



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:27 AM UTC

PDB ID : 3TW7 / pdb_00003tw7
Title : Structure of Rhizobium etli pyruvate carboxylase T882A crystallized without acetyl coenzyme-A
Authors : St Maurice, M.; Kumar, S.; Lietzan, A.D.
Deposited on : 2011-09-21
Resolution : 3.10 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

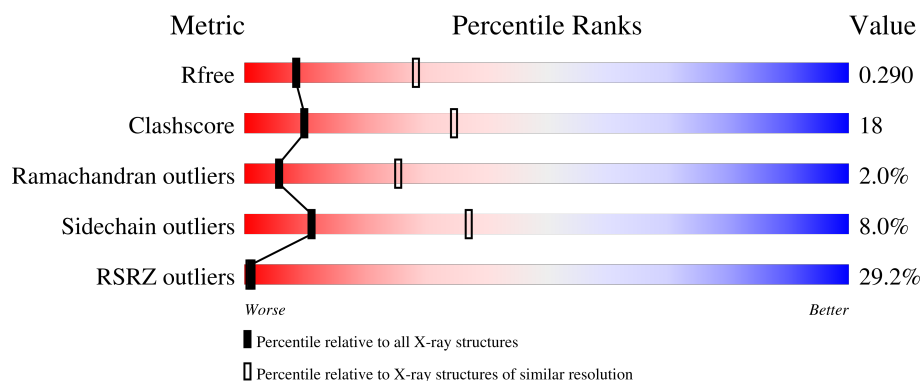
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	1165	28% 54% 29% • 14%
1	B	1165	22% 54% 28% • 14%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15185 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 Pyruvate carboxylase protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1004	Total	C	N	O	S	0	15	0
			7544	4804	1275	1434	31			
1	B	1002	Total	C	N	O	S	0	16	0
			7623	4853	1290	1449	31			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP Q2K340
A	-9	HIS	-	expression tag	UNP Q2K340
A	-8	HIS	-	expression tag	UNP Q2K340
A	-7	HIS	-	expression tag	UNP Q2K340
A	-6	HIS	-	expression tag	UNP Q2K340
A	-5	HIS	-	expression tag	UNP Q2K340
A	-4	HIS	-	expression tag	UNP Q2K340
A	-3	HIS	-	expression tag	UNP Q2K340
A	-2	HIS	-	expression tag	UNP Q2K340
A	-1	HIS	-	expression tag	UNP Q2K340
A	0	GLY	-	expression tag	UNP Q2K340
A	1	GLY	-	expression tag	UNP Q2K340
A	882	ALA	THR	engineered mutation	UNP Q2K340
B	-10	MET	-	expression tag	UNP Q2K340
B	-9	HIS	-	expression tag	UNP Q2K340
B	-8	HIS	-	expression tag	UNP Q2K340
B	-7	HIS	-	expression tag	UNP Q2K340
B	-6	HIS	-	expression tag	UNP Q2K340
B	-5	HIS	-	expression tag	UNP Q2K340
B	-4	HIS	-	expression tag	UNP Q2K340
B	-3	HIS	-	expression tag	UNP Q2K340
B	-2	HIS	-	expression tag	UNP Q2K340
B	-1	HIS	-	expression tag	UNP Q2K340
B	0	GLY	-	expression tag	UNP Q2K340
B	1	GLY	-	expression tag	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
B	882	ALA	THR	engineered mutation	UNP Q2K340

- 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 ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	5	Total	O	0	0
			5	5		





4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	264.16Å 264.16Å 91.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.10) 99.9 (50.00-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.13 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.250 , 0.292 0.248 , 0.290	Depositor DCC
R_{free} test set	2964 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	15185	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ZN, KCX, 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	0.94	6/7719 (0.1%)	1.12	28/10500 (0.3%)
1	B	0.96	2/7799 (0.0%)	1.18	42/10603 (0.4%)
All	All	0.95	8/15518 (0.1%)	1.15	70/21103 (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	1
1	B	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1045	GLN	CD-NE2	7.97	1.50	1.33
1	A	749	HIS	CA-C	-6.75	1.44	1.52
1	A	1043	ASP	CA-C	6.33	1.56	1.53
1	A	573	HIS	CG-CD2	5.89	1.42	1.35
1	A	1045	GLN	CG-CD	5.88	1.66	1.52
1	A	269	LYS	CE-NZ	5.87	1.67	1.49
1	B	713	HIS	ND1-CE1	5.01	1.37	1.32
1	B	745	HIS	CG-CD2	5.00	1.41	1.35

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	499	GLU	N-CA-C	9.06	121.98	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	626	VAL	N-CA-C	-8.20	105.33	113.20
1	B	125	VAL	N-CA-C	-8.18	105.05	112.90
1	B	851	GLN	N-CA-C	-8.15	103.28	113.55
1	A	1043	ASP	N-CA-C	7.84	116.28	108.75
1	A	764	GLU	N-CA-C	-7.48	103.14	111.82
1	B	269	LYS	N-CA-C	7.24	118.95	111.14
1	B	1065	ASP	N-CA-C	7.01	118.43	108.54
1	A	1044	SER	N-CA-C	7.01	119.14	109.54
1	B	409	ALA	CA-C-N	-7.00	112.34	120.12
1	B	409	ALA	C-N-CA	-7.00	112.34	120.12
1	A	1042	THR	N-CA-C	6.59	120.23	110.48
1	B	29	THR	N-CA-C	6.50	119.33	108.73
1	B	403	VAL	N-CA-C	6.48	117.44	107.78
1	A	848	LEU	N-CA-C	6.44	117.96	111.07
1	B	604	LEU	N-CA-C	-6.38	104.41	111.36
1	A	303	GLN	N-CA-C	6.34	119.46	110.14
1	B	881	VAL	N-CA-C	-6.26	99.46	108.42
1	B	736	LEU	N-CA-C	-6.26	104.34	112.23
1	B	444	HIS	CA-C-N	6.25	126.45	119.32
1	B	444	HIS	C-N-CA	6.25	126.45	119.32
1	B	478	THR	N-CA-C	-6.24	104.02	111.69
1	B	143	GLU	CA-C-N	6.22	127.62	119.84
1	B	143	GLU	C-N-CA	6.22	127.62	119.84
1	A	567	ILE	CB-CA-C	6.12	118.50	110.84
1	B	391	GLY	N-CA-C	-6.05	107.28	114.48
1	B	94	SER	N-CA-C	6.03	118.65	111.71
1	A	368	GLY	N-CA-C	5.98	118.80	111.45
1	B	474	THR	N-CA-C	-5.97	104.69	111.14
1	B	499	GLU	CA-C-N	5.94	132.39	121.70
1	B	499	GLU	C-N-CA	5.94	132.39	121.70
1	B	364	ILE	CA-C-N	-5.88	112.31	120.25
1	B	364	ILE	C-N-CA	-5.88	112.31	120.25
1	A	409	ALA	N-CA-C	5.78	114.95	108.25
1	A	692	ARG	CA-C-N	5.64	126.13	120.04
1	A	692	ARG	C-N-CA	5.64	126.13	120.04
1	B	829	LYS	N-CA-C	5.61	120.28	113.38
1	A	55	GLY	CA-C-N	5.58	126.81	119.84
1	A	55	GLY	C-N-CA	5.58	126.81	119.84
1	A	163	VAL	N-CA-C	5.56	116.74	108.46
1	A	364	ILE	CA-C-N	5.54	126.77	119.84
1	A	364	ILE	C-N-CA	5.54	126.77	119.84
1	A	94	SER	N-CA-C	5.54	119.54	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	VAL	N-CA-C	5.51	116.66	108.23
1	B	141	ALA	N-CA-C	5.46	115.23	108.19
1	B	85	ALA	N-CA-C	5.44	117.35	108.76
1	B	534	MET	N-CA-C	-5.41	105.39	111.28
1	B	95	GLU	N-CA-C	5.40	119.56	112.92
1	B	579	LEU	N-CA-C	-5.33	104.36	111.24
1	A	627	GLY	N-CA-C	5.32	125.80	113.18
1	B	55	GLY	CA-C-N	5.30	125.38	119.87
1	B	55	GLY	C-N-CA	5.30	125.38	119.87
1	B	477	LEU	N-CA-C	-5.29	106.83	113.28
1	A	907[A]	SER	CA-C-N	5.29	125.60	119.47
1	A	907[A]	SER	C-N-CA	5.29	125.60	119.47
1	A	907[B]	SER	CA-C-N	5.29	125.60	119.47
1	A	907[B]	SER	C-N-CA	5.29	125.60	119.47
1	A	987	TYR	CB-CA-C	-5.28	104.61	111.15
1	A	845	PHE	N-CA-C	-5.27	106.87	113.72
1	B	358	ASP	CA-C-N	5.23	124.90	119.56
1	B	358	ASP	C-N-CA	5.23	124.90	119.56
1	B	603	ARG	N-CA-C	-5.21	105.50	111.07
1	B	928	GLN	N-CA-C	5.21	117.73	109.40
1	B	218	GLU	N-CA-C	5.20	116.97	108.55
1	B	531	GLY	N-CA-C	-5.19	106.47	112.50
1	A	902	VAL	N-CA-C	5.14	116.60	111.00
1	A	115	ALA	N-CA-C	5.13	116.51	111.02
1	B	363	PHE	N-CA-C	5.12	119.37	113.38
1	A	474	THR	N-CA-C	-5.08	105.39	111.03
1	B	270	ILE	CB-CA-C	-5.04	105.34	112.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1046	GLY	Peptide
1	B	1065	ASP	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	7544	0	7261	257	0
1	B	7623	0	7393	269	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	7	0	0	0	0
5	B	5	0	0	0	0
All	All	15185	0	14654	522	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 18.

