



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 09:48 PM EDT

PDB ID : 3TW7  
Title : Structure of Rhizobium etli pyruvate carboxylase T882A crystallized without acetyl coenzyme-A  
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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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

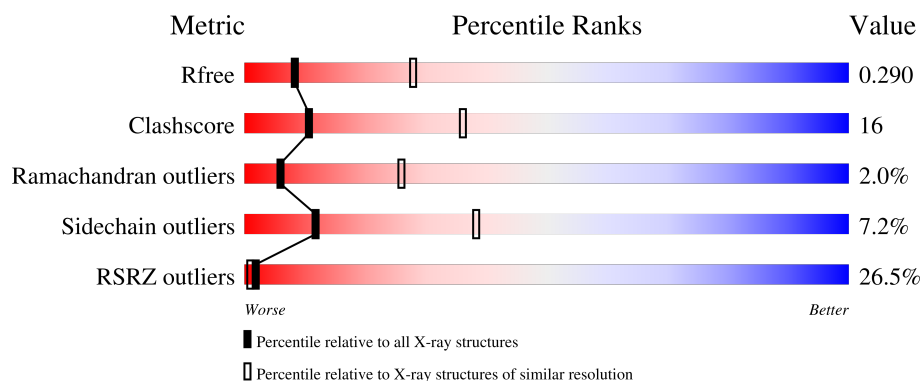
# 1 Overall quality at a glance

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))
$R_{free}$	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (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  $\geq 3$ , 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	
1	B	1165	

## 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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

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







## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	54.7	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 66.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, CL, 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	0.69	8/7719 (0.1%)	0.79	7/10500 (0.1%)
1	B	0.70	2/7799 (0.0%)	0.84	6/10603 (0.1%)
All	All	0.70	10/15518 (0.1%)	0.82	13/21103 (0.1%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98[A]	GLU	CD-OE1	7.78	1.34	1.25
1	A	98[B]	GLU	CD-OE1	7.78	1.34	1.25
1	A	269	LYS	CE-NZ	7.16	1.67	1.49
1	A	1045	GLN	CD-NE2	6.86	1.50	1.32
1	A	1045	GLN	CG-CD	6.82	1.66	1.51
1	A	814	TRP	CD2-CE2	6.09	1.48	1.41
1	A	408	TRP	CD2-CE2	6.01	1.48	1.41
1	A	659	TRP	CD2-CE2	5.40	1.47	1.41
1	B	814	TRP	CD2-CE2	5.18	1.47	1.41
1	B	933	TRP	CD2-CE2	5.01	1.47	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	LEU	CA-CB-CG	7.13	131.69	115.30
1	A	548	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	A	542	LEU	CA-CB-CG	-6.47	100.42	115.30
1	A	798	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	542	LEU	CA-CB-CG	-6.16	101.13	115.30
1	A	383	LEU	CA-CB-CG	5.80	128.64	115.30
1	B	423	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	145	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	737	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	590	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	B	535	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	737	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	627	GLY	N-CA-C	5.08	125.80	113.10

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	7260	247	0
1	B	7623	0	7392	249	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	14652	492	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 16.

