



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:25 PM GMT

PDB ID : 3TW7
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

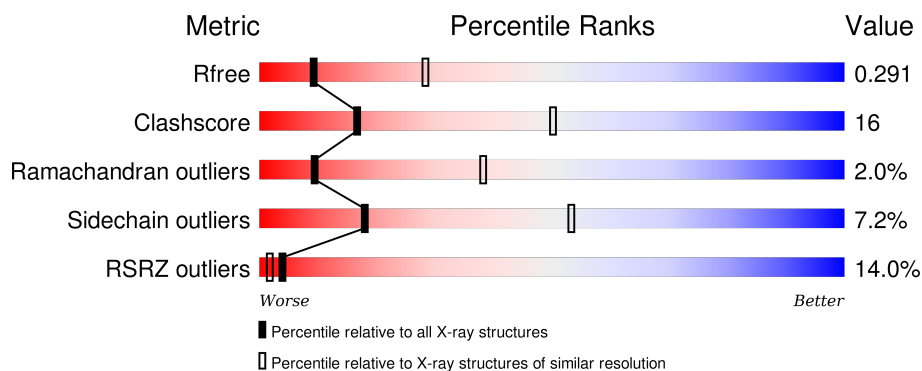
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

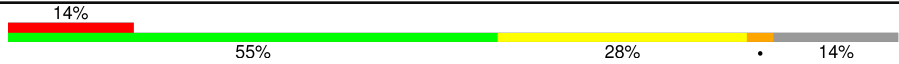

The reported resolution of this entry is 3.10 Å.

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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	1200	-	-	-	X
2	MG	B	1200	-	-	-	X

2 Entry composition

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	B	1	Total Mg 1 1	0	0
2	A	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	B	1	Total Zn 1 1	0	0
3	A	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	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

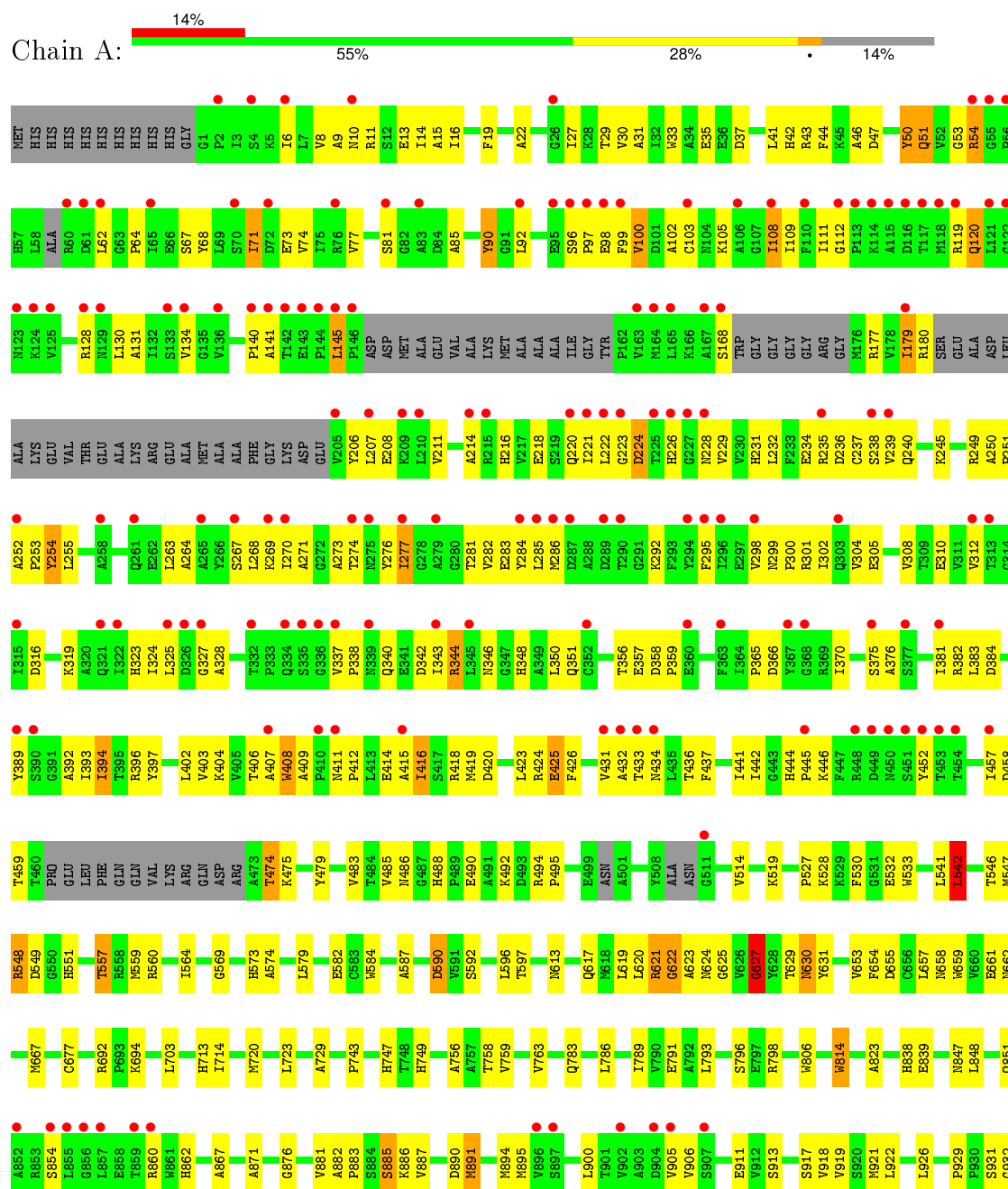
- Molecule 5 is water.