All (522) 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:4:SER:O	1:B:28:LYS:HG3	1.53	1.08
1:A:359:PRO:HD3	1:A:433:THR:O	1.55	1.06
1:A:90:TYR:HB2	1:A:301:ARG:HH11	1.21	1.05
1:A:1029:GLY:HA3	1:A:1030:LYS:HB2	1.39	1.04
1:B:1029:GLY:CA	1:B:1030:LYS:HB2	1.88	1.04
1:B:1029:GLY:HA3	1:B:1030:LYS:HB2	1.06	1.03
1:A:90:TYR:HB2	1:A:301:ARG:NH1	1.75	1.00
1:B:361:HIS:CD2	1:B:364:ILE:HD12	1.99	0.98
1:A:221:ILE:HG21	1:A:267:SER:HB3	1.46	0.97
1:B:239:VAL:HG13	1:B:457:ILE:HD11	1.47	0.96
1:A:1042:THR:HB	1:A:1048:VAL:HG22	1.47	0.94
1:A:1029:GLY:HA3	1:A:1030:LYS:CB	1.98	0.93
1:B:1029:GLY:HA3	1:B:1030:LYS:CB	1.99	0.92
1:B:677:CYS:H	1:B:713:HIS:HD2	1.07	0.92
1:B:357:GLU:HG2	1:B:363:PHE:O	1.71	0.90
1:A:356:THR:O	1:A:365:PRO:HA	1.72	0.89
1:B:320:ALA:O	1:B:324:ILE:HB	1.74	0.88
1:A:384:ASP:HB2	1:A:404[B]:LYS:HE2	1.55	0.88
1:B:117:THR:HG21	1:B:276:TYR:CD1	2.10	0.87
1:A:677:CYS:H	1:A:713:HIS:HD2	1.19	0.86
1:B:117:THR:HG21	1:B:276:TYR:HD1	1.38	0.86
1:B:376:ALA:HB2	1:B:425:GLU:HB3	1.55	0.85
1:B:299:ASN:HD22	1:B:303:GLN:NE2	1.74	0.84
1:B:318:VAL:O	1:B:322:ILE:HG13	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLU:O	1:B:77:VAL:HG23	1.78	0.84
1:B:16:ILE:HD13	1:B:386:GLY:HA3	1.60	0.83
1:A:1029:GLY:CA	1:A:1030:LYS:HB2	2.08	0.82
1:B:41:LEU:HB3	1:B:386:GLY:O	1.79	0.81
1:B:860:ARG:C	1:B:862:HIS:H	1.84	0.81
1:B:677:CYS:H	1:B:713:HIS:CD2	1.97	0.79
1:A:35:GLU:HG3	1:A:54:ARG:HD2	1.64	0.79
1:B:52:VAL:HG12	1:B:77:VAL:HG21	1.64	0.78
1:A:13:GLU:O	1:A:16:ILE:N	2.18	0.77
1:A:71:ILE:HA	1:A:74:VAL:HG23	1.64	0.77
1:A:420:ASP:O	1:A:424:ARG:HG3	1.83	0.77
1:A:969:GLU:HG2	1:A:975:GLU:HA	1.65	0.77
1:A:51:GLN:HE22	1:A:54:ARG:CB	1.97	0.77
1:A:1003:PRO:O	1:A:1006:VAL:HG22	1.85	0.77
1:B:299:ASN:ND2	1:B:303:GLN:NE2	2.34	0.76
1:A:862:HIS:CB	1:B:812:PHE:HE2	1.99	0.75
1:B:812:PHE:HD1	1:B:812:PHE:O	1.70	0.75
1:B:414:GLU:OE2	1:B:418:ARG:NH1	2.19	0.75
1:B:860:ARG:O	1:B:862:HIS:N	2.19	0.75
1:A:8:VAL:HG11	1:A:15:ALA:HA	1.67	0.74
1:A:921:MET:HG3	1:A:926:LEU:HD12	1.69	0.74
1:A:359:PRO:CD	1:A:433:THR:O	2.34	0.74
1:A:221:ILE:CG2	1:A:267:SER:HB3	2.18	0.73
1:B:218:GLU:O	1:B:234:GLU:HA	1.89	0.73
1:A:282:VAL:HG13	1:A:298:VAL:HG22	1.70	0.73
1:B:1052:PHE:CD2	1:B:1061:ILE:HD13	2.23	0.73
1:A:224:ASP:HB3	1:A:324:ILE:HG12	1.71	0.72
1:A:338:PRO:HB2	1:A:342:ASP:HB2	1.71	0.72
1:B:547:MET:HG2	1:B:564:ILE:HG23	1.70	0.72
1:B:921:MET:HG3	1:B:926:LEU:HD12	1.69	0.72
1:B:677:CYS:N	1:B:713:HIS:HD2	1.86	0.72
1:A:479:TYR:HB2	1:A:1001:TYR:CD1	2.25	0.71
1:B:429:ARG:HH22	1:B:1058:PRO:HA	1.55	0.71
1:A:74:VAL:HG11	1:A:99:PHE:HE1	1.55	0.71
1:B:922:LEU:HD13	1:B:938:GLN:HA	1.73	0.71
1:B:812:PHE:HD1	1:B:812:PHE:C	1.99	0.71
1:B:221:ILE:HG13	1:B:280:GLY:O	1.91	0.70
1:B:299:ASN:ND2	1:B:303:GLN:HE21	1.90	0.70
1:A:276:TYR:OH	1:A:300:PRO:HA	1.91	0.69
1:B:901:THR:O	1:B:904:ASP:HB2	1.92	0.69
1:B:283:GLU:OE2	1:B:299:ASN:ND2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:CYS:H	1:A:713:HIS:CD2	2.09	0.68
1:A:211:VAL:CG1	1:A:214:ALA:HB2	2.23	0.68
1:A:350:LEU:HD22	1:A:415:ALA:HB1	1.76	0.68
1:A:1029:GLY:HA3	1:A:1030:LYS:CG	2.24	0.68
1:B:114:LYS:H	1:B:277:ILE:HD12	1.59	0.68
1:A:211:VAL:HG12	1:A:214:ALA:HB2	1.76	0.68
1:B:8:VAL:HG11	1:B:15:ALA:HA	1.74	0.67
1:A:90:TYR:CB	1:A:301:ARG:HH11	2.03	0.67
1:B:351[B]:GLN:OE1	1:B:404[B]:LYS:HD2	1.95	0.67
1:A:384:ASP:HB2	1:A:404[A]:LYS:HE2	1.76	0.67
1:B:239:VAL:HG13	1:B:457:ILE:CD1	2.22	0.67
1:B:7:LEU:HA	1:B:30:VAL:HB	1.77	0.66
1:A:862:HIS:CB	1:B:812:PHE:CE2	2.78	0.66
1:B:354:VAL:HG23	1:B:403:VAL:O	1.95	0.66
1:B:52:VAL:CG1	1:B:77:VAL:HG21	2.25	0.65
1:B:427:ARG:HH12	1:B:1037:GLN:HE21	1.44	0.65
1:B:452:TYR:H	1:B:452:TYR:HD2	1.42	0.65
1:B:1048:VAL:N	1:B:1063:VAL:O	2.23	0.65
1:B:136:VAL:HG22	1:B:266:TYR:HB3	1.79	0.65
1:A:667:MET:HG2	1:A:677:CYS:SG	2.37	0.65
1:B:240:GLN:HA	1:B:244:GLN:O	1.97	0.65
1:B:1052:PHE:HD2	1:B:1061:ILE:HD13	1.61	0.64
1:A:569:GLY:O	1:A:573:HIS:HD2	1.81	0.64
1:A:624:ASN:HB2	1:A:627:GLY:HA3	1.79	0.63
1:B:838:HIS:O	1:B:839:GLU:HB2	1.97	0.63
1:A:134:VAL:HG11	1:A:273:ALA:HB2	1.81	0.63
1:B:479:TYR:HB2	1:B:1001:TYR:HB3	1.79	0.63
1:B:234:GLU:OE2	1:B:252:ALA:N	2.31	0.63
1:B:838:HIS:ND1	1:B:840:MET:HG3	2.14	0.63
1:A:411[B]:ASN:HB2	1:A:412:PRO:HD2	1.81	0.63
1:A:972:LEU:O	1:A:973:GLU:HB2	1.98	0.62
1:A:74:VAL:HG11	1:A:99:PHE:CE1	2.34	0.62
1:A:223:GLY:HA2	1:A:228:ASN:O	1.99	0.62
1:B:1044:SER:O	1:B:1045:GLN:HB2	1.98	0.62
1:A:350:LEU:HD23	1:A:407:ALA:O	1.99	0.62
1:A:359:PRO:HG2	1:A:436:THR:OG1	1.99	0.62
1:A:1021:GLU:HB2	1:A:1035:VAL:HG22	1.81	0.62
1:B:312:VAL:CG1	1:B:349:ALA:HB2	2.30	0.62
1:B:892:ALA:O	1:B:896:VAL:HG23	1.99	0.62
1:B:860:ARG:CB	1:B:863:GLN:HE22	2.13	0.61
1:B:53:GLY:N	1:B:73:GLU:OE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:LEU:HD13	1:B:1003:PRO:HD2	1.82	0.61
1:A:283:GLU:OE2	1:A:299:ASN:ND2	2.33	0.61
1:A:381:ILE:HD11	1:A:418:ARG:HG2	1.83	0.60
1:A:96:SER:O	1:A:100:VAL:HG23	2.01	0.60
1:B:235:ARG:HG2	1:B:250:ALA:HB2	1.84	0.60
1:A:444:HIS:HD2	1:A:446:LYS:H	1.49	0.60
1:B:1029:GLY:CA	1:B:1030:LYS:CB	2.65	0.59
1:B:408:TRP:O	1:B:418:ARG:HD2	2.02	0.59
1:A:661:GLU:HA	1:A:661:GLU:OE2	2.01	0.59
1:A:582:GLU:HA	1:A:617:GLN:HB3	1.84	0.59
1:A:494:ARG:HB3	1:A:495:PRO:HD2	1.84	0.59
1:A:530:PHE:O	1:A:533:TRP:HB3	2.01	0.59
1:B:5:LYS:HE2	1:B:28:LYS:HB2	1.83	0.59
1:A:51:GLN:HE22	1:A:54:ARG:HB3	1.68	0.59
1:A:359:PRO:HG3	1:A:434:ASN:HA	1.84	0.59
1:B:33:TRP:HA	1:B:68:TYR:OH	2.02	0.59
1:A:485:VAL:HG12	1:A:486:ASN:ND2	2.18	0.58
1:A:312:VAL:O	1:A:346:ASN:HB3	2.03	0.58
1:B:346:ASN:ND2	1:B:408:TRP:HZ2	2.01	0.58
1:A:231:HIS:CD2	1:A:264:ALA:HB1	2.39	0.58
1:B:427:ARG:NH1	1:B:429:ARG:HH21	2.02	0.58
1:B:812:PHE:C	1:B:812:PHE:CD1	2.72	0.57
1:A:1039:VAL:HG13	1:A:1050:VAL:HG22	1.87	0.57
