



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:01 PM UTC

PDB ID : 6TS8 / pdb_00006ts8
Title : Chaetomium thermophilum UDP-Glucose Glucosyl Transferase (UGGT) double cysteine mutant G177C/A786C.
Authors : Roversi, P.; Zitzmann, N.; Ibba, R.; Hensen, M.; Chandran, A.
Deposited on : 2019-12-20
Resolution : 4.60 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
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

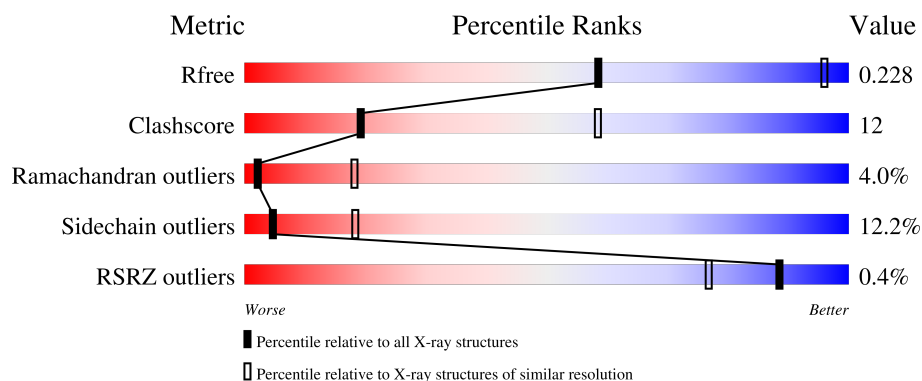
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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	1007 (5.28-3.92)
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
Sidechain outliers	187428	1051 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)

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	1382	
1	B	1382	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20112 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 UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1254	Total	C	N	O	S	0	0	0
			10056	6439	1711	1879	27			
1	B	1254	Total	C	N	O	S	0	0	0
			10056	6439	1711	1879	27			

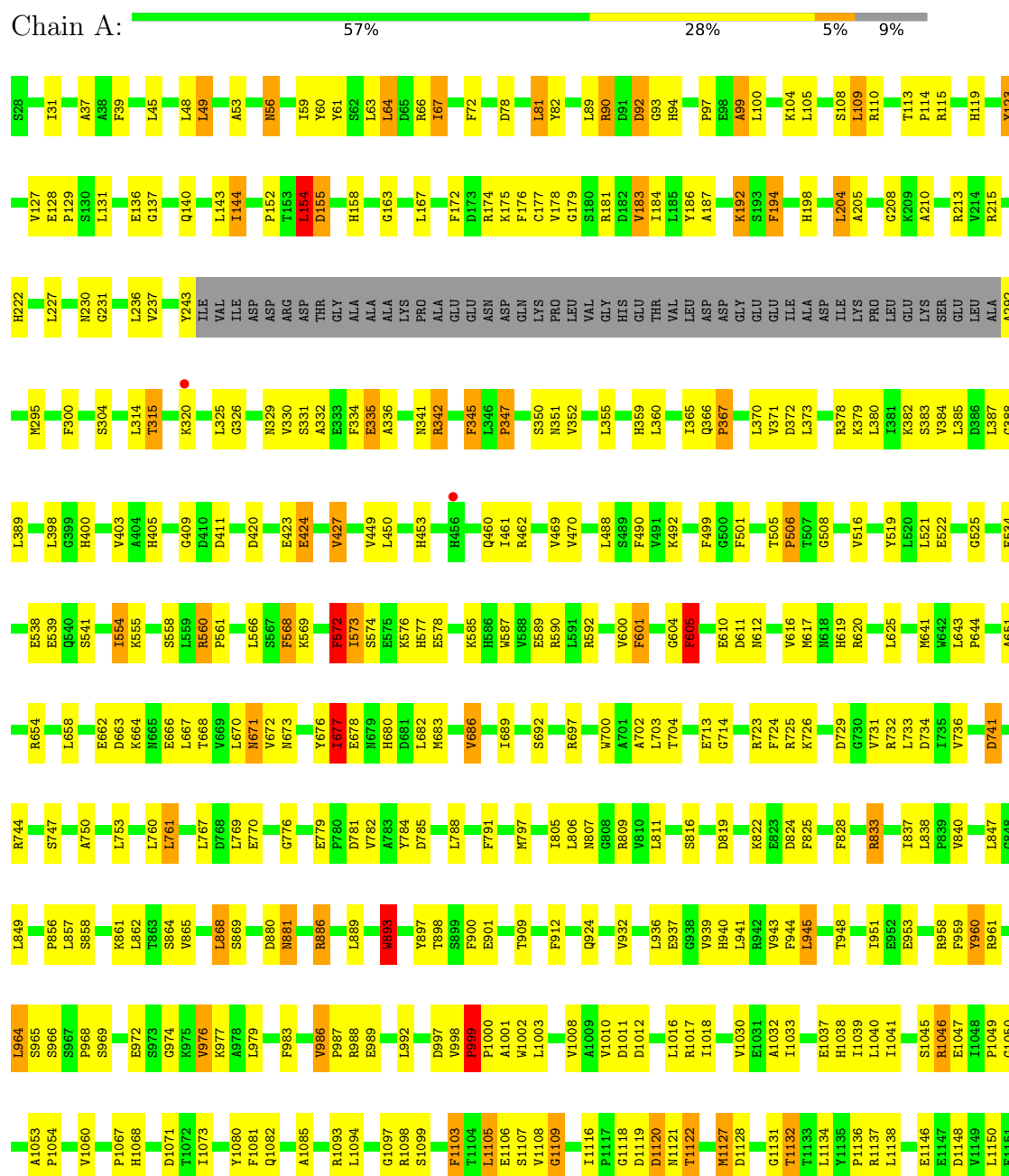
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	CYS	GLY	engineered mutation	UNP G0SB58
A	786	CYS	ALA	engineered mutation	UNP G0SB58
B	177	CYS	GLY	engineered mutation	UNP G0SB58
B	786	CYS	ALA	engineered mutation	UNP G0SB58

