



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:11 AM UTC

PDB ID : 1A3X / pdb_00001a3x
Title : PYRUVATE KINASE FROM SACCHAROMYCES CEREVISIAE COM-
PLEXED WITH PG, MN2+ AND K+
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Deposited on : 1998-01-26
Resolution : 3.00 Å(reported)

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

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

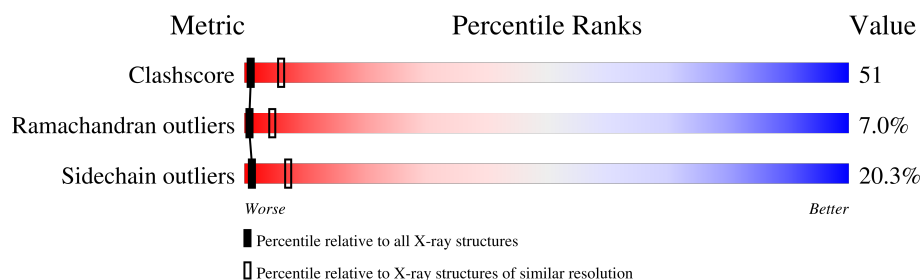
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

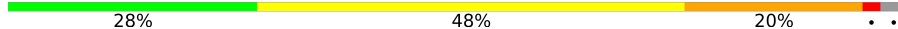
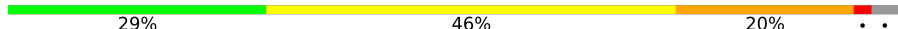
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	500	
1	B	500	

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	PGA	A	1005	-	-	X	-
2	PGA	B	1006	-	X	-	-

2 Entry composition [i](#)

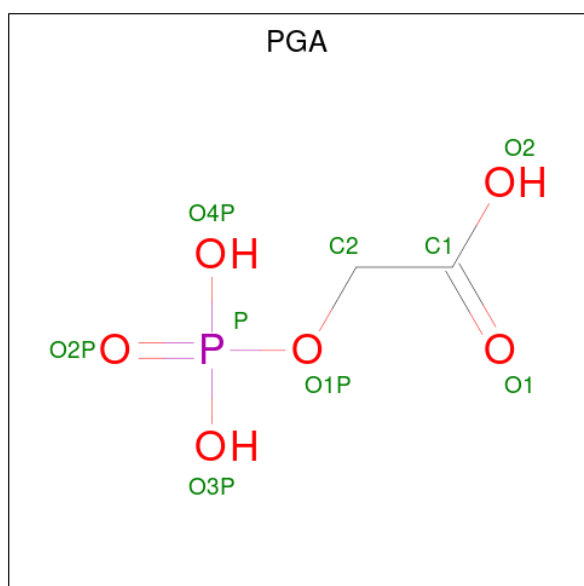
There are 4 unique types of molecules in this entry. The entry contains 7472 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3725	2347	642	718	18			
1	B	487	Total	C	N	O	S	0	0	0
			3725	2347	642	718	18			

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (CCD ID: PGA) (formula: $C_2H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	2	6	1		
2	B	1	Total	C	O	P	0	0
			9	2	6	1		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

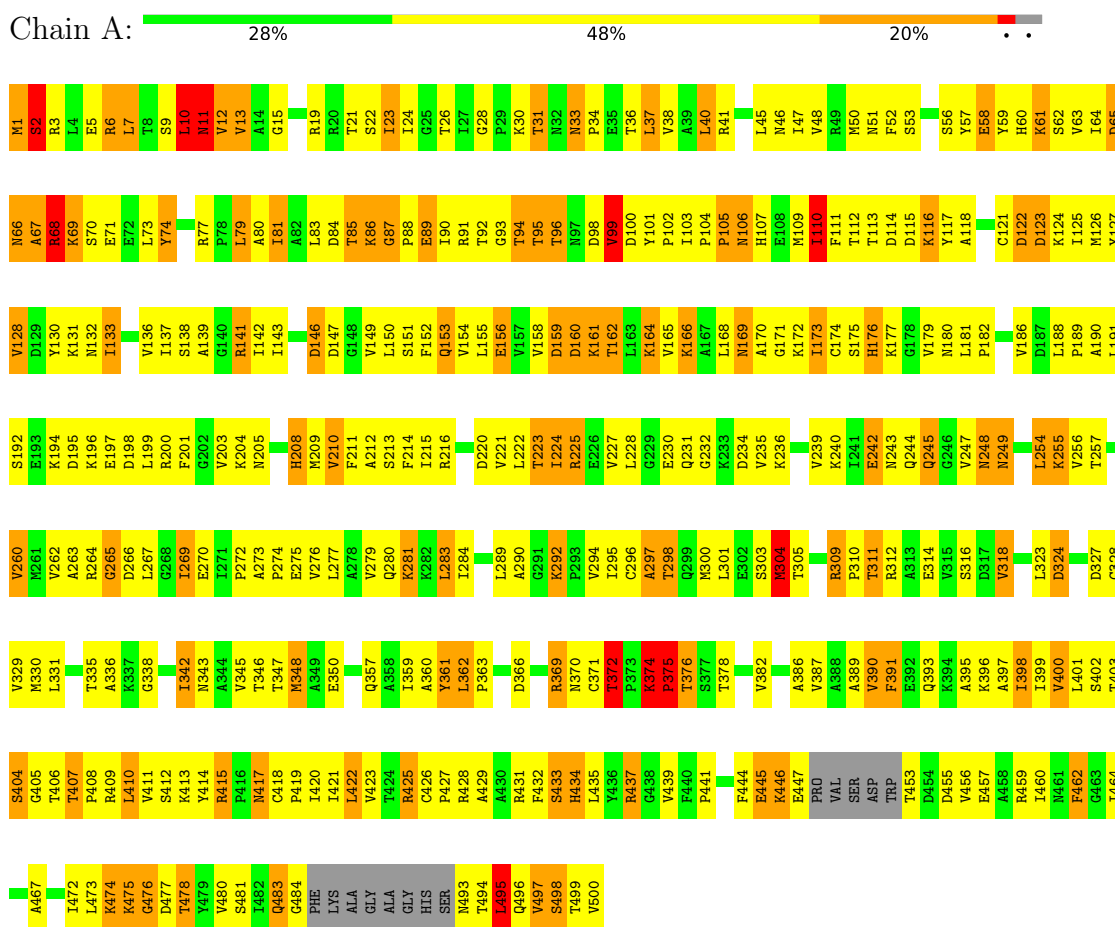
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	K 1	0	0
4	B	1	Total 1	K 1	0	0

3 Residue-property plots

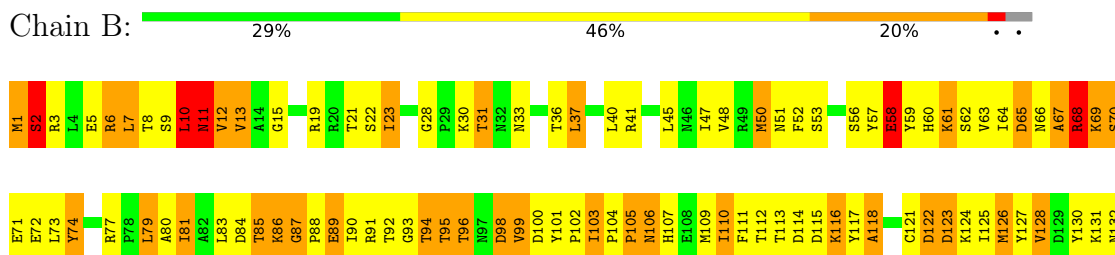
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: PYRUVATE KINASE



• Molecule 1: PYRUVATE KINASE



D477	T478	V411	S412	K342	L267	I133
T479	V479	K413	K343	I343	G268	V136
V480	V480	V414	A344	E270	D198	I137
S481	V481	R415	V345	I271	L199	S138
I482	V482	P416	T346	P272	R200	A139
Q483	V483	M417	T347	A273	G140	I401
G484	V484	C418	M348	P274	F201	R141
PHE	V485	P419	A349	E275	H208	I142
LYS	V486	L420	E350	V276	M209	I143
ALA	V487	I421	Q357	L277	V210	I144
GLY	V488	L422	A358	A278	F211	V145
ALA	V489	V423	I359	Q280	A212	D146
GLY	V490	T424	A360	K281	S213	D147
HIS	V491	R425	A361	V294	F214	G148
SER	V492	C426	Y361	K282	I215	G148
N493	V493	P427	L362	L283	R216	V149
T494	V494	R428	P363	I284	L150	L150
L495	V495	A429	D366	N288	F152	S151
Q496	V496	A430	D367	L289	D220	Q153
V497	V497	R431	M368	K292	V221	Q153
S498	V498	F432	R369	P293	L222	V154
T499	V499	S433	N370	V294	I224	L155
V500	V500	L435	C371	K296	R225	E156
		V436	T372	I295	E226	V157
		R437	F373	C296	V227	V158
		G438	K374	A297	L228	D159
		V439	P375	T298	G229	D160
		F440	T376	Q299	E230	K161
		P441	S377	M300	Q231	T162
			T378	L301	G232	L163
				E302	V235	K165
		F444	V382	S303	K236	K166
		E445		M304		A167
		K446		T305		L168
		E447	A386	P308	V239	N169
	PRO	VAL	V387	R309	K240	A170
	SER	SER	A389	E242	I241	G171
	ASP	ASP	V390	P310	N243	K172
	TRP	TRP	F391	T311	Q244	I173
			E392		G245	C174
	T453	D454	Q393	E314	G246	H176
	D455	V456	K394	V315	V247	K177
	V456	A395	A395	S316	N248	G178
	E457	K396	K396	D317	N249	V179
	A458	A458	A397	V318		N180
	R459	R459	I398	L323	L254	L181
	I460	I460	I399	D324	K255	P182
	N461	N461	V400		V256	G183
	F462	F462	L401	D327	T257	T184
	G463	G463	S402	C328	D258	D185
	I464	I464	T403	V329	G259	V186
			S404	M330	V260	D187
			G405	L331	M261	L188
	A467	A467	T406	A336	V262	P189
	L473	L473	P408	K337	A263	A190
	K474	K474	R409	G338	R264	L191
	G476	G476	L410	D265	G266	K194

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.30Å 106.40Å 105.50Å 90.00° 110.80° 90.00°	Depositor
Resolution (Å)	100.00 – 3.00	Depositor
% Data completeness (in resolution range)	85.0 (100.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.227 , 0.341	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7472	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGA, K, MN

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	2/3781 (0.1%)	1.24	38/5124 (0.7%)
1	B	0.51	2/3781 (0.1%)	1.31	37/5124 (0.7%)
All	All	0.57	4/7562 (0.1%)	1.27	75/10248 (0.7%)

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	2
1	B	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	LYS	C-N	-21.01	0.84	1.33
1	A	375	PRO	C-N	8.96	1.46	1.33
1	B	375	PRO	C-N	-6.05	1.25	1.33
1	B	188	LEU	CA-C	-5.23	1.47	1.53

