42
1:B:290:THR:OG1	1:B:474:PHE:HB2	2.18	0.42
1:C:557:ARG:O	1:C:616:GLU:HG2	2.20	0.42
1:D:80:GLY:O	1:D:84:LEU:HG	2.19	0.42
1:A:56:PRO:HA	1:A:59:ILE:HD12	2.01	0.42
1:B:148:ARG:NH1	2:B:704:HOH:O	2.44	0.42
1:C:226:ASP:OD1	1:C:590:THR:HB	2.19	0.42
1:D:343:MET:HG2	1:D:355:THR:HG23	2.01	0.42
1:B:332:ARG:HD3	1:B:389:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:562:THR:HG22	1:D:612:ILE:HG22	2.01	0.42
1:A:329:ASP:HB2	1:A:338:SER:HB3	2.01	0.42
1:A:585:ILE:H	1:A:585:ILE:CD1	2.24	0.42
1:C:245:ARG:HB2	1:C:300:SER:HB2	2.02	0.42
1:D:223:THR:HG22	1:D:592:ARG:HH12	1.85	0.42
1:C:107:GLN:HB3	1:C:177:GLN:HE21	1.85	0.41
1:C:66:PHE:CE1	1:C:70:GLU:HB2	2.55	0.41
1:D:102:GLU:HG2	1:D:108:ARG:HA	2.02	0.41
1:B:152:ARG:NH1	1:B:203:TRP:O	2.43	0.41
1:B:165:ARG:HG2	1:B:165:ARG:HH21	1.86	0.41
1:C:394:ILE:HG22	1:C:395:GLY:H	1.84	0.41
1:B:301:PHE:CE1	1:B:469:ILE:HD11	2.55	0.41
1:C:469:ILE:O	1:C:470:ARG:HD2	2.20	0.41
1:A:389:ARG:NH2	1:A:398:ASN:OD1	2.53	0.41
1:A:558:VAL:HB	1:A:579:LEU:HD11	2.03	0.41
1:B:61:LEU:HD21	1:B:259:LEU:HD22	2.03	0.41
1:C:568:GLY:O	1:C:570:GLY:N	2.53	0.41
1:B:81:LEU:HB3	1:B:86:TRP:HD1	1.85	0.41
1:C:73:PRO:HG2	1:C:198:PHE:CD2	2.56	0.41
1:D:317:LEU:HD23	1:D:317:LEU:HA	1.84	0.41
1:A:288:ILE:CD1	1:A:434:ILE:CD1	2.99	0.41
1:A:347:VAL:HG23	2:A:706:HOH:O	2.21	0.41
1:A:381:ARG:HB3	1:A:410:ALA:HB3	2.03	0.41
1:A:429:ASP:O	1:A:432:ASP:HB2	2.20	0.41
1:A:522:ARG:HD3	1:A:631:TYR:CE1	2.56	0.41
1:C:155:PHE:CE2	1:C:196:VAL:HG11	2.56	0.41
1:C:553:SER:C	1:C:581:LYS:HG3	2.42	0.41
1:D:77:PHE:CE1	1:D:81:LEU:HD11	2.56	0.41
1:A:505:GLY:O	1:A:523:ARG:NH2	2.53	0.41
1:B:551:ALA:O	1:B:630:LEU:HD12	2.21	0.41
1:B:619:LEU:HD12	1:B:620:PHE:H	1.86	0.41
1:C:389:ARG:O	1:C:390:ARG:HD3	2.21	0.41
1:C:520:ILE:HG22	1:C:633:ASP:HA	2.02	0.41
1:C:121:LEU:HD11	1:C:181:VAL:CG1	2.44	0.40
1:C:566:SER:O	1:C:567:THR:OG1	2.31	0.40
1:A:548:PHE:CE1	1:A:635:ILE:HG22	2.56	0.40
1:B:470:ARG:HD3	1:B:470:ARG:HA	1.83	0.40
1:D:398:ASN:OD1	1:D:398:ASN:C	2.60	0.40
1:D:561:LEU:HA	1:D:572:GLN:O	2.21	0.40
1:A:500:GLY:HA2	1:A:532:LEU:HB3	2.02	0.40
1:C:577:MET:HE1	1:C:597:THR:OG1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:SER:HB2	1:B:473:MET:HB3	2.03	0.40
1:D:546:LEU:HA	1:D:636:GLU:O	2.22	0.40