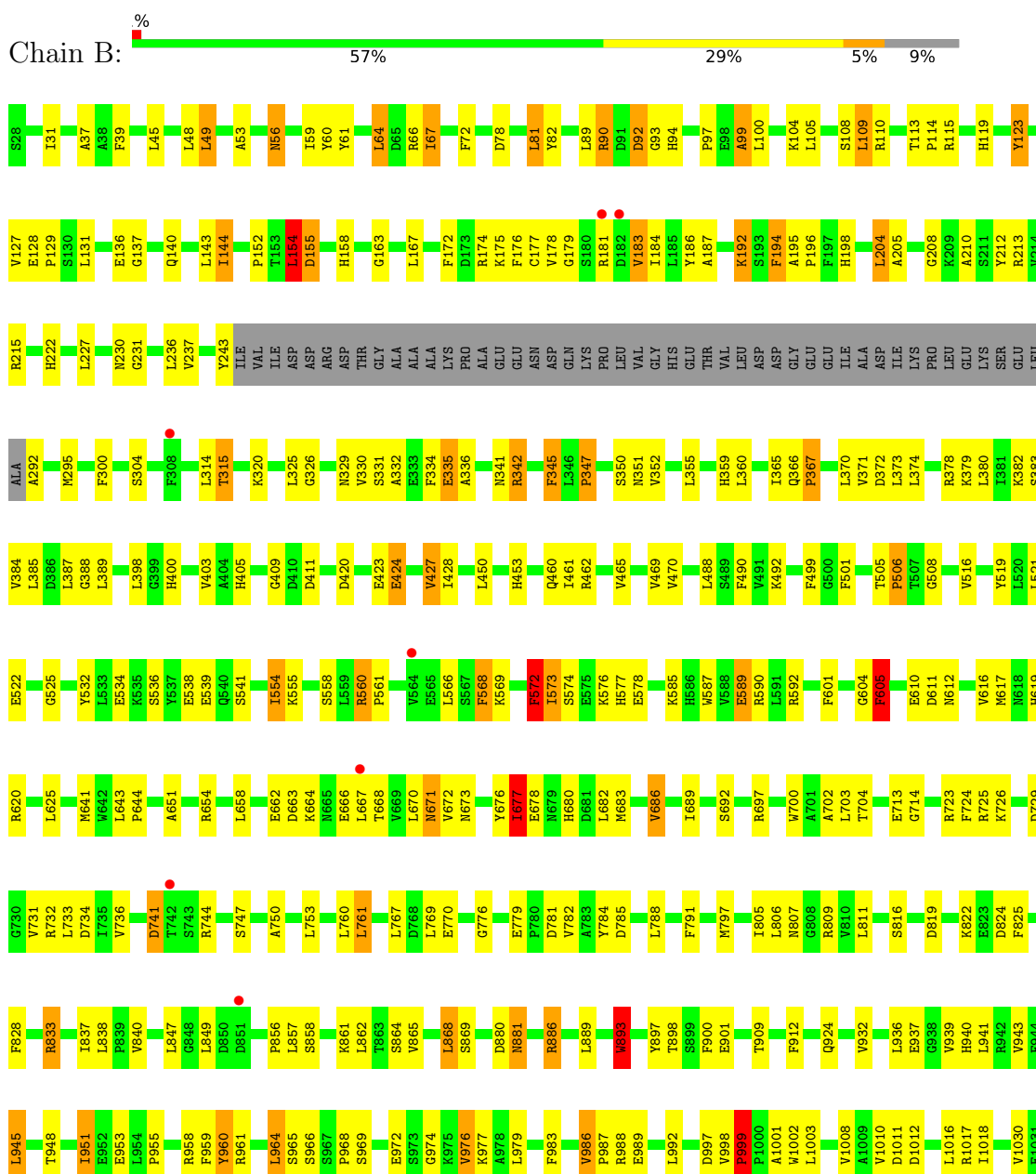
3 Residue-property plots

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: UDP-glucose-glycoprotein glucosyltransferase-like protein



- Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	139.05Å 139.05Å 176.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	139.04 – 4.60 139.04 – 4.77	Depositor EDS
% Data completeness (in resolution range)	32.1 (139.04-4.60) 36.0 (139.04-4.77)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 4.88Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.203 , 0.234 0.202 , 0.228	Depositor DCC
R_{free} test set	339 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	206.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 718.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.369 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20112	wwPDB-VP
Average B, all atoms (Å ²)	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.97	5/10293 (0.0%)	1.27	13/13959 (0.1%)
1	B	0.97	5/10293 (0.0%)	1.27	12/13959 (0.1%)
All	All	0.97	10/20586 (0.0%)	1.27	25/27918 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	750	ALA	C-O	-6.34	1.16	1.24
1	B	750	ALA	C-O	-6.10	1.16	1.24
1	A	519	TYR	C-O	-6.05	1.17	1.24
1	B	519	TYR	C-O	-5.82	1.17	1.24
1	A	152	PRO	C-O	-5.53	1.17	1.24
1	A	525	GLY	C-O	5.41	1.27	1.23
1	B	152	PRO	C-O	-5.22	1.17	1.24
1	B	525	GLY	C-O	5.22	1.27	1.23
1	A	833	ARG	C-O	-5.22	1.18	1.24
1	B	833	ARG	C-O	-5.18	1.18	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	SER	CA-C-N	5.85	130.67	122.08
1	B	304	SER	C-N-CA	5.85	130.67	122.08
1	A	304	SER	CA-C-N	5.81	130.62	122.08
1	A	304	SER	C-N-CA	5.81	130.62	122.08
1	B	345	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	345	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	154	LEU	CA-C-N	5.50	132.04	121.54
1	A	154	LEU	C-N-CA	5.50	132.04	121.54
1	B	154	LEU	CA-C-N	5.46	131.98	121.54
1	B	154	LEU	C-N-CA	5.46	131.98	121.54
1	B	999	PRO	N-CA-C	5.36	117.24	110.70
1	A	999	PRO	N-CA-C	5.33	117.20	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	VAL	CA-C-O	-5.23	115.51	120.95
1	A	314	LEU	CA-C-N	5.23	127.81	120.28
1	A	314	LEU	C-N-CA	5.23	127.81	120.28
1	B	516	VAL	CA-C-O	-5.21	115.53	120.95
1	B	314	LEU	CA-C-N	5.21	127.78	120.28
1	B	314	LEU	C-N-CA	5.21	127.78	120.28
1	A	1208	GLY	CA-C-O	-5.16	117.34	121.77
1	B	1208	GLY	CA-C-O	-5.10	117.38	121.77
1	B	601	PHE	CA-CB-CG	-5.08	108.72	113.80
1	A	601	PHE	CA-CB-CG	-5.08	108.72	113.80
1	A	1000	PRO	N-CA-C	5.03	119.28	112.48
1	B	605	PHE	CA-CB-CG	5.03	118.83	113.80
1	A	605	PHE	CA-CB-CG	5.03	118.83	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10056	0	9955	233	0
1	B	10056	0	9955	236	0
All	All	20112	0	19910	469	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (469) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:GLY:H	1:A:1136:PRO:HA	1.12	1.11
1:B:1109:GLY:H	1:B:1136:PRO:HA	1.12	1.06
1:A:382:LYS:HA	1:A:385:LEU:HG	1.51	0.93
1:B:382:LYS:HA	1:B:385:LEU:HG	1.51	0.92
1:B:833:ARG:HA	1:B:837:ILE:HB	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:ARG:HA	1:A:837:ILE:HB	1.55	0.85
1:B:704:THR:HB	1:B:805:ILE:HB	1.59	0.85
1:A:704:THR:HB	1:A:805:ILE:HB	1.59	0.84
1:A:123:TYR:HA	1:A:127:VAL:HB	1.60	0.83
1:B:345:PHE:HB3	1:B:893:TRP:NE1	1.94	0.82
1:A:345:PHE:HB3	1:A:893:TRP:NE1	1.95	0.82
1:A:342:ARG:HG2	1:A:347:PRO:HA	1.63	0.81
1:B:123:TYR:HA	1:B:127:VAL:HB	1.60	0.81
1:B:342:ARG:HG2	1:B:347:PRO:HA	1.64	0.80
1:A:901:GLU:OE1	1:A:940:HIS:NE2	2.16	0.78
1:A:676:TYR:HA	1:A:683:MET:HG3	1.68	0.75
1:B:676:TYR:HA	1:B:683:MET:HG3	1.67	0.75
1:A:932:VAL:HG21	1:A:964:LEU:HB3	1.69	0.74
1:B:932:VAL:HG21	1:B:964:LEU:HB3	1.69	0.73
1:A:671:ASN:HA	1:A:864:SER:HB3	1.72	0.72
1:B:1109:GLY:N	1:B:1136:PRO:HA	1.97	0.72
1:A:31:ILE:HA	1:A:1030:VAL:HB	1.72	0.72
1:A:1109:GLY:N	1:A:1136:PRO:HA	1.97	0.71
1:B:671:ASN:HA	1:B:864:SER:HB3	1.71	0.71
1:B:384:VAL:HA	1:B:387:LEU:HG	1.73	0.71
1:B:901:GLU:OE1	1:B:940:HIS:NE2	2.16	0.70
1:A:61:TYR:OH	1:A:174:ARG:O	2.08	0.70
1:B:61:TYR:OH	1:B:174:ARG:O	2.08	0.70
1:A:384:VAL:HA	1:A:387:LEU:HG	1.73	0.70
1:B:31:ILE:HA	1:B:1030:VAL:HB	1.73	0.70
1:B:115:ARG:HA	1:B:1127:MET:HB2	1.73	0.69
1:A:342:ARG:CG	1:A:347:PRO:HA	2.23	0.69
1:A:115:ARG:HA	1:A:1127:MET:HB2	1.75	0.68
1:B:64:LEU:HD23	1:B:198:HIS:CE1	2.29	0.68
1:A:64:LEU:HD23	1:A:198:HIS:CE1	2.28	0.67
1:B:342:ARG:CG	1:B:347:PRO:HA	2.23	0.67
1:B:1201:ASN:HB3	1:B:1233:TRP:HE1	1.59	0.67
1:A:1201:ASN:HB3	1:A:1233:TRP:HE1	1.60	0.66
1:B:898:THR:HB	1:B:945:LEU:HB3	1.78	0.66
1:B:1225:HIS:CD2	1:B:1308:ARG:HA	2.30	0.66
1:B:1109:GLY:H	1:B:1136:PRO:CA	2.01	0.66
1:A:898:THR:HB	1:A:945:LEU:HB3	1.78	0.66
1:A:988:ARG:HA	1:A:1018:ILE:HB	1.78	0.66
1:B:988:ARG:HA	1:B:1018:ILE:HB	1.78	0.65
1:A:1225:HIS:CD2	1:A:1308:ARG:HA	2.31	0.65
1:B:658:LEU:HB3	1:B:811:LEU:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:HB3	1:A:992:LEU:HB3	1.79	0.65
1:A:78:ASP:HB2	1:A:974:GLY:O	1.97	0.65
1:A:398:LEU:HB3	1:A:886:ARG:HD3	1.79	0.65
1:B:236:LEU:HB3	1:B:992:LEU:HB3	1.79	0.64
1:B:378:ARG:HE	1:B:909:THR:HG21	1.62	0.64
1:A:378:ARG:HE	1:A:909:THR:HG21	1.61	0.64
1:B:78:ASP:HB2	1:B:974:GLY:O	1.97	0.64
1:B:105:LEU:HD12	1:B:966:SER:HA	1.79	0.64
1:B:398:LEU:HB3	1:B:886:ARG:HD3	1.79	0.64
1:A:658:LEU:HB3	1:A:811:LEU:HB3	1.79	0.64
1:A:858:SER:O	1:A:862:LEU:HG	1.98	0.64
1:B:858:SER:O	1:B:862:LEU:HG	1.98	0.63
1:A:105:LEU:HD12	1:A:966:SER:HA	1.79	0.63
1:A:192:LYS:HE2	1:A:192:LYS:HA	1.81	0.62
1:A:411:ASP:HA	1:A:664:LYS:HB3	1.80	0.62
1:B:411:ASP:HA	1:B:664:LYS:HB3	1.80	0.62
1:B:1311:MET:HA	1:B:1314:LEU:HD13	1.81	0.61
1:B:192:LYS:HA	1:B:192:LYS:HE2	1.81	0.61
1:A:1311:MET:HA	1:A:1314:LEU:HD13	1.83	0.61
1:B:140:GLN:HG3	1:B:187:ALA:HA	1.83	0.61
1:A:341:ASN:O	1:A:893:TRP:NE1	2.33	0.60
1:A:1109:GLY:H	1:A:1136:PRO:CA	2.01	0.60
1:B:341:ASN:O	1:B:893:TRP:NE1	2.33	0.60
1:A:686:VAL:HG11	1:A:736:VAL:HG22	1.84	0.60
1:A:237:VAL:O	1:A:992:LEU:HA	2.02	0.60
1:A:1362:TYR:CD1	1:A:1362:TYR:C	2.81	0.59
1:A:352:VAL:HG13	1:A:359:HIS:HD2	1.67	0.59
1:A:689:ILE:HG21	1:A:761:LEU:HD21	1.85	0.59