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	374	LYS	O-C-N	-36.18	79.71	121.32
1	A	375	PRO	O-C-N	-30.03	82.10	122.64
1	B	375	PRO	O-C-N	-26.03	71.64	121.10
1	A	374	LYS	CA-C-N	-22.84	91.29	119.84
1	A	374	LYS	C-N-CA	-22.84	91.29	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	374	LYS	C-N-CD	-21.33	73.68	120.60
1	A	374	LYS	C-N-CD	-12.25	74.79	125.00
1	B	374	LYS	CA-C-N	-10.88	100.89	127.00
1	B	374	LYS	C-N-CA	-10.88	100.89	127.00
1	B	375	PRO	CA-C-N	-9.81	102.79	121.54
1	B	375	PRO	C-N-CA	-9.81	102.79	121.54
1	B	103	ILE	N-CA-C	9.09	117.32	107.60
1	B	188	LEU	CA-C-N	-8.84	110.62	119.90
1	B	188	LEU	C-N-CA	-8.84	110.62	119.90
1	B	317	ASP	N-CA-C	-8.00	105.50	114.62
1	A	58	GLU	N-CA-C	-7.62	102.11	111.40
1	B	476	GLY	N-CA-C	-7.60	100.70	114.46
1	A	375	PRO	CA-C-N	7.46	133.11	121.26
1	A	375	PRO	C-N-CA	7.46	133.11	121.26
1	B	58	GLU	N-CA-C	-7.42	102.35	111.40
1	B	161	LYS	N-CA-C	-7.32	103.51	114.64
1	A	161	LYS	N-CA-C	-7.31	103.53	114.64
1	A	476	GLY	N-CA-C	-7.28	101.28	114.46
1	A	208	HIS	N-CA-C	7.27	120.25	111.82
1	A	318	VAL	N-CA-C	-7.15	103.81	110.53
1	B	86	LYS	N-CA-C	-6.96	99.18	109.62
1	A	434	HIS	N-CA-C	-6.93	104.82	113.20
1	B	434	HIS	N-CA-C	-6.84	104.92	113.20
1	A	86	LYS	N-CA-C	-6.63	99.67	109.62
1	A	462	PHE	N-CA-C	-6.62	103.68	111.03
1	A	6	ARG	N-CA-C	-6.46	103.75	111.69
1	B	318	VAL	N-CA-C	-6.28	104.63	110.53
1	A	116	LYS	N-CA-C	-6.26	105.13	112.89
1	B	67	ALA	N-CA-C	-6.17	104.48	111.14
1	A	67	ALA	N-CA-C	-6.14	104.51	111.14
1	B	74	TYR	CA-C-N	6.14	125.62	119.24
1	B	74	TYR	C-N-CA	6.14	125.62	119.24
1	B	6	ARG	N-CA-C	-6.12	104.16	111.69
1	B	297	ALA	N-CA-C	6.09	118.55	108.99
1	B	208	HIS	N-CA-C	6.06	119.87	112.23
1	B	361	TYR	N-CA-C	6.05	118.38	111.11
1	B	256	VAL	N-CA-C	5.95	120.37	112.04
1	B	190	ALA	N-CA-C	-5.83	104.29	111.75
1	B	462	PHE	N-CA-C	-5.83	104.56	111.03
1	A	188	LEU	CA-C-N	5.78	125.54	119.76
1	A	188	LEU	C-N-CA	5.78	125.54	119.76
1	B	116	LYS	N-CA-C	-5.77	105.50	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ILE	N-CA-C	-5.75	106.10	111.45
1	B	348	MET	N-CA-C	-5.71	104.05	111.02
1	A	256	VAL	N-CA-C	5.70	120.02	112.04
1	B	98	ASP	CB-CA-C	-5.68	110.05	116.63
1	A	348	MET	N-CA-C	-5.67	104.11	111.02
1	A	74	TYR	CA-C-N	5.56	125.03	119.24
1	A	74	TYR	C-N-CA	5.56	125.03	119.24
1	A	361	TYR	N-CA-C	5.53	117.75	111.11
1	A	372	THR	CA-C-N	-5.52	113.62	120.79
1	A	372	THR	C-N-CA	-5.52	113.62	120.79
1	B	159	ASP	CB-CA-C	-5.51	110.20	116.54
1	A	297	ALA	N-CA-C	5.51	117.64	108.99
1	A	405	GLY	N-CA-C	-5.48	106.47	114.90
1	A	214	PHE	N-CA-C	5.47	118.93	111.39
1	B	236	LYS	N-CA-C	5.42	119.08	109.96
1	A	425	ARG	N-CA-C	-5.40	107.06	113.97
1	A	159	ASP	CB-CA-C	-5.37	110.37	116.54
1	B	68	ARG	N-CA-C	-5.36	105.54	111.71
1	A	437	ARG	N-CA-C	5.27	117.96	110.10
1	B	140	GLY	N-CA-C	-5.22	107.99	113.58
1	A	23	ILE	N-CA-C	5.22	115.29	107.51
1	A	68	ARG	N-CA-C	-5.16	105.78	111.71
1	A	292	LYS	CA-C-N	5.12	125.92	119.98
1	A	292	LYS	C-N-CA	5.12	125.92	119.98
1	B	425	ARG	N-CA-C	-5.12	107.59	113.88
1	A	236	LYS	N-CA-C	5.08	118.50	109.96
1	B	23	ILE	N-CA-C	5.05	115.03	107.51
1	B	214	PHE	N-CA-C	5.00	118.29	111.39

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	LYS	Peptide
1	A	375	PRO	Mainchain
1	B	374	LYS	Peptide,Mainchain

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	3725	0	3804	382	1
1	B	3725	0	3804	393	1
2	A	9	0	2	6	0
2	B	9	0	2	2	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
All	All	7472	0	7612	775	1

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 51.

