



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:22 PM UTC

PDB ID : 4QG6 / pdb_00004qg6
Title : crystal structure of PKM2-Y105E mutant
Authors : Wang, P.; Sun, C.; Zhu, T.; Xu, Y.
Deposited on : 2014-05-22
Resolution : 3.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

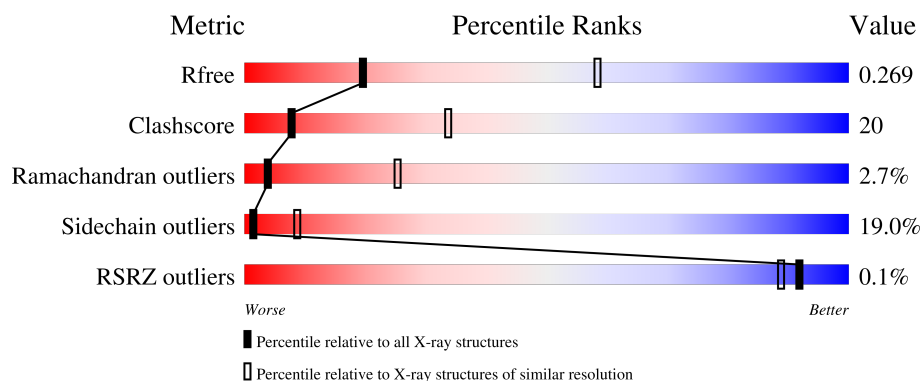
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	535	
1	B	535	
1	C	535	
1	D	535	

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	PRO	C	1001	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13991 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.

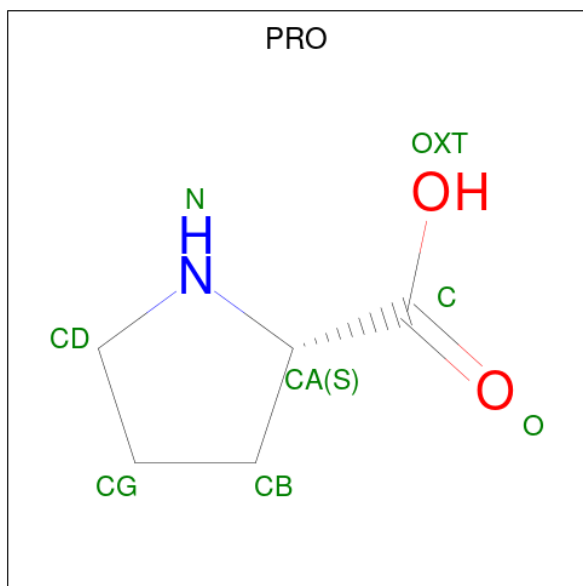
- Molecule 1 is a protein called Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3122	1958	564	579	21			
1	B	502	Total	C	N	O	S	0	0	0
			3849	2420	682	723	24			
1	C	406	Total	C	N	O	S	0	0	0
			3122	1958	564	579	21			
1	D	505	Total	C	N	O	S	0	0	0
			3870	2434	686	726	24			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P14618
A	-2	PRO	-	expression tag	UNP P14618
A	-1	GLY	-	expression tag	UNP P14618
A	0	SER	-	expression tag	UNP P14618
A	105	GLU	TYR	engineered mutation	UNP P14618
B	-3	GLY	-	expression tag	UNP P14618
B	-2	PRO	-	expression tag	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
B	105	GLU	TYR	engineered mutation	UNP P14618
C	-3	GLY	-	expression tag	UNP P14618
C	-2	PRO	-	expression tag	UNP P14618
C	-1	GLY	-	expression tag	UNP P14618
C	0	SER	-	expression tag	UNP P14618
C	105	GLU	TYR	engineered mutation	UNP P14618
D	-3	GLY	-	expression tag	UNP P14618
D	-2	PRO	-	expression tag	UNP P14618
D	-1	GLY	-	expression tag	UNP P14618
D	0	SER	-	expression tag	UNP P14618
D	105	GLU	TYR	engineered mutation	UNP P14618

- Molecule 2 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).

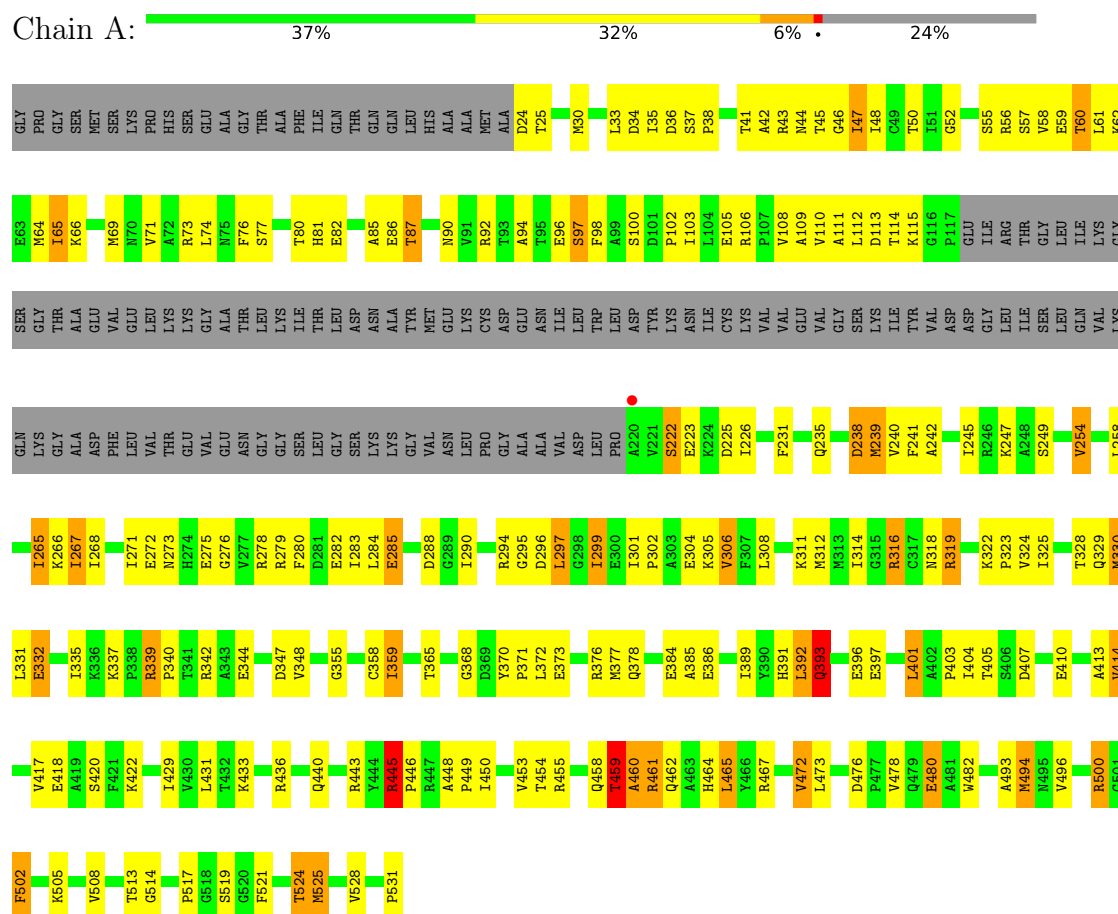


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	5	1	1		
2	B	1	Total	C	N	O	0	0
			7	5	1	1		
2	C	1	Total	C	N	O	0	0
			7	5	1	1		
2	D	1	Total	C	N	O	0	0
			7	5	1	1		

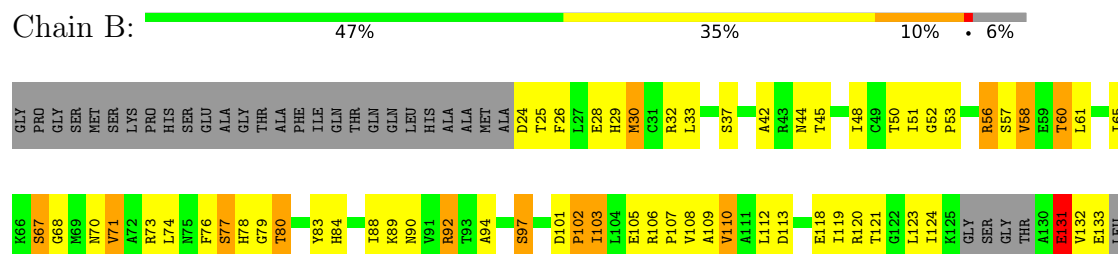
3 Residue-property plots

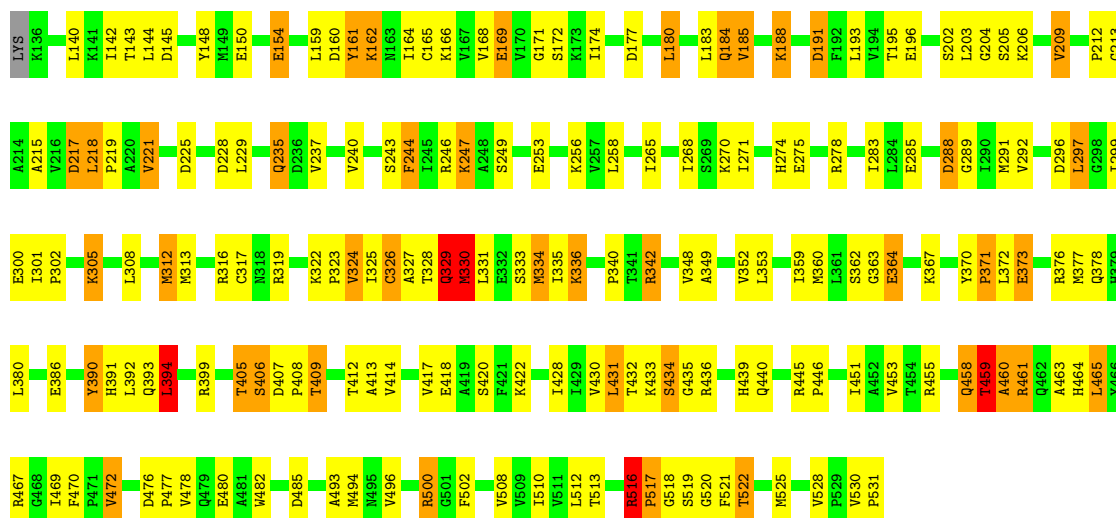
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Pyruvate kinase PKM