1:B:366:GLN:HB2	1:B:367:PRO:HD2	1.83	0.59
1:B:1322:ALA:HA	1:B:1408:PRO:HB2	1.85	0.59
1:B:686:VAL:HG11	1:B:736:VAL:HG22	1.84	0.59
1:A:56:ASN:HB3	1:A:59:ILE:HB	1.83	0.59
1:A:140:GLN:HG3	1:A:187:ALA:HA	1.83	0.59
1:A:1362:TYR:C	1:A:1362:TYR:HD1	2.10	0.59
1:B:689:ILE:HG21	1:B:761:LEU:HD21	1.85	0.59
1:A:366:GLN:HB2	1:A:367:PRO:HD2	1.84	0.59
1:B:1362:TYR:HD1	1:B:1362:TYR:C	2.10	0.59
1:B:237:VAL:O	1:B:992:LEU:HA	2.02	0.58
1:B:352:VAL:HG13	1:B:359:HIS:HD2	1.68	0.58
1:B:1205:VAL:HG11	1:B:1283:LYS:HE2	1.85	0.58
1:A:450:LEU:HD11	1:A:461:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:HB2	1:A:959:PHE:HB2	1.86	0.58
1:A:1322:ALA:HA	1:A:1408:PRO:HB2	1.84	0.58
1:B:833:ARG:HG3	1:B:838:LEU:HG	1.86	0.58
1:A:676:TYR:OH	1:A:704:THR:OG1	2.18	0.58
1:B:1362:TYR:C	1:B:1362:TYR:CD1	2.81	0.58
1:B:1039:ILE:O	1:B:1085:ALA:O	2.22	0.57
1:B:236:LEU:HB2	1:B:959:PHE:HB2	1.86	0.57
1:A:1039:ILE:O	1:A:1085:ALA:O	2.21	0.57
1:B:450:LEU:HD11	1:B:461:ILE:HD13	1.87	0.57
1:A:411:ASP:HA	1:A:664:LYS:CB	2.35	0.57
1:B:179:GLY:HA3	1:B:210:ALA:HA	1.86	0.57
1:B:360:LEU:HB2	1:B:365:ILE:HD11	1.87	0.57
1:B:725:ARG:HD3	1:B:731:VAL:HB	1.86	0.57
1:A:179:GLY:HA3	1:A:210:ALA:HA	1.86	0.57
1:B:411:ASP:HA	1:B:664:LYS:CB	2.35	0.57
1:A:1223:MET:HG3	1:A:1256:PHE:HB3	1.87	0.57
1:A:725:ARG:HD3	1:A:731:VAL:HB	1.86	0.56
1:B:56:ASN:HB3	1:B:59:ILE:HB	1.85	0.56
1:B:1296:ASP:HA	1:B:1366:LEU:HB2	1.88	0.56
1:B:1108:VAL:HA	1:B:1136:PRO:HB3	1.87	0.56
1:A:360:LEU:HB2	1:A:365:ILE:HD11	1.87	0.56
1:A:822:LYS:HA	1:A:825:PHE:HD2	1.71	0.56
1:B:49:LEU:HD11	1:B:64:LEU:HD12	1.88	0.56
1:B:379:LYS:O	1:B:383:SER:OG	2.23	0.56
1:A:833:ARG:HG3	1:A:838:LEU:HG	1.87	0.56
1:A:1205:VAL:HG11	1:A:1283:LYS:HE2	1.88	0.56
1:A:1272:GLN:HB2	1:A:1278:GLU:HG3	1.88	0.56
1:B:676:TYR:OH	1:B:704:THR:OG1	2.18	0.56
1:A:1011:ASP:OD2	1:A:1030:VAL:HG13	2.06	0.55
1:B:1011:ASP:OD2	1:B:1030:VAL:HG13	2.06	0.55
1:B:1223:MET:HG3	1:B:1256:PHE:HB3	1.87	0.55
1:B:1272:GLN:HB2	1:B:1278:GLU:HG3	1.88	0.55
1:A:379:LYS:O	1:A:383:SER:OG	2.23	0.55
1:B:366:GLN:HB2	1:B:367:PRO:CD	2.37	0.55
1:B:822:LYS:HA	1:B:825:PHE:HD2	1.70	0.55
1:A:1080:TYR:CE2	1:A:1266:PRO:HG3	2.42	0.55
1:B:1041:ILE:HD11	1:B:1085:ALA:HB3	1.88	0.55
1:A:315:THR:HG23	1:A:924:GLN:HB3	1.88	0.55
1:A:380:LEU:HG	1:A:865:VAL:HG13	1.88	0.55
1:A:1041:ILE:HD11	1:A:1085:ALA:HB3	1.89	0.55
1:B:315:THR:HG23	1:B:924:GLN:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:LEU:HB2	1:B:1038:HIS:HB2	1.89	0.55
1:B:1283:LYS:O	1:B:1287:LEU:HG	2.07	0.55
1:A:470:VAL:O	1:A:501:PHE:HB2	2.07	0.55
1:A:366:GLN:HB2	1:A:367:PRO:CD	2.37	0.55
1:A:1296:ASP:HA	1:A:1366:LEU:HB2	1.89	0.54
1:A:1202:ILE:HD11	1:A:1311:MET:HE2	1.88	0.54
1:B:1235:ILE:O	1:B:1239:LEU:HG	2.08	0.54
1:B:807:ASN:O	1:B:864:SER:OG	2.26	0.54
1:A:49:LEU:HD11	1:A:64:LEU:HD12	1.89	0.54
1:A:1108:VAL:HA	1:A:1136:PRO:HB3	1.87	0.54
1:B:380:LEU:HG	1:B:865:VAL:HG13	1.88	0.54
1:B:1080:TYR:CE2	1:B:1266:PRO:HG3	2.42	0.54
1:B:1202:ILE:HD11	1:B:1311:MET:HE2	1.89	0.54
1:A:144:ILE:HG13	1:A:183:VAL:HB	1.89	0.53
1:A:325:LEU:HA	1:A:330:VAL:HG21	1.89	0.53
1:B:355:LEU:HB2	1:B:360:LEU:HD11	1.89	0.53
1:B:355:LEU:HD13	1:B:912:PHE:CZ	2.44	0.53
1:A:1235:ILE:O	1:A:1239:LEU:HG	2.08	0.53
1:A:1283:LYS:O	1:A:1287:LEU:HG	2.07	0.53
1:B:470:VAL:O	1:B:501:PHE:HB2	2.08	0.53
1:A:1107:SER:HB3	1:A:1120:ASP:HA	1.91	0.53
1:A:355:LEU:HB2	1:A:360:LEU:HD11	1.89	0.53
1:A:89:LEU:HA	1:A:94:HIS:CD2	2.43	0.53
1:A:807:ASN:O	1:A:864:SER:OG	2.26	0.53
1:B:89:LEU:HA	1:B:94:HIS:CD2	2.43	0.53
1:B:144:ILE:HG13	1:B:183:VAL:HB	1.91	0.53
1:B:869:SER:HB2	1:B:886:ARG:HD2	1.90	0.53
1:A:1003:LEU:HB2	1:A:1038:HIS:HB2	1.90	0.53
1:A:610:GLU:O	1:A:1050:GLY:HA2	2.09	0.52
1:A:741:ASP:HB2	1:A:744:ARG:HB2	1.89	0.52
1:B:998:VAL:O	1:B:999:PRO:O	2.27	0.52
1:B:113:THR:N	1:B:114:PRO:HD2	2.25	0.52
1:A:869:SER:HB2	1:A:886:ARG:HD2	1.90	0.52
1:B:292:ALA:HA	1:B:295:MET:SD	2.50	0.52
1:A:113:THR:N	1:A:114:PRO:HD2	2.25	0.52
1:A:747:SER:HB3	1:A:784:TYR:HB3	1.92	0.52
1:B:960:TYR:O	1:B:961:ARG:HG2	2.10	0.52
1:A:355:LEU:HD13	1:A:912:PHE:CZ	2.43	0.52
1:B:325:LEU:HA	1:B:330:VAL:HG21	1.90	0.52
1:A:177:CYS:HB3	1:A:205:ALA:HB1	1.91	0.52
1:A:1221:SER:HB2	1:A:1306:ILE:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:PHE:HB3	1:B:893:TRP:CE2	2.45	0.52
1:B:741:ASP:HB2	1:B:744:ARG:HB2	1.90	0.52
1:A:960:TYR:O	1:A:961:ARG:HG2	2.10	0.52
1:A:998:VAL:O	1:A:999:PRO:O	2.27	0.52
1:B:610:GLU:O	1:B:1050:GLY:HA2	2.10	0.52
1:B:1107:SER:HB3	1:B:1120:ASP:HA	1.91	0.52
1:B:572:PHE:HA	1:B:577:HIS:ND1	2.25	0.51
1:B:1108:VAL:HB	1:B:1122:THR:HA	1.92	0.51
1:A:998:VAL:CG2	1:A:999:PRO:HD2	2.41	0.51
1:B:1221:SER:HB2	1:B:1306:ILE:HG23	1.92	0.51
1:A:292:ALA:HA	1:A:295:MET:SD	2.51	0.51
1:A:572:PHE:HA	1:A:577:HIS:ND1	2.26	0.51
1:B:858:SER:HA	1:B:861:LYS:HD2	1.92	0.51
1:B:1216:ASN:HA	1:B:1219:MET:SD	2.51	0.51
1:A:1108:VAL:HB	1:A:1122:THR:HA	1.93	0.51
1:A:1228:HIS:NE2	1:A:1310:ASP:OD1	2.44	0.51
1:A:858:SER:HA	1:A:861:LYS:HD2	1.92	0.50
1:A:1134:LEU:C	1:A:1136:PRO:HD3	2.36	0.50
1:B:747:SER:HB3	1:B:784:TYR:HB3	1.93	0.50
1:B:177:CYS:HB3	1:B:205:ALA:HB1	1.92	0.50
1:B:1134:LEU:C	1:B:1136:PRO:HD3	2.36	0.50
1:B:998:VAL:CG2	1:B:999:PRO:HD2	2.41	0.50
1:B:1200:ILE:CD1	1:B:1228:HIS:CD2	2.95	0.50
1:B:1226:THR:OG1	1:B:1228:HIS:CD2	2.65	0.50
1:B:1228:HIS:NE2	1:B:1310:ASP:OD1	2.44	0.50
1:A:1226:THR:OG1	1:A:1228:HIS:CD2	2.65	0.50
1:A:345:PHE:HB3	1:A:893:TRP:CE2	2.45	0.50
1:A:1216:ASN:HA	1:A:1219:MET:SD	2.51	0.50
1:B:208:GLY:HA3	1:B:782:VAL:HB	1.94	0.49
1:A:352:VAL:HG13	1:A:359:HIS:CD2	2.47	0.49
1:B:352:VAL:HG13	1:B:359:HIS:CD2	2.46	0.49
1:B:989:GLU:HA	1:B:1017:ARG:HG2	1.95	0.49
1:A:208:GLY:HA3	1:A:782:VAL:HB	1.94	0.49
1:A:387:LEU:HD21	1:A:861:LYS:HD3	1.95	0.49
1:A:560:ARG:N	1:A:561:PRO:HD3	2.28	0.49
1:B:108:SER:OG	1:B:965:SER:O	2.21	0.49
1:B:1080:TYR:OH	1:B:1082:GLN:NE2	2.42	0.49
1:B:1282:TYR:O	1:B:1286:PHE:O	2.31	0.49