All (775) 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:374:LYS:HG2	1:A:375:PRO:HD3	1.25	1.11
1:B:186:VAL:HG23	1:B:216:ARG:HE	1.19	1.06
1:A:272:PRO:HB2	1:A:275:GLU:HG3	1.28	1.06
1:B:272:PRO:HB2	1:B:275:GLU:HG3	1.37	1.05
1:A:390:VAL:HB	1:A:395:ALA:HB3	1.37	1.02
1:A:263:ALA:CA	2:A:1005:PGA:O2	2.08	1.02
1:A:378:THR:HG22	1:A:493:ASN:HD21	1.18	1.01
1:A:263:ALA:HB1	2:A:1005:PGA:O2	1.58	1.00
1:B:378:THR:HG22	1:B:493:ASN:HD21	1.21	0.98
1:B:375:PRO:HB2	1:B:376:THR:OG1	1.61	0.98
1:B:390:VAL:HB	1:B:395:ALA:HB3	1.45	0.96
1:A:374:LYS:HG2	1:A:375:PRO:CD	1.89	0.96
1:A:263:ALA:CB	2:A:1005:PGA:O2	2.14	0.96
1:A:220:ASP:O	1:A:224:ILE:HG22	1.63	0.95
1:B:374:LYS:H	1:B:375:PRO:HB3	1.31	0.95
1:B:374:LYS:N	1:B:375:PRO:HB3	1.82	0.94
1:B:220:ASP:O	1:B:224:ILE:HG22	1.69	0.93
1:B:342:ILE:HD13	1:B:342:ILE:H	1.33	0.91
1:A:374:LYS:CG	1:A:375:PRO:HD3	2.03	0.89
1:A:342:ILE:HD13	1:A:342:ILE:H	1.36	0.89
1:B:375:PRO:CB	1:B:376:THR:OG1	2.19	0.89
1:A:369:ARG:HE	1:A:370:ASN:HD21	1.22	0.87
1:B:310:PRO:HG3	1:B:347:THR:HG21	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:HH21	1:A:280:GLN:HE22	1.24	0.84
1:B:395:ALA:HA	1:B:478:THR:HG23	1.57	0.84
1:A:224:ILE:O	1:A:228:LEU:HD23	1.78	0.84
1:A:265:GLY:N	2:A:1005:PGA:O1	2.12	0.83
1:A:378:THR:HG22	1:A:493:ASN:ND2	1.93	0.83
1:A:395:ALA:HA	1:A:478:THR:HG23	1.61	0.83
1:B:224:ILE:O	1:B:228:LEU:HD23	1.79	0.83
1:A:310:PRO:HG3	1:A:347:THR:HG21	1.61	0.83
1:B:369:ARG:HE	1:B:370:ASN:HD21	1.24	0.82
1:B:378:THR:HG22	1:B:493:ASN:ND2	1.95	0.82
1:B:51:ASN:HD21	1:B:53:SER:HB2	1.44	0.82
1:A:106:ASN:HD21	1:A:166:LYS:NZ	1.78	0.81
1:B:153:GLN:HB2	1:B:168:LEU:HD21	1.60	0.81
1:A:151:SER:H	1:A:169:ASN:HD21	1.25	0.81
1:A:158:VAL:HB	1:A:162:THR:HB	1.60	0.81
1:A:155:LEU:HB2	1:A:164:LYS:HG2	1.62	0.81
1:B:216:ARG:HB3	1:B:245:GLN:HG2	1.61	0.81
1:A:56:SER:N	1:A:59:TYR:HB2	1.97	0.80
1:B:309:ARG:HD3	1:B:309:ARG:N	1.93	0.80
1:B:104:PRO:HD2	1:B:171:GLY:O	1.82	0.79
1:B:481:SER:HB2	1:B:496:GLN:HB3	1.62	0.79
1:B:69:LYS:HZ2	1:B:73:LEU:HG	1.47	0.79
1:B:158:VAL:HB	1:B:162:THR:HB	1.64	0.79
1:A:254:LEU:O	1:A:292:LYS:HE3	1.83	0.79
1:B:56:SER:N	1:B:59:TYR:HB2	1.98	0.79
1:A:151:SER:N	1:A:169:ASN:HD21	1.80	0.79
1:B:90:ILE:HD12	1:B:130:TYR:HB2	1.64	0.79
1:B:52:PHE:O	1:B:86:LYS:HB2	1.82	0.78
1:A:369:ARG:HE	1:A:370:ASN:ND2	1.80	0.78
1:B:366:ASP:O	1:B:369:ARG:HG3	1.83	0.78
1:A:481:SER:HB2	1:A:496:GLN:HB3	1.65	0.78
1:B:51:ASN:ND2	1:B:53:SER:HB2	1.99	0.78
1:B:396:LYS:O	1:B:418:CYS:HB2	1.83	0.78
1:B:254:LEU:O	1:B:292:LYS:HE3	1.82	0.77
1:A:51:ASN:HD21	1:A:53:SER:HB2	1.49	0.77
1:A:90:ILE:HD12	1:A:130:TYR:HB2	1.65	0.77
1:B:139:ALA:HA	1:B:154:VAL:HG12	1.67	0.77
1:B:141:ARG:HH12	1:B:181:LEU:HB3	1.50	0.76
1:B:408:PRO:HG3	1:B:422:LEU:HD13	1.66	0.76
1:B:297:ALA:HB1	1:B:330:MET:HE2	1.65	0.76
1:A:284:ILE:HG23	1:A:294:VAL:HG11	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLU:O	1:A:279:VAL:HG23	1.86	0.75
1:A:295:ILE:HG12	1:A:328:CYS:HB2	1.68	0.75
1:A:33:ASN:HD21	1:A:36:THR:H	1.32	0.75
1:B:90:ILE:HB	1:B:179:VAL:HB	1.67	0.75
1:B:496:GLN:HE21	1:B:498:SER:HB2	1.50	0.75
1:B:189:PRO:HB2	1:B:191:LEU:O	1.87	0.75
1:A:297:ALA:HB1	1:A:330:MET:HE2	1.69	0.75
1:A:263:ALA:C	2:A:1005:PGA:O2	2.29	0.75
1:A:216:ARG:HB3	1:A:245:GLN:HG2	1.68	0.75
1:A:51:ASN:ND2	1:A:53:SER:HB2	2.02	0.74
1:A:52:PHE:O	1:A:86:LYS:HB2	1.87	0.74
1:A:125:ILE:HG12	1:A:126:MET:H	1.53	0.74
1:A:117:TYR:O	1:A:121:CYS:HB3	1.88	0.74
1:A:408:PRO:HG3	1:A:422:LEU:HD13	1.69	0.74
1:A:263:ALA:HA	2:A:1005:PGA:O2	1.87	0.74
1:B:151:SER:H	1:B:169:ASN:HD21	1.36	0.74
1:B:369:ARG:HE	1:B:370:ASN:ND2	1.85	0.74
1:A:366:ASP:O	1:A:369:ARG:HG3	1.88	0.74
1:A:496:GLN:HG3	1:A:497:VAL:N	2.02	0.73
1:A:346:THR:O	1:A:350:GLU:HG3	1.87	0.73
1:B:117:TYR:O	1:B:121:CYS:HB3	1.89	0.73
1:B:151:SER:N	1:B:169:ASN:HD21	1.86	0.73
1:B:155:LEU:HB2	1:B:164:LYS:HG2	1.71	0.73
1:B:496:GLN:HG3	1:B:497:VAL:H	1.53	0.73
1:B:372:THR:HG22	1:B:372:THR:O	1.87	0.73
1:A:247:VAL:C	1:A:249:ASN:H	1.97	0.72
1:B:398:ILE:HG23	1:B:420:ILE:HA	1.71	0.72
1:B:496:GLN:HG3	1:B:497:VAL:N	2.04	0.72
1:B:417:ASN:HD22	1:B:417:ASN:H	1.36	0.72
1:A:396:LYS:O	1:A:418:CYS:HB2	1.88	0.72
1:A:423:VAL:HG11	1:A:459:ARG:HB3	1.72	0.72
1:A:151:SER:H	1:A:169:ASN:ND2	1.88	0.72
1:B:295:ILE:HG12	1:B:328:CYS:HB2	1.70	0.72
1:B:125:ILE:HG12	1:B:126:MET:H	1.55	0.72
1:A:311:THR:OG1	1:A:314:GLU:HG3	1.90	0.71
1:A:398:ILE:HG23	1:A:420:ILE:HA	1.71	0.71
1:B:213:SER:HA	1:B:240:LYS:HD3	1.73	0.71
1:A:417:ASN:HD22	1:A:417:ASN:H	1.39	0.71
1:B:86:LYS:HG2	1:B:89:GLU:OE2	1.91	0.71
1:A:125:ILE:HG12	1:A:126:MET:N	2.06	0.71
1:A:372:THR:O	1:A:372:THR:HG22	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:GLN:HG3	1:A:497:VAL:H	1.55	0.71
1:B:346:THR:O	1:B:350:GLU:HG3	1.91	0.70
1:B:499:THR:HG22	1:B:500:VAL:N	2.07	0.70
1:B:79:LEU:HD12	1:B:80:ALA:H	1.55	0.70
1:A:153:GLN:HB2	1:A:168:LEU:HD21	1.74	0.70
1:B:456:VAL:O	1:B:460:ILE:HG13	1.92	0.70
1:A:496:GLN:HE21	1:A:498:SER:HB2	1.56	0.70
1:A:121:CYS:O	1:A:122:ASP:HB3	1.92	0.70
1:A:476:GLY:H	1:A:500:VAL:HB	1.57	0.70
1:B:67:ALA:HB1	1:B:79:LEU:HD21	1.74	0.70
1:B:284:ILE:HG23	1:B:294:VAL:HG11	1.73	0.70
1:A:48:VAL:HG23	1:A:79:LEU:HD11	1.72	0.69
1:B:308:PRO:C	1:B:309:ARG:HD3	2.18	0.69
1:A:106:ASN:HD21	1:A:166:LYS:HZ3	1.41	0.69
1:B:209:MET:O	1:B:210:VAL:HG23	1.91	0.69
1:B:243:ASN:HA	1:B:270:GLU:HG2	1.75	0.69
1:B:499:THR:HG22	1:B:500:VAL:H	1.56	0.69
1:A:104:PRO:HD2	1:A:171:GLY:O	1.93	0.69
1:B:263:ALA:C	2:B:1006:PGA:O1	2.36	0.68
1:A:86:LYS:HG2	1:A:89:GLU:OE2	1.93	0.68
1:A:141:ARG:HH12	1:A:181:LEU:HB3	1.58	0.68
1:B:247:VAL:C	1:B:249:ASN:H	2.02	0.68
1:A:375:PRO:O	1:A:376:THR:C	2.36	0.68
1:A:499:THR:HG22	1:A:500:VAL:H	1.59	0.68
1:A:90:ILE:HG23	1:A:130:TYR:HB2	1.75	0.68
1:A:369:ARG:NE	1:A:370:ASN:HD21	1.92	0.68
1:A:499:THR:HG22	1:A:500:VAL:N	2.08	0.68
1:A:208:HIS:NE2	1:A:431:ARG:HD3	2.10	0.67
1:B:125:ILE:HG12	1:B:126:MET:N	2.09	0.67
1:B:264:ARG:HH21	1:B:280:GLN:HE22	1.40	0.67
1:A:213:SER:HA	1:A:240:LYS:HD3	1.77	0.67
1:A:304:MET:HG3	1:A:310:PRO:HB3	1.76	0.67
1:B:301:LEU:HD23	1:B:314:GLU:HB3	1.75	0.67
1:B:124:LYS:N	1:B:124:LYS:HD2	2.10	0.67
1:B:311:THR:OG1	1:B:314:GLU:HG3	1.95	0.67
1:B:476:GLY:H	1:B:500:VAL:HB	1.59	0.67
1:A:243:ASN:HA	1:A:270:GLU:HG2	1.76	0.67
1:B:53:SER:HA	1:B:86:LYS:CG	2.24	0.66
1:B:475:LYS:HA	1:B:500:VAL:HB	1.78	0.66
1:B:360:ALA:HB1	1:B:363:PRO:HG2	1.78	0.66
1:B:133:ILE:HA	1:B:136:VAL:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:GLU:O	1:B:279:VAL:HG23	1.95	0.66
1:A:53:SER:HA	1:A:86:LYS:CG	2.24	0.66
1:A:33:ASN:ND2	1:A:36:THR:H	1.93	0.66
1:B:216:ARG:HG2	1:B:243:ASN:HD21	1.61	0.66
1:A:56:SER:H	1:A:59:TYR:HB2	1.60	0.65
1:A:216:ARG:HG2	1:A:243:ASN:HD21	1.61	0.65