1:B:376:ALA:CB	1:B:425:GLU:HB3	2.30	0.57
1:B:361:HIS:O	1:B:363:PHE:N	2.37	0.57
1:A:621:ARG:O	1:A:622:GLY:C	2.46	0.56
1:B:33:TRP:CD1	1:B:49:SER:HB2	2.40	0.56
1:A:416:ILE:CG2	1:A:442:ILE:HB	2.35	0.56
1:B:121:LEU:HD13	1:B:298:VAL:HG11	1.87	0.56
1:B:427:ARG:HH12	1:B:1037:GLN:NE2	2.03	0.56
1:A:41:LEU:O	1:A:44:PHE:N	2.38	0.56
1:A:403:VAL:HG22	1:A:404[A]:LYS:H	1.71	0.56
1:B:887:VAL:HG22	1:B:917:SER:HB2	1.88	0.56
1:B:94:SER:O	1:B:118:MET:HE1	2.05	0.55
1:A:416:ILE:HG22	1:A:442:ILE:HB	1.88	0.55
1:B:263[A]:LEU:HG	1:B:293:PHE:CE2	2.42	0.55
1:B:857:LEU:O	1:B:860:ARG:N	2.40	0.55
1:A:847:ASN:O	1:A:851:GLN:HG2	2.06	0.55
1:A:921:MET:CG	1:A:926:LEU:HD12	2.35	0.55
1:B:31:ALA:O	1:B:49:SER:HA	2.07	0.55
1:A:51:GLN:HE22	1:A:54:ARG:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ASP:HB3	1:B:249:ARG:HB2	1.88	0.55
1:B:299:ASN:HD22	1:B:303:GLN:HE22	1.52	0.55
1:B:560:ARG:NH1	1:B:1009:THR:HA	2.20	0.55
1:B:25:LEU:HD11	1:B:319:LYS:HG2	1.87	0.55
1:A:546:THR:HG21	1:A:814:TRP:NE1	2.22	0.54
1:B:229:VAL:HG11	1:B:271:ALA:HB3	1.88	0.54
1:B:555:LEU:HD11	1:B:818:ARG:HG3	1.89	0.54
1:B:634:ASN:CG	1:B:958:GLU:HG3	2.32	0.54
1:A:50:TYR:N	1:A:50:TYR:CD2	2.75	0.54
1:A:560:ARG:NH1	1:A:1009:THR:HA	2.22	0.54
1:A:211:VAL:HG21	1:A:285:LEU:HD13	1.90	0.54
1:B:423:LEU:HD22	1:B:435:LEU:HD23	1.90	0.54
1:B:427:ARG:NH1	1:B:1037:GLN:HE21	2.06	0.54
1:B:860:ARG:CB	1:B:863:GLN:NE2	2.71	0.54
1:A:629:THR:HG23	1:A:630:ASN:N	2.23	0.54
1:A:723:LEU:HD11	1:A:839:GLU:HG2	1.89	0.54
1:A:488:HIS:CE1	1:A:490:GLU:HB2	2.43	0.53
1:A:1048:VAL:N	1:A:1063:VAL:O	2.31	0.53
1:B:296[B]:ILE:HG13	1:B:297:GLU:H	1.73	0.53
1:A:224:ASP:OD1	1:A:224:ASP:N	2.42	0.53
1:A:131:ALA:HA	1:A:270:ILE:HD11	1.90	0.53
1:A:263[B]:LEU:HD11	1:A:284:TYR:CG	2.43	0.53
1:B:667:MET:HG2	1:B:677:CYS:SG	2.48	0.53
1:B:255:LEU:HD11	1:B:293:PHE:HZ	1.74	0.53
1:B:385:GLY:HA2	1:B:403:VAL:HG23	1.91	0.53
1:A:403:VAL:HG22	1:A:404[B]:LYS:H	1.71	0.53
1:A:1043:ASP:CG	1:A:1044:SER:H	2.17	0.53
1:B:71:ILE:HG13	1:B:93:LEU:HD11	1.90	0.53
1:A:396:ARG:O	1:A:397:TYR:CD1	2.62	0.53
1:B:319:LYS:HA	1:B:322:ILE:HD12	1.91	0.53
1:A:423:LEU:HD12	1:A:442:ILE:HD11	1.91	0.52
1:A:282:VAL:HG13	1:A:298:VAL:CG2	2.37	0.52
1:B:12:SER:O	1:B:16:ILE:HD12	2.10	0.52
1:B:279:ALA:HB3	1:B:321:GLN:NE2	2.24	0.52
1:A:340:GLN:HA	1:A:343:ILE:HD12	1.92	0.52
1:B:559:MET:CG	1:B:564:ILE:HD11	2.39	0.52
1:B:62:LEU:O	1:B:63:GLY:O	2.28	0.52
1:B:900:LEU:HD22	1:B:904:ASP:HB3	1.90	0.52
1:A:229:VAL:HG11	1:A:271:ALA:HB3	1.91	0.52
1:A:206:TYR:HE1	1:A:208:GLU:HB2	1.74	0.52
1:A:236:ASP:OD1	1:A:254:TYR:OH	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:PRO:O	1:A:415:ALA:HB3	2.10	0.52
1:A:479:TYR:C	1:A:479:TYR:CD2	2.88	0.52
1:B:113:PRO:HD2	1:B:118:MET:HE3	1.90	0.52
1:A:542:LEU:HD22	1:A:786:LEU:CD1	2.40	0.51
1:B:229:VAL:HG11	1:B:271:ALA:CB	2.40	0.51
1:B:282:VAL:HG13	1:B:295:PHE:HE1	1.75	0.51
1:B:551:HIS:CE1	1:B:559:MET:HB3	2.45	0.51
1:A:111:ILE:HA	1:A:325[B]:LEU:HG	1.91	0.51
1:A:252:ALA:HB3	1:A:255:LEU:HD22	1.93	0.51
1:A:624:ASN:CB	1:A:627:GLY:HA3	2.40	0.51
1:A:867:ALA:O	1:A:871:ALA:N	2.36	0.51
1:B:775:ASP:HB2	1:B:811:SER:OG	2.11	0.51
1:A:97:PRO:HG3	1:A:119:ARG:HG3	1.92	0.51
1:B:429:ARG:HH22	1:B:1058:PRO:CA	2.23	0.51
1:B:450:ASN:HA	1:B:452:TYR:CE2	2.45	0.51
1:A:514:VAL:HG13	1:A:613:ASN:ND2	2.25	0.51
1:B:97:PRO:HB2	1:B:119:ARG:NH1	2.25	0.51
1:B:590:ASP:HB3	1:B:987:TYR:CZ	2.46	0.51
1:B:650:LEU:HA	1:B:676:LEU:HB2	1.92	0.51
1:A:8:VAL:C	1:A:10:ASN:H	2.17	0.51
1:A:838:HIS:O	1:A:839:GLU:HB2	2.10	0.51
1:B:486:ASN:HD21	1:B:1065:ASP:HA	1.76	0.51
1:A:22:ALA:HB1	1:A:27:ILE:HG22	1.93	0.51
1:A:220:GLN:HE21	1:A:235:ARG:HH12	1.58	0.51
1:B:251:PRO:HG3	1:B:345:LEU:HD13	1.93	0.51
1:A:559:MET:CG	1:A:564:ILE:HD11	2.41	0.51
1:B:656:CYS:O	1:B:657:LEU:HD23	2.11	0.51
1:A:130:LEU:HD21	1:A:274:THR:CG2	2.40	0.50
1:A:749:HIS:CE1	1:A:783:GLN:HE22	2.29	0.50
1:B:117:THR:HG22	1:B:121:LEU:HD12	1.91	0.50
1:A:621:ARG:HG3	1:A:625:GLY:O	2.12	0.50
1:A:890:ASP:O	1:A:894:MET:HG2	2.11	0.50
1:A:343:ILE:C	1:A:344:ARG:HG2	2.37	0.50
1:A:657:LEU:O	1:A:658:ASN:HB2	2.12	0.50
1:B:353:ARG:O	1:B:438:LEU:HD11	2.12	0.50
1:B:429:ARG:HD2	1:B:1051:PHE:HB3	1.94	0.50
1:B:1060:ARG:O	1:B:1060:ARG:NH1	2.41	0.50
1:A:359:PRO:HB3	1:A:437:PHE:HB2	1.93	0.50
1:B:57:HIS:CE1	1:B:73:GLU:OE1	2.64	0.50
1:B:356:THR:HG21	1:B:394:ILE:HG21	1.94	0.50
1:A:19:PHE:CD1	1:A:29:THR:HB	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LYS:HE2	1:A:532:GLU:OE2	2.12	0.50
1:A:619:LEU:HD11	1:A:654:PHE:CD2	2.46	0.50
1:B:302:ILE:CD1	1:B:318:VAL:HG22	2.41	0.50
1:B:310:GLU:HG2	1:B:317:ILE:H	1.76	0.50
1:A:270:ILE:HG13	1:A:295:PHE:CE1	2.47	0.49
1:B:812:PHE:O	1:B:812:PHE:CD1	2.58	0.49
1:A:423:LEU:HD12	1:A:442:ILE:CD1	2.42	0.49
1:B:70:SER:O	1:B:74:VAL:HG23	2.12	0.49
1:A:356:THR:HG22	1:A:402:LEU:HD11	1.95	0.49
1:A:694:LYS:NZ	1:A:876:GLY:O	2.44	0.49
1:B:11:ARG:HE	1:B:37:ASP:CG	2.21	0.49
1:B:422:ALA:O	1:B:426:PHE:HD1	1.95	0.49
1:A:474:THR:O	1:A:475:LYS:C	2.55	0.49
1:B:140:PRO:O	1:B:209:LYS:HB2	2.13	0.49
1:A:324:ILE:HG22	1:A:325[B]:LEU:HD22	1.95	0.49
1:A:359:PRO:HD3	1:A:433:THR:C	2.35	0.49
1:B:950:VAL:HG21	1:B:955:LEU:HD21	1.94	0.49
1:B:432:ALA:O	1:B:433:THR:HG22	2.13	0.49
1:A:370:ILE:HD11	1:A:394:ILE:HD11	1.95	0.48
1:B:357:GLU:CG	1:B:363:PHE:O	2.55	0.48
1:B:559:MET:HG3	1:B:564:ILE:HD11	1.95	0.48
1:B:218:GLU:O	1:B:234:GLU:CA	2.61	0.48
1:A:1021:GLU:OE1	1:A:1033:VAL:HG13	2.13	0.48
1:B:5:LYS:HB3	1:B:83:ALA:HA	1.95	0.48
1:A:622:GLY:O	1:A:624:ASN:N	2.46	0.48
1:B:312:VAL:HG12	1:B:408:TRP:HD1	1.78	0.48
1:A:131:ALA:HB2	1:A:295:PHE:CD2	2.49	0.48
1:B:16:ILE:HD13	1:B:386:GLY:CA	2.38	0.48
1:B:323:HIS:HA	1:B:326:ASP:HB2	1.94	0.48
1:A:264:ALA:O	1:A:268:LEU:HG	2.13	0.48
1:A:759:VAL:HG11	1:A:789:ILE:HD13	1.94	0.48