All (492) 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
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: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:860:ARG:C	1:B:862:HIS:H	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:812:PHE:HD1	1:B:812:PHE:C	1.99	0.66
1:B:354:VAL:HG23	1:B:403:VAL:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:661:GLU:HA	1:A:661:GLU:OE2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:95:GLU:HA	1:B:118:MET:HE1	1.87	0.57
1:B:361:HIS:O	1:B:363:PHE:N	2.37	0.57
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:VAL:N	1:A:1063:VAL:O	2.31	0.53
1:B:812:PHE:C	1:B:812:PHE:CD1	2.72	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: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:A:621:ARG:O	1:A:622:GLY:C	2.46	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
1:A:412:PRO:O	1:A:415:ALA:HB3	2.10	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:B:812:PHE:O	1:B:812:PHE:CD1	2.58	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:A:891:MET:HE1	1:A:905:VAL:HG13	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:350:LEU:O	1:A:419:MET:HE2	2.11	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:B:634:ASN:CG	1:B:958:GLU:HG3	2.32	0.50
1:A:19:PHE:CD1	1:A:29:THR:HB	2.47	0.50
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: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:422:ALA:O	1:B:426:PHE:HD1	1.95	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: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:A:1043:ASP:CG	1:A:1044:SER:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:891:MET:HE1	1:A:905:VAL:CG1	2.43	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: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: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:8:VAL:O	1:A:10:ASN:N	2.38	0.48
1:B:131:ALA:HA	1:B:270:ILE:CD1	2.44	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: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:A:479:TYR:CD2	1:A:479:TYR:C	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:16:ILE:HA	1:B:19:PHE:CD2	2.51	0.46
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:8:VAL:C	1:A:10:ASN:H	2.17	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: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:343:ILE:C	1:A:344:ARG:HG2	2.37	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1027:GLU:O	1:A:1029:GLY:N	2.50	0.45
1:B:110:PHE:CE2	1:B:112:GLY:HA3	2.51	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
1:B:11:ARG:HE	1:B:37:ASP:CG	2.21	0.44
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: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:A:474:THR:O	1:A:475:LYS:C	2.55	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:350:LEU:CD2	1:A:415:ALA:HB1	2.48	0.43
1:A:756:ALA:HB1	1:B:754:ILE:HG22	2.01	0.43
1:B:361:HIS:O	1:B:362:ASN:C	2.56	0.43
1:B:1032:LEU:HD22	1:B:1054:LEU:HD11	2.00	0.43
1:B:41:LEU:O	1:B:42:HIS:C	2.55	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: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: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:A:624:ASN:CG	1:A:627:GLY:HA3	2.39	0.43
1:B:272:GLY:C	1:B:274:THR:H	2.22	0.43
1:B:304:VAL:HG21	1:B:353:ARG:HE	1.83	0.43
1:B:316:ASP:OD1	1:B:316:ASP:C	2.56	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:218:GLU:CD	1:A:237:CYS:HG	2.22	0.43
1:B:308:VAL:O	1:B:312:VAL:HG22	2.19	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:A:881:VAL:C	1:A:885:SER:OG	2.57	0.42
1:B:41:LEU:HD12	1:B:44:PHE:HB2	2.01	0.42
1:B:416:ILE:O	1:B:420:ASP:HB2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:724:LEU:HD23	1:B:746:PHE:CZ	2.55	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:886:LYS:O	1:A:887:VAL:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:114:LYS:HG3	1:B:277:ILE:CD1	2.51	0.41
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: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: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:A:940:LYS:O	1:A:941:ALA:C	2.59	0.41
1:B:249:ARG:CZ	1:B:253:PRO:HG3	2.50	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:99:PHE:O	1:B:100:VAL:C	2.57	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: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: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:519:LYS:HA	1:B:615:LEU:HD23	2.03	0.40
1:A:424:ARG:O	1:A:426:PHE:N	2.55	0.40
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
1:B:1044:SER:C	1:B:1046:GLY:H	2.24	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	26

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
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

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Mol	Chain	Res	Type
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%)	699 (93%)	50 (7%)	13	40
1	B	769/933 (82%)	709 (92%)	60 (8%)	10	35
All	All	1518/1866 (81%)	1408 (93%)	110 (7%)	12	38

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	50	TYR
1	A	51	GLN
1	A	54	ARG
1	A	71	ILE

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Mol	Chain	Res	Type
1	A	81	SER
1	A	90	TYR
1	A	100	VAL
1	A	108	ILE
1	A	120	GLN
1	A	128	ARG
1	A	145	LEU
1	A	168	SER
1	A	179	ILE
1	A	224	ASP
1	A	232	LEU
1	A	234	GLU
1	A	239	VAL
1	A	254	TYR
1	A	277	ILE
1	A	286	MET
1	A	304	VAL
1	A	344	ARG
1	A	393	ILE
1	A	394	ILE
1	A	416	ILE
1	A	459	THR
1	A	474	THR
1	A	542	LEU
1	A	557	THR
1	A	584	TRP
1	A	590	ASP
1	A	597	THR
1	A	621	ARG
1	A	630	ASN
1	A	692	ARG
1	A	720	MET
1	A	796	SER
1	A	848	LEU
1	A	854	SER
1	A	860	ARG
1	A	885	SER
1	A	891	MET
1	A	913	SER
1	A	919	VAL
1	A	931	SER
1	A	958	GLU