1:B:53:SER:HA	1:B:86:LYS:HG3	1.77	0.65
1:A:3:ARG:HG2	1:A:7:LEU:HD22	1.77	0.65
1:A:53:SER:HA	1:A:86:LYS:HG3	1.77	0.65
1:A:483:GLN:HE21	1:A:483:GLN:N	1.94	0.65
1:A:360:ALA:HB1	1:A:363:PRO:HG2	1.79	0.65
1:B:139:ALA:HA	1:B:154:VAL:CG1	2.26	0.65
1:A:107:HIS:CE1	1:A:109:MET:HB3	2.32	0.65
1:A:390:VAL:CB	1:A:395:ALA:HB3	2.21	0.65
1:B:56:SER:H	1:B:59:TYR:HB2	1.60	0.65
1:B:64:ILE:HG12	1:B:81:ILE:HG21	1.79	0.65
1:B:369:ARG:NE	1:B:370:ASN:HD21	1.94	0.65
1:A:475:LYS:HA	1:A:500:VAL:HB	1.79	0.65
1:B:423:VAL:HG11	1:B:459:ARG:HB3	1.78	0.65
1:B:483:GLN:N	1:B:483:GLN:HE21	1.94	0.65
1:B:211:PHE:O	1:B:240:LYS:HD2	1.97	0.65
1:B:387:VAL:O	1:B:390:VAL:HG13	1.97	0.64
1:B:33:ASN:HD21	1:B:36:THR:H	1.45	0.64
1:A:107:HIS:HE1	1:A:109:MET:HB3	1.61	0.64
1:A:130:TYR:O	1:A:133:ILE:HG22	1.97	0.64
1:B:112:THR:HG23	1:B:161:LYS:O	1.98	0.64
1:B:260:VAL:HG13	1:B:294:VAL:HG23	1.79	0.64
1:A:67:ALA:HB1	1:A:79:LEU:HD21	1.80	0.64
1:A:133:ILE:HA	1:A:136:VAL:HG22	1.79	0.63
1:A:196:LYS:HB3	1:A:200:ARG:HH21	1.63	0.63
1:A:86:LYS:HZ2	1:A:89:GLU:HG3	1.63	0.63
1:B:69:LYS:NZ	1:B:73:LEU:HG	2.12	0.63
1:B:208:HIS:NE2	1:B:431:ARG:HD3	2.13	0.63
1:B:297:ALA:O	1:B:298:THR:HB	1.98	0.63
1:A:9:SER:O	1:A:11:ASN:N	2.31	0.63
1:A:211:PHE:O	1:A:240:LYS:HD2	1.97	0.63
1:B:398:ILE:HD13	1:B:411:VAL:HG11	1.80	0.63
1:B:3:ARG:HG2	1:B:7:LEU:HD22	1.78	0.63
1:A:64:ILE:HG12	1:A:81:ILE:HG21	1.80	0.63
1:B:107:HIS:HE1	1:B:109:MET:HB3	1.63	0.63
1:B:304:MET:HG3	1:B:310:PRO:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:THR:O	1:A:292:LYS:HD3	1.99	0.63
1:A:303:SER:C	1:A:305:THR:H	2.07	0.63
1:B:257:THR:O	1:B:292:LYS:HD3	1.98	0.63
1:A:429:ALA:HA	1:A:432:PHE:CZ	2.33	0.63
1:B:429:ALA:HA	1:B:432:PHE:CZ	2.34	0.63
1:A:209:MET:O	1:A:210:VAL:HG23	1.99	0.62
1:B:186:VAL:CG2	1:B:216:ARG:HE	2.06	0.62
1:A:92:THR:HG22	1:A:177:LYS:H	1.64	0.62
1:A:113:THR:HG22	1:A:128:VAL:O	1.98	0.62
1:A:141:ARG:HH22	1:A:181:LEU:HA	1.63	0.62
1:B:101:TYR:CD1	1:B:174:CYS:HA	2.33	0.62
1:B:92:THR:HG22	1:B:177:LYS:H	1.65	0.62
1:A:112:THR:HG23	1:A:161:LYS:O	1.99	0.62
1:A:110:ILE:HD11	1:A:162:THR:HG23	1.82	0.62
1:B:111:PHE:CZ	1:B:126:MET:SD	2.93	0.61
1:B:232:GLY:O	1:B:235:VAL:HG22	2.00	0.61
1:A:101:TYR:HB3	1:A:172:LYS:HG3	1.82	0.61
1:A:12:VAL:O	1:A:13:VAL:HB	2.00	0.61
1:A:180:ASN:O	1:A:182:PRO:HD3	2.01	0.61
1:B:113:THR:HG22	1:B:128:VAL:O	2.00	0.61
1:B:375:PRO:HB3	1:B:376:THR:OG1	1.99	0.61
1:B:9:SER:O	1:B:11:ASN:N	2.33	0.61
1:B:56:SER:O	1:B:59:TYR:HB2	2.01	0.61
1:B:92:THR:OG1	1:B:126:MET:HE2	2.01	0.61
1:B:151:SER:H	1:B:169:ASN:ND2	1.98	0.61
1:B:375:PRO:HB2	1:B:376:THR:HG1	1.66	0.60
1:B:2:SER:HB2	1:B:5:GLU:HB2	1.83	0.60
1:B:141:ARG:HH22	1:B:181:LEU:HA	1.65	0.60
1:B:362:LEU:HB2	1:B:363:PRO:CD	2.31	0.60
1:A:301:LEU:HD23	1:A:314:GLU:HB3	1.82	0.60
1:B:398:ILE:HG12	1:B:398:ILE:O	2.01	0.60
1:A:2:SER:HB2	1:A:5:GLU:HB2	1.82	0.60
1:A:93:GLY:HA3	1:A:127:TYR:HB3	1.82	0.60
1:B:102:PRO:HB3	1:B:123:ASP:OD2	2.01	0.60
1:A:297:ALA:O	1:A:298:THR:HB	2.02	0.60
1:A:112:THR:HB	1:A:125:ILE:HD11	1.82	0.60
1:A:69:LYS:HZ2	1:A:73:LEU:HG	1.67	0.60
1:A:403:THR:HG23	1:A:426:CYS:HB2	1.83	0.60
1:B:107:HIS:CE1	1:B:109:MET:HB3	2.37	0.60
1:B:141:ARG:HH12	1:B:181:LEU:CB	2.14	0.60
1:A:409:ARG:O	1:A:412:SER:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LYS:O	1:A:475:LYS:HB3	2.00	0.60
1:B:396:LYS:O	1:B:419:PRO:HD2	2.02	0.60
1:B:242:GLU:HA	1:B:267:LEU:HD13	1.84	0.59
1:B:475:LYS:HA	1:B:500:VAL:CG1	2.32	0.59
1:B:48:VAL:HG23	1:B:79:LEU:HD11	1.83	0.59
1:B:151:SER:HB2	1:B:168:LEU:HB2	1.84	0.59
1:A:65:ASP:HA	1:A:68:ARG:HB2	1.84	0.59
1:A:41:ARG:NH2	1:A:74:TYR:O	2.36	0.59
1:B:95:THR:HA	1:B:121:CYS:O	2.03	0.59
1:A:56:SER:O	1:A:59:TYR:HB2	2.03	0.59
1:B:495:LEU:HD23	1:B:495:LEU:C	2.28	0.59
1:A:242:GLU:HA	1:A:267:LEU:HD13	1.84	0.59
1:A:300:MET:O	1:A:314:GLU:HB3	2.03	0.59
1:B:15:GLY:H	1:B:357:GLN:HE22	1.51	0.59
1:A:139:ALA:HA	1:A:154:VAL:HG12	1.85	0.58
1:A:101:TYR:HD2	1:A:172:LYS:HZ1	1.49	0.58
1:A:398:ILE:HD13	1:A:411:VAL:HG11	1.83	0.58
1:B:84:ASP:CG	1:B:240:LYS:HZ2	2.10	0.58
1:A:15:GLY:H	1:A:357:GLN:HE22	1.52	0.58
1:A:387:VAL:O	1:A:390:VAL:HG13	2.03	0.58
1:B:156:GLU:HB2	1:B:164:LYS:HE2	1.86	0.58
1:A:151:SER:HB2	1:A:168:LEU:HB2	1.85	0.58
1:B:121:CYS:O	1:B:122:ASP:HB3	2.03	0.58
1:B:474:LYS:O	1:B:475:LYS:HB3	2.04	0.58
1:A:12:VAL:HG23	1:A:13:VAL:HG23	1.85	0.58
1:B:151:SER:HB3	1:B:168:LEU:HD12	1.85	0.58
1:B:195:ASP:HA	1:B:198:ASP:OD2	2.03	0.58
1:B:477:ASP:O	1:B:478:THR:HB	2.03	0.58
1:A:101:TYR:CE1	1:A:174:CYS:HB3	2.39	0.58
1:B:94:THR:HA	1:B:175:SER:HB2	1.85	0.58
1:A:69:LYS:NZ	1:A:73:LEU:HG	2.18	0.58
1:A:94:THR:HA	1:A:175:SER:HB2	1.84	0.57
1:B:105:PRO:HD2	1:B:107:HIS:CD2	2.39	0.57
1:B:417:ASN:HD22	1:B:417:ASN:N	2.01	0.57
1:A:91:ARG:HH11	1:A:91:ARG:HG2	1.69	0.57
1:A:475:LYS:HA	1:A:500:VAL:CG1	2.34	0.57
1:B:303:SER:C	1:B:305:THR:H	2.11	0.57
1:B:110:ILE:HD11	1:B:162:THR:HG23	1.86	0.57
1:B:264:ARG:HB2	1:B:297:ALA:O	2.05	0.57
1:B:480:VAL:HG13	1:B:496:GLN:O	2.03	0.57
1:A:101:TYR:CD1	1:A:174:CYS:HA	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASN:ND2	1:A:166:LYS:NZ	2.50	0.57
1:A:112:THR:HA	1:A:161:LYS:O	2.05	0.57
1:A:189:PRO:HB2	1:A:191:LEU:O	2.05	0.57
1:B:403:THR:HG23	1:B:426:CYS:HB2	1.87	0.57
1:B:10:LEU:O	1:B:11:ASN:C	2.47	0.57
1:B:65:ASP:HA	1:B:68:ARG:HB2	1.87	0.57
1:B:112:THR:HB	1:B:125:ILE:HD11	1.87	0.57
1:B:431:ARG:O	1:B:434:HIS:HD2	1.88	0.57
1:A:456:VAL:O	1:A:460:ILE:HG13	2.05	0.57
1:A:141:ARG:HH12	1:A:181:LEU:CB	2.16	0.56
1:B:33:ASN:ND2	1:B:36:THR:H	2.02	0.56
1:B:409:ARG:O	1:B:412:SER:HB3	2.05	0.56
1:A:84:ASP:OD1	1:A:240:LYS:NZ	2.37	0.56
1:A:92:THR:O	1:A:176:HIS:HD2	1.87	0.56
1:A:141:ARG:HE	1:A:142:ILE:N	2.04	0.56
1:B:180:ASN:O	1:B:182:PRO:HD3	2.05	0.56
1:A:401:LEU:HD12	1:A:401:LEU:N	2.21	0.56
1:B:110:ILE:HD13	1:B:125:ILE:HG13	1.87	0.56
1:B:86:LYS:HZ1	1:B:89:GLU:HG3	1.71	0.56
1:A:101:TYR:HD2	1:A:172:LYS:NZ	2.03	0.55
1:A:110:ILE:HD13	1:A:125:ILE:HG13	1.88	0.55
1:A:247:VAL:O	1:A:249:ASN:N	2.39	0.55
1:A:264:ARG:HB2	1:A:297:ALA:O	2.06	0.55
1:B:432:PHE:CD1	1:B:432:PHE:C	2.84	0.55
1:A:50:MET:HE3	1:A:63:VAL:HB	1.88	0.55
1:A:79:LEU:HD12	1:A:80:ALA:H	1.71	0.55
1:A:153:GLN:HG3	1:A:168:LEU:HD21	1.88	0.55
1:A:232:GLY:O	1:A:235:VAL:HG22	2.05	0.55
1:A:396:LYS:O	1:A:419:PRO:HD2	2.06	0.55
1:A:495:LEU:C	1:A:495:LEU:HD23	2.31	0.55
1:B:362:LEU:HB2	1:B:363:PRO:HD3	1.87	0.55
1:A:480:VAL:HG13	1:A:496:GLN:O	2.05	0.55
1:B:112:THR:HA	1:B:161:LYS:O	2.07	0.55
1:B:67:ALA:HB1	1:B:79:LEU:CD2	2.36	0.55
1:B:141:ARG:HE	1:B:142:ILE:N	2.05	0.55
1:B:300:MET:O	1:B:314:GLU:HB3	2.06	0.55
1:B:153:GLN:CB	1:B:168:LEU:HD21	2.32	0.55
1:A:67:ALA:HB1	1:A:79:LEU:CD2	2.36	0.55
1:A:247:VAL:C	1:A:249:ASN:N	2.63	0.55