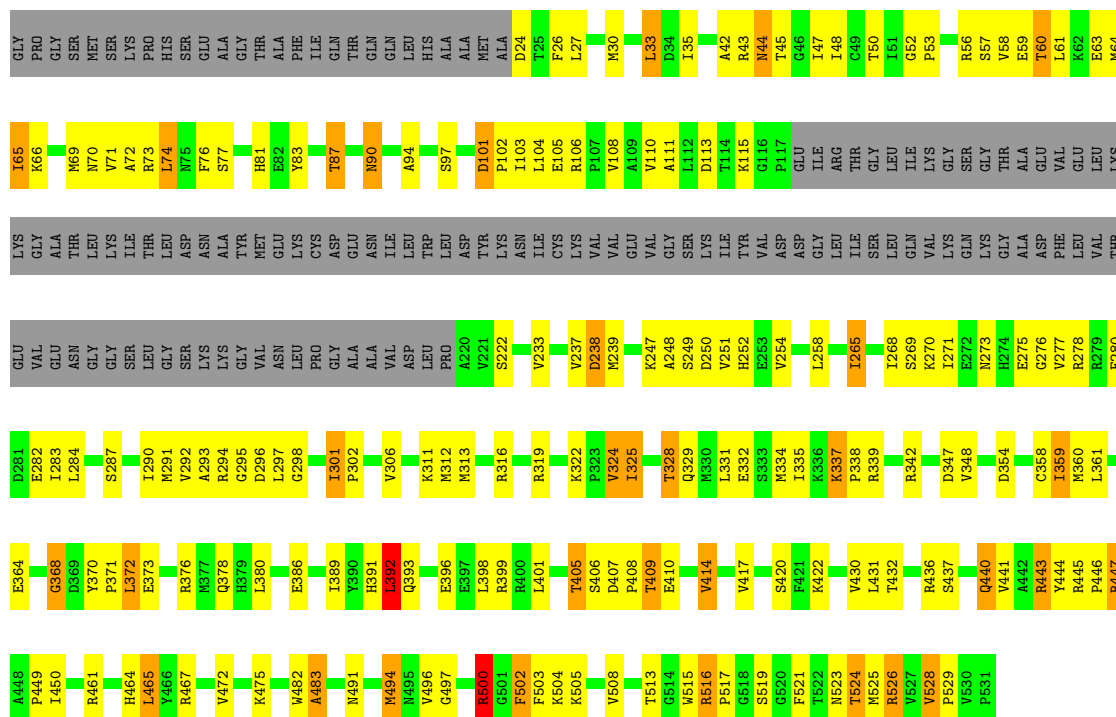
• Molecule 1: Pyruvate kinase PKM





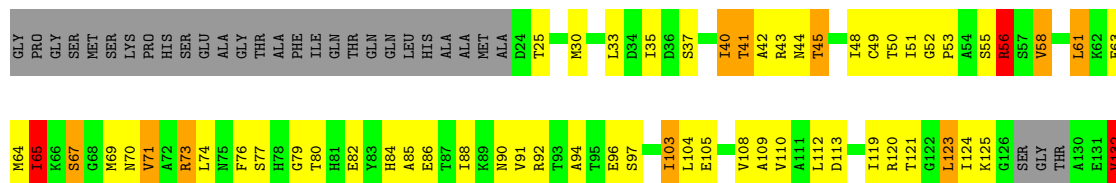
● Molecule 1: Pyruvate kinase PKM

Chain C: 41% 29% 6% 24%



● Molecule 1: Pyruvate kinase PKM

Chain D: 46% 39% 8% 6%



E133	K207	V306	E384	R461
L134	G208	F307	A385	Q462
K135	V209	K311	E386	A463
K136	N210	M312	Y390	H464
	L211	M313	H391	L465
T139	P212		L392	Y466
L140		R316	Q393	R467
K141	V216		L394	
I142	D217	P323	F395	F470
T143	L218	V324		P471
		I325	L398	V472
N146	V221	C326	R399	L473
A147		A327	R400	C474
Y148	K224	T328	L401	
M149		Q329		V478
E150	D228	M330	T405	
K151	L229	L331	S406	A481
C152	K230	E332	D407	W482
D153	F231	S333	P408	A483
		M334		E484
I156	Q235	I335	T412	D485
L157	D236	K336	V414	V486
W158	V237			D487
L159	D238	R339	V417	L488
D160	M239	P340	E418	R489
		T341	A419	V490
V167	F244	R342	S420	M491
V168	R246	E344	F421	F492
E169		G345	K422	A493
V170	E253	D347	I428	M494
G171	V254	V348	I429	W495
S172		N350	V430	V496
K173		A351	L431	G497
I174	V257	V352	T432	K498
Y175	K261	L353	K433	
V176		D354	S434	F502
D177	L265		R436	V508
D178	K266	I359	Q440	
G179	L267	M360	V441	L512
L180	I268	L361	A442	T513
I181	S269	G363	R443	
S182		E364	Y444	R516
L183	K270	T365	P446	P517
		A366		G518
K186		L372	P449	S519
Q187	E275		I450	G520
K188		V375	I451	F521
	R279	R376	A452	T522
D191	E265	M377	V453	N523
		Q378	T454	T524
			R455	M525
T195	G289	I381	Q458	
E196	L290	A382		T528
V197	M291	R383		P529
E198	V292			W530
N199	A293			P531
	R294			
L203				
G204	L297			
S205	K305			
K206				

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	124.45Å 124.45Å 257.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.62 – 3.21 45.62 – 3.21	Depositor EDS
% Data completeness (in resolution range)	98.2 (45.62-3.21) 98.3 (45.62-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.220 , 0.265 0.223 , 0.269	Depositor DCC
R_{free} test set	3637 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	95.0	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 71.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.438 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13991	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	1/3175 (0.0%)	1.04	10/4287 (0.2%)
1	B	0.62	0/3909	1.08	12/5276 (0.2%)
1	C	0.61	0/3175	1.02	6/4287 (0.1%)
1	D	0.63	0/3931	1.08	12/5306 (0.2%)
All	All	0.62	1/14190 (0.0%)	1.06	40/19156 (0.2%)

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	D	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	ARG	C-O	-6.05	1.21	1.23

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	516	ARG	CA-C-N	-13.27	103.25	119.84
1	B	516	ARG	C-N-CA	-13.27	103.25	119.84
1	B	461	ARG	N-CA-C	-9.29	101.72	113.43
1	D	218	LEU	N-CA-C	9.11	122.88	109.04
1	B	288	ASP	N-CA-C	-7.29	104.54	113.50
1	B	131	GLU	N-CA-C	6.88	117.67	108.38
1	A	429	ILE	CB-CA-C	-6.79	102.32	111.15
1	D	37	SER	CA-C-N	6.79	127.37	120.38
1	D	37	SER	C-N-CA	6.79	127.37	120.38
1	B	406	SER	N-CA-C	-6.72	103.47	112.94
1	C	406	SER	N-CA-C	-6.68	103.59	113.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	SER	CA-C-N	6.56	127.13	120.38
1	B	37	SER	C-N-CA	6.56	127.13	120.38
1	B	52	GLY	CA-C-N	6.55	128.03	119.84
1	B	52	GLY	C-N-CA	6.55	128.03	119.84
1	D	406	SER	N-CA-C	-6.45	104.09	114.09
1	D	56	ARG	N-CA-C	6.39	120.67	113.01
1	A	461	ARG	N-CA-C	-6.38	104.25	111.14
1	A	476	ASP	CA-C-N	6.07	126.39	119.83
1	A	476	ASP	C-N-CA	6.07	126.39	119.83
1	C	447	ARG	N-CA-C	-6.06	104.59	112.23
1	C	52	GLY	CA-C-N	5.83	127.13	119.84
1	C	52	GLY	C-N-CA	5.83	127.13	119.84
1	C	516	ARG	N-CA-C	-5.78	102.87	110.39
1	D	52	GLY	CA-C-N	5.71	126.98	119.84
1	D	52	GLY	C-N-CA	5.71	126.98	119.84
1	D	167	VAL	CB-CA-C	-5.57	106.97	111.71
1	A	450	ILE	CB-CA-C	-5.54	104.73	111.88
1	A	502	PHE	N-CA-C	5.50	117.98	111.33
1	D	153	ASP	N-CA-C	5.42	114.99	107.73
1	D	520	GLY	N-CA-C	-5.42	105.02	111.36
1	A	52	GLY	CA-C-N	5.41	126.60	119.84
1	A	52	GLY	C-N-CA	5.41	126.60	119.84
1	C	502	PHE	N-CA-C	5.31	117.75	111.33
1	B	107	PRO	CA-C-O	-5.23	115.37	123.16
1	A	47	ILE	N-CA-C	5.15	115.75	107.98
1	D	65	ILE	CB-CA-C	-5.07	105.48	111.97
1	A	254	VAL	CB-CA-C	-5.04	105.42	112.02
1	D	77	SER	N-CA-C	-5.03	107.10	113.18
1	B	352	VAL	CB-CA-C	-5.02	105.54	111.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	217	ASP	Peptide
1	D	218	LEU	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	3122	0	3177	144	0
1	B	3849	0	3929	162	0
1	C	3122	0	3177	125	0
1	D	3870	0	3957	166	0
2	A	7	0	7	2	0
2	B	7	0	7	3	0
2	C	7	0	7	4	0
2	D	7	0	7	0	0
All	All	13991	0	14268	562	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 20.