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Mol	Chain	Res	Type
1	A	998	SER
1	A	1021	GLU
1	A	1045	GLN
1	B	10	ASN
1	B	30	VAL
1	B	54	ARG
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	179	ILE
1	B	206	TYR
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	289	ASP
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
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	521	LEU
1	B	542	LEU
1	B	557	THR

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Mol	Chain	Res	Type
1	B	584	TRP
1	B	590	ASP
1	B	597	THR
1	B	720	MET
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	1021	GLU
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 (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	220	GLN
1	A	226	HIS
1	A	299	ASN
1	A	348	HIS
1	A	444	HIS
1	A	486	ASN
1	A	573	HIS
1	A	630	ASN
1	A	713	HIS
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	299	ASN

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Mol	Chain	Res	Type
1	B	346	ASN
1	B	361	HIS
1	B	444	HIS
1	B	486	ASN
1	B	630	ASN
1	B	713	HIS
1	B	863	GLN
1	B	873	GLN
1	B	1037	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	A	718[A]	1,3	10,11,12	0.72	0	6,12,14	1.02	1 (16%)
1	KCX	B	718[A]	1,3	10,11,12	0.94	0	6,12,14	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	718[A]	1,3	-	1/9/10/12	-
1	KCX	B	718[A]	1,3	-	3/9/10/12	-

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1003/1165 (86%)	1.02	302 (30%)  	16, 71, 162, 191	22 (2%)
1	B	1001/1165 (85%)	0.78	230 (22%)  	17, 56, 139, 190	22 (2%)
All	All	2004/2330 (86%)	0.90	532 (26%)  	16, 64, 156, 191	44 (2%)