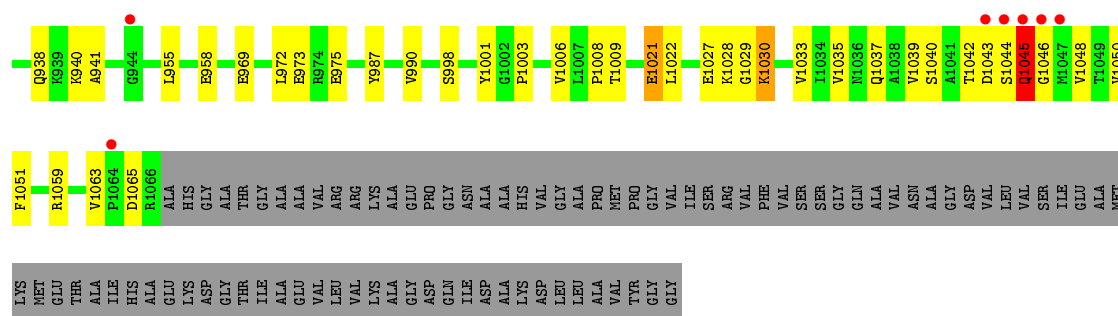
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	7	Total O 7 7	0	0
5	B	5	Total O 5 5	0	0

3 Residue-property plots

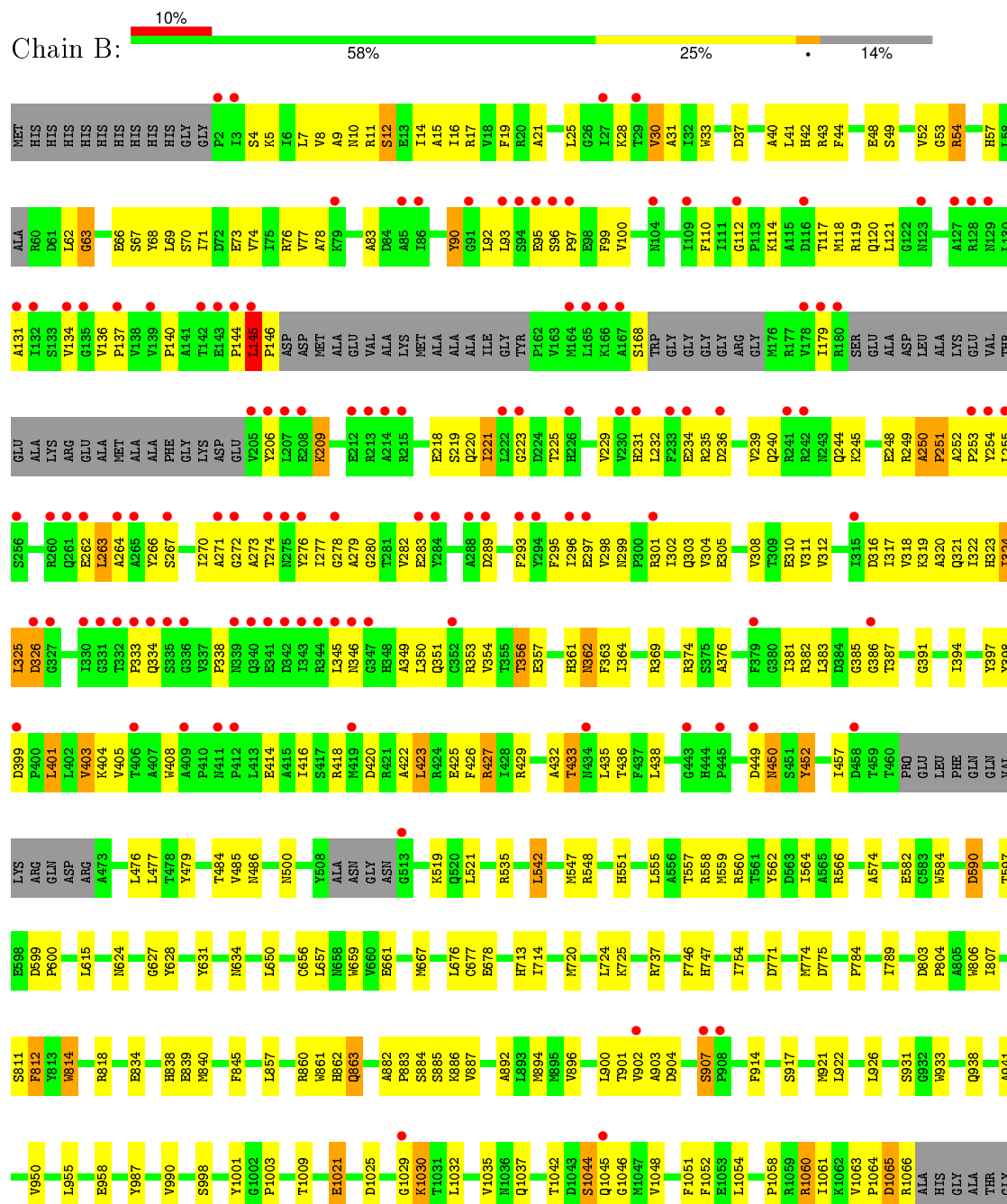
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Pyruvate carboxylase protein