1:A:195:ASP:HA	1:A:198:ASP:OD2	2.07	0.55
1:A:444:PHE:CE2	1:A:459:ARG:HG2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LEU:HD12	1:B:80:ALA:N	2.22	0.55
1:A:114:ASP:O	1:A:115:ASP:HB2	2.06	0.54
1:A:208:HIS:CE1	1:A:431:ARG:HD3	2.43	0.54
1:A:398:ILE:HG12	1:A:398:ILE:O	2.07	0.54
1:B:102:PRO:O	1:B:173:ILE:HG22	2.06	0.54
1:A:57:TYR:O	1:A:61:LYS:HB2	2.08	0.54
1:A:401:LEU:HD23	1:A:459:ARG:HD2	1.89	0.54
1:B:460:ILE:O	1:B:464:ILE:HG13	2.08	0.54
1:B:399:ILE:HA	1:B:421:ILE:O	2.07	0.54
1:A:477:ASP:O	1:A:478:THR:HB	2.07	0.54
1:B:41:ARG:NH2	1:B:74:TYR:O	2.40	0.54
1:B:86:LYS:NZ	1:B:89:GLU:HG3	2.22	0.54
1:A:476:GLY:N	1:A:500:VAL:HB	2.21	0.54
1:B:12:VAL:O	1:B:13:VAL:HB	2.06	0.54
1:B:141:ARG:HH21	1:B:143:ILE:HA	1.73	0.54
1:B:208:HIS:CE1	1:B:431:ARG:HD3	2.43	0.54
1:A:457:GLU:H	1:A:457:GLU:CD	2.16	0.54
1:A:47:ILE:HG12	1:A:80:ALA:HB3	1.89	0.54
1:B:45:LEU:HD21	1:B:48:VAL:CG2	2.38	0.54
1:B:110:ILE:HD11	1:B:112:THR:OG1	2.07	0.54
1:B:402:SER:HB3	1:B:422:LEU:HD11	1.89	0.54
1:A:362:LEU:HB2	1:A:363:PRO:CD	2.38	0.53
1:A:52:PHE:CD2	1:A:198:ASP:HB3	2.44	0.53
1:A:146:ASP:OD1	1:A:177:LYS:HD2	2.08	0.53
1:A:431:ARG:O	1:A:434:HIS:HD2	1.90	0.53
1:B:159:ASP:HB2	1:B:162:THR:OG1	2.09	0.53
1:B:444:PHE:CE2	1:B:459:ARG:HG2	2.43	0.53
1:B:47:ILE:HG12	1:B:80:ALA:HB3	1.91	0.53
1:B:130:TYR:O	1:B:133:ILE:HG22	2.08	0.53
1:A:399:ILE:HA	1:A:421:ILE:O	2.09	0.53
1:A:427:PRO:O	1:A:431:ARG:HG3	2.09	0.53
1:A:453:THR:HG22	1:A:453:THR:O	2.09	0.53
1:B:45:LEU:HD21	1:B:48:VAL:HG22	1.91	0.53
1:B:273:ALA:N	1:B:274:PRO:HD2	2.24	0.53
1:A:478:THR:HG23	1:A:478:THR:O	2.09	0.53
1:B:196:LYS:HB3	1:B:200:ARG:HH21	1.74	0.53
1:B:445:GLU:O	1:B:446:LYS:CB	2.56	0.53
1:B:114:ASP:O	1:B:115:ASP:HB2	2.08	0.53
1:A:52:PHE:HZ	1:A:201:PHE:CE2	2.27	0.53
1:A:112:THR:CB	1:A:125:ILE:HD11	2.39	0.53
1:A:496:GLN:CG	1:A:497:VAL:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:GLN:HG3	1:B:168:LEU:HD21	1.91	0.52
1:B:50:MET:HE3	1:B:63:VAL:HB	1.90	0.52
1:B:362:LEU:HD13	1:B:362:LEU:N	2.24	0.52
1:A:45:LEU:HD21	1:A:48:VAL:HG22	1.91	0.52
1:B:476:GLY:N	1:B:500:VAL:HB	2.23	0.52
1:A:102:PRO:HB3	1:A:123:ASP:OD2	2.09	0.52
1:A:432:PHE:C	1:A:432:PHE:CD1	2.87	0.52
1:B:427:PRO:O	1:B:431:ARG:HG3	2.09	0.52
1:A:1:MET:O	1:A:3:ARG:N	2.43	0.52
1:B:496:GLN:CG	1:B:497:VAL:H	2.19	0.52
1:B:105:PRO:CD	1:B:107:HIS:HD2	2.23	0.52
1:B:123:ASP:HB3	1:B:124:LYS:HD2	1.92	0.52
1:B:425:ARG:HA	1:B:444:PHE:O	2.10	0.52
1:B:457:GLU:CD	1:B:457:GLU:H	2.17	0.52
1:A:103:ILE:HA	1:A:172:LYS:HA	1.92	0.52
1:B:6:ARG:NE	1:B:360:ALA:HB2	2.25	0.52
1:B:398:ILE:HG22	1:B:419:PRO:O	2.10	0.52
1:A:6:ARG:NE	1:A:360:ALA:HB2	2.24	0.52
1:A:10:LEU:O	1:A:11:ASN:C	2.52	0.52
1:B:95:THR:H	1:B:175:SER:HB3	1.74	0.52
1:B:456:VAL:HG12	1:B:459:ARG:NH2	2.25	0.52
1:A:111:PHE:CD1	1:A:165:VAL:HG21	2.45	0.52
1:A:151:SER:HB3	1:A:168:LEU:HD12	1.91	0.52
1:A:296:CYS:SG	1:A:300:MET:HE3	2.50	0.52
1:B:1:MET:O	1:B:3:ARG:N	2.43	0.52
1:B:429:ALA:HA	1:B:432:PHE:CE2	2.45	0.52
1:A:45:LEU:HD21	1:A:48:VAL:CG2	2.41	0.51
1:A:105:PRO:HD2	1:A:107:HIS:CD2	2.45	0.51
1:A:264:ARG:HE	1:A:280:GLN:NE2	2.08	0.51
1:A:362:LEU:HB2	1:A:363:PRO:HD3	1.91	0.51
1:A:425:ARG:HA	1:A:444:PHE:O	2.09	0.51
1:A:95:THR:HA	1:A:121:CYS:O	2.09	0.51
1:A:159:ASP:HB2	1:A:162:THR:OG1	2.10	0.51
1:A:223:THR:O	1:A:227:VAL:HG23	2.10	0.51
1:B:410:LEU:O	1:B:413:LYS:HB3	2.10	0.51
1:B:496:GLN:CG	1:B:497:VAL:N	2.73	0.51
1:A:52:PHE:HZ	1:A:201:PHE:HE2	1.59	0.51
1:B:213:SER:CA	1:B:240:LYS:HD3	2.41	0.51
1:A:114:ASP:C	1:A:116:LYS:H	2.18	0.51
1:A:361:TYR:CG	1:A:417:ASN:HB3	2.45	0.51
1:B:122:ASP:O	1:B:124:LYS:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:GLN:CG	1:A:497:VAL:N	2.73	0.51
1:B:247:VAL:C	1:B:249:ASN:N	2.67	0.51
1:B:28:GLY:N	1:B:336:ALA:HA	2.26	0.51
1:B:223:THR:O	1:B:227:VAL:HG23	2.11	0.51
1:B:106:ASN:HD21	1:B:166:LYS:NZ	2.09	0.51
1:A:446:LYS:O	1:A:447:GLU:CB	2.58	0.50
1:B:86:LYS:HZ2	1:B:89:GLU:CD	2.19	0.50
1:A:19:ARG:NH1	1:A:21:THR:O	2.42	0.50
1:A:429:ALA:HA	1:A:432:PHE:CE2	2.45	0.50
1:B:382:VAL:HG21	1:B:493:ASN:ND2	2.26	0.50
1:A:84:ASP:CG	1:A:240:LYS:HZ2	2.20	0.50
1:B:401:LEU:HD12	1:B:401:LEU:N	2.26	0.50
1:A:432:PHE:O	1:A:435:LEU:HB2	2.12	0.50
1:B:279:VAL:HG12	1:B:279:VAL:O	2.10	0.50
1:A:156:GLU:HB2	1:A:164:LYS:HE2	1.94	0.50
1:A:247:VAL:HG13	1:A:248:ASN:N	2.26	0.50
1:A:445:GLU:O	1:A:446:LYS:CB	2.60	0.50
1:B:23:ILE:HG21	1:B:345:VAL:HG13	1.94	0.50
1:B:52:PHE:CD2	1:B:198:ASP:HB3	2.47	0.50
1:B:359:ILE:HG22	1:B:360:ALA:N	2.26	0.50
1:B:475:LYS:HA	1:B:500:VAL:CB	2.40	0.50
1:A:34:PRO:O	1:A:38:VAL:HG23	2.11	0.50
1:A:92:THR:OG1	1:A:126:MET:HE2	2.12	0.50
1:A:398:ILE:CG2	1:A:420:ILE:HA	2.40	0.50
1:A:410:LEU:O	1:A:413:LYS:HB3	2.12	0.50
1:B:398:ILE:CG2	1:B:420:ILE:HA	2.39	0.50
1:A:399:ILE:O	1:A:481:SER:HA	2.11	0.49
1:B:361:TYR:CG	1:B:417:ASN:HB3	2.46	0.49
1:B:374:LYS:N	1:B:375:PRO:CB	2.67	0.49
1:B:141:ARG:NH2	1:B:143:ILE:HA	2.28	0.49
1:B:390:VAL:CB	1:B:395:ALA:HB3	2.29	0.49
1:B:439:VAL:O	1:B:441:PRO:HD3	2.12	0.49
1:A:425:ARG:HH21	1:A:447:GLU:N	2.09	0.49
1:B:483:GLN:HG2	1:B:484:GLY:N	2.25	0.49
1:A:273:ALA:N	1:A:274:PRO:HD2	2.26	0.49
1:B:57:TYR:O	1:B:61:LYS:HB2	2.12	0.49
1:B:90:ILE:CB	1:B:179:VAL:HB	2.40	0.49
1:A:279:VAL:O	1:A:283:LEU:HD22	2.12	0.49
1:B:81:ILE:HD13	1:B:81:ILE:N	2.28	0.49
1:B:93:GLY:HA3	1:B:127:TYR:HB3	1.95	0.49
1:B:425:ARG:HH21	1:B:447:GLU:N	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:HH21	1:A:143:ILE:HA	1.76	0.49
1:B:112:THR:CB	1:B:125:ILE:HD11	2.42	0.49
1:B:188:LEU:HD23	1:B:189:PRO:HD2	1.94	0.49
1:B:266:ASP:O	1:B:269:ILE:N	2.41	0.49
1:B:499:THR:CG2	1:B:500:VAL:N	2.75	0.49
1:A:28:GLY:N	1:A:336:ALA:HA	2.27	0.49
1:A:31:THR:O	1:A:37:LEU:HD22	2.13	0.49
1:A:386:ALA:O	1:A:389:ALA:HB3	2.12	0.49
1:B:85:THR:HG22	1:B:87:GLY:N	2.27	0.49
1:B:103:ILE:HG12	1:B:172:LYS:HB2	1.94	0.49
1:B:288:ASN:HB3	1:B:368:MET:HE1	1.94	0.49
1:A:122:ASP:O	1:A:124:LYS:N	2.43	0.49
1:B:146:ASP:O	1:B:149:VAL:HG13	2.12	0.49
1:B:264:ARG:HE	1:B:280:GLN:NE2	2.11	0.49
1:B:499:THR:CG2	1:B:500:VAL:H	2.25	0.49
1:A:212:ALA:O	1:A:240:LYS:HB2	2.12	0.49
1:A:460:ILE:O	1:A:464:ILE:HG13	2.13	0.49
1:B:105:PRO:HD2	1:B:107:HIS:HD2	1.78	0.49
1:A:89:GLU:O	1:A:90:ILE:HD13	2.12	0.48
1:A:141:ARG:HH12	1:A:181:LEU:CA	2.26	0.48
1:A:266:ASP:O	1:A:269:ILE:N	2.45	0.48
1:A:305:THR:HG23	1:A:338:GLY:HA2	1.95	0.48
1:B:247:VAL:HG13	1:B:248:ASN:N	2.28	0.48
1:A:231:GLN:H	1:A:231:GLN:NE2	2.11	0.48
1:B:258:ASP:O	1:B:293:PRO:HD2	2.13	0.48
1:A:139:ALA:HA	1:A:154:VAL:CG1	2.43	0.48
1:B:400:VAL:O	1:B:422:LEU:HA	2.14	0.48
1:B:52:PHE:HZ	1:B:201:PHE:CE2	2.32	0.48
1:B:375:PRO:CB	1:B:376:THR:HG1	2.23	0.48
1:A:301:LEU:O	1:A:304:MET:HB2	2.13	0.48
1:A:475:LYS:HA	1:A:500:VAL:CB	2.42	0.48
1:B:12:VAL:HG23	1:B:13:VAL:HG23	1.94	0.48