All (1) 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)
1:A:629:GLU:OE1	1:D:522:ARG:NH2[8_545]	2.19	0.01

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	587/591 (99%)	549 (94%)	27 (5%)	11 (2%)	8	36
1	B	587/591 (99%)	551 (94%)	30 (5%)	6 (1%)	15	53
1	C	586/591 (99%)	542 (92%)	34 (6%)	10 (2%)	9	39
1	D	587/591 (99%)	548 (93%)	29 (5%)	10 (2%)	9	39
All	All	2347/2364 (99%)	2190 (93%)	120 (5%)	37 (2%)	9	40

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	393	ASN
1	A	564	ALA
1	A	601	ASN
1	B	396	ILE
1	C	171	ILE
1	C	396	ILE
1	C	566	SER
1	C	601	ASN

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Mol	Chain	Res	Type
1	C	626	SER
1	D	393	ASN
1	D	396	ILE
1	D	465	SER
1	D	564	ALA
1	D	570	GLY
1	D	585	ILE
1	A	149	GLU
1	A	396	ILE
1	A	463	ASN
1	A	569	VAL
1	B	465	SER
1	C	569	VAL
1	D	601	ASN
1	B	566	SER
1	B	567	THR
1	B	601	ASN
1	C	417	LEU
1	A	148	ARG
1	A	465	SER
1	A	570	GLY
1	C	465	SER
1	D	587	GLU
1	C	622	ALA
1	A	91	PRO
1	B	91	PRO
1	C	565	ALA
1	D	394	ILE
1	D	563	GLY

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	505/508 (99%)	493 (98%)	12 (2%)	49	79
1	B	505/508 (99%)	492 (97%)	13 (3%)	46	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	504/508 (99%)	498 (99%)	6 (1%)	71	90
1	D	505/508 (99%)	486 (96%)	19 (4%)	33	69
All	All	2019/2032 (99%)	1969 (98%)	50 (2%)	49	79

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	SER
1	A	172	GLN
1	A	286	ARG
1	A	332	ARG
1	A	370	ARG
1	A	385	SER
1	A	414	SER
1	A	463	ASN
1	A	489	SER
1	A	490	ASP
1	A	523	ARG
1	A	552	SER
1	B	108	ARG
1	B	163	SER
1	B	202	ARG
1	B	244	SER
1	B	286	ARG
1	B	304	SER
1	B	338	SER
1	B	345	SER
1	B	385	SER
1	B	508	SER
1	B	511	THR
1	B	557	ARG
1	B	577	MET
1	C	167	SER
1	C	286	ARG
1	C	311	SER
1	C	345	SER
1	C	523	ARG
1	C	608	ASN
1	D	71	PHE
1	D	140	ARG
1	D	202	ARG

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Mol	Chain	Res	Type
1	D	244	SER
1	D	273	SER
1	D	286	ARG
1	D	304	SER
1	D	383	LEU
1	D	390	ARG
1	D	467	SER
1	D	490	ASP
1	D	511	THR
1	D	543[A]	ARG
1	D	543[B]	ARG
1	D	574	SER
1	D	577	MET
1	D	608	ASN
1	D	615	SER
1	D	624	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	ASN
1	C	542	GLN
1	D	291	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	588/591 (99%)	-0.05	6 (1%) 82 59	19, 36, 65, 93	0
1	B	588/591 (99%)	-0.25	5 (0%) 84 63	19, 33, 58, 88	0
1	C	588/591 (99%)	-0.23	5 (0%) 84 63	20, 35, 57, 93	0
1	D	588/591 (99%)	-0.12	6 (1%) 82 59	19, 35, 63, 94	0
All	All	2352/2364 (99%)	-0.16	22 (0%) 84 63	19, 35, 61, 94	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	624	SER	8.1
1	B	624	SER	5.9
1	C	623	GLY	4.5
1	B	393	ASN	3.5
1	D	387	LEU	3.3
1	B	623	GLY	3.0
1	B	53	GLY	2.9
1	D	335	TYR	2.5
1	D	140	ARG	2.5
1	C	393	ASN	2.5
1	A	362	MET	2.4
1	A	393	ASN	2.4
1	D	298	ASP	2.4
1	A	140	ARG	2.3
1	A	405	ASP	2.3
1	C	463	ASN	2.3
1	B	616	GLU	2.3
1	D	388	TYR	2.3
1	D	392	PHE	2.3
1	C	53	GLY	2.2
1	A	390	ARG	2.0
1	A	463	ASN	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.