● Molecule 1: Pyruvate carboxylase protein



ALA VAL VAL ARG ARG LYS ALA GLU PRO GLY ASN ALA ALA HIS VAL VAL ALA ALA PRO PRO GLY VAL ILE SER ARG VAL PHE VAL SER SER GLY GLN VAL VAL ALA ALA ASN ALA ALA GLY ASP VAL VAL LEU VAL SER ILE GLU ALA ALA MET MET LYS MET GLU THR ALA ILE HIS ALA GLY LYS ASP GLY THR ILE

ALA
GLU
VAL
LEU
VAL
LYS
ALA
GLY
ASP
GLN
ILE
ASP
ALA
LYS
ASP
LEU
LEU
ALA
VAL
TYR
GLY
GLY

4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	264.16 Å 264.16 Å 91.79 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 45.30 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.10) 100.0 (45.30-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.13 (at 3.12 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.250 , 0.292 0.248 , 0.291	Depositor DCC
R_{free} test set	2964 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 66.1	EDS
Estimated twinning fraction	0.023 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 57689 reflections	Xtriage
F_o, F_c correlation	0.86	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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ZN, KCX, CL

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:969:GLU:HG2	1:A:975:GLU:HA	1.65	0.77
1:A:420:ASP:O	1:A:424:ARG:HG3	1.83	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:921:MET:HG3	1:B:926:LEU:HD12	1.69	0.72
1:B:547:MET:HG2	1:B:564:ILE:HG23	1.70	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:350:LEU:HD22	1:A:415:ALA:HB1	1.76	0.68
1:A:211:VAL:CG1	1:A:214:ALA:HB2	2.23	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:B:812:PHE:HD1	1:B:812:PHE:C	1.99	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