1:B:1108:VAL:HG13	1:B:1136:PRO:HG3	1.95	0.49
1:A:1200:ILE:CD1	1:A:1228:HIS:CD2	2.95	0.49
1:B:1099:SER:O	1:B:1103:PHE:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1307:VAL:HG11	1:B:1311:MET:SD	2.53	0.48
1:A:604:GLY:O	1:A:605:PHE:O	2.32	0.48
1:A:811:LEU:HD11	1:A:828:PHE:CE2	2.48	0.48
1:B:560:ARG:N	1:B:561:PRO:HD3	2.29	0.48
1:B:697:ARG:HA	1:B:700:TRP:CE3	2.48	0.48
1:B:811:LEU:HD11	1:B:828:PHE:CE2	2.48	0.48
1:A:1099:SER:O	1:A:1103:PHE:O	2.30	0.48
1:A:1282:TYR:O	1:A:1286:PHE:O	2.31	0.48
1:B:92:ASP:OD1	1:B:92:ASP:N	2.46	0.48
1:B:387:LEU:HD21	1:B:861:LYS:HD3	1.96	0.48
1:B:105:LEU:HD11	1:B:932:VAL:HG12	1.96	0.48
1:A:1047:GLU:HA	1:A:1138:LEU:O	2.14	0.48
1:B:1239:LEU:HB2	1:B:1244:LYS:HE3	1.96	0.48
1:A:53:ALA:HB1	1:A:60:TYR:HA	1.95	0.48
1:A:366:GLN:O	1:A:370:LEU:HB2	2.14	0.48
1:B:53:ALA:HB1	1:B:60:TYR:HA	1.96	0.48
1:B:1030:VAL:HG12	1:B:1032:ALA:H	1.79	0.48
1:A:1030:VAL:HG12	1:A:1032:ALA:H	1.79	0.48
1:A:1239:LEU:HB2	1:A:1244:LYS:HE3	1.96	0.48
1:B:366:GLN:O	1:B:370:LEU:HB2	2.14	0.48
1:B:1047:GLU:HA	1:B:1138:LEU:O	2.14	0.48
1:A:989:GLU:HA	1:A:1017:ARG:HG2	1.95	0.48
1:B:724:PHE:HA	1:B:822:LYS:HE2	1.95	0.48
1:B:1040:LEU:O	1:B:1131:GLY:HA2	2.14	0.48
1:A:1073:ILE:HG12	1:A:1289:VAL:HG12	1.96	0.47
1:A:92:ASP:N	1:A:92:ASP:OD1	2.46	0.47
1:A:724:PHE:HA	1:A:822:LYS:HE2	1.95	0.47
1:B:154:LEU:O	1:B:155:ASP:CG	2.57	0.47
1:B:604:GLY:O	1:B:605:PHE:O	2.31	0.47
1:B:97:PRO:O	1:B:937:GLU:OE1	2.33	0.47
1:B:1280:TRP:HB3	1:B:1395:LEU:HG	1.95	0.47
1:A:154:LEU:O	1:A:155:ASP:CG	2.56	0.47
1:A:724:PHE:HA	1:A:822:LYS:CE	2.44	0.47
1:A:998:VAL:O	1:A:999:PRO:C	2.58	0.47
1:B:724:PHE:HA	1:B:822:LYS:CE	2.44	0.47
1:B:791:PHE:CZ	1:B:797:MET:SD	3.07	0.47
1:B:998:VAL:O	1:B:999:PRO:C	2.58	0.47
1:B:1073:ILE:HG12	1:B:1289:VAL:HG12	1.97	0.47
1:A:1108:VAL:HG13	1:A:1136:PRO:HG3	1.96	0.47
1:A:1307:VAL:HG11	1:A:1311:MET:SD	2.54	0.47
1:B:703:LEU:HD12	1:B:806:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1119:ASP:C	1:B:1121:ASN:H	2.23	0.47
1:B:1376:ASP:OD1	1:B:1376:ASP:N	2.47	0.47
1:A:176:PHE:CD2	1:A:205:ALA:HB3	2.50	0.47
1:A:697:ARG:HA	1:A:700:TRP:CE3	2.49	0.47
1:A:1119:ASP:C	1:A:1121:ASN:H	2.23	0.47
1:B:176:PHE:CD2	1:B:205:ALA:HB3	2.50	0.47
1:B:643:LEU:N	1:B:644:PRO:HD2	2.30	0.47
1:A:97:PRO:O	1:A:937:GLU:OE1	2.33	0.46
1:A:791:PHE:CZ	1:A:797:MET:SD	3.08	0.46
1:A:1280:TRP:HB3	1:A:1395:LEU:HG	1.95	0.46
1:A:986:VAL:HG22	1:A:987:PRO:HD2	1.97	0.46
1:A:1040:LEU:O	1:A:1131:GLY:HA2	2.14	0.46
1:A:167:LEU:HA	1:A:184:ILE:HD11	1.96	0.46
1:A:643:LEU:N	1:A:644:PRO:HD2	2.30	0.46
1:A:1001:ALA:HB1	1:A:1040:LEU:HB2	1.97	0.46
1:B:186:TYR:HE1	1:B:215:ARG:HD2	1.81	0.46
1:B:723:ARG:HA	1:B:726:LYS:HE3	1.97	0.46
1:B:1001:ALA:HB1	1:B:1040:LEU:HB2	1.97	0.46
1:A:403:VAL:C	1:A:405:HIS:H	2.24	0.46
1:A:105:LEU:HD11	1:A:932:VAL:HG12	1.96	0.46
1:A:713:GLU:HB3	1:A:816:SER:HA	1.98	0.46
1:A:767:LEU:HA	1:A:770:GLU:HG2	1.97	0.46
1:B:403:VAL:C	1:B:405:HIS:H	2.24	0.46
1:B:713:GLU:HB3	1:B:816:SER:HA	1.98	0.46
1:B:104:LYS:HB3	1:B:968:PRO:HD3	1.98	0.46
1:B:167:LEU:HA	1:B:184:ILE:HD11	1.96	0.46
1:B:1201:ASN:O	1:B:1202:ILE:HG13	2.16	0.46
1:A:1200:ILE:HD11	1:A:1312:TYR:HD1	1.81	0.45
1:A:723:ARG:HA	1:A:726:LYS:HE3	1.97	0.45
1:B:560:ARG:N	1:B:561:PRO:CD	2.80	0.45
1:A:969:SER:HB2	1:A:977:LYS:HD3	1.98	0.45
1:A:1046:ARG:HE	1:A:1137:ARG:HG2	1.80	0.45
1:B:961:ARG:HG2	1:B:983:PHE:CE2	2.52	0.45
1:B:1046:ARG:HE	1:B:1137:ARG:HG2	1.80	0.45
1:A:186:TYR:HE1	1:A:215:ARG:HD2	1.81	0.45
1:A:702:ALA:HA	1:A:732:ARG:HB3	1.99	0.45
1:A:1080:TYR:OH	1:A:1082:GLN:NE2	2.42	0.45
1:A:45:LEU:HD12	1:A:81:LEU:HD21	1.99	0.45
1:A:119:HIS:NE2	1:A:172:PHE:CD1	2.85	0.45
1:A:573:ILE:HG22	1:A:574:SER:H	1.81	0.45
1:A:998:VAL:HG21	1:A:1002:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1201:ASN:O	1:A:1202:ILE:HG13	2.16	0.45
1:A:1376:ASP:N	1:A:1376:ASP:OD1	2.47	0.45
1:B:767:LEU:HA	1:B:770:GLU:HG2	1.98	0.45
1:A:108:SER:OG	1:A:965:SER:O	2.21	0.45
1:A:900:PHE:CZ	1:A:943:VAL:HB	2.52	0.45
1:A:1241:PRO:O	1:A:1245:ASP:OD1	2.35	0.45
1:B:66:ARG:HB2	1:B:72:PHE:CE2	2.52	0.45
1:B:986:VAL:HG22	1:B:987:PRO:HD2	1.99	0.45
1:B:998:VAL:HG21	1:B:1002:TRP:CE3	2.52	0.45
1:A:961:ARG:HG2	1:A:983:PHE:CE2	2.52	0.45
1:B:900:PHE:CZ	1:B:943:VAL:HB	2.52	0.45
1:B:1008:VAL:HB	1:B:1033:ILE:HB	1.99	0.45
1:A:66:ARG:HB2	1:A:72:PHE:CE2	2.52	0.45
1:A:560:ARG:N	1:A:561:PRO:CD	2.80	0.45
1:B:45:LEU:HD12	1:B:81:LEU:HD21	1.99	0.45
1:B:119:HIS:NE2	1:B:172:PHE:CD1	2.85	0.45
1:B:382:LYS:HG2	1:B:385:LEU:HD21	1.98	0.45
1:A:104:LYS:HB3	1:A:968:PRO:HD3	1.99	0.45
1:A:616:VAL:HA	1:A:619:HIS:CD2	2.52	0.45
1:B:573:ILE:HG22	1:B:574:SER:H	1.81	0.44
1:B:969:SER:HB2	1:B:977:LYS:HD3	1.98	0.44
1:B:1241:PRO:O	1:B:1245:ASP:OD1	2.35	0.44
1:A:382:LYS:HG2	1:A:385:LEU:HD21	1.98	0.44
1:A:334:PHE:C	1:A:336:ALA:H	2.25	0.44
1:B:702:ALA:HA	1:B:732:ARG:HB3	2.00	0.44
1:A:703:LEU:HD12	1:A:806:LEU:HB2	1.98	0.44
1:A:732:ARG:HB2	1:A:856:PRO:HG2	1.99	0.44
1:B:128:GLU:N	1:B:129:PRO:HD2	2.33	0.44
1:B:334:PHE:C	1:B:336:ALA:H	2.25	0.44
1:B:732:ARG:HB2	1:B:856:PRO:HG2	1.99	0.44
1:A:1008:VAL:HB	1:A:1033:ILE:HB	2.00	0.44
1:B:89:LEU:HA	1:B:94:HIS:HB2	1.99	0.44
1:A:110:ARG:CZ	1:A:976:VAL:HG11	2.48	0.44
1:A:1265:TRP:HE1	1:A:1269:LEU:HG	1.83	0.44
1:B:589:GLU:OE1	1:B:589:GLU:HA	2.17	0.44
1:B:1378:LEU:HA	1:B:1381:GLN:HB2	2.00	0.44
1:A:89:LEU:HA	1:A:94:HIS:HB2	1.99	0.44
1:A:554:ILE:HG21	1:A:568:PHE:CE1	2.53	0.44
1:B:110:ARG:CZ	1:B:976:VAL:HG11	2.48	0.44
1:B:1200:ILE:HD11	1:B:1312:TYR:HD1	1.82	0.44
1:A:128:GLU:N	1:A:129:PRO:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:PHE:HZ	1:A:1134:LEU:HB2	1.82	0.44
1:A:1297:LYS:HD2	1:A:1315:VAL:HG13	1.99	0.43
1:A:1399:LEU:N	1:A:1400:PRO:HD2	2.32	0.43
1:B:616:VAL:HA	1:B:619:HIS:CD2	2.52	0.43
1:B:1081:PHE:HZ	1:B:1134:LEU:HB2	1.82	0.43
1:B:1399:LEU:N	1:B:1400:PRO:HD2	2.32	0.43
1:A:380:LEU:HD13	1:A:868:LEU:HD22	2.00	0.43
1:B:90:ARG:HG3	1:B:100:LEU:HD11	2.00	0.43