1:B:41:LEU:O	1:B:42:HIS:C	2.55	0.48
1:B:90:TYR:CE2	1:B:304:VAL:HA	2.48	0.48
1:B:131:ALA:HA	1:B:270:ILE:HD11	1.96	0.48
1:B:361:HIS:O	1:B:362:ASN:C	2.56	0.48
1:A:179:ILE:CG2	1:A:180:ARG:N	2.77	0.48
1:A:906:VAL:HG23	1:A:906:VAL:O	2.14	0.48
1:B:302:ILE:CD1	1:B:318:VAL:CG2	2.91	0.48
1:A:677:CYS:N	1:A:713:HIS:HD2	2.00	0.48
1:A:408:TRP:O	1:A:418:ARG:NH2	2.46	0.48
1:A:624:ASN:CG	1:A:627:GLY:HA3	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:O	1:A:10:ASN:N	2.38	0.48
1:A:874:MET:HE1	1:A:891:MET:SD	2.54	0.48
1:B:131:ALA:HA	1:B:270:ILE:CD1	2.44	0.48
1:B:272:GLY:C	1:B:274:THR:H	2.22	0.48
1:B:316:ASP:OD1	1:B:316:ASP:C	2.56	0.48
1:A:224:ASP:HA	1:A:324:ILE:HG23	1.95	0.47
1:A:411[A]:ASN:HB3	1:A:412:PRO:HD2	1.96	0.47
1:A:376:ALA:HB3	1:A:426:PHE:CE1	2.49	0.47
1:B:25:LEU:HG	1:B:319:LYS:HE2	1.96	0.47
1:B:369:ARG:HE	1:B:391:GLY:HA2	1.79	0.47
1:B:477:LEU:HD11	1:B:1054:LEU:HD22	1.96	0.47
1:B:774:MET:HG3	1:B:814:TRP:CD1	2.49	0.47
1:A:627:GLY:HA2	1:A:631:TYR:CE2	2.49	0.47
1:A:881:VAL:C	1:A:885:SER:OG	2.57	0.47
1:B:33:TRP:NE1	1:B:49:SER:HB2	2.29	0.47
1:B:21:ALA:HB1	1:B:319:LYS:HG3	1.97	0.47
1:A:19:PHE:HE2	1:A:42:HIS:HB2	1.79	0.47
1:A:33:TRP:CG	1:A:43:ARG:HD2	2.50	0.47
1:A:131:ALA:HB2	1:A:295:PHE:CE2	2.49	0.47
1:A:308:VAL:HG13	1:A:351[A]:GLN:HE21	1.79	0.47
1:A:350:LEU:O	1:A:419:MET:CE	2.63	0.47
1:A:403:VAL:CG2	1:A:404[A]:LYS:H	2.27	0.47
1:B:309:THR:O	1:B:313:THR:OG1	2.31	0.47
1:A:250:ALA:HB3	1:A:308:VAL:O	2.14	0.47
1:B:137:PRO:O	1:B:295:PHE:HB3	2.15	0.47
1:B:278:GLY:HA2	1:B:324:ILE:HG21	1.97	0.47
1:A:547:MET:O	1:A:551:HIS:NE2	2.45	0.47
1:B:427:ARG:NH1	1:B:1037:GLN:NE2	2.62	0.47
1:A:437:PHE:O	1:A:441:ILE:HG13	2.14	0.47
1:B:52:VAL:HA	1:B:76:ARG:HH22	1.80	0.47
1:B:903:ALA:O	1:B:907[B]:SER:HB3	2.16	0.47
1:A:987:TYR:HB3	1:A:990:VAL:HB	1.97	0.46
1:B:574:ALA:HB1	1:B:806:TRP:CG	2.50	0.46
1:B:921:MET:CG	1:B:926:LEU:HD12	2.42	0.46
1:A:403:VAL:CG2	1:A:404[B]:LYS:H	2.27	0.46
1:A:620:LEU:O	1:A:653:VAL:HA	2.15	0.46
1:B:562:TYR:O	1:B:566:ARG:HG3	2.15	0.46
1:A:29:THR:OG1	1:A:47:ASP:N	2.44	0.46
1:A:551:HIS:CE1	1:A:559:MET:HB3	2.51	0.46
1:A:886:LYS:O	1:A:887:VAL:C	2.58	0.46
1:B:16:ILE:HA	1:B:19:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:TYR:O	1:B:628:TYR:CD1	2.68	0.46
1:A:655:ASP:OD1	1:A:662:ASN:HB3	2.15	0.46
1:B:450:ASN:HA	1:B:452:TYR:CD2	2.50	0.46
1:B:634:ASN:ND2	1:B:958:GLU:CG	2.79	0.46
1:B:90:TYR:HE2	1:B:304:VAL:HA	1.81	0.46
1:A:31:ALA:HB2	1:A:46:ALA:HB2	1.97	0.46
1:B:485:VAL:HG11	1:B:1048:VAL:HG21	1.96	0.46
1:A:206:TYR:CE1	1:A:208:GLU:HB2	2.50	0.46
1:A:887:VAL:CG1	1:A:918:VAL:HA	2.45	0.46
1:B:397:TYR:HB2	1:B:398:TYR:CD2	2.50	0.46
1:B:484:THR:O	1:B:484:THR:HG22	2.15	0.46
1:B:784:PRO:HB2	1:B:789:ILE:HD11	1.98	0.46
1:A:714:ILE:HG12	1:A:743:PRO:HG2	1.98	0.46
1:B:548:ARG:HB3	1:B:582:GLU:OE1	2.16	0.46
1:A:569:GLY:O	1:A:573:HIS:CD2	2.65	0.46
1:A:251:PRO:HD2	1:A:348:HIS:CD2	2.51	0.45
1:A:791:GLU:OE2	1:B:725:LYS:NZ	2.49	0.45
1:A:940:LYS:O	1:A:941:ALA:C	2.59	0.45
1:B:231:HIS:CE1	1:B:264:ALA:HB1	2.50	0.45
1:B:838:HIS:CE1	1:B:845:PHE:CE1	3.04	0.45
1:A:407:ALA:H	1:A:419:MET:HE2	1.82	0.45
1:B:838:HIS:O	1:B:839:GLU:CB	2.64	0.45
1:B:882:ALA:HA	1:B:883:PRO:HA	1.77	0.45
1:A:389:TYR:CE2	1:A:392:ALA:HB2	2.52	0.45
1:B:99:PHE:O	1:B:100:VAL:C	2.57	0.45
1:B:834:GLU:HG3	1:B:838:HIS:NE2	2.32	0.45
1:A:519:LYS:HD2	1:A:519:LYS:O	2.17	0.45
1:A:759:VAL:O	1:A:763:VAL:HG23	2.16	0.45
1:B:30:VAL:HA	1:B:48:GLU:HG3	1.99	0.45
1:B:401:LEU:HD21	1:B:404[B]:LYS:HG3	1.98	0.45
1:A:8:VAL:C	1:A:10:ASN:N	2.75	0.45
1:A:1027:GLU:O	1:A:1029:GLY:N	2.50	0.45
1:B:860:ARG:C	1:B:862:HIS:N	2.55	0.45
1:B:110:PHE:CE2	1:B:112:GLY:HA3	2.51	0.45
1:B:1044:SER:C	1:B:1046:GLY:H	2.24	0.45
1:A:286:MET:HE2	1:A:291:GLY:HA2	1.97	0.45
1:A:629:THR:HG23	1:A:630:ASN:H	1.81	0.45
1:B:117:THR:HG21	1:B:276:TYR:CE1	2.51	0.45
1:B:121:LEU:HD22	1:B:298:VAL:HB	1.99	0.45
1:B:361:HIS:O	1:B:364:ILE:HG13	2.15	0.45
1:A:22:ALA:HB1	1:A:27:ILE:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:VAL:CG1	1:B:349:ALA:CB	2.95	0.44
1:B:678:GLU:OE1	1:B:714:ILE:HG21	2.16	0.44
1:A:574:ALA:HB1	1:A:806:TRP:CG	2.53	0.44
1:B:113:PRO:CD	1:B:118:MET:HE3	2.47	0.44
1:B:263[A]:LEU:HD23	1:B:263[A]:LEU:HA	1.83	0.44
1:A:270:ILE:HG21	1:A:298:VAL:HG21	1.98	0.44
1:A:358:ASP:HB2	1:A:432:ALA:HB1	1.99	0.44
1:A:474:THR:HG23	1:A:1059:ARG:NH2	2.32	0.44
1:B:7:LEU:HD13	1:B:78:ALA:HA	1.99	0.44
1:A:6:ILE:O	1:A:30:VAL:N	2.51	0.44
1:A:895:MET:O	1:A:900:LEU:N	2.47	0.44
1:B:220:GLN:HE21	1:B:235:ARG:HH12	1.65	0.44
1:A:549:ASP:OD2	1:A:747:HIS:CE1	2.71	0.44
1:A:922:LEU:HD13	1:A:938:GLN:HA	2.00	0.44
1:A:281:THR:O	1:A:298:VAL:HG13	2.18	0.44
1:A:810:ILE:O	1:A:811:SER:C	2.58	0.44
1:B:16:ILE:HA	1:B:19:PHE:HD2	1.83	0.44
1:A:103:CYS:SG	1:A:108:ILE:HB	2.58	0.44
1:A:249:ARG:HD3	1:A:253:PRO:HG3	2.00	0.44
1:A:411[B]:ASN:HB2	1:A:412:PRO:CD	2.47	0.44
1:A:559:MET:HG2	1:A:564:ILE:HD11	1.99	0.44
1:A:592:SER:HA	1:A:596:LEU:HB2	2.00	0.44
1:B:474:THR:O	1:B:475:LYS:C	2.60	0.44
1:A:216:HIS:NE2	1:A:283:GLU:HB3	2.32	0.44
1:A:376:ALA:HB2	1:A:425:GLU:HG2	2.00	0.44
1:A:627:GLY:HA2	1:A:631:TYR:HE2	1.83	0.44
1:B:449:ASP:O	1:B:450:ASN:HB2	2.18	0.44
1:A:299:ASN:HA	1:A:300:PRO:HD3	1.70	0.44
1:A:381:ILE:CD1	1:A:407:ALA:HB2	2.48	0.44
1:A:729:ALA:HB2	1:A:758:THR:HG23	1.99	0.44
1:B:282:VAL:HG13	1:B:295:PHE:CE1	2.51	0.44
1:A:222:LEU:HD13	1:A:337:VAL:HG21	2.00	0.43
1:A:240:GLN:HG2	1:A:245:LYS:HA	2.00	0.43
1:A:316:ASP:HB3	1:A:319:LYS:HB2	2.00	0.43
1:B:100:VAL:HG22	1:B:110:PHE:CZ	2.52	0.43
1:B:239:VAL:CG1	1:B:457:ILE:HD11	2.32	0.43
1:B:627:GLY:HA3	1:B:631:TYR:CE2	2.53	0.43
1:B:248:GLU:HG2	1:B:305:GLU:HB3	2.01	0.43
1:B:628:TYR:CD1	1:B:628:TYR:C	2.96	0.43
1:A:350:LEU:CD2	1:A:415:ALA:HB1	2.48	0.43