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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:359:PRO:HG2	1:A:436:THR:OG1	1.99	0.62
1:A:350:LEU:HD23	1:A:407:ALA:O	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:OE2	1:A:661:GLU:HA	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:B:5:LYS:HE2	1:B:28:LYS:HB2	1.83	0.59
1:A:530:PHE:O	1:A:533:TRP:HB3	2.01	0.59
1:A:494:ARG:HB3	1:A:495:PRO:HD2	1.84	0.59
1:A:359:PRO:HG3	1:A:434:ASN:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLN:HE22	1:A:54:ARG:HB3	1.68	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: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:416:ILE:CG2	1:A:442:ILE:HB	2.35	0.56
1:A:403:VAL:HG22	1:A:404[A]:LYS:H	1.71	0.56
1:A:41:LEU:O	1:A:44:PHE:N	2.38	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:857:LEU:O	1:B:860:ARG:N	2.40	0.55
1:B:263[A]:LEU:HG	1:B:293:PHE:CE2	2.42	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:B:299:ASN:HD22	1:B:303:GLN:HE22	1.52	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: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:555:LEU:HD11	1:B:818:ARG:HG3	1.89	0.54
1:B:229:VAL:HG11	1:B:271:ALA:HB3	1.88	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:860:ARG:CB	1:B:863:GLN:NE2	2.71	0.54
1:B:427:ARG:NH1	1:B:1037:GLN:HE21	2.06	0.54
1:A:723:LEU:HD11	1:A:839:GLU:HG2	1.89	0.54
1:A:629:THR:HG23	1:A:630:ASN:N	2.23	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:B:667:MET:HG2	1:B:677:CYS:SG	2.48	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:385:GLY:HA2	1:B:403:VAL:HG23	1.91	0.53
1:B:255:LEU:HD11	1:B:293:PHE:HZ	1.74	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:B:319:LYS:HA	1:B:322:ILE:HD12	1.91	0.53
1:A:396:ARG:O	1:A:397:TYR:CD1	2.62	0.53
1:A:423:LEU:HD12	1:A:442:ILE:HD11	1.91	0.52
1:B:12:SER:O	1:B:16:ILE:HD12	2.10	0.52
1:A:282:VAL:HG13	1:A:298:VAL:CG2	2.37	0.52
1:B:279:ALA:HB3	1:B:321:GLN:NE2	2.24	0.52
1:B:559:MET:CG	1:B:564:ILE:HD11	2.39	0.52
1:A:621:ARG:O	1:A:622:GLY:C	2.46	0.52
1:A:340:GLN:HA	1:A:343:ILE:HD12	1.92	0.52
1:B:900:LEU:HD22	1:B:904:ASP:HB3	1.90	0.52
1:B:62:LEU:O	1:B:63:GLY:O	2.28	0.52
1:A:229:VAL:HG11	1:A:271:ALA:HB3	1.91	0.52
1:A:412:PRO:O	1:A:415:ALA:HB3	2.10	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:B:229:VAL:HG11	1:B:271:ALA:CB	2.40	0.51
1:A:542:LEU:HD22	1:A:786:LEU:CD1	2.40	0.51
1:B:282:VAL:HG13	1:B:295:PHE:HE1	1.75	0.51
1:B:812:PHE:CD1	1:B:812:PHE:O	2.58	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:624:ASN:CB	1:A:627:GLY:HA3	2.40	0.51
1:A:252:ALA:HB3	1:A:255:LEU:HD22	1.93	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: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:891:MET:HE1	1:A:905:VAL:HG13	1.93	0.51
1:A:97:PRO:HG3	1:A:119:ARG:HG3	1.92	0.51
1:B:650:LEU:HA	1:B:676:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:ASP:HB3	1:B:987:TYR:CZ	2.46	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: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:B:117:THR:HG22	1:B:121:LEU:HD12	1.91	0.50
1:A:749:HIS:CE1	1:A:783:GLN:HE22	2.29	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:NH1	1:B:1060:ARG:O	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:A:350:LEU:O	1:A:419:MET:HE2	2.11	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:B:302:ILE:CD1	1:B:318:VAL:HG22	2.41	0.50
1:A:528:LYS:HE2	1:A:532:GLU:OE2	2.12	0.50
1:A:19:PHE:CD1	1:A:29:THR:HB	2.47	0.50
1:A:619:LEU:HD11	1:A:654:PHE:CD2	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:218:GLU:O	1:B:234:GLU:CA	2.61	0.48
1:B:5:LYS:HB3	1:B:83:ALA:HA	1.95	0.48
1:A:1021:GLU:OE1	1:A:1033:VAL:HG13	2.13	0.48
1:A:891:MET:HE1	1:A:905:VAL:CG1	2.43	0.48
1:B:312:VAL:HG12	1:B:408:TRP:HD1	1.78	0.48
1:A:622:GLY:O	1:A:624:ASN:N	2.46	0.48
1:B:16:ILE:HD13	1:B:386:GLY:CA	2.38	0.48
1:A:131:ALA:HB2	1:A:295:PHE:CD2	2.49	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: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:759:VAL:HG11	1:A:789:ILE:HD13	1.94	0.48
1:B:302:ILE:CD1	1:B:318:VAL:CG2	2.91	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: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:B:25:LEU:HG	1:B:319:LYS:HE2	1.96	0.47