All (532) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	LEU	10.7
1	B	335	SER	9.1
1	A	285	LEU	8.7
1	B	167	ALA	8.0
1	A	367	TYR	6.9
1	A	313	THR	6.7
1	B	386	GLY	6.6
1	A	146	PRO	6.5
1	B	376	ALA	6.3
1	B	95	GLU	6.3
1	B	377	SER	6.1
1	A	121	LEU	5.8
1	B	132	ILE	5.6
1	A	322	ILE	5.5
1	B	144	PRO	5.5
1	B	27	ILE	5.4
1	B	206	TYR	5.4
1	A	144	PRO	5.3
1	A	10	ASN	5.1
1	A	434	ASN	5.0
1	A	214	ALA	5.0
1	B	341[A]	GLU	5.0
1	A	298	VAL	5.0
1	A	225	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	232	LEU	4.9
1	A	279	ALA	4.9
1	A	432	ALA	4.9
1	B	86	ILE	4.8
1	A	401	LEU	4.8
1	A	221	ILE	4.8
1	B	91	GLY	4.8
1	A	389	TYR	4.8
1	A	180	ARG	4.8
1	A	335	SER	4.7
1	B	134	VAL	4.7
1	A	904	ASP	4.7
1	A	96	SER	4.7
1	A	315	ILE	4.7
1	B	861	TRP	4.7
1	A	164	MET	4.6
1	A	431	VAL	4.6
1	A	99	PHE	4.6
1	A	336	GLY	4.6
1	A	296[A]	ILE	4.6
1	B	315	ILE	4.6
1	A	290	THR	4.6
1	A	123	ASN	4.6
1	A	386	GLY	4.6
1	A	168	SER	4.5
1	B	123	ASN	4.5
1	B	346	ASN	4.5
1	B	434	ASN	4.5
1	A	360	GLU	4.5
1	A	457	ILE	4.5
1	B	379	PHE	4.5
1	A	1043	ASP	4.5
1	B	165	LEU	4.4
1	B	180	ARG	4.4
1	A	454	THR	4.4
1	B	168	SER	4.4
1	A	222	LEU	4.4
1	A	303	GLN	4.3
1	A	284	TYR	4.3
1	B	345	LEU	4.3
1	B	419	MET	4.3
1	B	29	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	334	GLN	4.3
1	A	98[A]	GLU	4.2
1	B	241	ARG	4.2
1	B	277	ILE	4.2
1	A	270	ILE	4.2
1	A	117	THR	4.2
1	A	176	MET	4.2
1	B	179	ILE	4.2
1	B	222	LEU	4.2
1	B	125	VAL	4.1
1	B	146	PRO	4.1
1	A	6	ILE	4.1
1	B	352[A]	CYS	4.1
1	A	399	ASP	4.1
1	A	406	THR	4.1
1	B	387	THR	4.1
1	B	128	ARG	4.1
1	A	275	ASN	4.1
1	A	108	ILE	4.1
1	B	296[A]	ILE	4.1
1	B	348	HIS	4.1
1	B	96	SER	4.1
1	B	278	GLY	4.0
1	A	334	GLN	4.0
1	B	301	ARG	4.0
1	A	115	ALA	4.0
1	A	312	VAL	4.0
1	A	114	LYS	4.0
1	B	145	LEU	4.0
1	A	231	HIS	4.0
1	B	124	LYS	4.0
1	B	285	LEU	4.0
1	A	136	VAL	4.0
1	A	267	SER	4.0
1	B	331	GLY	4.0
1	A	295	PHE	3.9
1	B	131	ALA	3.9
1	B	166	LYS	3.9
1	A	450	ASN	3.9
1	A	460	THR	3.9
1	A	211	VAL	3.9
1	B	211	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	909	ASP	3.9
1	A	416	ILE	3.9
1	B	25	LEU	3.9
1	A	394	ILE	3.9
1	B	162	PRO	3.9
1	A	274	THR	3.9
1	A	132	ILE	3.9
1	B	267	SER	3.8
1	B	272	GLY	3.8
1	A	85	ALA	3.8
1	B	127	ALA	3.8
1	A	325[A]	LEU	3.8
1	A	411[A]	ASN	3.8
1	A	119	ARG	3.8
1	B	336	GLY	3.8
1	A	855	LEU	3.8
1	B	270	ILE	3.8
1	B	112	GLY	3.8
1	A	92	LEU	3.8
1	A	849	LYS	3.8
1	A	110	PHE	3.7
1	A	363	PHE	3.7
1	B	113	PRO	3.7
1	A	3	ILE	3.7
1	A	215	ARG	3.7
1	A	226	HIS	3.7
1	B	323	HIS	3.7