1:A:667:MET:HE1	1:A:710:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:ALA:HB1	1:B:754:ILE:HG22	2.01	0.43
1:B:1032:LEU:HD22	1:B:1054:LEU:HD11	2.00	0.43
1:B:634:ASN:ND2	1:B:958:GLU:HG2	2.33	0.43
1:A:226:HIS:HE1	1:A:327:GLY:O	2.01	0.43
1:A:414:GLU:OE2	1:A:418:ARG:NH1	2.51	0.43
1:B:1060:ARG:C	1:B:1061:ILE:HD12	2.43	0.43
1:A:1065:ASP:OD2	1:A:1065:ASP:C	2.61	0.43
1:B:62:LEU:O	1:B:67:SER:OG	2.37	0.43
1:B:279:ALA:HB3	1:B:321:GLN:HE21	1.83	0.43
1:B:560:ARG:HH11	1:B:1009:THR:HA	1.83	0.43
1:B:599:ASP:HA	1:B:600:PRO:HD2	1.89	0.43
1:B:929:PRO:O	1:B:930:PRO:C	2.61	0.43
1:A:108:ILE:H	1:A:108:ILE:HG13	1.70	0.43
1:A:141:ALA:HA	1:A:207:LEU:O	2.18	0.43
1:B:304:VAL:HG21	1:B:353:ARG:HE	1.83	0.43
1:B:914:PHE:CD2	1:B:941:ALA:HA	2.54	0.43
1:A:11:ARG:HB3	1:A:68:TYR:CE1	2.53	0.43
1:A:310:GLU:OE1	1:A:382:ARG:NH1	2.34	0.43
1:A:557:THR:HG21	1:A:587:ALA:HB3	2.01	0.43
1:A:874:MET:HB3	1:A:874:MET:HE2	1.58	0.43
1:B:308:VAL:O	1:B:312:VAL:HG22	2.19	0.43
1:B:871:ALA:O	1:B:872:ASN:C	2.61	0.43
1:B:881:VAL:O	1:B:882:ALA:C	2.62	0.43
1:B:803:ASP:O	1:B:807:ILE:HG13	2.19	0.43
1:A:90:TYR:CB	1:A:301:ARG:NH1	2.65	0.42
1:A:382:ARG:HB3	1:A:406:THR:HB	2.01	0.42
1:A:546:THR:HG21	1:A:814:TRP:CE2	2.54	0.42
1:B:282:VAL:HA	1:B:298:VAL:HG22	2.01	0.42
1:B:449:ASP:C	1:B:449:ASP:OD1	2.62	0.42
1:B:41:LEU:HD12	1:B:44:PHE:HB2	2.01	0.42
1:A:671:ALA:O	1:A:672:GLU:C	2.62	0.42
1:B:416:ILE:O	1:B:420:ASP:HB2	2.20	0.42
1:B:421:ARG:C	1:B:421:ARG:HD2	2.44	0.42
1:B:987:TYR:HB3	1:B:990:VAL:HB	2.02	0.42
1:A:53:GLY:N	1:A:73:GLU:OE2	2.47	0.42
1:A:1037:GLN:HB2	1:A:1051:PHE:O	2.19	0.42
1:B:272:GLY:O	1:B:274:THR:N	2.52	0.42
1:A:85:ALA:HA	1:A:109:ILE:O	2.19	0.42
1:A:90:TYR:HB3	1:A:302:ILE:O	2.19	0.42
1:B:245:LYS:HB3	1:B:248:GLU:OE2	2.19	0.42
1:B:263[A]:LEU:HG	1:B:293:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:724:LEU:HD23	1:B:746:PHE:CZ	2.55	0.42
1:B:894:MET:HE2	1:B:894:MET:HB3	1.88	0.42
1:A:14:ILE:HD12	1:A:14:ILE:HA	1.89	0.42
1:B:7:LEU:HD13	1:B:78:ALA:CA	2.49	0.42
1:B:14:ILE:HD12	1:B:17:ARG:HB3	2.00	0.42
1:B:324:ILE:HG22	1:B:325[A]:LEU:HD12	2.01	0.42
1:A:218:GLU:OE2	1:A:305:GLU:HG3	2.20	0.42
1:B:311:VAL:HG13	1:B:382:ARG:HH11	1.85	0.42
1:B:312:VAL:HG11	1:B:349:ALA:CB	2.49	0.42
1:A:220:GLN:HB2	1:A:235:ARG:HH12	1.85	0.42
1:A:479:TYR:O	1:A:483:VAL:HG12	2.19	0.42
1:A:929:PRO:HG2	1:A:932:GLY:O	2.20	0.42
1:A:33:TRP:CD1	1:A:43:ARG:HD2	2.55	0.42
1:A:238:SER:HB2	1:A:452:TYR:CE1	2.54	0.42
1:A:882:ALA:HA	1:A:883:PRO:HA	1.87	0.42
1:B:96:SER:O	1:B:100:VAL:HG23	2.20	0.42
1:B:551:HIS:ND1	1:B:559:MET:HB3	2.35	0.42
1:B:834:GLU:HG3	1:B:838:HIS:HE2	1.85	0.42
1:A:548:ARG:HB3	1:A:582:GLU:OE1	2.19	0.42
1:B:40:ALA:O	1:B:43:ARG:HG2	2.20	0.42
1:B:838:HIS:NE2	1:B:845:PHE:HE1	2.18	0.42
1:B:1021:GLU:HB2	1:B:1035:VAL:HG22	2.02	0.42
1:A:358:ASP:HB2	1:A:432:ALA:CB	2.50	0.41
1:A:494:ARG:HB2	1:A:823:ALA:HB1	2.02	0.41
1:B:145:LEU:HA	1:B:146:PRO:HD2	1.90	0.41
1:B:270:ILE:O	1:B:274:THR:HG23	2.19	0.41
1:B:452:TYR:CD2	1:B:452:TYR:N	2.83	0.41
1:A:622:GLY:O	1:A:623:ALA:C	2.62	0.41
1:A:1008:PRO:HG2	1:A:1022:LEU:HD11	2.02	0.41
1:B:17:ARG:NH1	1:B:21:ALA:HB2	2.35	0.41
1:A:366:ASP:HB3	1:A:431:VAL:HB	2.01	0.41
1:A:541:LEU:HB3	1:A:579:LEU:HB2	2.03	0.41
1:A:112:GLY:O	1:A:277:ILE:HB	2.19	0.41
1:A:282:VAL:HG12	1:A:284:TYR:CE2	2.55	0.41
1:B:25:LEU:CD1	1:B:319:LYS:HG2	2.50	0.41
1:B:346:ASN:ND2	1:B:408:TRP:CZ2	2.85	0.41
1:B:1046:GLY:O	1:B:1064:PRO:HA	2.19	0.41
1:A:323:HIS:HB3	1:A:328:ALA:HB3	2.02	0.41
1:A:375:SER:HA	1:A:426:PHE:CE2	2.56	0.41
1:A:871:ALA:O	1:A:872:ASN:C	2.63	0.41
1:B:114:LYS:HG3	1:B:277:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:GLU:O	1:B:308:VAL:HG22	2.19	0.41
1:A:62:LEU:HB2	1:A:67:SER:OG	2.21	0.41
1:A:546:THR:HG21	1:A:814:TRP:CD1	2.55	0.41
1:A:955:LEU:HD23	1:A:955:LEU:HA	1.91	0.41
1:B:71:ILE:HG23	1:B:99:PHE:HD1	1.84	0.41
1:A:19:PHE:HD1	1:A:29:THR:HB	1.84	0.41
1:A:350:LEU:O	1:A:419:MET:HE2	2.20	0.41
1:B:54:ARG:HE	1:B:54:ARG:HB2	1.56	0.41
1:B:252:ALA:HA	1:B:253:PRO:HD2	1.95	0.41
1:B:374[A]:ARG:NH2	1:B:427:ARG:HD3	2.36	0.41
1:B:659:TRP:CE2	1:B:661:GLU:HB3	2.56	0.41
1:B:1052:PHE:CE2	1:B:1061:ILE:HD13	2.55	0.41
1:A:348:HIS:O	1:A:409:ALA:N	2.44	0.41
1:B:664:ARG:O	1:B:665:VAL:C	2.61	0.41
1:A:102:ALA:HA	1:A:105:LYS:HB3	2.03	0.41
1:A:220:GLN:HE21	1:A:235:ARG:NH1	2.17	0.41
1:A:419:MET:O	1:A:423:LEU:HG	2.20	0.41
1:A:444:HIS:HA	1:A:445:PRO:HD3	1.88	0.41
1:A:887:VAL:HG22	1:A:917:SER:HB2	2.02	0.41
1:B:99:PHE:C	1:B:101:ASP:N	2.77	0.41
1:B:249:ARG:CZ	1:B:253:PRO:HG3	2.50	0.41
1:B:373:TYR:C	1:B:374[B]:ARG:HG3	2.46	0.41
1:B:383:LEU:HD22	1:B:405:VAL:HG22	2.03	0.41
1:B:296[B]:ILE:HG13	1:B:297:GLU:N	2.35	0.41
1:B:747:HIS:HB2	1:B:771:ASP:OD2	2.21	0.41
1:A:703:LEU:HD23	1:A:703:LEU:HA	1.81	0.40
1:A:793:LEU:HD23	1:A:793:LEU:HA	1.85	0.40
1:B:91:GLY:O	1:B:92:LEU:C	2.63	0.40
1:B:558:ARG:HA	1:B:558:ARG:HD3	1.88	0.40
1:B:1052:PHE:HD2	1:B:1061:ILE:CD1	2.31	0.40
1:A:357:GLU:O	1:A:434:ASN:HB3	2.21	0.40
1:B:63:GLY:O	1:B:67:SER:OG	2.39	0.40
1:B:223:GLY:O	1:B:277:ILE:HA	2.21	0.40
1:B:382:ARG:O	1:B:383:LEU:HD23	2.20	0.40
1:B:843:GLY:C	1:B:844:GLN:HG3	2.46	0.40
1:A:50:TYR:HB2	1:A:77:VAL:HG13	2.03	0.40
1:A:527:PRO:HB2	1:A:713:HIS:CE1	2.56	0.40
1:B:113:PRO:O	1:B:114:LYS:C	2.64	0.40
1:B:519:LYS:HA	1:B:615:LEU:HD23	2.03	0.40
1:A:218:GLU:CD	1:A:237:CYS:SG	3.04	0.40
1:A:424:ARG:O	1:A:426:PHE:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLN:HE21	1:A:120:GLN:HB3	1.66	0.40
1:B:248:GLU:HB3	1:B:305:GLU:HB2	2.04	0.40
1:B:624:ASN:HB2	1:B:631:TYR:CD2	2.56	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	1001/1165 (86%)	875 (87%)	107 (11%)	19 (2%)	6	27
1	B	1002/1165 (86%)	899 (90%)	82 (8%)	21 (2%)	5	25
All	All	2003/2330 (86%)	1774 (89%)	189 (9%)	40 (2%)	6	25