1:A:376:ALA:HB3	1:A:426:PHE:CE1	2.49	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:403:VAL:CG2	1:A:404[A]:LYS:H	2.27	0.47
1:A:131:ALA:HB2	1:A:295:PHE:CE2	2.49	0.47
1:A:479:TYR:CD2	1:A:479:TYR:C	2.88	0.47
1:A:350:LEU:O	1:A:419:MET:CE	2.63	0.47
1:A:19:PHE:HE2	1:A:42:HIS:HB2	1.79	0.47
1:A:308:VAL:HG13	1:A:351[A]:GLN:HE21	1.79	0.47
1:A:33:TRP:CG	1:A:43:ARG:HD2	2.50	0.47
1:B:278:GLY:HA2	1:B:324:ILE:HG21	1.97	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:A:250:ALA:HB3	1:A:308:VAL:O	2.14	0.47
1:B:427:ARG:NH1	1:B:1037:GLN:NE2	2.62	0.47
1:A:547:MET:O	1:A:551:HIS:NE2	2.45	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:B:921:MET:CG	1:B:926:LEU:HD12	2.42	0.46
1:B:574:ALA:HB1	1:B:806:TRP:CG	2.50	0.46
1:A:987:TYR:HB3	1:A:990:VAL:HB	1.97	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:B:16:ILE:HA	1:B:19:PHE:CD2	2.51	0.46
1:A:551:HIS:CE1	1:A:559:MET:HB3	2.51	0.46
1:A:29:THR:OG1	1:A:47:ASP:N	2.44	0.46
1:B:628:TYR:O	1:B:628:TYR:CD1	2.68	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:A:655:ASP:OD1	1:A:662:ASN:HB3	2.15	0.46
1:B:90:TYR:HE2	1:B:304:VAL:HA	1.81	0.46
1:B:485:VAL:HG11	1:B:1048:VAL:HG21	1.96	0.46
1:A:31:ALA:HB2	1:A:46:ALA:HB2	1.97	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:B:397:TYR:HB2	1:B:398:TYR:CD2	2.50	0.46
1:A:887:VAL:CG1	1:A:918:VAL:HA	2.45	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:B:548:ARG:HB3	1:B:582:GLU:OE1	2.16	0.46
1:A:714:ILE:HG12	1:A:743:PRO:HG2	1.98	0.46
1:A:569:GLY:O	1:A:573:HIS:CD2	2.65	0.46
1:B:838:HIS:CE1	1:B:845:PHE:CE1	3.04	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:A:251:PRO:HD2	1:A:348:HIS:CD2	2.51	0.45
1:B:838:HIS:O	1:B:839:GLU:CB	2.64	0.45
1:A:343:ILE:C	1:A:344:ARG:HG2	2.37	0.45
1:B:882:ALA:HA	1:B:883:PRO:HA	1.77	0.45
1:B:834:GLU:HG3	1:B:838:HIS:NE2	2.32	0.45
1:A:389:TYR:CE2	1:A:392:ALA:HB2	2.52	0.45
1:A:759:VAL:O	1:A:763:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:LYS:HD2	1:A:519:LYS:O	2.17	0.45
1:B:401:LEU:HD21	1:B:404[B]:LYS:HG3	1.98	0.45
1:B:30:VAL:HA	1:B:48:GLU:HG3	1.99	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:B:361:HIS:O	1:B:364:ILE:HG13	2.15	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:A:629:THR:HG23	1:A:630:ASN:H	1.81	0.45
1:B:312:VAL:CG1	1:B:349:ALA:CB	2.95	0.44
1:A:22:ALA:HB1	1:A:27:ILE:CG2	2.48	0.44
1:B:678:GLU:OE1	1:B:714:ILE:HG21	2.16	0.44
1:B:11:ARG:HE	1:B:37:ASP:CG	2.21	0.44
1:B:263[A]:LEU:HA	1:B:263[A]:LEU:HD23	1.83	0.44
1:A:574:ALA:HB1	1:A:806:TRP:CG	2.53	0.44
1:A:270:ILE:HG21	1:A:298:VAL:HG21	1.98	0.44
1:B:7:LEU:HD13	1:B:78:ALA:HA	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:A:358:ASP:HB2	1:A:432:ALA:HB1	1.99	0.44
1:B:220:GLN:HE21	1:B:235:ARG:HH12	1.65	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: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:B:16:ILE:HA	1:B:19:PHE:HD2	1.83	0.44
1:A:281:THR:O	1:A:298:VAL:HG13	2.18	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: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:376:ALA:HB2	1:A:425:GLU:HG2	2.00	0.44
1:A:216:HIS:NE2	1:A:283:GLU:HB3	2.32	0.44
1:B:449:ASP:O	1:B:450:ASN:HB2	2.18	0.44
1:A:627:GLY:HA2	1:A:631:TYR:HE2	1.83	0.44
1:B:282:VAL:HG13	1:B:295:PHE:CE1	2.51	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:239:VAL:CG1	1:B:457:ILE:HD11	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:VAL:HG22	1:B:110:PHE:CZ	2.52	0.43
1:B:627:GLY:HA3	1:B:631:TYR:CE2	2.53	0.43
1:A:222:LEU:HD13	1:A:337:VAL:HG21	2.00	0.43
1:A:316:ASP:HB3	1:A:319:LYS:HB2	2.00	0.43
1:A:240:GLN:HG2	1:A:245:LYS:HA	2.00	0.43
1:B:248:GLU:HG2	1:B:305:GLU:HB3	2.01	0.43
1:B:361:HIS:O	1:B:362:ASN:C	2.56	0.43
1:A:350:LEU:CD2	1:A:415:ALA:HB1	2.48	0.43
1:B:1032:LEU:HD22	1:B:1054:LEU:HD11	2.00	0.43
1:A:756:ALA:HB1	1:B:754:ILE:HG22	2.01	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:414:GLU:OE2	1:A:418:ARG:NH1	2.51	0.43
1:A:226:HIS:HE1	1:A:327:GLY:O	2.01	0.43
1:B:560:ARG:HH11	1:B:1009:THR:HA	1.83	0.43
1:B:279:ALA:HB3	1:B:321:GLN:HE21	1.83	0.43