1	A	321	GLN	3.7
1	A	167	ALA	3.7
1	A	223	GLY	3.7
1	A	317	ILE	3.7
1	A	415	ALA	3.7
1	B	283	GLU	3.7
1	B	142	THR	3.7
1	A	65	ILE	3.7
1	A	112	GLY	3.6
1	B	423	LEU	3.6
1	A	116[A]	ASP	3.6
1	B	178	VAL	3.6
1	A	304	VAL	3.6
1	B	230	VAL	3.6
1	A	292	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	130	LEU	3.6
1	B	297	GLU	3.6
1	A	124	LYS	3.6
1	B	269	LYS	3.6
1	B	21	ALA	3.6
1	B	413	LEU	3.6
1	A	238	SER	3.6
1	A	437	PHE	3.6
1	A	857	LEU	3.5
1	A	239	VAL	3.5
1	A	273	ALA	3.5
1	A	351[A]	GLN	3.5
1	A	408	TRP	3.5
1	A	179	ILE	3.5
1	A	364	ILE	3.5
1	A	294	TYR	3.5
1	A	207	LEU	3.5
1	A	848	LEU	3.5
1	B	130	LEU	3.5
1	A	388	SER	3.5
1	A	87	HIS	3.5
1	B	258	ALA	3.5
1	A	344	ARG	3.5
1	B	455	ARG	3.5
1	A	113	PRO	3.5
1	A	145	LEU	3.5
1	A	442	ILE	3.5
1	A	338	PRO	3.4
1	A	265	ALA	3.4
1	B	109	ILE	3.4
1	B	326	ASP	3.4
1	A	407	ALA	3.4
1	A	337	VAL	3.4
1	B	138	VAL	3.4
1	B	6	ILE	3.4
1	A	90	TYR	3.4
1	A	109	ILE	3.4
1	A	302	ILE	3.4
1	A	58	LEU	3.4
1	A	286	MET	3.4
1	A	852	ALA	3.4
1	A	410	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	399	ASP	3.4
1	A	309	THR	3.4
1	A	28	LYS	3.3
1	B	137	PRO	3.3
1	A	850	GLU	3.3
1	A	453	THR	3.3
1	B	140	PRO	3.3
1	B	242	ARG	3.3
1	A	314	GLY	3.3
1	B	234	GLU	3.3
1	B	94	SER	3.3
1	B	339	ASN	3.3
1	A	412	PRO	3.3
1	B	2	PRO	3.3
1	B	231	HIS	3.3
1	A	413	LEU	3.3
1	A	326	ASP	3.3
1	B	85	ALA	3.3
1	A	300	PRO	3.3
1	A	111	ILE	3.3
1	A	846	THR	3.3
1	B	233	PHE	3.3
1	A	129	ASN	3.3
1	B	412	PRO	3.3
1	A	381	ILE	3.3
1	A	233	PHE	3.2
1	B	343	ILE	3.2
1	A	125	VAL	3.2
1	A	230	VAL	3.2
1	B	271	ALA	3.2
1	B	121	LEU	3.2
1	B	375	SER	3.2
1	A	13	GLU	3.2
1	B	205	VAL	3.2
1	B	288	ALA	3.2
1	B	426	PHE	3.2
1	B	327	GLY	3.2
1	A	390	SER	3.2
1	A	276	TYR	3.2
1	A	1042	THR	3.2
1	B	135	GLY	3.2
1	B	385	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	287	ASP	3.2
1	B	116[A]	ASP	3.2
1	A	133	SER	3.2
1	A	1044	SER	3.2
1	A	118	MET	3.2
1	B	284	TYR	3.2
1	A	387	THR	3.2
1	A	455	ARG	3.1
1	B	330	ILE	3.1
1	A	353	ARG	3.1
1	B	308	VAL	3.1
1	A	140	PRO	3.1
1	A	81	SER	3.1
1	B	408	TRP	3.1
1	B	97	PRO	3.1
1	A	249	ARG	3.1
1	A	853	ARG	3.1
1	B	353	ARG	3.1
1	A	861	TRP	3.1
1	A	246	VAL	3.1
1	B	208	GLU	3.0
1	B	417	SER	3.0
1	A	2	PRO	3.0
1	A	62	LEU	3.0
1	B	360	GLU	3.0
1	A	371	THR	3.0
1	A	435	LEU	3.0
1	B	260	ARG	3.0
1	B	344	ARG	3.0
1	B	265	ALA	3.0
1	A	333	PRO	3.0
1	A	405	VAL	3.0
1	A	370	ILE	3.0
1	B	324	ILE	3.0
1	B	381	ILE	3.0
1	B	409	ALA	3.0
1	A	268	LEU	3.0
1	B	337	VAL	3.0
1	B	384	ASP	3.0