All (562) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:HG23	1:A:69:MET:HE3	1.48	0.94
1:B:73:ARG:NH1	1:B:113:ASP:OD2	2.03	0.92
1:D:73:ARG:NH1	1:D:113:ASP:OD2	2.03	0.91
1:C:65:ILE:HG23	1:C:69:MET:HE3	1.56	0.85
1:C:73:ARG:NH1	1:C:113:ASP:OD2	2.10	0.83
1:D:147:ALA:O	1:D:151:LYS:NZ	2.12	0.83
1:C:422:LYS:HG3	1:D:414:VAL:HG21	1.62	0.82
1:A:445:ARG:HE	1:A:467:ARG:HD3	1.43	0.82
1:C:287:SER:O	1:C:322:LYS:NZ	2.10	0.82
1:C:56:ARG:HG3	1:C:87:THR:HG23	1.62	0.82
1:A:445:ARG:HH11	1:A:445:ARG:HG2	1.44	0.81
1:B:417:VAL:HG13	1:B:446:PRO:HB3	1.63	0.80
1:D:394:LEU:HD12	1:D:445:ARG:HD3	1.65	0.79
1:D:414:VAL:HG22	1:D:444:TYR:HE2	1.48	0.79
1:C:325:ILE:HG22	1:C:358:CYS:HB2	1.64	0.78
1:B:171:GLY:H	1:B:185:VAL:HG23	1.49	0.77
1:C:516:ARG:NH2	1:D:487:ASP:OD2	2.18	0.77
1:D:92:ARG:NH1	1:D:235:GLN:O	2.17	0.77
1:B:118:GLU:OE1	1:B:120:ARG:NH1	2.18	0.77
1:C:42:ALA:O	1:C:44:ASN:ND2	2.18	0.77
1:B:386:GLU:OE2	1:B:467:ARG:NH2	2.16	0.76
1:D:71:VAL:HG22	1:D:109:ALA:HB3	1.68	0.76
1:A:42:ALA:O	1:A:44:ASN:ND2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:THR:HG22	1:D:207:LYS:H	1.49	0.75
1:D:451:ILE:HD11	1:D:502:PHE:HD2	1.51	0.75
1:C:386:GLU:OE2	1:C:467:ARG:NH2	2.20	0.75
1:D:70:ASN:HD22	1:D:464:HIS:HD2	1.34	0.74
1:B:58:VAL:HG23	1:B:90:ASN:HD22	1.53	0.74
1:D:70:ASN:HD22	1:D:464:HIS:CD2	2.04	0.74
1:D:354:ASP:OD1	1:D:354:ASP:N	2.18	0.74
1:A:86:GLU:O	1:A:90:ASN:ND2	2.21	0.73
1:A:223:GLU:HA	1:A:226:ILE:HD12	1.69	0.73
1:C:280:PHE:HA	1:C:283:ILE:HD12	1.71	0.73
1:A:328:THR:HG22	1:A:329:GLN:HG3	1.69	0.73
1:C:268:ILE:HG21	1:C:325:ILE:HD11	1.71	0.72
1:D:386:GLU:OE2	1:D:467:ARG:NH2	2.23	0.72
1:D:482:TRP:CD1	1:D:517:PRO:HD3	2.24	0.71
1:C:292:VAL:HG22	1:C:313:MET:HE3	1.73	0.71
1:A:325:ILE:HG22	1:A:358:CYS:HB2	1.71	0.71
1:D:239:MET:HB3	1:D:266:LYS:HB2	1.73	0.71
1:A:370:TYR:HB3	1:A:373:GLU:HB2	1.73	0.70
1:A:449:PRO:HG3	1:A:502:PHE:HD2	1.56	0.70
1:B:370:TYR:HD1	1:B:373:GLU:HG3	1.55	0.69
1:C:337:LYS:HE2	1:C:338:PRO:HD2	1.73	0.69
1:A:464:HIS:HD2	2:A:1001:PRO:HB2	1.57	0.69
1:C:392:LEU:H	1:C:392:LEU:HD22	1.56	0.69
1:A:71:VAL:HG21	1:A:239:MET:HE1	1.75	0.69
1:B:328:THR:HG22	1:B:329:GLN:HG2	1.75	0.69
1:C:311:LYS:NZ	1:C:354:ASP:OD1	2.25	0.68
1:B:451:ILE:HD11	1:B:502:PHE:HD2	1.58	0.68
1:B:133:GLU:HG2	1:B:203:LEU:H	1.59	0.68
1:C:370:TYR:HB3	1:C:373:GLU:HB2	1.76	0.68
1:A:73:ARG:NH1	1:A:113:ASP:OD2	2.26	0.68
1:D:270:LYS:HA	1:D:291:MET:HB3	1.76	0.68
1:B:390:TYR:CZ	1:B:394:LEU:HD22	2.29	0.67
1:C:464:HIS:HD2	2:C:1001:PRO:CB	2.08	0.67
1:C:405:THR:HB	1:C:407:ASP:H	1.59	0.67
1:D:170:VAL:HG23	1:D:188:LYS:HE2	1.74	0.67
1:B:92:ARG:NH1	1:B:235:GLN:O	2.28	0.67
1:B:191:ASP:N	1:B:191:ASP:OD1	2.29	0.66
1:A:418:GLU:HG2	1:B:418:GLU:HG3	1.78	0.66
1:D:50:THR:HG22	1:D:366:ALA:HB2	1.77	0.66
1:A:378:GLN:O	1:A:378:GLN:NE2	2.29	0.66
1:B:102:PRO:HA	1:B:105:GLU:HG2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:ILE:HD11	1:D:378:GLN:OE1	1.95	0.65
1:A:372:LEU:HG	1:A:376:ARG:HD2	1.78	0.65
1:D:312:MET:HE2	1:D:316:ARG:HH21	1.59	0.65
1:C:414:VAL:HG21	1:D:422:LYS:HD3	1.77	0.65
1:D:42:ALA:O	1:D:44:ASN:ND2	2.30	0.65
1:A:417:VAL:O	1:A:420:SER:OG	2.12	0.65
1:B:312:MET:HE1	1:B:316:ARG:HH21	1.62	0.64
1:B:433:LYS:O	1:B:459:THR:OG1	2.11	0.64
1:A:417:VAL:HG22	1:A:446:PRO:HG3	1.79	0.64
1:D:65:ILE:HD12	1:D:108:VAL:HG21	1.79	0.64
1:C:399:ARG:NH2	1:D:399:ARG:HH12	1.97	0.63
1:B:409:THR:OG1	1:B:440:GLN:NE2	2.27	0.63
1:B:68:GLY:O	1:B:70:ASN:ND2	2.30	0.63
1:A:472:VAL:HG21	1:A:496:VAL:HG11	1.80	0.63
1:B:229:LEU:HD22	1:B:258:LEU:HD21	1.81	0.63
1:B:244:PHE:HD2	1:B:246:ARG:HH11	1.44	0.63
1:C:58:VAL:HG23	1:C:90:ASN:ND2	2.12	0.63
1:D:55:SER:O	1:D:61:LEU:HD23	1.98	0.63
1:C:482:TRP:HZ3	1:C:515:TRP:C	2.07	0.63
1:D:61:LEU:HD12	1:D:91:VAL:HA	1.81	0.63
1:C:238:ASP:OD2	1:C:461:ARG:NE	2.26	0.62
1:A:464:HIS:HD2	2:A:1001:PRO:CB	2.11	0.62
1:D:229:LEU:HD21	1:D:254:VAL:HG13	1.81	0.62
1:A:238:ASP:OD1	1:A:238:ASP:N	2.32	0.62
1:A:332:GLU:O	1:A:335:ILE:HG13	1.99	0.62
1:B:292:VAL:HG22	1:B:313:MET:HE3	1.81	0.62
1:D:294:ARG:NH2	1:D:347:ASP:OD2	2.30	0.61
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.81	0.61
1:C:359:ILE:HD13	1:C:359:ILE:H	1.65	0.61
1:D:61:LEU:HD11	1:D:91:VAL:HG22	1.82	0.61
1:D:88:ILE:HG22	1:D:92:ARG:HE	1.66	0.61
1:C:391:HIS:C	1:C:393:GLN:H	2.08	0.61
1:A:482:TRP:CD1	1:A:517:PRO:HB3	2.36	0.61
1:A:64:MET:HB3	1:A:69:MET:HE2	1.83	0.61
1:B:51:ILE:HD13	1:B:61:LEU:HD21	1.83	0.61
1:B:119:ILE:HB	1:B:209:VAL:HG22	1.82	0.61
1:A:445:ARG:NE	1:A:467:ARG:HD3	2.14	0.60
1:A:403:PRO:O	1:B:422:LYS:NZ	2.33	0.60
1:B:145:ASP:HB3	1:B:148:TYR:HD2	1.67	0.60
1:A:85:ALA:HB2	1:A:231:PHE:HZ	1.66	0.60
1:B:370:TYR:CD1	1:B:373:GLU:HG3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:ASP:OD2	1:C:409:THR:HG22	2.01	0.60
1:D:173:LYS:NZ	1:D:198:GLU:OE2	2.29	0.60
1:A:403:PRO:HG2	1:A:405:THR:HG23	1.84	0.60
1:A:414:VAL:HG21	1:B:422:LYS:HG2	1.84	0.60
1:A:273:ASN:HD21	1:A:275:GLU:HB3	1.67	0.60
1:B:405:THR:HB	1:B:407:ASP:H	1.67	0.59
1:B:330:MET:HE2	1:B:359:ILE:HB	1.83	0.59
1:A:247:LYS:NZ	1:A:275:GLU:OE1	2.35	0.59
1:B:253:GLU:HA	1:B:256:LYS:HE2	1.84	0.59
1:C:391:HIS:O	1:C:393:GLN:N	2.35	0.59
1:C:399:ARG:NE	1:D:399:ARG:HH22	2.00	0.59
1:D:70:ASN:HB3	1:D:464:HIS:HD2	1.66	0.59
1:A:301:ILE:HG13	1:A:306:VAL:HG23	1.85	0.59
1:D:431:LEU:HD22	1:D:513:THR:HA	1.84	0.59
1:B:458:GLN:O	1:B:460:ALA:N	2.36	0.59
1:C:399:ARG:NH1	1:D:418:GLU:OE2	2.34	0.59
1:A:305:LYS:NZ	1:D:384:GLU:OE1	2.30	0.59
1:B:70:ASN:OD1	1:B:464:HIS:HD2	1.85	0.59
1:D:451:ILE:HD11	1:D:502:PHE:CD2	2.37	0.59
1:A:275:GLU:HA	1:A:278:ARG:HB2	1.85	0.59
1:D:70:ASN:HB3	1:D:464:HIS:CD2	2.37	0.59
1:D:132:VAL:HG23	1:D:203:LEU:HB3	1.85	0.59
1:A:325:ILE:CG2	1:A:358:CYS:HB2	2.33	0.58
1:B:359:ILE:HD11	1:B:378:GLN:CD	2.27	0.58
1:C:445:ARG:HH11	1:C:467:ARG:HD3	1.68	0.58
1:B:431:LEU:HD22	1:B:513:THR:HA	1.86	0.58
1:A:459:THR:HA	1:A:462:GLN:HB2	1.86	0.58
1:B:406:SER:O	1:B:408:PRO:HD3	2.03	0.58
1:A:35:ILE:O	1:D:305:LYS:NZ	2.31	0.58
1:B:26:PHE:CZ	1:B:30:MET:HE2	2.39	0.58
1:C:325:ILE:CG2	1:C:358:CYS:HB2	2.31	0.58
1:A:240:VAL:HG21	1:A:258:LEU:HD21	1.86	0.57
1:A:431:LEU:HD22	1:A:513:THR:HG22	1.87	0.57
1:D:191:ASP:N	1:D:191:ASP:OD1	2.37	0.57
1:A:55:SER:HA	1:A:60:THR:HG21	1.87	0.57
1:B:428:ILE:HG23	1:B:510:ILE:HB	1.87	0.57
1:C:290:ILE:HB	1:C:324:VAL:HG23	1.85	0.57
1:C:399:ARG:CZ	1:D:399:ARG:HH12	2.18	0.57
1:A:297:LEU:HD12	1:A:301:ILE:HD11	1.85	0.56
1:A:311:LYS:HD3	1:D:30:MET:HE1	1.87	0.56
1:A:513:THR:O	1:A:524:THR:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ILE:HB	1:B:193:LEU:HB2	1.86	0.56
1:D:141:LYS:HB3	1:D:156:ILE:HG23	1.87	0.56
1:C:238:ASP:OD1	1:C:238:ASP:N	2.38	0.56
1:B:390:TYR:CE2	1:B:394:LEU:HD22	2.41	0.56
1:D:109:ALA:HA	1:D:461:ARG:HD2	1.87	0.56
1:A:318:ASN:HD21	1:A:355:GLY:HA3	1.70	0.56
1:A:422:LYS:HG3	1:B:414:VAL:HG21	1.88	0.56
1:D:124:ILE:HG12	1:D:132:VAL:HG22	1.88	0.56
1:A:61:LEU:HD23	1:A:69:MET:HE1	1.86	0.56
1:D:88:ILE:HG21	1:D:92:ARG:HH11	1.71	0.56
1:C:399:ARG:CD	1:D:399:ARG:HH22	2.18	0.56
1:B:218:LEU:HD23	1:B:246:ARG:HH21	1.70	0.55
1:C:64:MET:HG2	1:C:372:LEU:HD23	1.88	0.55
1:A:238:ASP:OD2	1:A:461:ARG:NE	2.26	0.55
1:B:48:ILE:HG12	1:B:71:VAL:HB	1.89	0.55
1:D:432:THR:HG21	1:D:435:GLY:HA2	1.89	0.55
1:A:273:ASN:ND2	1:A:275:GLU:HB3	2.21	0.55
1:D:430:VAL:HG22	1:D:512:LEU:HD12	1.87	0.55
1:D:43:ARG:NH1	1:D:45:THR:O	2.40	0.55
1:A:384:GLU:CD	1:D:305:LYS:HD3	2.32	0.55
1:B:28:GLU:O	1:B:32:ARG:HG2	2.07	0.55
1:C:312:MET:SD	1:C:316:ARG:NH1	2.76	0.55
1:B:61:LEU:O	1:B:65:ILE:HG12	2.07	0.55
1:D:146:ASN:N	1:D:146:ASN:OD1	2.40	0.54
1:A:71:VAL:HG22	1:A:109:ALA:HB3	1.88	0.54
1:C:83:TYR:O	1:C:87:THR:OG1	2.25	0.54
1:C:254:VAL:O	1:C:258:LEU:HD12	2.06	0.54
1:C:417:VAL:HG23	1:C:446:PRO:HG3	1.89	0.54
1:D:395:PHE:O	1:D:398:LEU:HD22	2.07	0.54
1:B:221:VAL:HG12	1:B:225:ASP:HB3	1.89	0.54
1:B:464:HIS:CD2	2:B:1001:PRO:HB2	2.42	0.54
1:B:101:ASP:OD1	1:B:103:ILE:N	2.41	0.54
1:B:472:VAL:HG21	1:B:496:VAL:HG11	1.88	0.54
1:D:481:ALA:HB3	1:D:484:GLU:HG2	1.89	0.54
1:D:494:MET:HG2	1:D:531:PRO:HD2	1.87	0.54
1:B:218:LEU:HB3	1:B:219:PRO:HA	1.90	0.54
1:B:323:PRO:HB3	1:B:465:LEU:O	2.08	0.54
1:B:459:THR:OG1	1:B:459:THR:O	2.22	0.54
1:D:70:ASN:ND2	1:D:464:HIS:HD2	2.05	0.54
1:C:26:PHE:HE1	1:C:30:MET:HE2	1.72	0.54
1:B:106:ARG:NH2	1:B:500:ARG:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:VAL:HG22	1:D:253:GLU:HG2	1.90	0.54