1:B:62:LEU:O	1:B:67:SER:OG	2.37	0.43
1:B:599:ASP:HA	1:B:600:PRO:HD2	1.89	0.43
1:A:624:ASN:CG	1:A:627:GLY:HA3	2.39	0.43
1:B:304:VAL:HG21	1:B:353:ARG:HE	1.83	0.43
1:B:272:GLY:C	1:B:274:THR:H	2.22	0.43
1:A:108:ILE:H	1:A:108:ILE:HG13	1.70	0.43
1:B:914:PHE:CD2	1:B:941:ALA:HA	2.54	0.43
1:B:316:ASP:C	1:B:316:ASP:OD1	2.56	0.43
1:A:141:ALA:HA	1:A:207:LEU:O	2.18	0.43
1:A:557:THR:HG21	1:A:587:ALA:HB3	2.01	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:B:308:VAL:O	1:B:312:VAL:HG22	2.19	0.43
1:A:218:GLU:CD	1:A:237:CYS:HG	2.22	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:B:282:VAL:HA	1:B:298:VAL:HG22	2.01	0.42
1:A:546:THR:HG21	1:A:814:TRP:CE2	2.54	0.42
1:A:382:ARG:HB3	1:A:406:THR:HB	2.01	0.42
1:B:41:LEU:HD12	1:B:44:PHE:HB2	2.01	0.42
1:A:881:VAL:C	1:A:885:SER:OG	2.57	0.42
1:B:987:TYR:HB3	1:B:990:VAL:HB	2.02	0.42
1:B:416:ILE:O	1:B:420:ASP:HB2	2.20	0.42
1:B:272:GLY:O	1:B:274:THR:N	2.52	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:A:53:GLY:N	1:A:73:GLU:OE2	2.47	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:A:85:ALA:HA	1:A:109:ILE:O	2.19	0.42
1:B:724:LEU:HD23	1:B:746:PHE:CZ	2.55	0.42
1:B:324:ILE:HG22	1:B:325[A]:LEU:HD12	2.01	0.42
1:B:14:ILE:HD12	1:B:17:ARG:HB3	2.00	0.42
1:B:7:LEU:HD13	1:B:78:ALA:CA	2.49	0.42
1:A:14:ILE:HD12	1:A:14:ILE:HA	1.89	0.42
1:B:312:VAL:HG11	1:B:349:ALA:CB	2.49	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:A:479:TYR:O	1:A:483:VAL:HG12	2.19	0.42
1:A:220:GLN:HB2	1:A:235:ARG:HH12	1.85	0.42
1:A:929:PRO:HG2	1:A:932:GLY:O	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:B:96:SER:O	1:B:100:VAL:HG23	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:838:HIS:NE2	1:B:845:PHE:HE1	2.18	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:1021:GLU:HB2	1:B:1035:VAL:HG22	2.02	0.42
1:B:452:TYR:N	1:B:452:TYR:CD2	2.83	0.41
1:A:494:ARG:HB2	1:A:823:ALA:HB1	2.02	0.41
1:B:270:ILE:O	1:B:274:THR:HG23	2.19	0.41
1:A:358:ASP:HB2	1:A:432:ALA:CB	2.50	0.41
1:B:145:LEU:HA	1:B:146:PRO:HD2	1.90	0.41
1:B:17:ARG:NH1	1:B:21:ALA:HB2	2.35	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:A:541:LEU:HB3	1:A:579:LEU:HB2	2.03	0.41
1:A:366:ASP:HB3	1:A:431:VAL:HB	2.01	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:A:282:VAL:HG12	1:A:284:TYR:CE2	2.55	0.41
1:B:1046:GLY:O	1:B:1064:PRO:HA	2.19	0.41
1:A:112:GLY:O	1:A:277:ILE:HB	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:SER:HA	1:A:426:PHE:CE2	2.56	0.41
1:B:305:GLU:O	1:B:308:VAL:HG22	2.19	0.41
1:B:114:LYS:HG3	1:B:277:ILE:CD1	2.51	0.41
1:A:323:HIS:HB3	1:A:328:ALA:HB3	2.02	0.41
1:A:546:THR:HG21	1:A:814:TRP:CD1	2.55	0.41
1:B:71:ILE:HG23	1:B:99:PHE:HD1	1.84	0.41
1:A:62:LEU:HB2	1:A:67:SER:OG	2.21	0.41
1:A:955:LEU:HA	1:A:955:LEU:HD23	1.91	0.41
1:B:252:ALA:HA	1:B:253:PRO:HD2	1.95	0.41
1:B:1052:PHE:CE2	1:B:1061:ILE:HD13	2.55	0.41
1:B:374[A]:ARG:NH2	1:B:427:ARG:HD3	2.36	0.41
1:A:19:PHE:HD1	1:A:29:THR:HB	1.84	0.41
1:B:659:TRP:CE2	1:B:661:GLU:HB3	2.56	0.41
1:B:54:ARG:HE	1:B:54:ARG:HB2	1.56	0.41
1:A:348:HIS:O	1:A:409:ALA:N	2.44	0.41
1:B:249:ARG:CZ	1:B:253:PRO:HG3	2.50	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:220:GLN:HE21	1:A:235:ARG:NH1	2.17	0.41
1:A:887:VAL:HG22	1:A:917:SER:HB2	2.02	0.41
1:B:383:LEU:HD22	1:B:405:VAL:HG22	2.03	0.41
1:A:102:ALA:HA	1:A:105:LYS:HB3	2.03	0.41
1:A:940:LYS:O	1:A:941:ALA:C	2.59	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:B:1052:PHE:HD2	1:B:1061:ILE:CD1	2.31	0.40
1:B:99:PHE:O	1:B:100:VAL:C	2.57	0.40
1:A:793:LEU:HD23	1:A:793:LEU:HA	1.85	0.40
1:A:703:LEU:HD23	1:A:703:LEU:HA	1.81	0.40
1:B:558:ARG:HD3	1:B:558:ARG:HA	1.88	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:527:PRO:HB2	1:A:713:HIS:CE1	2.56	0.40
1:A:50:TYR:HB2	1:A:77:VAL:HG13	2.03	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:B:248:GLU:HB3	1:B:305:GLU:HB2	2.04	0.40
1:B:1044:SER:C	1:B:1046:GLY:H	2.24	0.40
1:B:624:ASN:HB2	1:B:631:TYR:CD2	2.56	0.40
1:A:120:GLN:HE21	1:A:120:GLN:HB3	1.66	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%)	10	40
1	B	1002/1165 (86%)	899 (90%)	82 (8%)	21 (2%)	9	37
All	All	2003/2330 (86%)	1774 (89%)	189 (9%)	40 (2%)	9	38