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	622	GLY
1	A	623	ALA
1	A	1030	LYS
1	B	92	LEU
1	B	145	LEU
1	B	362	ASN
1	B	500	ASN
1	B	861	TRP
1	B	1030	LYS
1	A	425	GLU
1	A	492	LYS
1	A	627	GLY
1	A	1028	LYS
1	A	1040	SER

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Mol	Chain	Res	Type
1	A	1045	GLN
1	B	63	GLY
1	B	66	GLU
1	B	144	PRO
1	B	273	ALA
1	A	9	ALA
1	A	458	ASP
1	A	1065	ASP
1	B	209	LYS
1	B	301	ARG
1	B	886	LYS
1	A	177	ARG
1	A	292	LYS
1	B	9	ALA
1	B	12	SER
1	A	911	GLU
1	B	250	ALA
1	B	356	THR
1	B	333	PRO
1	B	450	ASN
1	A	64	PRO
1	A	140	PRO
1	B	338	PRO
1	A	457	ILE
1	B	251	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	749/933 (80%)	695 (93%)	54 (7%)	13	40
1	B	769/933 (82%)	701 (91%)	68 (9%)	9	33
All	All	1518/1866 (81%)	1396 (92%)	122 (8%)	11	37

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ILE
1	A	37	ASP
1	A	50	TYR
1	A	51	GLN
1	A	54	ARG
1	A	71	ILE
1	A	81	SER
1	A	90	TYR
1	A	100	VAL
1	A	108	ILE
1	A	128	ARG
1	A	145	LEU
1	A	168	SER
1	A	179	ILE
1	A	217	VAL
1	A	224	ASP
1	A	232	LEU
1	A	234	GLU
1	A	239	VAL
1	A	277	ILE
1	A	282	VAL
1	A	286	MET
1	A	304	VAL
1	A	344	ARG
1	A	364	ILE
1	A	370	ILE
1	A	393	ILE
1	A	394	ILE
1	A	416	ILE
1	A	459	THR
1	A	474	THR
1	A	514	VAL
1	A	521	LEU
1	A	542	LEU
1	A	557	THR
1	A	584	TRP
1	A	597	THR
1	A	621	ARG
1	A	630	ASN
1	A	720	MET
1	A	796	SER
1	A	848	LEU
1	A	854	SER