1:B:144:ILE:HD13	1:B:154:LEU:HD21	2.01	0.43
1:B:1148:ASP:OD1	1:B:1148:ASP:O	2.36	0.43
1:B:1205:VAL:HG21	1:B:1279:ILE:HG23	2.00	0.43
1:B:1297:LYS:HD2	1:B:1315:VAL:HG13	1.99	0.43
1:A:144:ILE:HD13	1:A:154:LEU:HD21	2.00	0.43
1:B:380:LEU:HD13	1:B:868:LEU:HD22	2.01	0.43
1:B:572:PHE:N	1:B:572:PHE:CD1	2.86	0.43
1:A:208:GLY:HA3	1:A:782:VAL:CG1	2.49	0.43
1:A:572:PHE:N	1:A:572:PHE:CD1	2.87	0.43
1:B:371:VAL:C	1:B:373:LEU:H	2.26	0.43
1:B:532:TYR:O	1:B:536:SER:N	2.47	0.43
1:B:37:ALA:HB3	1:B:227:LEU:HB3	2.01	0.43
1:A:67:ILE:HB	1:A:194:PHE:HZ	1.84	0.43
1:B:53:ALA:HB2	1:B:59:ILE:HG22	2.00	0.43
1:B:97:PRO:HA	1:B:100:LEU:HG	1.99	0.43
1:A:1105:LEU:O	1:A:1105:LEU:HD12	2.19	0.43
1:B:654:ARG:NH1	1:B:824:ASP:OD2	2.52	0.43
1:A:505:THR:N	1:A:506:PRO:HD3	2.34	0.43
1:B:554:ILE:HG21	1:B:568:PHE:CE1	2.54	0.43
1:A:110:ARG:O	1:A:113:THR:OG1	2.28	0.43
1:A:1148:ASP:OD1	1:A:1148:ASP:O	2.36	0.43
1:A:37:ALA:HB3	1:A:227:LEU:HB3	2.00	0.42
1:B:505:THR:N	1:B:506:PRO:HD3	2.34	0.42
1:B:1265:TRP:HE1	1:B:1269:LEU:HG	1.83	0.42
1:A:654:ARG:NH1	1:A:824:ASP:OD2	2.52	0.42
1:A:1378:LEU:HA	1:A:1381:GLN:HB2	2.00	0.42
1:B:673:ASN:OD1	1:B:677:ILE:HD12	2.20	0.42
1:A:53:ALA:HB2	1:A:59:ILE:HG22	2.01	0.42
1:A:97:PRO:HA	1:A:100:LEU:HG	2.00	0.42
1:A:1060:VAL:HB	1:A:1093:ARG:HG2	2.00	0.42
1:B:67:ILE:HB	1:B:194:PHE:HZ	1.84	0.42
1:B:208:GLY:HA3	1:B:782:VAL:CG1	2.49	0.42
1:B:936:LEU:HB2	1:B:939:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:HG3	1:A:100:LEU:HD11	2.01	0.42
1:B:682:LEU:HD13	1:B:788:LEU:HB2	2.01	0.42
1:A:1116:ILE:HG22	1:A:1118:GLY:H	1.85	0.42
1:A:1403:MET:HB3	1:A:1406:THR:OG1	2.20	0.42
1:A:682:LEU:HD22	1:A:788:LEU:HA	2.02	0.42
1:A:1203:PHE:CD2	1:A:1300:PHE:HB2	2.55	0.42
1:B:389:LEU:HG	1:B:849:LEU:HD22	2.01	0.42
1:B:747:SER:HB2	1:B:781:ASP:HB3	2.02	0.42
1:B:1103:PHE:CD1	1:B:1138:LEU:HD22	2.55	0.42
1:B:1206:ALA:HB3	1:B:1239:LEU:CD2	2.50	0.42
1:A:371:VAL:C	1:A:373:LEU:H	2.27	0.42
1:A:747:SER:HB2	1:A:781:ASP:HB3	2.01	0.42
1:B:143:LEU:HD23	1:B:184:ILE:HD12	2.02	0.42
1:B:332:ALA:HB1	1:B:334:PHE:CE2	2.55	0.42
1:B:1060:VAL:HB	1:B:1093:ARG:HG2	2.00	0.42
1:A:204:LEU:HG	1:A:210:ALA:HB3	2.02	0.42
1:A:689:ILE:HD11	1:A:760:LEU:HD13	2.02	0.42
1:B:335:GLU:HB3	1:B:897:TYR:HB3	2.02	0.42
1:B:1116:ILE:HG22	1:B:1118:GLY:H	1.84	0.42
1:A:109:LEU:HA	1:A:230:ASN:HD21	1.85	0.41
1:B:371:VAL:HA	1:B:374:LEU:HG	2.02	0.41
1:A:490:PHE:HB3	1:A:499:PHE:CE2	2.56	0.41
1:A:1205:VAL:HG21	1:A:1279:ILE:HG23	2.02	0.41
1:B:109:LEU:HA	1:B:230:ASN:HD21	1.85	0.41
1:B:97:PRO:C	1:B:99:ALA:H	2.28	0.41
1:B:427:VAL:HG21	1:B:587:TRP:HB3	2.01	0.41
1:B:572:PHE:N	1:B:572:PHE:HD1	2.18	0.41
1:B:1105:LEU:HD12	1:B:1105:LEU:O	2.20	0.41
1:A:589:GLU:HA	1:A:589:GLU:OE1	2.19	0.41
1:B:204:LEU:HG	1:B:210:ALA:HB3	2.02	0.41
1:B:400:HIS:HE2	1:B:847:LEU:HD13	1.86	0.41
1:B:423:GLU:O	1:B:424:GLU:HB2	2.20	0.41
1:B:1403:MET:HB3	1:B:1406:THR:OG1	2.20	0.41
1:A:1204:SER:HB3	1:A:1215:LEU:HD12	2.03	0.41
1:B:951:ILE:HG21	1:B:955:PRO:HG3	2.01	0.41
1:B:1203:PHE:CD2	1:B:1300:PHE:HB2	2.55	0.41
1:B:1250:MET:HG3	1:B:1256:PHE:CZ	2.56	0.41
1:A:423:GLU:O	1:A:424:GLU:HB2	2.21	0.41
1:A:1103:PHE:CD1	1:A:1138:LEU:HD22	2.55	0.41
1:A:1107:SER:CB	1:A:1120:ASP:HA	2.50	0.41
1:A:1206:ALA:HB3	1:A:1239:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1378:LEU:HD22	1:A:1399:LEU:HD23	2.02	0.41
1:B:39:PHE:CE2	1:B:227:LEU:HD22	2.56	0.41
1:B:682:LEU:HD22	1:B:788:LEU:HA	2.01	0.41
1:A:39:PHE:CE2	1:A:227:LEU:HD22	2.55	0.41
1:A:97:PRO:C	1:A:99:ALA:H	2.28	0.41
1:A:342:ARG:HG2	1:A:347:PRO:CA	2.44	0.41
1:A:488:LEU:O	1:A:492:LYS:HB2	2.21	0.41
1:A:1201:ASN:HB3	1:A:1233:TRP:NE1	2.33	0.41
1:B:176:PHE:HB3	1:B:212:TYR:HB3	2.02	0.41
1:B:231:GLY:HA2	1:B:964:LEU:CD1	2.50	0.41
1:B:490:PHE:HB3	1:B:499:PHE:CE2	2.55	0.41
1:A:231:GLY:HA2	1:A:964:LEU:CD1	2.51	0.41
1:A:335:GLU:HB3	1:A:897:TYR:HB3	2.02	0.41
1:A:350:SER:C	1:A:351:ASN:HD22	2.28	0.41
1:A:385:LEU:HD12	1:A:385:LEU:C	2.46	0.41
1:A:682:LEU:HD13	1:A:788:LEU:HB2	2.01	0.41
1:B:1200:ILE:O	1:B:1230:VAL:HA	2.21	0.41
1:B:1399:LEU:N	1:B:1400:PRO:CD	2.84	0.41
1:A:427:VAL:HG21	1:A:587:TRP:HB3	2.02	0.41
1:A:554:ILE:O	1:A:558:SER:HB2	2.21	0.41
1:A:673:ASN:OD1	1:A:677:ILE:HD12	2.20	0.41
1:A:893:TRP:HB3	1:A:944:PHE:CZ	2.56	0.41
1:B:195:ALA:HB3	1:B:196:PRO:HD3	2.03	0.41
1:B:998:VAL:HG22	1:B:999:PRO:HD2	2.02	0.41
1:B:1132:THR:O	1:B:1134:LEU:HG	2.21	0.41
1:A:936:LEU:HB2	1:A:939:VAL:HG21	2.02	0.41
1:B:465:VAL:HG22	1:B:643:LEU:HD13	2.03	0.41
1:B:488:LEU:O	1:B:492:LYS:HB2	2.21	0.41
1:A:143:LEU:HD23	1:A:184:ILE:HD12	2.02	0.40
1:A:572:PHE:N	1:A:572:PHE:HD1	2.18	0.40
1:B:350:SER:C	1:B:351:ASN:HD22	2.29	0.40
1:B:427:VAL:HG13	1:B:428:ILE:H	1.86	0.40
1:A:961:ARG:HG2	1:A:983:PHE:CZ	2.56	0.40
1:B:1246:PHE:HA	1:B:1249:HIS:ND1	2.36	0.40
1:A:332:ALA:HB1	1:A:334:PHE:CE2	2.56	0.40
1:A:420:ASP:HA	1:A:423:GLU:OE1	2.21	0.40
1:A:1246:PHE:HA	1:A:1249:HIS:ND1	2.36	0.40
1:B:420:ASP:HA	1:B:423:GLU:OE1	2.21	0.40
1:B:689:ILE:HD11	1:B:760:LEU:HD13	2.02	0.40
1:B:961:ARG:HG2	1:B:983:PHE:CZ	2.56	0.40
1:B:1201:ASN:CB	1:B:1233:TRP:HE1	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1378:LEU:HD22	1:B:1399:LEU:HD23	2.02	0.40
1:A:389:LEU:HG	1:A:849:LEU:HD22	2.02	0.40
1:A:600:VAL:HG12	1:A:601:PHE:N	2.36	0.40
1:A:1053:ALA:HA	1:A:1054:PRO:HD3	1.92	0.40
1:A:1132:THR:O	1:A:1134:LEU:HG	2.21	0.40
1:A:1250:MET:HG3	1:A:1256:PHE:CZ	2.56	0.40
1:B:382:LYS:HA	1:B:385:LEU:CG	2.37	0.40
1:A:53:ALA:HB2	1:A:63:LEU:HD12	2.03	0.40
1:A:400:HIS:HE2	1:A:847:LEU:HD13	1.86	0.40
1:A:449:VAL:HB	1:A:461:ILE:HD12	2.04	0.40
1:B:554:ILE:O	1:B:558:SER:HB2	2.22	0.40
1:B:1201:ASN:HB3	1:B:1233:TRP:NE1	2.33	0.40
1:B:1231:LYS:HE3	1:B:1257:LYS:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1246/1382 (90%)	988 (79%)	208 (17%)	50 (4%)	2	18
1	B	1246/1382 (90%)	989 (79%)	207 (17%)	50 (4%)	2	18
All	All	2492/2764 (90%)	1977 (79%)	415 (17%)	100 (4%)	2	18