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%)	20	56
1	B	769/933 (82%)	709 (92%)	60 (8%)	16	49
All	All	1518/1866 (81%)	1408 (93%)	110 (7%)	18	53

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

Some 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	7,11,12	0.76	0	7,12,14	1.24	1 (14%)
1	KCX	B	718[A]	1,3	7,11,12	0.98	0	7,12,14	1.11	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	-	0/6/10/12	0/0/0/0
1	KCX	B	718[A]	1,3	-	0/6/10/12	0/0/0/0

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	-2.37	105.24	113.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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%)	0.55	161 (16%)	3 1	19, 72, 163, 191	8 (0%)
1	B	1001/1165 (85%)	0.33	120 (11%)	6 2	19, 56, 139, 190	7 (0%)
All	All	2004/2330 (86%)	0.44	281 (14%)	4 2	19, 65, 156, 191	15 (0%)

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	SER	11.4
1	A	142	THR	8.3
1	B	288	ALA	7.9
1	A	285	LEU	7.7
1	B	346	ASN	7.2
1	B	341[A]	GLU	7.1
1	A	136	VAL	6.9
1	A	215	ARG	6.6
1	B	207	LEU	6.6
1	A	334	GLN	6.4
1	A	294	TYR	6.2
1	B	331	GLY	6.2
1	A	124	LYS	6.0
1	B	167	ALA	6.0
1	B	96	SER	5.9
1	A	290	THR	5.8
1	A	115	ALA	5.8
1	A	108	ILE	5.8
1	B	135	GLY	5.8
1	A	225	THR	5.7
1	A	1043	ASP	5.7
1	B	206	TYR	5.7
1	A	141	ALA	5.6
1	A	116[A]	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	133	SER	5.5
1	A	144	PRO	5.4
1	A	313	THR	5.3
1	A	454	THR	5.3
1	B	272	GLY	5.2
1	A	164	MET	5.2
1	A	296[A]	ILE	5.2
1	A	145	LEU	5.2
1	A	336	GLY	5.1
1	A	275	ASN	5.1
1	B	132	ILE	5.1
1	B	278	GLY	5.0
1	A	1046	GLY	4.9
1	A	457	ILE	4.9
1	A	214	ALA	4.8
1	B	97	PRO	4.8
1	A	335	SER	4.7
1	A	450	ASN	4.7
1	A	852	ALA	4.7
1	A	274	THR	4.7
1	A	453	THR	4.7
1	A	411[A]	ASN	4.6
1	A	367	TYR	4.5
1	A	168	SER	4.5
1	A	449	ASP	4.5
1	A	286	MET	4.4
1	A	56	PRO	4.4
1	B	128	ARG	4.4
1	A	511	GLY	4.3
1	A	1044	SER	4.3
1	A	339	ASN	4.3
1	B	95	GLU	4.3
1	A	221	ILE	4.3
1	A	855	LEU	4.3
1	A	167	ALA	4.2
1	B	214	ALA	4.1
1	B	334	GLN	4.1
1	B	255	LEU	4.1
1	B	289	ASP	4.1
1	A	99	PHE	4.1
1	B	213	ARG	4.1
1	B	253	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	142	THR	4.0
1	A	415	ALA	4.0
1	A	96	SER	4.0
1	B	127	ALA	3.9
1	B	275	ASN	3.9
1	B	276	TYR	3.9
1	B	271	ALA	3.9
1	B	131	ALA	3.9
1	B	179	ILE	3.9
1	A	238	SER	3.9
1	B	212	GLU	3.8
1	B	139	VAL	3.8
1	A	856	GLY	3.8
1	A	434	ASN	3.8
1	B	226	HIS	3.7
1	B	166	LYS	3.7
1	A	431	VAL	3.7
1	A	326	ASP	3.7
1	B	294	TYR	3.6
1	A	55	GLY	3.6
1	B	345	LEU	3.6
1	A	315	ILE	3.6
1	B	336	GLY	3.6
1	A	1045	GLN	3.6
1	A	298	VAL	3.6
1	A	287	ASP	3.6
1	B	165	LEU	3.6
1	B	223	GLY	3.6
1	A	322	ILE	3.6
1	A	332	THR	3.6
1	B	205	VAL	3.5
1	A	60	ARG	3.5
1	A	452	TYR	3.5
1	A	1047	MET	3.5
1	A	179	ILE	3.5
1	A	113	PRO	3.5
1	A	312	VAL	3.5
1	A	432	ALA	3.5
1	B	116[A]	ASP	3.4
1	B	145	LEU	3.4
1	B	261	GLN	3.4
1	A	337	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	363	PHE	3.4
1	B	137	PRO	3.4
1	A	451	SER	3.3
1	A	210	LEU	3.3
1	A	209	LYS	3.3
1	B	352[A]	CYS	3.3
1	A	143	GLU	3.3
1	A	904	ASP	3.3
1	B	27	ILE	3.3
1	B	178	VAL	3.3
1	A	279	ALA	3.3
1	A	123	ASN	3.3
1	B	399	ASP	3.3
1	A	258	ALA	3.3
1	B	409	ALA	3.3
1	A	83	ALA	3.2
1	B	86	ILE	3.2
1	A	72	ASP	3.2
1	B	386	GLY	3.2
1	A	228	ASN	3.2
1	B	342	ASP	3.1