1:A:295:GLY:HA3	1:A:328:THR:HG21	1.90	0.54
1:B:342:ARG:HD3	1:C:294:ARG:HB3	1.90	0.54
1:C:73:ARG:HA	1:C:111:ALA:HB3	1.88	0.54
1:C:248:ALA:N	1:C:282:GLU:OE2	2.42	0.53
1:A:280:PHE:HA	1:A:283:ILE:HD12	1.89	0.53
1:D:76:PHE:CE1	1:D:84:HIS:CD2	2.96	0.53
1:B:109:ALA:HA	1:B:461:ARG:HD2	1.90	0.53
1:A:271:ILE:HG23	1:A:276:GLY:HA3	1.91	0.53
1:C:361:LEU:HD21	1:C:378:GLN:HE21	1.72	0.53
1:A:111:ALA:HB2	1:A:239:MET:HE2	1.91	0.53
1:B:335:ILE:HG22	1:B:336:LYS:HG2	1.89	0.53
1:A:247:LYS:NZ	1:A:279:ARG:HG3	2.24	0.53
1:B:330:MET:HG3	1:B:348:VAL:HG22	1.89	0.53
1:C:513:THR:O	1:C:524:THR:HB	2.09	0.52
1:D:119:ILE:HB	1:D:209:VAL:HG22	1.91	0.52
1:B:80:THR:HG23	1:B:83:TYR:HB2	1.90	0.52
1:C:417:VAL:O	1:C:420:SER:OG	2.21	0.52
1:A:407:ASP:HB3	1:A:410:GLU:H	1.74	0.52
1:A:294:ARG:NH2	1:A:347:ASP:OD1	2.32	0.52
1:B:268:ILE:HG21	1:B:325:ILE:HD12	1.90	0.52
1:B:275:GLU:HG3	1:B:278:ARG:HH21	1.75	0.52
1:C:431:LEU:HD22	1:C:513:THR:HG22	1.92	0.52
1:B:327:ALA:HB1	1:B:360:MET:HE2	1.92	0.51
1:C:43:ARG:NH1	1:C:47:ILE:HG13	2.26	0.51
1:A:30:MET:HE1	1:D:311:LYS:HD3	1.91	0.51
1:C:57:SER:HB3	1:C:60:THR:HB	1.91	0.51
1:C:250:ASP:O	1:C:254:VAL:HG23	2.10	0.51
1:D:48:ILE:HG12	1:D:71:VAL:HB	1.92	0.51
1:C:293:ALA:O	1:C:297:LEU:HB2	2.10	0.51
1:C:464:HIS:HD2	2:C:1001:PRO:HB3	1.75	0.51
1:D:40:ILE:HD13	1:D:40:ILE:H	1.75	0.51
1:A:391:HIS:C	1:A:393:GLN:H	2.19	0.51
1:A:43:ARG:NH1	1:A:47:ILE:HG13	2.25	0.51
1:B:124:ILE:HG21	1:B:132:VAL:HG13	1.92	0.51
1:B:494:MET:SD	1:B:530:VAL:HG22	2.51	0.51
1:D:103:ILE:HG22	1:D:104:LEU:HD12	1.92	0.51
1:C:482:TRP:CD2	1:C:517:PRO:HG3	2.46	0.51
1:A:50:THR:OG1	1:A:73:ARG:NE	2.41	0.51
1:A:386:GLU:OE2	1:A:467:ARG:NH2	2.40	0.51
1:D:455:ARG:NH2	1:D:485:ASP:OD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ALA:HB1	1:A:245:ILE:HD11	1.93	0.51
1:D:244:PHE:HE1	1:D:246:ARG:HD3	1.75	0.51
1:C:295:GLY:HA3	1:C:328:THR:HG21	1.92	0.51
1:D:349:ALA:C	1:D:351:ALA:H	2.19	0.51
1:D:482:TRP:CD2	1:D:516:ARG:HG3	2.44	0.51
1:A:372:LEU:HD21	1:A:376:ARG:NH1	2.25	0.50
1:B:29:HIS:CD2	1:B:390:TYR:HA	2.46	0.50
1:B:218:LEU:HD21	1:B:247:LYS:NZ	2.27	0.50
1:B:312:MET:HG3	1:B:313:MET:N	2.26	0.50
1:B:359:ILE:HD11	1:B:378:GLN:NE2	2.26	0.50
1:B:434:SER:HB2	1:B:436:ARG:HG3	1.94	0.50
1:D:218:LEU:HD21	1:D:246:ARG:CZ	2.41	0.50
1:A:494:MET:HG2	1:A:531:PRO:HD2	1.94	0.50
1:C:65:ILE:HD12	1:C:66:LYS:N	2.27	0.50
1:C:372:LEU:HD11	1:C:376:ARG:HH21	1.75	0.50
1:C:94:ALA:O	1:C:97:SER:OG	2.25	0.50
1:C:331:LEU:HB2	1:C:364:GLU:HG2	1.94	0.50
1:D:175:TYR:CE1	1:D:212:PRO:HG2	2.47	0.50
1:A:57:SER:HB3	1:A:60:THR:HB	1.94	0.50
1:A:365:THR:HA	1:A:371:PRO:HB3	1.94	0.50
1:B:371:PRO:HD2	1:B:372:LEU:H	1.75	0.50
1:D:168:VAL:HG13	1:D:172:SER:HB2	1.93	0.50
1:A:96:GLU:C	1:A:98:PHE:H	2.20	0.50
1:B:161:TYR:OH	1:B:217:ASP:HB2	2.12	0.50
1:B:195:THR:OG1	1:B:196:GLU:N	2.45	0.50
1:D:64:MET:HE3	1:D:69:MET:SD	2.52	0.50
1:D:244:PHE:CE1	1:D:246:ARG:HD3	2.47	0.50
1:A:319:ARG:HH11	1:A:319:ARG:HB3	1.77	0.50
1:B:30:MET:HE3	1:C:311:LYS:HD3	1.94	0.50
1:B:76:PHE:CE1	1:B:84:HIS:CD2	2.99	0.50
1:C:335:ILE:HG23	1:C:368:GLY:HA2	1.93	0.50
1:D:41:THR:O	1:D:383:ARG:NE	2.38	0.50
1:D:348:VAL:HG12	1:D:359:ILE:HD12	1.94	0.50
1:D:494:MET:SD	1:D:530:VAL:HG22	2.52	0.50
1:C:65:ILE:HG21	1:C:108:VAL:HG21	1.95	0.49
1:D:453:VAL:HG21	1:D:493:ALA:HB2	1.95	0.49
1:B:359:ILE:HD11	1:B:378:GLN:OE1	2.12	0.49
1:B:275:GLU:HG3	1:B:278:ARG:NH2	2.28	0.49
1:B:455:ARG:NH2	1:B:485:ASP:OD1	2.39	0.49
1:C:102:PRO:HA	1:C:105:GLU:OE2	2.11	0.49
1:A:239:MET:SD	1:A:465:LEU:HD21	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:SER:O	1:D:408:PRO:HD3	2.12	0.49
1:B:177:ASP:O	1:B:180:LEU:HB2	2.13	0.49
1:D:270:LYS:HE3	1:D:291:MET:SD	2.52	0.49
1:A:48:ILE:HG12	1:A:71:VAL:HB	1.94	0.49
1:B:131:GLU:HB3	1:B:204:GLY:HA2	1.94	0.49
1:B:312:MET:HE1	1:B:316:ARG:HE	1.78	0.49
1:D:333:SER:HB3	1:D:344:GLU:OE1	2.13	0.49
1:D:224:LYS:HG2	1:D:228:ASP:OD2	2.13	0.49
1:B:144:LEU:HD21	1:B:164:ILE:HG22	1.95	0.48
1:D:65:ILE:CD1	1:D:108:VAL:HG21	2.42	0.48
1:A:247:LYS:HE3	1:A:279:ARG:NE	2.27	0.48
1:A:410:GLU:O	1:A:413:ALA:N	2.46	0.48
1:D:61:LEU:O	1:D:65:ILE:HG12	2.12	0.48
1:D:266:LYS:HA	1:D:266:LYS:HD3	1.68	0.48
1:D:268:ILE:HD12	1:D:289:GLY:HA3	1.94	0.48
1:A:94:ALA:O	1:A:97:SER:OG	2.31	0.48
1:C:44:ASN:N	1:C:44:ASN:HD22	2.11	0.48
1:D:472:VAL:HG21	1:D:496:VAL:HG11	1.95	0.48
1:C:464:HIS:HD2	2:C:1001:PRO:HB2	1.78	0.48
1:B:271:ILE:HD11	1:B:283:ILE:HG21	1.95	0.48
1:C:496:VAL:O	1:C:500:ARG:HG2	2.13	0.48
1:C:294:ARG:O	1:C:298:GLY:N	2.47	0.48
1:D:464:HIS:CE1	1:D:471:PRO:HG2	2.49	0.48
1:A:58:VAL:HG23	1:A:90:ASN:OD1	2.14	0.48
1:B:469:ILE:O	2:B:1001:PRO:HB3	2.14	0.48
1:C:239:MET:SD	1:C:465:LEU:HD21	2.54	0.48
1:D:408:PRO:O	1:D:412:THR:OG1	2.30	0.48
1:B:291:MET:HE2	1:B:327:ALA:HB2	1.96	0.48
1:C:523:ASN:OD1	1:C:523:ASN:N	2.46	0.48
1:C:525:MET:HB3	1:D:525:MET:HB3	1.96	0.48
1:D:94:ALA:O	1:D:97:SER:HB3	2.13	0.48
1:C:56:ARG:HH22	1:C:83:TYR:HB3	1.78	0.47
1:B:161:TYR:CE1	1:B:217:ASP:HB2	2.48	0.47
1:B:436:ARG:O	1:B:439:HIS:HB2	2.15	0.47
1:C:301:ILE:HB	1:C:302:PRO:HD2	1.95	0.47
1:C:449:PRO:HG3	1:C:502:PHE:CD1	2.49	0.47
1:B:77:SER:C	1:B:78:HIS:HD1	2.23	0.47
1:C:482:TRP:CZ3	1:C:516:ARG:C	2.92	0.47
1:D:417:VAL:HG13	1:D:446:PRO:HB3	1.97	0.47
1:A:314:ILE:HA	1:A:324:VAL:HG11	1.95	0.47
1:B:244:PHE:CD2	1:B:246:ARG:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:HA	1:B:205:SER:HB2	1.96	0.47
1:D:352:VAL:HG12	1:D:353:LEU:HD23	1.95	0.47
1:A:312:MET:HB2	1:D:33:LEU:HB2	1.96	0.47
1:A:458:GLN:O	1:A:460:ALA:N	2.48	0.47
1:B:50:THR:HA	1:B:73:ARG:HB3	1.97	0.47
1:C:104:LEU:O	1:C:106:ARG:NH1	2.48	0.47
1:D:292:VAL:HG22	1:D:313:MET:HE3	1.95	0.47
1:C:65:ILE:HD12	1:C:66:LYS:H	1.79	0.47
1:C:74:LEU:HD11	1:C:87:THR:HB	1.97	0.47
1:D:331:LEU:HD12	1:D:340:PRO:HB3	1.97	0.47
1:A:519:SER:O	1:A:521:PHE:N	2.44	0.47
1:A:56:ARG:HB2	1:A:87:THR:HG23	1.97	0.46
1:B:174:ILE:N	1:B:183:LEU:O	2.42	0.46
1:B:296:ASP:O	1:B:299:ILE:HG13	2.14	0.46
1:B:413:ALA:O	1:B:417:VAL:HG23	2.15	0.46
1:A:34:ASP:OD1	1:A:36:ASP:N	2.38	0.46
1:A:241:PHE:CE1	1:A:268:ILE:HD13	2.50	0.46
1:C:494:MET:HE3	1:C:494:MET:HB2	1.74	0.46
1:D:178:ASP:C	1:D:180:LEU:H	2.23	0.46
1:A:319:ARG:HD3	1:A:401:LEU:HD22	1.97	0.46
1:A:85:ALA:HB2	1:A:231:PHE:CZ	2.49	0.46
1:C:526:ARG:HD3	1:D:524:THR:HG23	1.97	0.46
1:B:65:ILE:HD12	1:B:108:VAL:HG21	1.97	0.46
1:B:67:SER:OG	1:B:376:ARG:NE	2.42	0.46
1:B:407:ASP:CG	1:B:409:THR:HG23	2.40	0.46
1:A:454:THR:HG21	1:A:460:ALA:HB2	1.98	0.46
1:B:57:SER:O	1:B:60:THR:N	2.48	0.46
1:B:342:ARG:HH22	1:C:347:ASP:CG	2.24	0.46
1:B:464:HIS:HA	2:B:1001:PRO:HG3	1.96	0.46
1:C:103:ILE:HG23	1:C:496:VAL:HA	1.98	0.46
1:C:273:ASN:OD1	1:C:273:ASN:N	2.49	0.46
1:B:65:ILE:HD12	1:B:108:VAL:CG2	2.46	0.46
1:B:244:PHE:HD2	1:B:246:ARG:NH1	2.12	0.46
1:B:308:LEU:HD22	1:C:33:LEU:CD2	2.45	0.46
1:B:482:TRP:CD2	1:B:516:ARG:HG2	2.51	0.46
1:D:344:GLU:O	1:D:348:VAL:HG22	2.16	0.46
1:C:61:LEU:O	1:C:65:ILE:HG13	2.16	0.46
1:D:121:THR:O	1:D:206:LYS:HA	2.15	0.46
1:B:268:ILE:HD12	1:B:289:GLY:HA3	1.98	0.46
1:D:177:ASP:OD2	1:D:207:LYS:HD3	2.16	0.46
1:D:195:THR:OG1	1:D:196:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:PRO:HB2	1:A:304:GLU:OE1	2.16	0.45
1:A:329:GLN:OE1	1:D:342:ARG:NE	2.34	0.45
1:B:74:LEU:HD11	1:B:88:ILE:HG12	1.97	0.45
1:D:76:PHE:CD2	1:D:228:ASP:HB3	2.51	0.45
1:D:449:PRO:HB3	1:D:470:PHE:CE1	2.51	0.45
1:A:77:SER:HA	1:A:115:LYS:HB2	1.98	0.45
1:A:391:HIS:O	1:A:393:GLN:N	2.47	0.45
1:D:123:LEU:HD22	1:D:205:SER:HB3	1.97	0.45
1:D:413:ALA:O	1:D:417:VAL:HG23	2.17	0.45
1:A:65:ILE:HD12	1:A:66:LYS:H	1.81	0.45
1:B:430:VAL:HG22	1:B:512:LEU:HD12	1.98	0.45
1:C:525:MET:CB	1:D:525:MET:HE3	2.46	0.45
1:D:149:MET:HG3	1:D:158:TRP:CZ3	2.51	0.45
1:A:114:THR:HG22	1:A:242:ALA:HA	1.99	0.45
1:A:340:PRO:HD3	1:A:377:MET:HG2	1.98	0.45
1:B:76:PHE:CD2	1:B:228:ASP:HB3	2.52	0.45
1:C:398:LEU:HD13	1:C:443:ARG:O	2.16	0.45
1:C:505:LYS:HE2	1:C:505:LYS:HB3	1.80	0.45
1:D:56:ARG:H	1:D:56:ARG:HG3	1.44	0.45
1:A:453:VAL:HG21	1:A:493:ALA:HB2	1.99	0.45
1:B:342:ARG:HH21	1:C:329:GLN:HB3	1.82	0.45
1:C:48:ILE:HG23	1:C:71:VAL:HB	1.99	0.45
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.51	0.45
1:C:271:ILE:HG23	1:C:276:GLY:HA3	1.97	0.45
1:D:71:VAL:HG21	1:D:239:MET:HE1	1.99	0.45
1:D:85:ALA:HB2	1:D:231:PHE:CZ	2.52	0.45
1:B:184:GLN:O	1:B:195:THR:OG1	2.35	0.45