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ASP
1	A	424	GLU
1	A	427	VAL
1	A	506	PRO
1	A	541	SER

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Mol	Chain	Res	Type
1	A	592	ARG
1	A	605	PHE
1	A	651	ALA
1	A	880	ASP
1	A	972	GLU
1	A	999	PRO
1	A	1067	PRO
1	A	1236	GLU
1	B	155	ASP
1	B	424	GLU
1	B	427	VAL
1	B	506	PRO
1	B	541	SER
1	B	592	ARG
1	B	605	PHE
1	B	651	ALA
1	B	880	ASP
1	B	999	PRO
1	B	1067	PRO
1	B	1236	GLU
1	A	163	GLY
1	A	329	ASN
1	A	331	SER
1	A	367	PRO
1	A	508	GLY
1	A	572	PHE
1	A	578	GLU
1	A	881	ASN
1	A	1146	GLU
1	B	163	GLY
1	B	329	ASN
1	B	331	SER
1	B	367	PRO
1	B	508	GLY
1	B	572	PHE
1	B	578	GLU
1	B	881	ASN
1	B	972	GLU
1	B	1146	GLU
1	A	99	ALA
1	A	131	LEU
1	A	347	PRO

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Mol	Chain	Res	Type
1	A	569	LYS
1	A	611	ASP
1	A	666	GLU
1	A	714	GLY
1	A	776	GLY
1	A	857	LEU
1	A	893	TRP
1	B	99	ALA
1	B	131	LEU
1	B	347	PRO
1	B	569	LYS
1	B	611	ASP
1	B	666	GLU
1	B	714	GLY
1	B	776	GLY
1	B	857	LEU
1	B	893	TRP
1	A	154	LEU
1	A	566	LEU
1	A	671	ASN
1	A	677	ILE
1	A	692	SER
1	A	1049	PRO
1	A	1097	GLY
1	A	1109	GLY
1	A	1270	ARG
1	B	154	LEU
1	B	566	LEU
1	B	671	ASN
1	B	677	ILE
1	B	692	SER
1	B	1049	PRO
1	B	1097	GLY
1	B	1109	GLY
1	B	1270	ARG
1	A	1127	MET
1	B	568	PHE
1	B	1311	MET
1	A	137	GLY
1	A	568	PHE
1	A	1098	ARG
1	A	1311	MET