1:B:113:THR:CG2	1:B:128:VAL:HG23	2.43	0.48
1:B:114:ASP:OD2	1:B:116:LYS:HG3	2.12	0.48
1:B:422:LEU:HD23	1:B:441:PRO:HB3	1.94	0.48
1:B:186:VAL:HG23	1:B:216:ARG:NE	2.05	0.48
1:B:305:THR:HG23	1:B:338:GLY:HA2	1.96	0.48
1:B:386:ALA:O	1:B:389:ALA:HB3	2.14	0.48
1:B:122:ASP:C	1:B:122:ASP:OD1	2.56	0.48
1:B:477:ASP:O	1:B:478:THR:CB	2.61	0.48
1:A:94:THR:HG22	1:A:175:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ILE:H	1:B:342:ILE:CD1	2.10	0.48
1:B:401:LEU:HD23	1:B:459:ARG:HD2	1.94	0.48
1:A:175:SER:O	1:A:177:LYS:HG2	2.14	0.48
1:B:100:ASP:OD1	1:B:122:ASP:OD2	2.31	0.48
1:B:141:ARG:HH12	1:B:181:LEU:CA	2.27	0.48
1:B:478:THR:HG23	1:B:478:THR:O	2.13	0.48
1:A:86:LYS:NZ	1:A:89:GLU:HG3	2.27	0.47
1:A:146:ASP:O	1:A:149:VAL:HG22	2.14	0.47
1:A:279:VAL:O	1:A:279:VAL:HG12	2.13	0.47
1:B:84:ASP:OD1	1:B:240:LYS:NZ	2.42	0.47
1:B:296:CYS:SG	1:B:300:MET:HE3	2.53	0.47
1:B:399:ILE:O	1:B:481:SER:HA	2.15	0.47
1:B:110:ILE:HG13	1:B:162:THR:HG22	1.95	0.47
1:A:95:THR:H	1:A:175:SER:HB3	1.79	0.47
1:A:402:SER:HB3	1:A:422:LEU:HD11	1.96	0.47
1:B:188:LEU:CD2	1:B:189:PRO:HD2	2.44	0.47
1:A:361:TYR:HB3	1:A:391:PHE:CZ	2.49	0.47
1:A:425:ARG:NH2	1:A:447:GLU:N	2.62	0.47
1:A:433:SER:C	1:A:435:LEU:H	2.23	0.47
1:B:215:ILE:HG13	1:B:239:VAL:HG13	1.95	0.47
1:B:314:GLU:O	1:B:318:VAL:HG23	2.14	0.47
1:A:60:HIS:C	1:A:62:SER:N	2.72	0.47
1:A:456:VAL:HG12	1:A:459:ARG:NH2	2.29	0.47
1:B:30:LYS:HD3	1:B:30:LYS:C	2.38	0.47
1:B:247:VAL:O	1:B:249:ASN:N	2.45	0.47
1:A:153:GLN:CB	1:A:168:LEU:HD21	2.43	0.47
1:A:404:SER:HB2	1:A:406:THR:OG1	2.15	0.47
1:B:141:ARG:HE	1:B:142:ILE:H	1.63	0.47
1:B:156:GLU:OE1	1:B:164:LYS:NZ	2.48	0.47
1:B:231:GLN:H	1:B:231:GLN:NE2	2.13	0.47
1:B:415:ARG:NH1	1:B:437:ARG:HB3	2.29	0.47
1:B:432:PHE:C	1:B:432:PHE:HD1	2.22	0.47
1:B:130:TYR:CE1	1:B:132:ASN:HB2	2.49	0.47
1:A:48:VAL:HG23	1:A:79:LEU:CD1	2.42	0.47
1:B:19:ARG:NH1	1:B:21:THR:O	2.41	0.47
1:B:33:ASN:O	1:B:37:LEU:HB2	2.15	0.47
1:A:30:LYS:HD3	1:A:30:LYS:C	2.40	0.47
1:A:91:ARG:HG2	1:A:91:ARG:NH1	2.29	0.47
1:B:175:SER:O	1:B:177:LYS:HG2	2.15	0.47
1:B:247:VAL:CG1	1:B:248:ASN:N	2.78	0.47
1:B:467:ALA:HB1	1:B:473:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:MET:O	1:B:348:MET:HE1	2.13	0.46
1:B:425:ARG:NH2	1:B:447:GLU:N	2.63	0.46
1:A:400:VAL:O	1:A:422:LEU:HA	2.15	0.46
1:A:330:MET:O	1:A:348:MET:HE1	2.15	0.46
1:B:453:THR:O	1:B:453:THR:HG22	2.15	0.46
1:A:106:ASN:ND2	1:A:106:ASN:O	2.48	0.46
1:A:361:TYR:HB3	1:A:391:PHE:HZ	1.80	0.46
1:B:92:THR:O	1:B:176:HIS:HD2	1.99	0.46
1:B:132:ASN:O	1:B:133:ILE:C	2.58	0.46
1:A:110:ILE:HD13	1:A:110:ILE:O	2.15	0.46
1:A:415:ARG:NH1	1:A:437:ARG:HB3	2.31	0.46
1:A:281:LYS:HZ3	1:A:324:ASP:CG	2.24	0.46
1:B:41:ARG:HA	1:B:45:LEU:HB3	1.98	0.46
1:A:88:PRO:HG3	1:A:189:PRO:O	2.16	0.46
1:A:90:ILE:HB	1:A:179:VAL:HB	1.98	0.46
1:A:115:ASP:HA	1:A:118:ALA:HB2	1.97	0.46
1:A:122:ASP:OD1	1:A:122:ASP:C	2.58	0.46
1:A:362:LEU:H	1:A:362:LEU:HD22	1.81	0.46
1:A:382:VAL:HG21	1:A:493:ASN:ND2	2.31	0.46
1:A:401:LEU:HD21	1:A:459:ARG:HB2	1.97	0.46
1:A:456:VAL:HG12	1:A:459:ARG:CZ	2.46	0.46
1:B:88:PRO:HB2	1:B:188:LEU:HD13	1.96	0.46
1:B:111:PHE:CE2	1:B:126:MET:SD	3.09	0.46
1:B:329:VAL:HB	1:B:348:MET:SD	2.55	0.46
1:A:216:ARG:HH11	1:A:216:ARG:HG3	1.80	0.46
1:A:90:ILE:HD12	1:A:130:TYR:CB	2.39	0.46
1:A:132:ASN:O	1:A:133:ILE:C	2.59	0.46
1:A:499:THR:CG2	1:A:500:VAL:N	2.77	0.46
1:B:112:THR:HG22	1:B:113:THR:N	2.31	0.46
1:A:192:SER:H	1:A:195:ASP:HB2	1.81	0.45
1:A:359:ILE:HG22	1:A:360:ALA:N	2.32	0.45
1:B:87:GLY:O	1:B:89:GLU:HG2	2.15	0.45
1:B:110:ILE:CD1	1:B:112:THR:OG1	2.64	0.45
1:B:446:LYS:O	1:B:447:GLU:CB	2.63	0.45
1:A:180:ASN:C	1:A:182:PRO:HD3	2.42	0.45
1:B:133:ILE:O	1:B:137:ILE:HB	2.17	0.45
1:B:156:GLU:HB2	1:B:164:LYS:CE	2.46	0.45
1:B:185:ASP:OD1	1:B:245:GLN:NE2	2.49	0.45
1:B:327:ASP:HA	1:B:437:ARG:HB2	1.98	0.45
1:A:110:ILE:HD11	1:A:112:THR:OG1	2.16	0.45
1:A:141:ARG:NH2	1:A:143:ILE:HA	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:VAL:O	1:A:277:LEU:C	2.59	0.45
1:B:243:ASN:HA	1:B:270:GLU:CG	2.43	0.45
1:B:484:GLY:HA2	1:B:493:ASN:HA	1.99	0.45
1:A:85:THR:HG22	1:A:87:GLY:N	2.31	0.45
1:A:216:ARG:HD3	1:A:245:GLN:NE2	2.31	0.45
1:A:221:VAL:O	1:A:224:ILE:HG23	2.16	0.45
1:A:247:VAL:CG1	1:A:248:ASN:N	2.79	0.45
1:A:439:VAL:O	1:A:441:PRO:HD3	2.16	0.45
1:A:213:SER:CA	1:A:240:LYS:HD3	2.44	0.45
1:A:362:LEU:N	1:A:362:LEU:HD13	2.32	0.45
1:B:102:PRO:CG	1:B:122:ASP:OD2	2.65	0.45
1:A:303:SER:C	1:A:305:THR:N	2.73	0.45
1:B:90:ILE:CD1	1:B:130:TYR:HB2	2.41	0.45
1:A:141:ARG:HE	1:A:142:ILE:H	1.64	0.45
1:A:243:ASN:HA	1:A:270:GLU:CG	2.45	0.45
1:B:88:PRO:HB2	1:B:188:LEU:HB3	1.99	0.45
1:B:103:ILE:HA	1:B:172:LYS:HA	1.98	0.45
1:A:113:THR:CG2	1:A:128:VAL:HG23	2.46	0.45
1:A:260:VAL:HG13	1:A:294:VAL:HG23	1.98	0.44
1:B:105:PRO:O	1:B:106:ASN:HB2	2.17	0.44
1:B:158:VAL:CB	1:B:162:THR:HB	2.43	0.44
1:B:153:GLN:CG	1:B:168:LEU:HD21	2.47	0.44
1:A:81:ILE:N	1:A:81:ILE:HD13	2.32	0.44
1:A:99:VAL:HG12	1:A:101:TYR:CZ	2.53	0.44
1:A:159:ASP:HB3	1:A:160:ASP:H	1.60	0.44
1:A:204:LYS:HE3	1:A:204:LYS:HB2	1.78	0.44
1:A:444:PHE:HB2	1:A:462:PHE:CD2	2.53	0.44
1:B:28:GLY:HA3	1:B:336:ALA:O	2.17	0.44
1:B:45:LEU:HD11	1:B:47:ILE:O	2.18	0.44
1:B:330:MET:HG3	1:B:331:LEU:H	1.83	0.44
1:A:56:SER:H	1:A:59:TYR:CB	2.27	0.44
1:A:87:GLY:O	1:A:89:GLU:HG2	2.17	0.44
1:A:99:VAL:HG12	1:A:99:VAL:O	2.17	0.44
1:A:141:ARG:NH2	1:A:181:LEU:HA	2.32	0.44
1:A:397:ALA:HB2	1:A:473:LEU:HD11	1.99	0.44
1:B:48:VAL:HG23	1:B:79:LEU:CD1	2.47	0.44
1:B:158:VAL:O	1:B:162:THR:HB	2.18	0.44
1:A:103:ILE:HG12	1:A:172:LYS:HB2	2.00	0.44
1:A:124:LYS:N	1:A:124:LYS:HD2	2.33	0.44
1:A:216:ARG:HG3	1:A:216:ARG:NH1	2.32	0.44
1:A:477:ASP:O	1:A:478:THR:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ARG:HD3	1:B:79:LEU:HD22	1.99	0.44
1:B:415:ARG:HH11	1:B:437:ARG:HB3	1.82	0.44
1:A:89:GLU:HG2	1:A:89:GLU:H	1.62	0.44
1:A:432:PHE:C	1:A:432:PHE:HD1	2.26	0.44
1:B:94:THR:HG22	1:B:175:SER:HB2	2.00	0.44
1:B:145:VAL:O	1:B:149:VAL:HG22	2.17	0.44
1:B:456:VAL:HG12	1:B:459:ARG:CZ	2.48	0.44
1:B:114:ASP:C	1:B:116:LYS:H	2.26	0.44
1:B:216:ARG:HD3	1:B:245:GLN:NE2	2.33	0.44
1:B:407:THR:N	1:B:408:PRO:HD2	2.32	0.44
1:A:40:LEU:HD12	1:A:40:LEU:HA	1.81	0.44
1:B:91:ARG:HG2	1:B:91:ARG:HH11	1.83	0.44
1:B:301:LEU:O	1:B:304:MET:HB2	2.18	0.44
1:B:398:ILE:CD1	1:B:411:VAL:HG11	2.47	0.44
1:B:457:GLU:CD	1:B:457:GLU:N	2.75	0.44
1:A:133:ILE:O	1:A:137:ILE:HB	2.17	0.43
1:A:146:ASP:CG	1:A:177:LYS:HD2	2.43	0.43
1:A:263:ALA:O	1:A:267:LEU:HB2	2.18	0.43
1:A:457:GLU:CD	1:A:457:GLU:N	2.76	0.43
1:B:444:PHE:HB2	1:B:462:PHE:CD2	2.53	0.43
1:A:158:VAL:O	1:A:162:THR:HB	2.18	0.43
1:A:242:GLU:HA	1:A:267:LEU:HB2	1.99	0.43
1:B:191:LEU:HD22	1:B:195:ASP:HB3	1.98	0.43