1:A:267:ILE:HD13	1:A:267:ILE:H	1.82	0.44
1:C:30:MET:HA	1:C:33:LEU:CD1	2.47	0.44
1:D:474:CYS:HA	1:D:492:PHE:CE2	2.53	0.44
1:A:37:SER:HA	1:A:38:PRO:HD3	1.83	0.44
1:A:222:SER:HB2	1:A:225:ASP:CG	2.42	0.44
1:B:392:LEU:HD12	1:B:392:LEU:H	1.82	0.44
1:D:61:LEU:HD22	1:D:64:MET:HE2	1.98	0.44
1:D:70:ASN:CB	1:D:464:HIS:HD2	2.30	0.44
1:A:73:ARG:HA	1:A:111:ALA:HB3	1.99	0.44
1:A:302:PRO:HB3	1:D:339:ARG:HH22	1.81	0.44
1:A:525:MET:HB3	1:B:525:MET:HE3	2.00	0.44
1:B:33:LEU:HB2	1:C:312:MET:HB2	1.99	0.44
1:C:332:GLU:O	1:C:335:ILE:HG13	2.17	0.44
1:D:85:ALA:HB2	1:D:231:PHE:HZ	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:PRO:HD3	1:D:377:MET:HG3	2.00	0.44
1:D:494:MET:HE2	1:D:494:MET:HB2	1.80	0.44
1:A:339:ARG:HH21	1:A:377:MET:HE1	1.82	0.44
1:D:486:VAL:O	1:D:490:VAL:HG23	2.16	0.44
1:A:482:TRP:CG	1:A:517:PRO:HD3	2.52	0.44
1:B:162:LYS:HD2	1:B:162:LYS:HA	1.76	0.44
1:B:299:ILE:HD12	1:B:300:GLU:HG3	2.00	0.44
1:D:67:SER:OG	1:D:376:ARG:NE	2.43	0.44
1:D:470:PHE:CD1	1:D:470:PHE:N	2.85	0.44
1:A:61:LEU:O	1:A:65:ILE:HG13	2.18	0.44
1:A:272:GLU:HG2	1:A:296:ASP:HB2	2.00	0.44
1:B:326:CYS:HB3	1:B:330:MET:HE1	1.99	0.44
1:C:63:GLU:O	1:C:372:LEU:HD21	2.18	0.44
1:D:327:ALA:HB1	1:D:360:MET:HE2	2.00	0.44
1:D:372:LEU:HD12	1:D:372:LEU:HA	1.77	0.44
1:A:266:LYS:HD2	1:A:266:LYS:HA	1.73	0.44
1:A:359:ILE:H	1:A:359:ILE:HG12	1.68	0.44
1:B:517:PRO:HD2	1:B:518:GLY:H	1.82	0.44
1:C:444:TYR:OH	1:D:422:LYS:NZ	2.50	0.44
1:D:160:ASP:OD1	1:D:160:ASP:N	2.51	0.44
1:A:65:ILE:HD12	1:A:66:LYS:N	2.33	0.43
1:C:50:THR:OG1	1:C:73:ARG:NE	2.47	0.43
1:C:410:GLU:HA	1:C:440:GLN:HG2	2.00	0.43
1:C:432:THR:HB	1:C:437:SER:HB2	2.00	0.43
1:D:441:VAL:HG12	1:D:450:ILE:CD1	2.48	0.43
1:A:242:ALA:CB	1:A:245:ILE:HD11	2.48	0.43
1:A:335:ILE:HG23	1:A:368:GLY:HA2	2.00	0.43
1:A:347:ASP:CG	1:D:342:ARG:HH22	2.26	0.43
1:B:243:SER:HA	1:B:270:LYS:HD3	2.00	0.43
1:B:516:ARG:HB3	1:B:517:PRO:CD	2.48	0.43
1:D:348:VAL:HG11	1:D:378:GLN:HE22	1.83	0.43
1:A:330:MET:O	1:A:344:GLU:HG2	2.18	0.43
1:A:445:ARG:HG2	1:A:445:ARG:NH1	2.21	0.43
1:B:94:ALA:O	1:B:97:SER:HB3	2.18	0.43
1:B:407:ASP:OD2	1:B:409:THR:HG23	2.18	0.43
1:C:408:PRO:HG2	1:C:521:PHE:CD1	2.54	0.43
1:A:76:PHE:HZ	1:A:81:HIS:CE1	2.37	0.43
1:B:312:MET:HG3	1:B:313:MET:HG3	2.00	0.43
1:D:331:LEU:C	1:D:364:GLU:HG2	2.43	0.43
1:A:102:PRO:HA	1:A:105:GLU:OE2	2.18	0.43
1:B:322:LYS:HA	1:B:323:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:C	1:A:105:GLU:H	2.27	0.43
1:B:274:HIS:CD2	1:B:278:ARG:HG3	2.54	0.43
1:B:297:LEU:HD12	1:B:297:LEU:HA	1.87	0.43
1:B:432:THR:HG21	1:B:435:GLY:HA2	2.00	0.43
1:D:177:ASP:CG	1:D:207:LYS:HD3	2.43	0.43
1:B:76:PHE:HD2	1:B:228:ASP:CG	2.25	0.43
1:B:110:VAL:CG1	1:B:237:VAL:HG12	2.49	0.43
1:D:123:LEU:HA	1:D:205:SER:HB3	2.01	0.43
1:C:449:PRO:HG3	1:C:502:PHE:HD1	1.84	0.43
1:A:58:VAL:HG13	1:A:94:ALA:HB2	2.01	0.43
1:A:92:ARG:NH1	1:A:235:GLN:O	2.45	0.43
1:B:247:LYS:HD2	1:B:249:SER:HB2	2.00	0.43
1:B:312:MET:HB2	1:B:312:MET:HE2	1.54	0.43
1:C:482:TRP:CE3	1:C:517:PRO:HG3	2.54	0.43
1:A:288:ASP:O	1:A:323:PRO:HD2	2.19	0.42
1:B:305:LYS:HE3	1:C:35:ILE:O	2.18	0.42
1:A:290:ILE:HB	1:A:324:VAL:HG23	2.01	0.42
1:C:338:PRO:HB3	1:C:370:TYR:CE2	2.54	0.42
1:A:241:PHE:HE1	1:A:268:ILE:HD13	1.82	0.42
1:A:505:LYS:HE2	1:A:505:LYS:HB3	1.74	0.42
1:B:362:SER:O	1:B:364:GLU:N	2.51	0.42
1:C:464:HIS:CD2	2:C:1001:PRO:HB2	2.53	0.42
1:D:132:VAL:HB	1:D:133:GLU:H	1.40	0.42
1:B:312:MET:HE1	1:B:316:ARG:NH2	2.30	0.42
1:B:317:CYS:SG	1:B:324:VAL:HG23	2.60	0.42
1:D:157:LEU:HD21	1:D:203:LEU:HD21	2.02	0.42
1:C:56:ARG:O	1:C:90:ASN:ND2	2.52	0.42
1:D:86:GLU:O	1:D:90:ASN:ND2	2.42	0.42
1:D:203:LEU:HD12	1:D:204:GLY:H	1.84	0.42
1:D:312:MET:CE	1:D:316:ARG:HH21	2.27	0.42
1:D:345:GLY:HA2	1:D:381:ILE:HD13	2.02	0.42
1:A:312:MET:HE2	1:A:316:ARG:HH21	1.84	0.42
1:A:396:GLU:CD	1:B:399:ARG:HH22	2.26	0.42
1:C:239:MET:HE2	1:C:239:MET:HB3	1.90	0.42
1:C:528:VAL:HA	1:C:529:PRO:HD3	1.83	0.42
1:D:331:LEU:HB3	1:D:334:MET:HG3	2.02	0.42
1:B:212:PRO:HA	1:B:213:GLY:HA2	1.56	0.42
1:C:322:LYS:HB3	1:C:322:LYS:HE2	1.87	0.42
1:A:305:LYS:O	1:A:308:LEU:HB2	2.19	0.42
1:B:56:ARG:H	1:B:56:ARG:HG3	1.51	0.42
1:C:472:VAL:HG21	1:C:496:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:LYS:HA	1:D:186:LYS:HD3	1.82	0.42
1:B:70:ASN:HB3	1:B:464:HIS:CD2	2.55	0.42
1:B:218:LEU:HB3	1:B:219:PRO:CA	2.50	0.42
1:B:349:ALA:O	1:B:353:LEU:HG	2.20	0.42
1:C:284:LEU:O	1:C:322:LYS:NZ	2.49	0.42
1:D:330:MET:HG3	1:D:348:VAL:HG13	2.02	0.42
1:B:494:MET:HG2	1:B:531:PRO:HD2	2.01	0.41
1:D:124:ILE:HA	1:D:152:CYS:HB3	2.03	0.41
1:D:348:VAL:HG21	1:D:381:ILE:HG21	2.02	0.41
1:D:362:SER:O	1:D:364:GLU:N	2.53	0.41
1:A:448:ALA:HB1	1:A:449:PRO:HD2	2.02	0.41
1:B:26:PHE:HZ	1:B:30:MET:HE2	1.84	0.41
1:B:229:LEU:HD23	1:B:229:LEU:HA	1.93	0.41
1:C:69:MET:SD	1:C:72:ALA:HB2	2.59	0.41
1:C:249:SER:O	1:C:252:HIS:HB2	2.20	0.41
1:C:391:HIS:CG	1:C:447:ARG:HG3	2.55	0.41
1:C:482:TRP:O	1:C:483:ALA:C	2.63	0.41
1:A:431:LEU:HD12	1:A:453:VAL:HB	2.02	0.41
1:A:496:VAL:O	1:A:500:ARG:HB2	2.20	0.41
1:D:334:MET:HE2	1:D:334:MET:HB3	1.89	0.41
1:D:482:TRP:NE1	1:D:516:ARG:HA	2.35	0.41
1:A:46:GLY:O	1:A:358:CYS:HB3	2.20	0.41
1:B:331:LEU:HB3	1:B:334:MET:HG3	2.01	0.41
1:A:385:ALA:HA	1:D:307:PHE:HZ	1.85	0.41
1:A:500:ARG:HG2	1:A:502:PHE:HE1	1.86	0.41
1:B:340:PRO:HD3	1:B:377:MET:HG3	2.01	0.41
1:C:291:MET:HA	1:C:325:ILE:O	2.19	0.41
1:C:441:VAL:HG12	1:C:450:ILE:HD11	2.02	0.41
1:D:218:LEU:HA	1:D:218:LEU:HD23	1.69	0.41
1:A:267:ILE:HD13	1:A:288:ASP:OD2	2.21	0.41
1:A:502:PHE:H	1:A:502:PHE:HD1	1.66	0.41
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.81	0.41
1:B:476:ASP:HA	1:B:477:PRO:HD3	1.88	0.41
1:C:237:VAL:O	1:C:265:ILE:HD13	2.21	0.41
1:D:51:ILE:HA	1:D:55:SER:OG	2.20	0.41
1:D:182:SER:O	1:D:183:LEU:HD12	2.21	0.41
1:D:182:SER:OG	1:D:199:ASN:HB2	2.20	0.41
1:D:453:VAL:HG22	1:D:472:VAL:HG12	2.03	0.41
1:D:516:ARG:O	1:D:519:SER:HB2	2.21	0.41
1:A:65:ILE:HG21	1:A:108:VAL:CG2	2.51	0.41
1:A:71:VAL:CG2	1:A:239:MET:HE1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:VAL:HG22	1:B:109:ALA:HB3	2.03	0.41
1:B:168:VAL:HG12	1:B:169:GLU:O	2.21	0.41
1:B:370:TYR:HB3	1:B:373:GLU:HG3	2.03	0.41
1:A:325:ILE:HD13	1:A:325:ILE:HG21	1.84	0.41
1:A:393:GLN:O	1:A:397:GLU:HG3	2.21	0.41
1:A:480:GLU:CD	1:A:480:GLU:H	2.27	0.41
1:B:58:VAL:CG2	1:B:90:ASN:HD22	2.28	0.41
1:B:288:ASP:O	1:B:323:PRO:HD2	2.21	0.41
1:B:371:PRO:CD	1:B:372:LEU:H	2.33	0.41
1:B:520:GLY:C	1:B:522:THR:H	2.29	0.41
1:D:63:GLU:HB3	1:D:372:LEU:HD11	2.03	0.41
1:D:348:VAL:CG2	1:D:381:ILE:HG21	2.51	0.41
1:A:284:LEU:HD13	1:A:290:ILE:HG13	2.03	0.41
1:A:455:ARG:NH2	1:A:478:VAL:HA	2.36	0.41
1:D:465:LEU:HD23	1:D:465:LEU:HA	1.82	0.41
1:A:295:GLY:HA2	1:A:329:GLN:NE2	2.37	0.40
1:B:188:LYS:HB2	1:B:193:LEU:HD12	2.03	0.40
1:B:334:MET:HE2	1:B:334:MET:HB3	1.68	0.40
1:C:70:ASN:HB3	1:C:464:HIS:CG	2.57	0.40
1:D:275:GLU:O	1:D:279:ARG:HG3	2.21	0.40
1:D:434:SER:HB2	1:D:436:ARG:HG3	2.02	0.40
1:A:282:GLU:O	1:A:285:GLU:HB3	2.20	0.40
1:A:473:LEU:HD12	1:A:473:LEU:HA	1.87	0.40
1:B:60:THR:HG22	1:B:61:LEU:N	2.36	0.40
1:C:26:PHE:CE1	1:C:30:MET:HE2	2.55	0.40
1:D:323:PRO:HB3	1:D:465:LEU:O	2.21	0.40
1:A:254:VAL:O	1:A:258:LEU:HD12	2.21	0.40
1:A:482:TRP:HH2	1:A:514:GLY:O	2.04	0.40
1:B:184:GLN:HB3	1:B:185:VAL:H	1.77	0.40
1:B:301:ILE:HA	1:B:302:PRO:HD3	1.89	0.40
1:B:470:PHE:N	1:B:470:PHE:CD1	2.89	0.40
1:C:81:HIS:CD2	1:C:81:HIS:H	2.38	0.40
1:C:233:VAL:HG22	1:C:258:LEU:HD23	2.03	0.40
1:C:414:VAL:O	1:C:417:VAL:HG12	2.22	0.40
1:D:49:CYS:SG	1:D:375:VAL:HG22	2.61	0.40
1:B:105:GLU:O	1:B:105:GLU:HG3	2.20	0.40
1:C:101:ASP:HA	1:C:102:PRO:HD3	1.91	0.40
1:C:519:SER:C	1:C:521:PHE:H	2.29	0.40
1:D:73:ARG:O	1:D:74:LEU:HD23	2.21	0.40
1:D:179:GLY:O	1:D:181:ILE:N	2.53	0.40
1:D:237:VAL:HG23	1:D:265:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:ILE:HD13	1:D:428:ILE:HG21	1.91	0.40
1:A:339:ARG:HE	1:A:377:MET:HE1	1.86	0.40
1:B:42:ALA:O	1:B:44:ASN:ND2	2.55	0.40
1:B:121:THR:O	1:B:206:LYS:HA	2.20	0.40
1:D:205:SER:O	1:D:207:LYS:HG2	2.21	0.40
1:D:390:TYR:HD1	1:D:390:TYR:HA	1.61	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	402/535 (75%)	344 (86%)	49 (12%)	9 (2%)	5	29
1	B	496/535 (93%)	413 (83%)	61 (12%)	22 (4%)	2	15
1	C	402/535 (75%)	344 (86%)	51 (13%)	7 (2%)	7	35
1	D	501/535 (94%)	434 (87%)	57 (11%)	10 (2%)	6	31
All	All	1801/2140 (84%)	1535 (85%)	218 (12%)	48 (3%)	4	25