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Mol	Chain	Res	Type
1	B	137	GLY
1	B	1098	ARG
1	B	1127	MET
1	A	93	GLY
1	A	388	GLY
1	A	409	GLY
1	B	388	GLY
1	B	409	GLY
1	A	326	GLY
1	B	93	GLY
1	B	326	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1097/1197 (92%)	964 (88%)	133 (12%)	5	18
1	B	1097/1197 (92%)	963 (88%)	134 (12%)	5	18
All	All	2194/2394 (92%)	1927 (88%)	267 (12%)	5	18

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	49	LEU
1	A	56	ASN
1	A	64	LEU
1	A	67	ILE
1	A	81	LEU
1	A	82	TYR
1	A	90	ARG
1	A	92	ASP
1	A	109	LEU
1	A	123	TYR
1	A	136	GLU

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Mol	Chain	Res	Type
1	A	144	ILE
1	A	158	HIS
1	A	175	LYS
1	A	178	VAL
1	A	181	ARG
1	A	183	VAL
1	A	192	LYS
1	A	194	PHE
1	A	204	LEU
1	A	213	ARG
1	A	222	HIS
1	A	243	TYR
1	A	300	PHE
1	A	315	THR
1	A	320	LYS
1	A	335	GLU
1	A	342	ARG
1	A	372	ASP
1	A	453	HIS
1	A	460	GLN
1	A	462	ARG
1	A	469	VAL
1	A	521	LEU
1	A	522	GLU
1	A	534	GLU
1	A	538	GLU
1	A	539	GLU
1	A	554	ILE
1	A	555	LYS
1	A	560	ARG
1	A	572	PHE
1	A	573	ILE
1	A	576	LYS
1	A	585	LYS
1	A	590	ARG
1	A	605	PHE
1	A	612	ASN
1	A	617	MET
1	A	620	ARG
1	A	625	LEU
1	A	641	MET
1	A	662	GLU

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Mol	Chain	Res	Type
1	A	663	ASP
1	A	667	LEU
1	A	668	THR
1	A	670	LEU
1	A	672	VAL
1	A	677	ILE
1	A	678	GLU
1	A	680	HIS
1	A	686	VAL
1	A	729	ASP
1	A	733	LEU
1	A	734	ASP
1	A	741	ASP
1	A	753	LEU
1	A	761	LEU
1	A	769	LEU
1	A	779	GLU
1	A	785	ASP
1	A	809	ARG
1	A	819	ASP
1	A	840	VAL
1	A	868	LEU
1	A	881	ASN
1	A	886	ARG
1	A	889	LEU
1	A	893	TRP
1	A	941	LEU
1	A	945	LEU
1	A	948	THR
1	A	951	ILE
1	A	953	GLU
1	A	958	ARG
1	A	960	TYR
1	A	964	LEU
1	A	976	VAL
1	A	979	LEU
1	A	986	VAL
1	A	997	ASP
1	A	1010	VAL
1	A	1012	ASP
1	A	1016	LEU
1	A	1037	GLU

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Mol	Chain	Res	Type
1	A	1045	SER
1	A	1046	ARG
1	A	1068	HIS
1	A	1071	ASP
1	A	1094	LEU
1	A	1103	PHE
1	A	1105	LEU
1	A	1106	GLU
1	A	1120	ASP
1	A	1122	THR
1	A	1128	ASP
1	A	1132	THR
1	A	1150	LEU
1	A	1203	PHE
1	A	1204	SER
1	A	1211	TYR
1	A	1214	MET
1	A	1215	LEU
1	A	1218	MET
1	A	1224	HIS
1	A	1228	HIS
1	A	1245	ASP
1	A	1246	PHE
1	A	1247	ILE
1	A	1254	TYR
1	A	1258	TYR
1	A	1265	TRP
1	A	1290	LEU
1	A	1291	PHE
1	A	1297	LYS
1	A	1312	TYR
1	A	1362	TYR
1	A	1364	VAL
1	A	1376	ASP
1	A	1377	ARG
1	A	1381	GLN
1	A	1395	LEU
1	B	48	LEU
1	B	49	LEU
1	B	56	ASN
1	B	64	LEU
1	B	67	ILE

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Mol	Chain	Res	Type
1	B	81	LEU
1	B	82	TYR
1	B	90	ARG
1	B	92	ASP
1	B	109	LEU
1	B	123	TYR
1	B	136	GLU
1	B	144	ILE
1	B	158	HIS
1	B	175	LYS
1	B	178	VAL
1	B	181	ARG
1	B	183	VAL
1	B	192	LYS
1	B	194	PHE
1	B	204	LEU
1	B	213	ARG
1	B	222	HIS
1	B	243	TYR
1	B	300	PHE
1	B	315	THR
1	B	320	LYS
1	B	335	GLU
1	B	342	ARG
1	B	372	ASP
1	B	453	HIS
1	B	460	GLN
1	B	462	ARG
1	B	469	VAL
1	B	521	LEU
1	B	522	GLU
1	B	534	GLU
1	B	538	GLU
1	B	539	GLU
1	B	554	ILE
1	B	555	LYS
1	B	560	ARG
1	B	572	PHE
1	B	573	ILE
1	B	576	LYS
1	B	585	LYS
1	B	589	GLU

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Mol	Chain	Res	Type
1	B	590	ARG
1	B	605	PHE
1	B	612	ASN
1	B	617	MET
1	B	620	ARG
1	B	625	LEU
1	B	641	MET
1	B	662	GLU
1	B	663	ASP
1	B	667	LEU
1	B	668	THR
1	B	670	LEU
1	B	672	VAL
1	B	677	ILE
1	B	678	GLU
1	B	680	HIS
1	B	686	VAL
1	B	729	ASP
1	B	733	LEU
1	B	734	ASP
1	B	741	ASP
1	B	753	LEU
1	B	761	LEU
1	B	769	LEU
1	B	779	GLU
1	B	785	ASP
1	B	809	ARG
1	B	819	ASP
1	B	840	VAL
1	B	868	LEU
1	B	881	ASN
1	B	886	ARG
1	B	889	LEU
1	B	893	TRP
1	B	941	LEU
1	B	945	LEU
1	B	948	THR
1	B	951	ILE
1	B	953	GLU
1	B	958	ARG
1	B	960	TYR
1	B	964	LEU

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Mol	Chain	Res	Type
1	B	976	VAL
1	B	979	LEU
1	B	986	VAL
1	B	997	ASP
1	B	1010	VAL
1	B	1012	ASP
1	B	1016	LEU
1	B	1037	GLU
1	B	1045	SER
1	B	1046	ARG
1	B	1068	HIS
1	B	1071	ASP
1	B	1094	LEU
1	B	1103	PHE
1	B	1105	LEU
1	B	1106	GLU
1	B	1120	ASP
1	B	1122	THR
1	B	1128	ASP
1	B	1132	THR
1	B	1150	LEU
1	B	1203	PHE
1	B	1204	SER
1	B	1211	TYR
1	B	1214	MET
1	B	1215	LEU
1	B	1218	MET
1	B	1224	HIS
1	B	1228	HIS
1	B	1245	ASP
1	B	1246	PHE
1	B	1247	ILE
1	B	1254	TYR
1	B	1258	TYR
1	B	1265	TRP
1	B	1290	LEU
1	B	1291	PHE
1	B	1297	LYS
1	B	1312	TYR
1	B	1362	TYR
1	B	1364	VAL
1	B	1376	ASP

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Mol	Chain	Res	Type
1	B	1377	ARG
1	B	1381	GLN
1	B	1395	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	135	GLN
1	A	158	HIS
1	A	166	GLN
1	A	198	HIS
1	A	222	HIS
1	A	341	ASN
1	A	351	ASN
1	A	359	HIS
1	A	364	GLN
1	A	366	GLN
1	A	452	HIS
1	A	453	HIS
1	A	551	ASN
1	A	618	ASN
1	A	626	GLN
1	A	679	ASN
1	A	728	ASN
1	A	1044	HIS
1	A	1058	GLN
1	A	1082	GLN
1	A	1130	GLN
1	A	1225	HIS
1	A	1227	ASN
1	A	1394	ASN
1	A	1397	GLN
1	B	94	HIS
1	B	135	GLN
1	B	158	HIS
1	B	166	GLN
1	B	198	HIS
1	B	222	HIS
1	B	341	ASN
1	B	351	ASN
1	B	359	HIS

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Mol	Chain	Res	Type
1	B	366	GLN
1	B	618	ASN
1	B	626	GLN
1	B	629	GLN
1	B	679	ASN
1	B	728	ASN
1	B	946	ASN
1	B	1044	HIS
1	B	1058	GLN
1	B	1065	ASN
1	B	1082	GLN
1	B	1130	GLN
1	B	1225	HIS
1	B	1227	ASN
1	B	1397	GLN
1	B	1401	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1254/1382 (90%)	-0.90	2 (0%) 91 82	73, 141, 251, 333	0
1	B	1254/1382 (90%)	-0.81	7 (0%) 85 73	106, 188, 295, 398	0
All	All	2508/2764 (90%)	-0.85	9 (0%) 88 77	73, 168, 272, 398	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	181	ARG	3.6
1	B	851	ASP	3.2
1	B	308	PHE	3.0
1	A	456	HIS	3.0
1	B	667	LEU	2.7
1	B	182	ASP	2.4
1	A	320	LYS	2.3
1	B	742	THR	2.2
1	B	564	VAL	2.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.