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Mol	Chain	Res	Type
1	A	860	ARG
1	A	884	SER
1	A	885	SER
1	A	891	MET
1	A	913	SER
1	A	919	VAL
1	A	931	SER
1	A	958	GLU
1	A	1021	GLU
1	A	1031	THR
1	A	1045	GLN
1	B	6	ILE
1	B	10	ASN
1	B	30	VAL
1	B	69	LEU
1	B	90	TYR
1	B	120	GLN
1	B	134	VAL
1	B	145	LEU
1	B	168	SER
1	B	178	VAL
1	B	179	ILE
1	B	219	SER
1	B	221	ILE
1	B	225	THR
1	B	232	LEU
1	B	254	TYR
1	B	262	GLU
1	B	263[A]	LEU
1	B	263[B]	LEU
1	B	267	SER
1	B	270	ILE
1	B	274	THR
1	B	277	ILE
1	B	289	ASP
1	B	309	THR
1	B	324	ILE
1	B	325[A]	LEU
1	B	325[B]	LEU
1	B	326	ASP
1	B	334	GLN
1	B	350	LEU

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Mol	Chain	Res	Type
1	B	354	VAL
1	B	381	ILE
1	B	387	THR
1	B	399	ASP
1	B	401	LEU
1	B	403	VAL
1	B	427	ARG
1	B	433	THR
1	B	436	THR
1	B	452	TYR
1	B	457	ILE
1	B	514	VAL
1	B	521	LEU
1	B	524	THR
1	B	542	LEU
1	B	557	THR
1	B	584	TRP
1	B	590	ASP
1	B	597	THR
1	B	720	MET
1	B	748	THR
1	B	804	PRO
1	B	812	PHE
1	B	863	GLN
1	B	884	SER
1	B	885	SER
1	B	894	MET
1	B	902	VAL
1	B	907[A]	SER
1	B	907[B]	SER
1	B	931	SER
1	B	998	SER
1	B	1025	ASP
1	B	1042	THR
1	B	1044	SER
1	B	1060	ARG
1	B	1066	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN

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Mol	Chain	Res	Type
1	A	216	HIS
1	A	220	GLN
1	A	226	HIS
1	A	348	HIS
1	A	444	HIS
1	A	486	ASN
1	A	573	HIS
1	A	577	ASN
1	A	630	ASN
1	A	713	HIS
1	A	783	GLN
1	A	820	GLN
1	A	847	ASN
1	A	873	GLN
1	A	928	GLN
1	A	1057	GLN
1	B	10	ASN
1	B	57	HIS
1	B	120	GLN
1	B	220	GLN
1	B	231	HIS
1	B	240	GLN
1	B	299	ASN
1	B	334	GLN
1	B	339	ASN
1	B	346	ASN
1	B	361	HIS
1	B	486	ASN
1	B	536	ASN
1	B	630	ASN
1	B	713	HIS
1	B	847	ASN
1	B	863	GLN
1	B	1037	GLN
1	B	1057	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	KCX	B	718[A]	3,1	10,11,12	0.94	0	6,12,14	0.92	0
1	KCX	A	718[A]	3,1	10,11,12	0.72	0	6,12,14	1.02	1 (16%)

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
1	KCX	B	718[A]	3,1	-	3/9/10/12	-
1	KCX	A	718[A]	3,1	-	1/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	718[A]	KCX	CD-CG-CB	-2.22	105.24	113.62

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	718[A]	KCX	O-C-CA-CB
1	B	718[A]	KCX	O-C-CA-CB
1	B	718[A]	KCX	CG-CD-CE-NZ
1	B	718[A]	KCX	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	1003/1165 (86%)	1.17	330 (32%)  	16, 71, 162, 191	22 (2%)
1	B	1001/1165 (85%)	0.93	255 (25%)  	17, 56, 139, 190	22 (2%)
All	All	2004/2330 (86%)	1.05	585 (29%)  	16, 64, 156, 191	44 (2%)