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	ILE
1	A	299	ILE
1	B	58	VAL
1	B	102	PRO
1	B	371	PRO
1	B	394	LEU
1	B	460	ALA
1	B	516	ARG
1	B	517	PRO

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Mol	Chain	Res	Type
1	C	392	LEU
1	C	500	ARG
1	A	460	ALA
1	B	79	GLY
1	B	215	ALA
1	B	363	GLY
1	B	459	THR
1	B	463	ALA
1	D	58	VAL
1	D	180	LEU
1	D	463	ALA
1	A	97	SER
1	A	330	MET
1	A	436	ARG
1	B	53	PRO
1	B	161	TYR
1	B	330	MET
1	B	390	TYR
1	C	483	ALA
1	A	392	LEU
1	B	202	SER
1	D	53	PRO
1	D	79	GLY
1	D	363	GLY
1	D	440	GLN
1	A	393	GLN
1	B	103	ILE
1	B	154	GLU
1	B	329	GLN
1	B	521	PHE
1	A	459	THR
1	D	125	LYS
1	D	132	VAL
1	B	218	LEU
1	C	414	VAL
1	D	478	VAL
1	C	53	PRO
1	C	371	PRO
1	C	368	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/438 (76%)	278 (83%)	57 (17%)	2	11
1	B	415/438 (95%)	337 (81%)	78 (19%)	1	9
1	C	335/438 (76%)	273 (82%)	62 (18%)	1	9
1	D	417/438 (95%)	328 (79%)	89 (21%)	1	6
All	All	1502/1752 (86%)	1216 (81%)	286 (19%)	1	9