1	A	142	THR	3.0
1	B	302	ILE	3.0
1	A	383	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	139	VAL	2.9
1	A	426	PHE	2.9
1	A	71	ILE	2.9
1	B	332	THR	2.9
1	A	863	GLN	2.9
1	A	1047	MET	2.9
1	B	383	LEU	2.9
1	B	257	GLU	2.9
1	A	258	ALA	2.9
1	A	362	ASN	2.9
1	A	306	HIS	2.9
1	B	226	HIS	2.9
1	A	74	VAL	2.9
1	B	328	ALA	2.9
1	A	7	LEU	2.9
1	A	373	TYR	2.9
1	B	347	GLY	2.9
1	B	276	TYR	2.9
1	A	137	PRO	2.8
1	B	251	PRO	2.8
1	A	1041	ALA	2.8
1	B	858	GLU	2.8
1	B	274	THR	2.8
1	B	129	ASN	2.8
1	B	213	ARG	2.8
1	B	457	ILE	2.8
1	B	275	ASN	2.8
1	B	853	ARG	2.8
1	A	310	GLU	2.8
1	A	205	VAL	2.8
1	B	340	GLN	2.8
1	A	252	ALA	2.8
1	A	449	ASP	2.8
1	B	93	LEU	2.8
1	A	436	THR	2.8
1	B	322	ILE	2.8
1	A	64	PRO	2.7
1	A	359	PRO	2.7
1	B	87	HIS	2.7
1	B	253	PRO	2.7
1	A	452	TYR	2.7
1	A	345	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	217	VAL	2.7
1	B	392	ALA	2.7
1	B	209	LYS	2.7
1	A	438	LEU	2.7
1	B	217	VAL	2.7
1	B	311	VAL	2.7
1	A	293	PHE	2.7
1	A	330	ILE	2.7
1	B	3	ILE	2.7
1	B	108	ILE	2.7
1	B	295	PHE	2.7
1	B	224	ASP	2.7
1	A	95	GLU	2.7
1	B	1027	GLU	2.7
1	A	845	PHE	2.7
1	B	313	THR	2.7
1	B	374[A]	ARG	2.7
1	B	219	SER	2.7
1	B	89	GLY	2.7
1	A	165	LEU	2.7
1	B	28	LYS	2.6
1	B	141	ALA	2.6
1	A	178	VAL	2.6
1	A	235	ARG	2.6
1	A	380	GLY	2.6
1	B	342	ASP	2.6
1	A	83	ALA	2.6
1	A	127	ALA	2.6
1	B	445	PRO	2.6
1	A	307	THR	2.6
1	A	247	VAL	2.6
1	A	16	ILE	2.6
1	A	341[A]	GLU	2.6
1	A	93	LEU	2.6
1	A	400	PRO	2.6
1	B	349	ALA	2.6
1	B	411[A]	ASN	2.6
1	B	460	THR	2.6
1	A	844	GLN	2.6
1	A	441	ILE	2.6
1	B	367	TYR	2.6
1	B	122	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	232	LEU	2.6
1	A	248	GLU	2.6
1	A	236	ASP	2.6
1	A	902	VAL	2.6
1	B	114	LYS	2.6
1	B	416	ILE	2.6
1	B	58	LEU	2.6
1	B	350	LEU	2.6
1	B	438	LEU	2.6
1	A	56	PRO	2.6
1	B	60	ARG	2.6
1	B	410	PRO	2.6
1	A	100	VAL	2.6
1	B	229	VAL	2.6
1	A	433	THR	2.6
1	A	26	GLY	2.5
1	A	89	GLY	2.5
1	B	427	ARG	2.5
1	A	257	GLU	2.5
1	B	414	GLU	2.5
1	A	896	VAL	2.5
1	B	281	THR	2.5
1	A	244	GLN	2.5
1	A	856	GLY	2.5
1	B	843	GLY	2.5
1	A	448	ARG	2.5
1	A	36	GLU	2.5
1	A	97	PRO	2.5
1	B	164	MET	2.5
1	A	318	VAL	2.5
1	A	14	ILE	2.5
1	A	86	ILE	2.5
1	A	277	ILE	2.5
1	A	361	HIS	2.5
1	A	5	LYS	2.5
1	A	102	ALA	2.5
1	A	271	ALA	2.5
1	B	79	LYS	2.5
1	A	414	GLU	2.5
1	B	442	ILE	2.5
1	B	255	LEU	2.5
1	A	259	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	68	TYR	2.5
1	A	105	LYS	2.5
1	A	209	LYS	2.5
1	A	266	TYR	2.5
1	B	254	TYR	2.5
1	A	905	VAL	2.5
1	A	1026	ILE	2.5
1	A	323	HIS	2.5