1	A	226	HIS	3.1
1	B	180	ARG	3.1
1	A	284	TYR	3.1
1	B	347	GLY	3.1
1	A	114	LYS	3.1
1	A	343	ILE	3.1
1	B	143	GLU	3.1
1	A	125	VAL	3.1
1	A	896	VAL	3.1
1	B	333	PRO	3.1
1	A	267	SER	3.0
1	A	98[A]	GLU	3.0
1	A	239	VAL	3.0
1	A	106	ALA	3.0
1	A	905	VAL	3.0
1	B	129	ASN	2.9
1	A	134	VAL	2.9
1	A	146	PRO	2.9
1	B	445	PRO	2.9
1	A	128	ARG	2.9
1	B	301	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	208	GLU	2.9
1	B	91	GLY	2.9
1	B	296[A]	ILE	2.9
1	A	119	ARG	2.9
1	A	321	GLN	2.8
1	A	223	GLY	2.8
1	A	407	ALA	2.8
1	A	95	GLU	2.8
1	B	264	ALA	2.8
1	B	144	PRO	2.8
1	A	252	ALA	2.8
1	A	345	LEU	2.8
1	B	109	ILE	2.7
1	B	233	PHE	2.7
1	B	215	ARG	2.7
1	B	340	GLN	2.7
1	A	10	ASN	2.7
1	A	117	THR	2.7
1	B	241	ARG	2.7
1	B	123	ASN	2.7
1	B	339	ASN	2.7
1	B	284	TYR	2.7
1	A	445	PRO	2.7
1	B	267	SER	2.6
1	A	122	GLY	2.6
1	A	4	SER	2.6
1	B	907[A]	SER	2.6
1	A	410	PRO	2.6
1	A	1064	PRO	2.6
1	A	368	GLY	2.6
1	B	3	ILE	2.6
1	A	433	THR	2.6
1	B	94	SER	2.6
1	A	295	PHE	2.6
1	B	315	ILE	2.6
1	B	293	PHE	2.6
1	A	54	ARG	2.6
1	B	112	GLY	2.6
1	B	2	PRO	2.6
1	A	61	ASP	2.6
1	B	344	ARG	2.6
1	B	326	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	97	PRO	2.5
1	A	207	LEU	2.5
1	A	165	LEU	2.5
1	B	297	GLU	2.5
1	A	270	ILE	2.5
1	B	274	THR	2.5
1	B	332	THR	2.5
1	A	163	VAL	2.5
1	B	134	VAL	2.5
1	B	1045	GLN	2.5
1	A	360	GLU	2.5
1	A	327	GLY	2.5
1	A	261	GLN	2.4
1	B	419	MET	2.4
1	A	70	SER	2.4
1	A	265	ALA	2.4
1	B	79	LYS	2.4
1	A	227	GLY	2.4
1	A	205	VAL	2.4
1	A	303	GLN	2.4
1	A	377	SER	2.4
1	B	330	ILE	2.4
1	B	412	PRO	2.4
1	A	381	ILE	2.4
1	A	222	LEU	2.4
1	A	325[A]	LEU	2.4
1	B	29	THR	2.4
1	B	434	ASN	2.3
1	B	458	ASP	2.3
1	B	265	ALA	2.3
1	B	254	TYR	2.3
1	B	327	GLY	2.3
1	A	289	ASP	2.3
1	A	389	TYR	2.3
1	A	62	LEU	2.3
1	B	260	ARG	2.3
1	B	1029	GLY	2.3
1	A	277	ILE	2.3
1	A	375	SER	2.3
1	A	902	VAL	2.2
1	B	230	VAL	2.2
1	A	859	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	860	ARG	2.2
1	A	897	SER	2.2
1	B	262	GLU	2.2
1	A	103	CYS	2.2
1	A	2	PRO	2.2
1	A	110	PHE	2.2
1	B	513	GLY	2.2
1	A	76	ARG	2.2
1	A	81	SER	2.2
1	A	907[A]	SER	2.2
1	B	104	ASN	2.2
1	A	65	ILE	2.2
1	A	112	GLY	2.2
1	A	269	LYS	2.2
1	A	118	MET	2.2
1	A	235	ARG	2.2
1	B	234	GLU	2.2
1	B	93	LEU	2.1
1	A	26	GLY	2.1
1	B	443	GLY	2.1
1	A	6	ILE	2.1
1	B	164	MET	2.1
1	B	222	LEU	2.1
1	A	944	GLY	2.1
1	A	140	PRO	2.1
1	A	129	ASN	2.1
1	B	908	PRO	2.1
1	A	390	SER	2.1
1	B	231	HIS	2.1
1	B	256	SER	2.1
1	A	92	LEU	2.1
1	A	220	GLN	2.1
1	B	406	THR	2.1
1	B	449	ASP	2.1
1	A	857	LEU	2.1
1	B	343	ILE	2.1
1	B	236	ASP	2.1
1	A	448	ARG	2.1
1	A	854	SER	2.0
1	B	379	PHE	2.0
1	B	411[A]	ASN	2.0
1	B	902	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	242	ARG	2.0
1	A	121	LEU	2.0
1	B	85	ALA	2.0
1	A	352[A]	CYS	2.0
1	B	283	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	KCX	A	718[A]	12/13	0.98	0.13	-	20,21,22,22	0
1	KCX	B	718[A]	12/13	0.98	0.12	-	19,21,22,22	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	MG	B	1200	1/1	0.88	0.24	5.07	40,40,40,40	0
2	MG	A	1200	1/1	0.80	0.19	2.15	25,25,25,25	0
3	ZN	B	1201	1/1	0.98	0.06	-4.17	59,59,59,59	0
3	ZN	A	1201	1/1	0.97	0.09	-	56,56,56,56	0
4	CL	B	1202	1/1	0.97	0.11	-	30,30,30,30	0
4	CL	A	1202	1/1	0.97	0.17	-	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.