All (286) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	25	THR
1	A	33	LEU
1	A	41	THR
1	A	45	THR
1	A	59	GLU
1	A	60	THR
1	A	62	LYS
1	A	65	ILE
1	A	74	LEU
1	A	80	THR
1	A	82	GLU
1	A	87	THR
1	A	100	SER
1	A	106	ARG
1	A	110	VAL
1	A	112	LEU
1	A	222	SER
1	A	238	ASP
1	A	239	MET
1	A	249	SER
1	A	265	ILE
1	A	267	ILE
1	A	285	GLU

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Mol	Chain	Res	Type
1	A	297	LEU
1	A	299	ILE
1	A	306	VAL
1	A	316	ARG
1	A	319	ARG
1	A	322	LYS
1	A	331	LEU
1	A	332	GLU
1	A	337	LYS
1	A	339	ARG
1	A	342	ARG
1	A	348	VAL
1	A	359	ILE
1	A	389	ILE
1	A	392	LEU
1	A	393	GLN
1	A	401	LEU
1	A	404	ILE
1	A	414	VAL
1	A	433	LYS
1	A	440	GLN
1	A	443	ARG
1	A	445	ARG
1	A	459	THR
1	A	465	LEU
1	A	472	VAL
1	A	480	GLU
1	A	494	MET
1	A	500	ARG
1	A	508	VAL
1	A	524	THR
1	A	525	MET
1	A	528	VAL
1	B	24	ASP
1	B	25	THR
1	B	30	MET
1	B	45	THR
1	B	56	ARG
1	B	60	THR
1	B	67	SER
1	B	71	VAL
1	B	77	SER