1:B:62:SER:OG	1:B:63:VAL:N	2.51	0.43
1:B:433:SER:C	1:B:435:LEU:H	2.26	0.43
1:A:112:THR:HG22	1:A:113:THR:N	2.33	0.43
1:A:208:HIS:HA	1:A:428:ARG:HH12	1.84	0.43
1:A:231:GLN:N	1:A:231:GLN:CD	2.77	0.43
1:A:467:ALA:HB1	1:A:473:LEU:HD13	2.00	0.43
1:B:90:ILE:O	1:B:178:GLY:HA2	2.18	0.43
1:B:115:ASP:HA	1:B:118:ALA:HB2	2.00	0.43
1:A:141:ARG:HH22	1:A:181:LEU:HD23	1.84	0.43
1:A:331:LEU:HD23	1:A:331:LEU:HA	1.90	0.43
1:A:398:ILE:HG22	1:A:419:PRO:O	2.18	0.43
1:A:423:VAL:HG21	1:A:459:ARG:O	2.19	0.43
1:A:425:ARG:HG2	1:A:444:PHE:O	2.19	0.43
1:B:37:LEU:HD13	1:B:37:LEU:HA	1.77	0.43
1:B:156:GLU:HB2	1:B:164:LYS:NZ	2.34	0.43
1:B:242:GLU:HA	1:B:267:LEU:HB2	2.01	0.43
1:B:304:MET:HG3	1:B:310:PRO:CB	2.48	0.43
1:A:102:PRO:O	1:A:173:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:VAL:O	1:B:283:LEU:HD22	2.19	0.43
1:A:180:ASN:ND2	1:A:270:GLU:OE1	2.52	0.43
1:A:493:ASN:OD1	1:A:493:ASN:N	2.51	0.43
1:B:65:ASP:O	1:B:69:LYS:HB2	2.18	0.43
1:B:303:SER:C	1:B:305:THR:N	2.76	0.43
1:B:401:LEU:HD21	1:B:459:ARG:HB2	2.00	0.43
1:A:472:ILE:C	1:A:473:LEU:HD12	2.44	0.43
1:A:484:GLY:HA2	1:A:493:ASN:HA	2.01	0.43
1:B:222:LEU:O	1:B:225:ARG:HB3	2.18	0.43
1:B:243:ASN:CA	1:B:270:GLU:HG2	2.44	0.43
1:A:90:ILE:HG23	1:A:130:TYR:CB	2.48	0.43
1:A:327:ASP:HA	1:A:437:ARG:HB2	2.00	0.43
1:B:56:SER:C	1:B:58:GLU:N	2.77	0.43
1:B:60:HIS:C	1:B:62:SER:N	2.74	0.43
1:B:88:PRO:HG3	1:B:189:PRO:O	2.19	0.43
1:B:113:THR:HG22	1:B:128:VAL:HG23	2.00	0.43
1:B:133:ILE:O	1:B:137:ILE:N	2.47	0.43
1:B:146:ASP:O	1:B:149:VAL:HG22	2.19	0.43
1:B:391:PHE:HD1	1:B:391:PHE:HA	1.73	0.43
1:B:496:GLN:HE21	1:B:498:SER:CB	2.24	0.43
1:A:155:LEU:CB	1:A:164:LYS:HG2	2.39	0.43
1:B:117:TYR:N	1:B:117:TYR:CD1	2.86	0.43
1:B:181:LEU:HB3	1:B:184:THR:HB	2.00	0.43
1:B:387:VAL:HG21	1:B:414:TYR:HB2	2.01	0.42
1:A:41:ARG:HA	1:A:45:LEU:HB3	2.01	0.42
1:A:45:LEU:HD11	1:A:47:ILE:O	2.19	0.42
1:A:153:GLN:CG	1:A:168:LEU:HD21	2.49	0.42
1:B:8:THR:HG22	1:B:8:THR:O	2.19	0.42
1:B:115:ASP:OD1	1:B:131:LYS:HE3	2.19	0.42
1:B:496:GLN:HG3	1:B:498:SER:H	1.84	0.42
1:A:65:ASP:O	1:A:69:LYS:HB2	2.19	0.42
1:A:88:PRO:HD3	1:A:190:ALA:O	2.19	0.42
1:A:133:ILE:HD11	1:A:137:ILE:HD12	2.01	0.42
1:A:417:ASN:HD22	1:A:417:ASN:N	2.04	0.42
1:B:56:SER:H	1:B:59:TYR:CB	2.28	0.42
1:B:109:MET:HG3	1:B:110:ILE:N	2.34	0.42
1:B:405:GLY:C	1:B:408:PRO:HD2	2.45	0.42
1:A:314:GLU:O	1:A:318:VAL:HG23	2.18	0.42
1:B:189:PRO:C	1:B:191:LEU:N	2.74	0.42
1:B:194:LYS:O	1:B:197:GLU:HB2	2.20	0.42
1:A:276:VAL:O	1:A:280:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HA	1:B:10:LEU:HD22	2.01	0.42
1:B:28:GLY:H	1:B:31:THR:HG1	1.68	0.42
1:B:56:SER:OG	1:B:59:TYR:HD1	2.02	0.42
1:A:60:HIS:O	1:A:61:LYS:C	2.63	0.42
1:B:361:TYR:HB3	1:B:391:PHE:CZ	2.54	0.42
1:A:107:HIS:ND1	1:A:107:HIS:C	2.78	0.42
1:A:110:ILE:HG13	1:A:162:THR:HG22	2.01	0.42
1:A:143:ILE:HB	1:A:152:PHE:HB2	2.02	0.42
1:A:244:GLN:HA	1:A:247:VAL:HG12	2.01	0.42
1:A:499:THR:CG2	1:A:500:VAL:H	2.27	0.42
1:B:102:PRO:HG2	1:B:122:ASP:CG	2.44	0.42
1:B:407:THR:N	1:B:408:PRO:CD	2.82	0.42
1:A:23:ILE:HG21	1:A:345:VAL:HG13	2.02	0.42
1:A:37:LEU:HD13	1:A:37:LEU:HA	1.79	0.42
1:A:41:ARG:HG2	1:A:45:LEU:HD23	2.02	0.42
1:A:342:ILE:H	1:A:342:ILE:CD1	2.12	0.42
1:A:361:TYR:CD1	1:A:417:ASN:HB3	2.55	0.42
1:B:60:HIS:O	1:B:61:LYS:C	2.63	0.42
1:B:89:GLU:HG2	1:B:89:GLU:H	1.62	0.42
1:B:276:VAL:O	1:B:277:LEU:C	2.62	0.42
1:B:410:LEU:HD12	1:B:410:LEU:HA	1.90	0.42
1:B:432:PHE:O	1:B:435:LEU:HB2	2.20	0.42
1:A:213:SER:OG	1:A:240:LYS:NZ	2.51	0.42
1:B:289:LEU:HD12	1:B:289:LEU:HA	1.90	0.42
1:B:497:VAL:O	1:B:497:VAL:HG22	2.20	0.42
1:A:106:ASN:HD21	1:A:166:LYS:HZ1	1.60	0.41
1:A:243:ASN:CA	1:A:270:GLU:HG2	2.46	0.41
1:B:146:ASP:CG	1:B:177:LYS:HD2	2.45	0.41
1:A:110:ILE:HD11	1:A:162:THR:CG2	2.50	0.41
1:A:113:THR:HB	1:A:131:LYS:NZ	2.35	0.41
1:A:180:ASN:OD1	1:A:269:ILE:HG21	2.20	0.41
1:A:481:SER:CB	1:A:496:GLN:HB3	2.42	0.41
1:A:304:MET:HG3	1:A:310:PRO:CB	2.48	0.41
1:A:407:THR:N	1:A:408:PRO:HD2	2.35	0.41
1:A:12:VAL:O	1:A:13:VAL:CB	2.68	0.41
1:A:33:ASN:O	1:A:37:LEU:HB2	2.19	0.41
1:A:194:LYS:O	1:A:197:GLU:HB2	2.20	0.41
1:A:199:LEU:O	1:A:203:VAL:HG23	2.21	0.41
1:A:254:LEU:HD13	1:A:290:ALA:HB2	2.02	0.41
1:A:387:VAL:HG21	1:A:414:TYR:HB2	2.02	0.41
1:B:67:ALA:HA	1:B:70:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:GLN:HB2	1:B:168:LEU:CD2	2.41	0.41
1:B:263:ALA:O	1:B:267:LEU:HB2	2.21	0.41
1:A:24:ILE:HG12	1:A:47:ILE:HB	2.02	0.41
1:A:130:TYR:CE1	1:A:132:ASN:HB2	2.56	0.41
1:A:281:LYS:NZ	1:A:324:ASP:CG	2.79	0.41
1:A:472:ILE:HG22	1:A:473:LEU:HD12	2.02	0.41
1:B:88:PRO:CB	1:B:188:LEU:HB3	2.50	0.41
1:A:66:ASN:HD22	1:A:66:ASN:HA	1.64	0.41
1:B:144:TYR:HA	1:B:150:LEU:O	2.21	0.41
1:B:416:PRO:CG	1:B:420:ILE:HD11	2.51	0.41
1:A:46:ASN:O	1:A:79:LEU:HD12	2.21	0.41
1:A:100:ASP:OD1	1:A:122:ASP:OD2	2.38	0.41
1:B:239:VAL:HG23	1:B:257:THR:OG1	2.21	0.41
1:A:86:LYS:HD3	1:A:86:LYS:O	2.21	0.41
1:B:330:MET:CG	1:B:331:LEU:H	2.34	0.41
1:A:195:ASP:O	1:A:199:LEU:HG	2.20	0.41
1:A:215:ILE:HG13	1:A:239:VAL:HG13	2.03	0.41
1:B:41:ARG:HG2	1:B:45:LEU:HD23	2.02	0.41
1:B:52:PHE:HZ	1:B:201:PHE:HE2	1.67	0.41
1:B:144:TYR:HB3	1:B:148:GLY:HA2	2.02	0.41
1:B:208:HIS:HA	1:B:428:ARG:HH12	1.86	0.41
1:B:231:GLN:CD	1:B:231:GLN:N	2.79	0.41
1:B:281:LYS:H	1:B:281:LYS:HG3	1.55	0.41
1:B:330:MET:CG	1:B:331:LEU:N	2.84	0.41
1:B:362:LEU:HD13	1:B:362:LEU:H	1.85	0.41
1:B:362:LEU:H	1:B:362:LEU:HD22	1.86	0.41
1:A:146:ASP:O	1:A:147:ASP:C	2.64	0.41
1:A:234:ASP:OD1	1:A:234:ASP:N	2.53	0.41
1:A:304:MET:HE1	1:A:343:ASN:CB	2.51	0.41
1:B:47:ILE:HD13	1:B:209:MET:HE1	2.02	0.41
1:B:69:LYS:HA	1:B:72:GLU:OE2	2.20	0.41
1:B:342:ILE:HG12	1:B:343:ASN:N	2.36	0.41
1:A:125:ILE:CG1	1:A:126:MET:N	2.82	0.40
1:B:243:ASN:CB	1:B:270:GLU:HG2	2.51	0.40
1:B:262:VAL:O	1:B:264:ARG:N	2.53	0.40
1:B:304:MET:HE1	1:B:343:ASN:CB	2.51	0.40
1:A:26:THR:O	1:A:335:THR:HB	2.20	0.40
1:A:289:LEU:HD11	1:A:371:CYS:CB	2.52	0.40
1:A:415:ARG:HH11	1:A:437:ARG:HB3	1.86	0.40
1:B:114:ASP:CG	1:B:116:LYS:HG3	2.46	0.40
1:B:493:ASN:N	1:B:493:ASN:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLY:HA3	1:A:336:ALA:O	2.21	0.40
1:A:496:GLN:HG3	1:A:498:SER:H	1.86	0.40
1:B:1:MET:HG2	1:B:2:SER:N	2.36	0.40
1:B:263:ALA:O	2:B:1006:PGA:O1	2.39	0.40
1:B:315:VAL:C	1:B:317:ASP:H	2.30	0.40
1:B:361:TYR:CD1	1:B:417:ASN:HB3	2.56	0.40
1:A:222:LEU:O	1:A:225:ARG:HB3	2.22	0.40
1:A:372:THR:O	1:A:372:THR:CG2	2.60	0.40
1:B:151:SER:CB	1:B:168:LEU:HB2	2.48	0.40
1:A:191:LEU:HD22	1:A:195:ASP:HB3	2.04	0.40
1:A:201:PHE:O	1:A:205:ASN:ND2	2.52	0.40
1:A:433:SER:C	1:A:435:LEU:N	2.79	0.40
1:B:102:PRO:HG2	1:B:122:ASP:OD2	2.22	0.40
1:B:220:ASP:O	1:B:224:ILE:CG2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ARG:NH2	1:B:268:GLY:O[1_545]	2.06	0.14