All (585) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	LEU	10.9
1	B	335	SER	9.3
1	A	285	LEU	8.8
1	B	167	ALA	8.2
1	A	367	TYR	7.1
1	A	313	THR	6.8
1	B	386	GLY	6.8
1	A	146	PRO	6.8
1	B	376	ALA	6.5
1	B	95	GLU	6.3
1	B	377	SER	6.3
1	A	121	LEU	6.0
1	B	132	ILE	5.8
1	B	144	PRO	5.7
1	A	322	ILE	5.7
1	B	27	ILE	5.6
1	B	206	TYR	5.5
1	A	144	PRO	5.5
1	A	10	ASN	5.2
1	A	434	ASN	5.2
1	A	214	ALA	5.2
1	A	298	VAL	5.1
1	A	225	THR	5.1
1	B	341[A]	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	232	LEU	5.1
1	A	279	ALA	5.0
1	A	432	ALA	5.0
1	B	91	GLY	5.0
1	A	401	LEU	5.0
1	B	86	ILE	5.0
1	A	221	ILE	5.0
1	A	389	TYR	5.0
1	A	335	SER	4.9
1	B	861	TRP	4.9
1	A	904	ASP	4.9
1	A	96	SER	4.9
1	B	134	VAL	4.9
1	A	180	ARG	4.8
1	A	315	ILE	4.8
1	A	164	MET	4.8
1	A	99	PHE	4.8
1	A	336	GLY	4.8
1	A	431	VAL	4.8
1	A	386	GLY	4.7
1	A	290	THR	4.7
1	A	296[A]	ILE	4.7
1	B	315	ILE	4.7
1	A	168	SER	4.7
1	A	123	ASN	4.7
1	B	379	PHE	4.7
1	B	123	ASN	4.7
1	B	346	ASN	4.7
1	B	434	ASN	4.7
1	A	1043	ASP	4.6
1	A	457	ILE	4.6
1	A	360	GLU	4.6
1	B	168	SER	4.6
1	B	165	LEU	4.6
1	A	454	THR	4.6
1	A	222	LEU	4.5
1	B	180	ARG	4.5
1	A	284	TYR	4.5
1	B	419	MET	4.5
1	A	303	GLN	4.5
1	B	29	THR	4.4
1	B	345	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	334	GLN	4.4
1	B	277	ILE	4.4
1	A	176	MET	4.3
1	A	98[A]	GLU	4.3
1	A	117	THR	4.3
1	B	146	PRO	4.3
1	A	270	ILE	4.3
1	B	241	ARG	4.3
1	B	352[A]	CYS	4.3
1	B	222	LEU	4.3
1	B	179	ILE	4.3
1	B	125	VAL	4.3
1	A	6	ILE	4.3
1	A	399	ASP	4.3
1	A	406	THR	4.2
1	B	387	THR	4.2
1	B	96	SER	4.2
1	B	348	HIS	4.2
1	B	278	GLY	4.2
1	A	275	ASN	4.2
1	A	108	ILE	4.2
1	B	296[A]	ILE	4.2
1	B	128	ARG	4.2
1	A	334	GLN	4.2
1	A	115	ALA	4.2
1	A	231	HIS	4.2
1	A	312	VAL	4.1
1	B	145	LEU	4.1
1	A	295	PHE	4.1
1	A	267	SER	4.1
1	B	331	GLY	4.1
1	B	285	LEU	4.1
1	B	301	ARG	4.1
1	A	136	VAL	4.1
1	A	114	LYS	4.1
1	B	124	LYS	4.1
1	B	131	ALA	4.1
1	A	909	ASP	4.1
1	A	460	THR	4.1
1	B	162	PRO	4.1
1	A	211	VAL	4.0
1	A	450	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	211	VAL	4.0
1	A	416	ILE	4.0
1	B	25	LEU	4.0
1	B	166	LYS	4.0
1	B	267	SER	4.0
1	A	274	THR	4.0
1	A	394	ILE	4.0
1	B	272	GLY	4.0
1	A	132	ILE	4.0
1	A	85	ALA	4.0
1	B	127	ALA	4.0
1	A	325[A]	LEU	4.0
1	B	336	GLY	4.0
1	A	411[A]	ASN	4.0
1	B	112	GLY	3.9
1	A	855	LEU	3.9
1	B	270	ILE	3.9
1	A	110	PHE	3.9
1	A	363	PHE	3.9
1	A	92	LEU	3.9
1	B	113	PRO	3.9
1	A	119	ARG	3.9
1	A	226	HIS	3.9
1	B	323	HIS	3.9
1	A	223	GLY	3.9
1	A	3	ILE	3.9
1	A	849	LYS	3.9
1	A	321	GLN	3.8
1	A	167	ALA	3.8
1	A	112	GLY	3.8
1	B	142	THR	3.8
1	A	317	ILE	3.8
1	A	215	ARG	3.8
1	A	116[A]	ASP	3.8
1	A	415	ALA	3.8
1	A	65	ILE	3.8
1	B	423	LEU	3.8
1	B	283	GLU	3.8
1	B	178	VAL	3.8
1	A	408	TRP	3.8
1	A	437	PHE	3.8
1	A	304	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	230	VAL	3.7
1	A	238	SER	3.7
1	A	130	LEU	3.7
1	B	413	LEU	3.7
1	B	21	ALA	3.7
1	A	857	LEU	3.7
1	A	292	LYS	3.7
1	A	294	TYR	3.7
1	B	297	GLU	3.7
1	A	239	VAL	3.7
1	A	124	LYS	3.7
1	B	269	LYS	3.7
1	A	388	SER	3.7
1	A	273	ALA	3.7
1	A	351[A]	GLN	3.7
1	A	87	HIS	3.7
1	A	179	ILE	3.7
1	A	364	ILE	3.7
1	A	207	LEU	3.7
1	A	848	LEU	3.7
1	B	130	LEU	3.7
1	A	113	PRO	3.6
1	A	338	PRO	3.6
1	B	258	ALA	3.6
1	A	145	LEU	3.6
1	B	326	ASP	3.6
1	A	442	ILE	3.6
1	A	265	ALA	3.6
1	A	90	TYR	3.6
1	B	109	ILE	3.6
1	A	344	ARG	3.6
1	B	455	ARG	3.6
1	A	337	VAL	3.6
1	A	407	ALA	3.6
1	B	138	VAL	3.6
1	A	286	MET	3.6
1	B	6	ILE	3.6
1	A	410	PRO	3.5
1	A	58	LEU	3.5
1	A	109	ILE	3.5
1	A	302	ILE	3.5
1	B	399	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	852	ALA	3.5
1	B	137	PRO	3.5
1	A	309	THR	3.5
1	B	140	PRO	3.5
1	A	453	THR	3.5
1	A	314	GLY	3.5
1	B	94	SER	3.5
1	A	412	PRO	3.5
1	B	2	PRO	3.5
1	B	231	HIS	3.5
1	A	300	PRO	3.5
1	A	326	ASP	3.5
1	A	850	GLU	3.4
1	A	28	LYS	3.4
1	B	233	PHE	3.4
1	B	339	ASN	3.4
1	A	413	LEU	3.4
1	B	412	PRO	3.4
1	B	234	GLU	3.4
1	A	233	PHE	3.4
1	A	846	THR	3.4
1	B	85	ALA	3.4
1	B	242	ARG	3.4
1	A	111	ILE	3.4
1	A	129	ASN	3.4
1	A	381	ILE	3.4
1	B	375	SER	3.4
1	B	426	PHE	3.4
1	B	343	ILE	3.4
1	A	390	SER	3.4
1	A	125	VAL	3.4
1	A	230	VAL	3.4
1	B	121	LEU	3.4
1	A	276	TYR	3.4
1	B	271	ALA	3.4
1	B	327	GLY	3.4
1	A	133	SER	3.3
1	A	1044	SER	3.3
1	B	205	VAL	3.3
1	A	287	ASP	3.3
1	B	116[A]	ASP	3.3
1	A	118	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	135	GLY	3.3
1	B	284	TYR	3.3
1	B	288	ALA	3.3
1	B	385	GLY	3.3
1	A	1042	THR	3.3
1	B	408	TRP	3.3
1	A	13	GLU	3.3
1	A	387	THR	3.3
1	A	861	TRP	3.3
1	A	140	PRO	3.3
1	B	330	ILE	3.3
1	A	81	SER	3.3
1	B	97	PRO	3.3
1	B	308	VAL	3.3
1	A	455	ARG	3.2
1	A	353	ARG	3.2
1	B	417	SER	3.2
1	A	2	PRO	3.2
1	A	246	VAL	3.2
1	A	249	ARG	3.2
1	A	853	ARG	3.2
1	B	353	ARG	3.2
1	A	62	LEU	3.2
1	B	208	GLU	3.2
1	A	333	PRO	3.2
1	A	371	THR	3.2
1	A	435	LEU	3.1
1	B	265	ALA	3.1
1	B	384	ASP	3.1
1	B	360	GLU	3.1
1	A	405	VAL	3.1
1	A	426	PHE	3.1
1	A	370	ILE	3.1
1	B	324	ILE	3.1
1	B	381	ILE	3.1
1	B	409	ALA	3.1
1	A	142	THR	3.1
1	A	268	LEU	3.1
1	B	337	VAL	3.1
1	B	260	ARG	3.1
1	B	344	ARG	3.1
1	A	1047	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	302	ILE	3.1
1	A	383	LEU	3.1
1	B	332	THR	3.1
1	B	139	VAL	3.1
1	A	71	ILE	3.1
1	A	306	HIS	3.1
1	B	226	HIS	3.1
1	A	863	GLN	3.1
1	B	383	LEU	3.1
1	A	373	TYR	3.1
1	A	258	ALA	3.0
1	A	362	ASN	3.0
1	A	74	VAL	3.0
1	B	257	GLU	3.0
1	B	276	TYR	3.0
1	A	7	LEU	3.0
1	B	328	ALA	3.0
1	B	347	GLY	3.0
1	A	137	PRO	3.0
1	B	251	PRO	3.0
1	B	274	THR	3.0
1	A	1041	ALA	3.0
1	B	129	ASN	3.0
1	B	858	GLU	2.9
1	A	449	ASP	2.9
1	B	457	ILE	2.9
1	B	275	ASN	2.9
1	A	64	PRO	2.9
1	A	359	PRO	2.9
1	B	253	PRO	2.9
1	A	452	TYR	2.9
1	A	205	VAL	2.9
1	B	87	HIS	2.9
1	B	340	GLN	2.9
1	B	93	LEU	2.9
1	B	213	ARG	2.9
1	A	436	THR	2.9
1	A	252	ALA	2.9
1	A	310	GLU	2.9
1	A	293	PHE	2.9
1	B	295	PHE	2.9
1	B	322	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	345	LEU	2.9
1	B	853	ARG	2.9
1	A	217	VAL	2.9
1	A	845	PHE	2.9
1	A	438	LEU	2.9
1	B	224	ASP	2.9
1	B	392	ALA	2.9
1	B	217	VAL	2.9
1	B	311	VAL	2.9
1	A	330	ILE	2.9
1	B	3	ILE	2.9
1	B	108	ILE	2.9
1	B	219	SER	2.8
1	B	313	THR	2.8
1	B	89	GLY	2.8
1	B	209	LYS	2.8
1	A	95	GLU	2.8
1	B	1027	GLU	2.8
1	A	165	LEU	2.8
1	B	445	PRO	2.8
1	B	342	ASP	2.8
1	A	380	GLY	2.8
1	B	141	ALA	2.8
1	B	374[A]	ARG	2.8
1	A	178	VAL	2.8
1	A	400	PRO	2.8
1	A	307	THR	2.8
1	B	367	TYR	2.8
1	A	83	ALA	2.8
1	A	127	ALA	2.8
1	B	28	LYS	2.8
1	A	247	VAL	2.8
1	A	93	LEU	2.8
1	A	16	ILE	2.8
1	B	460	THR	2.8
1	A	236	ASP	2.7
1	B	122	GLY	2.7
1	B	411[A]	ASN	2.7
1	A	235	ARG	2.7
1	B	349	ALA	2.7
1	A	844	GLN	2.7
1	A	56	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	410	PRO	2.7
1	B	232	LEU	2.7
1	A	341[A]	GLU	2.7
1	A	441	ILE	2.7
1	A	902	VAL	2.7
1	B	58	LEU	2.7
1	B	350	LEU	2.7
1	B	438	LEU	2.7
1	B	416	ILE	2.7
1	A	248	GLU	2.7
1	A	26	GLY	2.7
1	A	89	GLY	2.7
1	A	433	THR	2.7
1	A	100	VAL	2.7
1	B	229	VAL	2.7
1	A	97	PRO	2.7
1	B	164	MET	2.7
1	A	856	GLY	2.7
1	B	843	GLY	2.7
1	B	114	LYS	2.7
1	B	281	THR	2.7
1	A	361	HIS	2.7
1	A	896	VAL	2.7
1	A	244	GLN	2.7
1	B	60	ARG	2.7
1	A	257	GLU	2.7
1	B	414	GLU	2.7
1	A	68	TYR	2.7
1	A	266	TYR	2.7
1	A	318	VAL	2.7
1	B	254	TYR	2.7
1	A	14	ILE	2.6
1	A	86	ILE	2.6
1	A	277	ILE	2.6
1	B	427	ARG	2.6
1	A	36	GLU	2.6
1	A	12	SER	2.6
1	A	102	ALA	2.6
1	A	271	ALA	2.6
1	B	255	LEU	2.6
1	A	323	HIS	2.6
1	B	442	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	448	ARG	2.6
1	B	286	MET	2.6
1	B	365	PRO	2.6
1	A	259	GLN	2.6
1	A	414	GLU	2.6
1	A	905	VAL	2.6
1	A	5	LYS	2.6
1	A	1026	ILE	2.6
1	B	79	LYS	2.6
1	A	220	GLN	2.6
1	B	84	ASP	2.6
1	B	261	GLN	2.6
1	A	107	GLY	2.6
1	A	134	VAL	2.6
1	A	105	LYS	2.6
1	A	209	LYS	2.6
1	B	325[A]	LEU	2.6
1	A	141	ALA	2.6
1	A	860	ARG	2.6
1	B	237	CYS	2.6
1	B	90	TYR	2.6
1	A	445	PRO	2.6
1	B	289	ASP	2.6
1	B	48	GLU	2.6
1	B	68	TYR	2.5
1	A	122	GLY	2.5
1	A	210	LEU	2.5
1	A	8	VAL	2.5
1	A	24	GLU	2.5
1	A	162	PRO	2.5
1	A	397	TYR	2.5
1	B	333	PRO	2.5
1	A	103	CYS	2.5
1	B	292	LYS	2.5
1	B	437	PHE	2.5
1	A	69	LEU	2.5
1	A	368	GLY	2.5
1	B	105	LYS	2.5
1	A	138	VAL	2.5
1	B	320	ALA	2.5
1	A	27	ILE	2.5
1	B	293	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	446	LYS	2.5
1	A	854	SER	2.5
1	B	83	ALA	2.5
1	A	393	ILE	2.5
1	B	111	ILE	2.5
1	A	166	LYS	2.5
1	A	324	ILE	2.4
1	A	263[A]	LEU	2.4
1	A	332	THR	2.4
1	B	92	LEU	2.4
1	B	268	LEU	2.4
1	A	139	VAL	2.4
1	B	312	VAL	2.4
1	B	248	GLU	2.4
1	A	366	ASP	2.4
1	B	30	VAL	2.4
1	B	247	VAL	2.4
1	B	176	MET	2.4
1	A	94	SER	2.4
1	B	7	LEU	2.4
1	A	859	THR	2.4
1	A	278	GLY	2.4
1	B	126	ALA	2.4
1	B	210	LEU	2.4
1	A	377	SER	2.4
1	A	229	VAL	2.4
1	B	23	ASN	2.4
1	A	340	GLN	2.4
1	A	944	GLY	2.3
1	A	32	ILE	2.3
1	A	348	HIS	2.3
1	B	862	HIS	2.3
1	A	906	VAL	2.3
1	B	82	GLY	2.3
1	B	407	ALA	2.3
1	B	228	ASN	2.3
1	A	72	ASP	2.3
1	A	120	GLN	2.3
1	B	245	LYS	2.3
1	B	4	SER	2.3
1	B	133	SER	2.3
1	B	1046	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	459	THR	2.3
1	A	57	HIS	2.3
1	A	847	ASN	2.3
1	A	456	PHE	2.3
1	B	1045	GLN	2.3
1	A	212	GLU	2.3
1	A	403	VAL	2.3
1	B	88	PRO	2.3
1	B	391	GLY	2.3
1	A	216	HIS	2.3
1	A	352[A]	CYS	2.3
1	A	316	ASP	2.3
1	A	52	VAL	2.3
1	A	242	ARG	2.3
1	B	239	VAL	2.3
1	B	282	VAL	2.3
1	A	430	GLY	2.3
1	B	102	ALA	2.3
1	A	281	THR	2.3
1	A	1049	THR	2.3
1	A	628	TYR	2.3
1	B	10	ASN	2.3
1	B	316	ASP	2.3
1	A	402	LEU	2.2
1	B	80	LEU	2.2
1	B	50	TYR	2.2
1	A	261	GLN	2.2
1	A	342	ASP	2.2
1	B	47	ASP	2.2
1	B	106	ALA	2.2
1	A	245	LYS	2.2
1	A	319	LYS	2.2
1	A	395	THR	2.2
1	A	77	VAL	2.2
1	A	1048	VAL	2.2
1	A	423	LEU	2.2
1	B	13	GLU	2.2
1	B	314	GLY	2.2
1	B	380	GLY	2.2
1	B	400	PRO	2.2
1	A	621	ARG	2.2
1	A	897	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	80	LEU	2.2
1	A	891	MET	2.2
1	A	1046	GLY	2.2
1	B	236	ASP	2.2
1	B	309	THR	2.1
1	A	264	ALA	2.1
1	B	359	PRO	2.1
1	A	289	ASP	2.1
1	B	449	ASP	2.1
1	B	163	VAL	2.1
1	B	246	VAL	2.1
1	B	403	VAL	2.1
1	A	428	ILE	2.1
1	B	373	TYR	2.1
1	A	269	LYS	2.1
1	A	9	ALA	2.1
1	A	213	ARG	2.1
1	A	297	GLU	2.1
1	B	81	SER	2.1
1	A	228	ASN	2.1
1	A	346	ASN	2.1
1	B	216	HIS	2.1
1	B	307	THR	2.1
1	A	1066	ARG	2.1
1	A	329	ALA	2.1
1	A	208	GLU	2.1
1	A	439	GLU	2.1
1	B	452	TYR	2.1
1	B	264	ALA	2.1
1	A	379	PHE	2.1
1	A	858	GLU	2.1
1	A	4	SER	2.1
1	A	219	SER	2.1
1	B	136	VAL	2.1
1	B	243	ASN	2.1
1	A	427	ARG	2.1
1	A	37	ASP	2.1
1	A	101	ASP	2.1
1	A	458	ASP	2.1
1	B	294	TYR	2.1
1	B	415	ALA	2.1
1	B	303	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	18	VAL	2.0
1	B	32	ILE	2.0
1	A	320	ALA	2.0
1	B	406	THR	2.0
1	A	1058	PRO	2.0
1	B	5	LYS	2.0
1	A	256	SER	2.0
1	A	343	ILE	2.0
1	A	512	ASN	2.0
1	B	362	ASN	2.0
1	A	15	ALA	2.0
1	B	290	THR	2.0
1	A	272	GLY	2.0
1	B	220	GLN	2.0
1	A	900	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	KCX	A	718[A]	12/13	0.97	0.07	20,21,22,22	0
1	KCX	B	718[A]	12/13	0.97	0.07	19,21,22,22	0

6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
2	MG	A	1200	1/1	0.88	0.14	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	1200	1/1	0.92	0.15	40,40,40,40	0
4	CL	A	1202	1/1	0.96	0.10	24,24,24,24	0
3	ZN	A	1201	1/1	0.98	0.04	56,56,56,56	0
3	ZN	B	1201	1/1	0.99	0.05	59,59,59,59	0
4	CL	B	1202	1/1	0.99	0.06	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.