1	A	860	ARG	2.5
1	A	12	SER	2.5
1	A	220	GLN	2.5
1	B	261	GLN	2.5
1	B	286	MET	2.5
1	A	134	VAL	2.5
1	B	365	PRO	2.5
1	A	107	GLY	2.4
1	A	141	ALA	2.4
1	B	84	ASP	2.4
1	B	48	GLU	2.4
1	B	325[A]	LEU	2.4
1	A	24	GLU	2.4
1	B	292	LYS	2.4
1	A	8	VAL	2.4
1	B	90	TYR	2.4
1	A	445	PRO	2.4
1	A	210	LEU	2.4
1	B	289	ASP	2.4
1	B	237	CYS	2.4
1	B	105	LYS	2.4
1	A	122	GLY	2.4
1	B	68	TYR	2.4
1	A	446	LYS	2.4
1	B	320	ALA	2.4
1	A	138	VAL	2.4
1	A	27	ILE	2.3
1	A	69	LEU	2.3
1	A	162	PRO	2.3
1	A	166	LYS	2.3
1	A	397	TYR	2.3
1	B	333	PRO	2.3
1	A	103	CYS	2.3
1	A	368	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	83	ALA	2.3
1	A	393	ILE	2.3
1	B	111	ILE	2.3
1	B	437	PHE	2.3
1	A	324	ILE	2.3
1	B	293	PHE	2.3
1	A	854	SER	2.3
1	B	248	GLU	2.3
1	A	139	VAL	2.3
1	B	312	VAL	2.3
1	A	263[A]	LEU	2.3
1	B	92	LEU	2.3
1	B	268	LEU	2.3
1	A	332	THR	2.3
1	B	30	VAL	2.3
1	B	247	VAL	2.3
1	B	126	ALA	2.3
1	B	7	LEU	2.3
1	A	366	ASP	2.2
1	A	859	THR	2.2
1	B	176	MET	2.2
1	A	229	VAL	2.2
1	A	278	GLY	2.2
1	B	210	LEU	2.2
1	A	94	SER	2.2
1	B	23	ASN	2.2
1	A	340	GLN	2.2
1	A	32	ILE	2.2
1	A	377	SER	2.2
1	B	245	LYS	2.2
1	A	906	VAL	2.2
1	B	407	ALA	2.2
1	A	944	GLY	2.2
1	A	348	HIS	2.2
1	B	862	HIS	2.2
1	B	228	ASN	2.2
1	A	120	GLN	2.2
1	B	82	GLY	2.2
1	A	212	GLU	2.2
1	A	242	ARG	2.2
1	A	847	ASN	2.2
1	A	72	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	403	VAL	2.2
1	A	459	THR	2.2
1	B	1045	GLN	2.2
1	B	1046	GLY	2.1
1	A	57	HIS	2.1
1	A	52	VAL	2.1
1	B	4	SER	2.1
1	B	133	SER	2.1
1	B	239	VAL	2.1
1	B	282	VAL	2.1
1	B	102	ALA	2.1
1	B	391	GLY	2.1
1	A	456	PHE	2.1
1	A	216	HIS	2.1
1	B	88	PRO	2.1
1	A	281	THR	2.1
1	A	1049	THR	2.1
1	B	10	ASN	2.1
1	A	316	ASP	2.1
1	A	430	GLY	2.1
1	A	352[A]	CYS	2.1
1	A	402	LEU	2.1
1	B	80	LEU	2.1
1	A	245	LYS	2.1
1	A	261	GLN	2.1
1	A	319	LYS	2.1
1	A	628	TYR	2.1
1	B	316	ASP	2.1
1	B	106	ALA	2.1
1	A	621	ARG	2.1
1	B	50	TYR	2.1
1	A	342	ASP	2.1
1	A	77	VAL	2.1
1	A	1048	VAL	2.1
1	B	13	GLU	2.1
1	A	395	THR	2.0
1	A	423	LEU	2.0
1	B	47	ASP	2.0
1	B	314	GLY	2.0
1	B	380	GLY	2.0
1	A	80	LEU	2.0
1	B	400	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	213	ARG	2.0
1	A	269	LYS	2.0
1	A	264	ALA	2.0
1	A	1046	GLY	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, 95<sup>th</sup> 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 <sup>2</sup> )	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MG	A	1200	1/1	0.87	0.14	25,25,25,25	0
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.