5.3 Torsion angles

5.3.1 Protein backbone

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	481/500 (96%)	382 (79%)	65 (14%)	34 (7%)	1	4
1	B	481/500 (96%)	377 (78%)	71 (15%)	33 (7%)	1	5
All	All	962/1000 (96%)	759 (79%)	136 (14%)	67 (7%)	1	4

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	12	VAL
1	A	96	THR
1	A	99	VAL
1	A	106	ASN
1	A	375	PRO
1	A	398	ILE
1	A	446	LYS
1	A	478	THR
1	A	497	VAL
1	B	10	LEU
1	B	96	THR
1	B	99	VAL
1	B	106	ASN
1	B	374	LYS
1	B	375	PRO
1	B	398	ILE
1	B	446	LYS
1	B	478	THR
1	B	497	VAL
1	A	2	SER
1	A	85	THR
1	A	87	GLY
1	A	123	ASP
1	A	146	ASP
1	A	176	HIS
1	A	265	GLY
1	A	374	LYS
1	B	2	SER
1	B	12	VAL
1	B	85	THR
1	B	123	ASP
1	B	146	ASP
1	B	176	HIS
1	B	265	GLY
1	A	11	ASN
1	A	248	ASN
1	A	249	ASN
1	A	494	THR
1	B	11	ASN
1	B	87	GLY
1	B	248	ASN
1	B	249	ASN

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Mol	Chain	Res	Type
1	B	494	THR
1	B	495	LEU
1	A	13	VAL
1	A	105	PRO
1	A	122	ASP
1	A	170	ALA
1	A	298	THR
1	A	304	MET
1	B	13	VAL
1	B	105	PRO
1	B	118	ALA
1	B	255	LYS
1	B	298	THR
1	A	255	LYS
1	A	475	LYS
1	A	495	LEU
1	B	170	ALA
1	B	304	MET
1	B	475	LYS
1	A	110	ILE
1	A	210	VAL
1	A	372	THR
1	B	372	THR
1	B	210	VAL

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	412/423 (97%)	328 (80%)	84 (20%)	1	7
1	B	412/423 (97%)	329 (80%)	83 (20%)	1	7
All	All	824/846 (97%)	657 (80%)	167 (20%)	1	7

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	SER
1	A	7	LEU
1	A	10	LEU
1	A	11	ASN
1	A	22	SER
1	A	31	THR
1	A	33	ASN
1	A	37	LEU
1	A	40	LEU
1	A	58	GLU
1	A	61	LYS
1	A	65	ASP
1	A	66	ASN
1	A	68	ARG
1	A	69	LYS
1	A	70	SER
1	A	71	GLU
1	A	77	ARG
1	A	79	LEU
1	A	81	ILE
1	A	83	LEU
1	A	89	GLU
1	A	94	THR
1	A	95	THR
1	A	96	THR
1	A	98	ASP
1	A	99	VAL
1	A	110	ILE
1	A	128	VAL
1	A	133	ILE
1	A	138	SER
1	A	141	ARG
1	A	150	LEU
1	A	153	GLN
1	A	156	GLU
1	A	160	ASP
1	A	162	THR
1	A	164	LYS
1	A	166	LYS
1	A	169	ASN
1	A	173	ILE
1	A	186	VAL

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Mol	Chain	Res	Type
1	A	223	THR
1	A	224	ILE
1	A	225	ARG
1	A	230	GLU
1	A	242	GLU
1	A	245	GLN
1	A	254	LEU
1	A	255	LYS
1	A	260	VAL
1	A	262	VAL
1	A	281	LYS
1	A	283	LEU
1	A	304	MET
1	A	309	ARG
1	A	311	THR
1	A	312	ARG
1	A	316	SER
1	A	323	LEU
1	A	324	ASP
1	A	329	VAL
1	A	342	ILE
1	A	362	LEU
1	A	369	ARG
1	A	376	THR
1	A	390	VAL
1	A	391	PHE
1	A	393	GLN
1	A	400	VAL
1	A	404	SER
1	A	407	THR
1	A	410	LEU
1	A	415	ARG
1	A	417	ASN
1	A	422	LEU
1	A	433	SER
1	A	445	GLU
1	A	455	ASP
1	A	474	LYS
1	A	483	GLN
1	A	495	LEU
1	A	498	SER
1	B	1	MET

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Mol	Chain	Res	Type
1	B	2	SER
1	B	7	LEU
1	B	10	LEU
1	B	11	ASN
1	B	22	SER
1	B	31	THR
1	B	37	LEU
1	B	40	LEU
1	B	50	MET
1	B	58	GLU
1	B	61	LYS
1	B	65	ASP
1	B	66	ASN
1	B	68	ARG
1	B	69	LYS
1	B	70	SER
1	B	71	GLU
1	B	77	ARG
1	B	79	LEU
1	B	81	ILE
1	B	83	LEU
1	B	89	GLU
1	B	94	THR
1	B	95	THR
1	B	96	THR
1	B	98	ASP
1	B	99	VAL
1	B	110	ILE
1	B	122	ASP
1	B	126	MET
1	B	128	VAL
1	B	138	SER
1	B	141	ARG
1	B	150	LEU
1	B	153	GLN
1	B	156	GLU
1	B	160	ASP
1	B	162	THR
1	B	164	LYS
1	B	169	ASN
1	B	173	ILE
1	B	186	VAL

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Mol	Chain	Res	Type
1	B	223	THR
1	B	224	ILE
1	B	225	ARG
1	B	230	GLU
1	B	242	GLU
1	B	254	LEU
1	B	255	LYS
1	B	260	VAL
1	B	262	VAL
1	B	281	LYS
1	B	283	LEU
1	B	304	MET
1	B	309	ARG
1	B	311	THR
1	B	316	SER
1	B	323	LEU
1	B	324	ASP
1	B	329	VAL
1	B	330	MET
1	B	342	ILE
1	B	362	LEU
1	B	369	ARG
1	B	376	THR
1	B	390	VAL
1	B	391	PHE
1	B	393	GLN
1	B	400	VAL
1	B	404	SER
1	B	407	THR
1	B	410	LEU
1	B	415	ARG
1	B	417	ASN
1	B	422	LEU
1	B	433	SER
1	B	445	GLU
1	B	455	ASP
1	B	474	LYS
1	B	483	GLN
1	B	495	LEU
1	B	498	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	60	HIS
1	A	66	ASN
1	A	106	ASN
1	A	169	ASN
1	A	176	HIS
1	A	243	ASN
1	A	244	GLN
1	A	245	GLN
1	A	280	GLN
1	A	320	ASN
1	A	343	ASN
1	A	357	GLN
1	A	370	ASN
1	A	417	ASN
1	A	434	HIS
1	A	461	ASN
1	A	483	GLN
1	A	493	ASN
1	A	496	GLN
1	B	33	ASN
1	B	60	HIS
1	B	66	ASN
1	B	106	ASN
1	B	132	ASN
1	B	169	ASN
1	B	176	HIS
1	B	231	GLN
1	B	243	ASN
1	B	244	GLN
1	B	280	GLN
1	B	320	ASN
1	B	343	ASN
1	B	357	GLN
1	B	370	ASN
1	B	417	ASN
1	B	434	HIS
1	B	461	ASN
1	B	483	GLN
1	B	493	ASN
1	B	496	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	PGA	B	1006	4,3	8,8,8	2.31	3 (37%)	10,11,11	2.98	4 (40%)
2	PGA	A	1005	4,3	8,8,8	3.04	3 (37%)	10,11,11	2.95	4 (40%)

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	PGA	B	1006	4,3	-	4/6/6/6	-
2	PGA	A	1005	4,3	-	2/6/6/6	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	PGA	O1P-C2	-6.62	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	PGA	P-O3P	4.25	1.70	1.54
2	B	1006	PGA	P-O3P	4.12	1.70	1.54
2	B	1006	PGA	O1P-C2	-3.62	1.39	1.43
2	B	1006	PGA	P-O2P	2.34	1.57	1.50
2	A	1005	PGA	P-O2P	2.18	1.57	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1006	PGA	O1P-P-O2P	7.23	125.98	106.44
2	A	1005	PGA	O1P-P-O2P	6.90	125.08	106.44
2	B	1006	PGA	O1P-C2-C1	3.78	116.24	110.54
2	A	1005	PGA	O1P-C2-C1	3.66	116.06	110.54
2	A	1005	PGA	O3P-P-O1P	2.96	114.39	106.67
2	B	1006	PGA	O3P-P-O1P	2.42	112.97	106.67
2	A	1005	PGA	O2-C1-O1	-2.40	117.17	123.33
2	B	1006	PGA	O2-C1-O1	-2.23	117.60	123.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1006	PGA	C2-O1P-P-O3P
2	A	1005	PGA	O2-C1-C2-O1P
2	A	1005	PGA	O1-C1-C2-O1P
2	B	1006	PGA	O2-C1-C2-O1P
2	B	1006	PGA	O1-C1-C2-O1P
2	B	1006	PGA	C2-O1P-P-O4P

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1006	PGA	2	0
2	A	1005	PGA	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	374:LYS	C	375:PRO	N	0.84

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.