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Mol	Chain	Res	Type
1	B	80	THR
1	B	89	LYS
1	B	92	ARG
1	B	97	SER
1	B	110	VAL
1	B	112	LEU
1	B	131	GLU
1	B	140	LEU
1	B	143	THR
1	B	150	GLU
1	B	154	GLU
1	B	159	LEU
1	B	160	ASP
1	B	162	LYS
1	B	165	CYS
1	B	166	LYS
1	B	169	GLU
1	B	172	SER
1	B	180	LEU
1	B	184	GLN
1	B	185	VAL
1	B	188	LYS
1	B	191	ASP
1	B	209	VAL
1	B	217	ASP
1	B	221	VAL
1	B	235	GLN
1	B	240	VAL
1	B	244	PHE
1	B	247	LYS
1	B	265	ILE
1	B	285	GLU
1	B	297	LEU
1	B	305	LYS
1	B	312	MET
1	B	319	ARG
1	B	324	VAL
1	B	326	CYS
1	B	329	GLN
1	B	330	MET
1	B	333	SER
1	B	334	MET

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Mol	Chain	Res	Type
1	B	336	LYS
1	B	342	ARG
1	B	364	GLU
1	B	367	LYS
1	B	373	GLU
1	B	391	HIS
1	B	393	GLN
1	B	394	LEU
1	B	405	THR
1	B	409	THR
1	B	412	THR
1	B	420	SER
1	B	431	LEU
1	B	434	SER
1	B	445	ARG
1	B	458	GLN
1	B	459	THR
1	B	465	LEU
1	B	472	VAL
1	B	478	VAL
1	B	480	GLU
1	B	500	ARG
1	B	508	VAL
1	B	516	ARG
1	B	519	SER
1	B	522	THR
1	B	528	VAL
1	C	24	ASP
1	C	27	LEU
1	C	33	LEU
1	C	44	ASN
1	C	45	THR
1	C	59	GLU
1	C	60	THR
1	C	65	ILE
1	C	74	LEU
1	C	76	PHE
1	C	77	SER
1	C	87	THR
1	C	90	ASN
1	C	101	ASP
1	C	110	VAL

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Mol	Chain	Res	Type
1	C	115	LYS
1	C	222	SER
1	C	238	ASP
1	C	247	LYS
1	C	251	VAL
1	C	265	ILE
1	C	269	SER
1	C	270	LYS
1	C	275	GLU
1	C	277	VAL
1	C	278	ARG
1	C	296	ASP
1	C	301	ILE
1	C	306	VAL
1	C	319	ARG
1	C	324	VAL
1	C	325	ILE
1	C	328	THR
1	C	334	MET
1	C	337	LYS
1	C	339	ARG
1	C	342	ARG
1	C	348	VAL
1	C	359	ILE
1	C	360	MET
1	C	372	LEU
1	C	380	LEU
1	C	389	ILE
1	C	392	LEU
1	C	396	GLU
1	C	401	LEU
1	C	405	THR
1	C	409	THR
1	C	430	VAL
1	C	436	ARG
1	C	440	GLN
1	C	443	ARG
1	C	465	LEU
1	C	475	LYS
1	C	491	ASN
1	C	494	MET
1	C	500	ARG

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Mol	Chain	Res	Type
1	C	504	LYS
1	C	508	VAL
1	C	524	THR
1	C	526	ARG
1	C	528	VAL
1	D	25	THR
1	D	35	ILE
1	D	40	ILE
1	D	41	THR
1	D	45	THR
1	D	56	ARG
1	D	58	VAL
1	D	61	LEU
1	D	65	ILE
1	D	67	SER
1	D	71	VAL
1	D	73	ARG
1	D	80	THR
1	D	82	GLU
1	D	96	GLU
1	D	103	ILE
1	D	105	GLU
1	D	110	VAL
1	D	112	LEU
1	D	120	ARG
1	D	123	LEU
1	D	132	VAL
1	D	135	LYS
1	D	136	LYS
1	D	139	THR
1	D	142	ILE
1	D	143	THR
1	D	146	ASN
1	D	151	LYS
1	D	152	CYS
1	D	156	ILE
1	D	157	LEU
1	D	159	LEU
1	D	173	LYS
1	D	176	VAL
1	D	178	ASP
1	D	188	LYS

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Mol	Chain	Res	Type
1	D	195	THR
1	D	197	VAL
1	D	207	LYS
1	D	209	VAL
1	D	210	ASN
1	D	211	LEU
1	D	216	VAL
1	D	229	LEU
1	D	239	MET
1	D	257	VAL
1	D	261	LYS
1	D	275	GLU
1	D	285	GLU
1	D	297	LEU
1	D	324	VAL
1	D	326	CYS
1	D	328	THR
1	D	330	MET
1	D	331	LEU
1	D	333	SER
1	D	336	LYS
1	D	342	ARG
1	D	348	VAL
1	D	350	ASN
1	D	354	ASP
1	D	364	GLU
1	D	391	HIS
1	D	392	LEU
1	D	393	GLN
1	D	394	LEU
1	D	398	LEU
1	D	400	ARG
1	D	401	LEU
1	D	405	THR
1	D	412	THR
1	D	414	VAL
1	D	420	SER
1	D	422	LYS
1	D	434	SER
1	D	440	GLN
1	D	443	ARG
1	D	453	VAL

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Mol	Chain	Res	Type
1	D	458	GLN
1	D	472	VAL
1	D	473	LEU
1	D	478	VAL
1	D	489	ARG
1	D	498	LYS
1	D	508	VAL
1	D	519	SER
1	D	522	THR
1	D	528	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	75	ASN
1	A	318	ASN
1	A	393	GLN
1	A	440	GLN
1	A	464	HIS
1	B	29	HIS
1	B	70	ASN
1	B	84	HIS
1	B	90	ASN
1	B	184	GLN
1	B	199	ASN
1	B	458	GLN
1	B	464	HIS
1	C	29	HIS
1	C	44	ASN
1	C	90	ASN
1	C	439	HIS
1	C	440	GLN
1	C	464	HIS
1	D	44	ASN
1	D	81	HIS
1	D	84	HIS
1	D	252	HIS
1	D	318	ASN
1	D	440	GLN
1	D	458	GLN
1	D	464	HIS

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Mol	Chain	Res	Type
1	D	491	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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$
2	PRO	B	1001	-	6,7,8	0.71	0	7,8,10	2.27	2 (28%)
2	PRO	A	1001	-	6,7,8	0.85	0	7,8,10	1.79	1 (14%)
2	PRO	C	1001	-	6,7,8	1.00	0	7,8,10	1.66	1 (14%)
2	PRO	D	1001	-	6,7,8	0.81	0	7,8,10	1.65	1 (14%)

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
2	PRO	B	1001	-	-	0/0/9/11	0/1/1/1
2	PRO	A	1001	-	-	0/0/9/11	0/1/1/1
2	PRO	C	1001	-	-	0/0/9/11	0/1/1/1
2	PRO	D	1001	-	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	1001	PRO	O-C-CA	-5.00	111.91	124.77
2	A	1001	PRO	O-C-CA	-3.86	114.86	124.77
2	C	1001	PRO	O-C-CA	-3.76	115.11	124.77
2	D	1001	PRO	O-C-CA	-3.56	115.61	124.77
2	B	1001	PRO	CB-CA-C	-2.51	109.21	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	PRO	3	0
2	A	1001	PRO	2	0
2	C	1001	PRO	4	0

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	406/535 (75%)	-1.42	1 (0%) 91 85	3, 36, 78, 121	0
1	B	502/535 (93%)	-1.35	0 100 100	1, 34, 101, 128	0
1	C	406/535 (75%)	-1.40	0 100 100	2, 35, 80, 134	0
1	D	505/535 (94%)	-1.41	0 100 100	2, 32, 97, 127	0
All	All	1819/2140 (85%)	-1.39	1 (0%) 92 89	1, 35, 91, 134	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ALA	2.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PRO	A	1001	7/8	1.00	0.05	19,19,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PRO	B	1001	7/8	1.00	0.05	9,9,19,19	0
2	PRO	C	1001	7/8	1.00	0.05	16,16,26,26	0
2	PRO	D	1001	7/8	1.00	0.04	23,23,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.