



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:17 AM GMT

PDB ID : 2GHO
Title : Recombinant *Thermus aquaticus* RNA polymerase for Structural Studies
Authors : Lamour, V.; Darst, S.A.
Deposited on : 2006-03-27
Resolution : 5.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

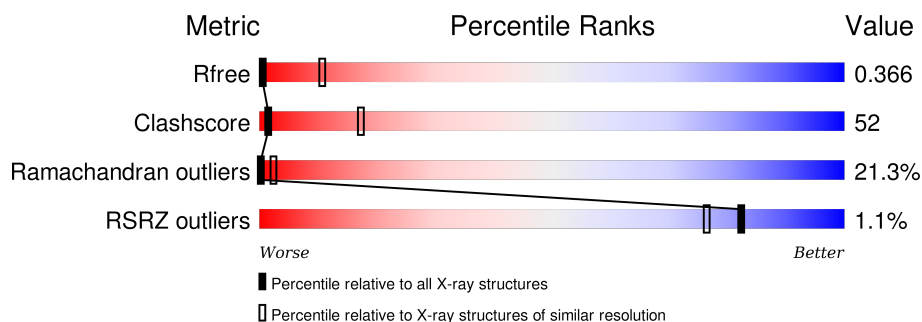
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 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))
R_{free}	91344	1119 (6.22-3.60)
Clashscore	102246	1019 (6.22-3.66)
Ramachandran outliers	100387	1158 (6.22-3.60)
RSRZ outliers	91569	1122 (6.22-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	314	<div> <div></div> <div> <div></div> <div>48%</div> <div>19%</div> <div>6%</div> <div>27%</div> </div> </div>
1	B	314	<div> <div></div> <div> <div></div> <div>51%</div> <div>17%</div> <div>•</div> <div>28%</div> </div> </div>
2	C	1119	<div> <div></div> <div> <div></div> <div>63%</div> <div>29%</div> <div>7%</div> </div> </div>
3	D	1233	<div> <div></div> <div> <div></div> <div>48%</div> <div>33%</div> <div>15%</div> <div>•</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11060 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 DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	0	0	0
			920	460	230	230			
1	B	225	Total	C	N	O	0	0	0
			900	450	225	225			

- Molecule 2 is a protein called DNA-directed RNA polymerase beta chain.

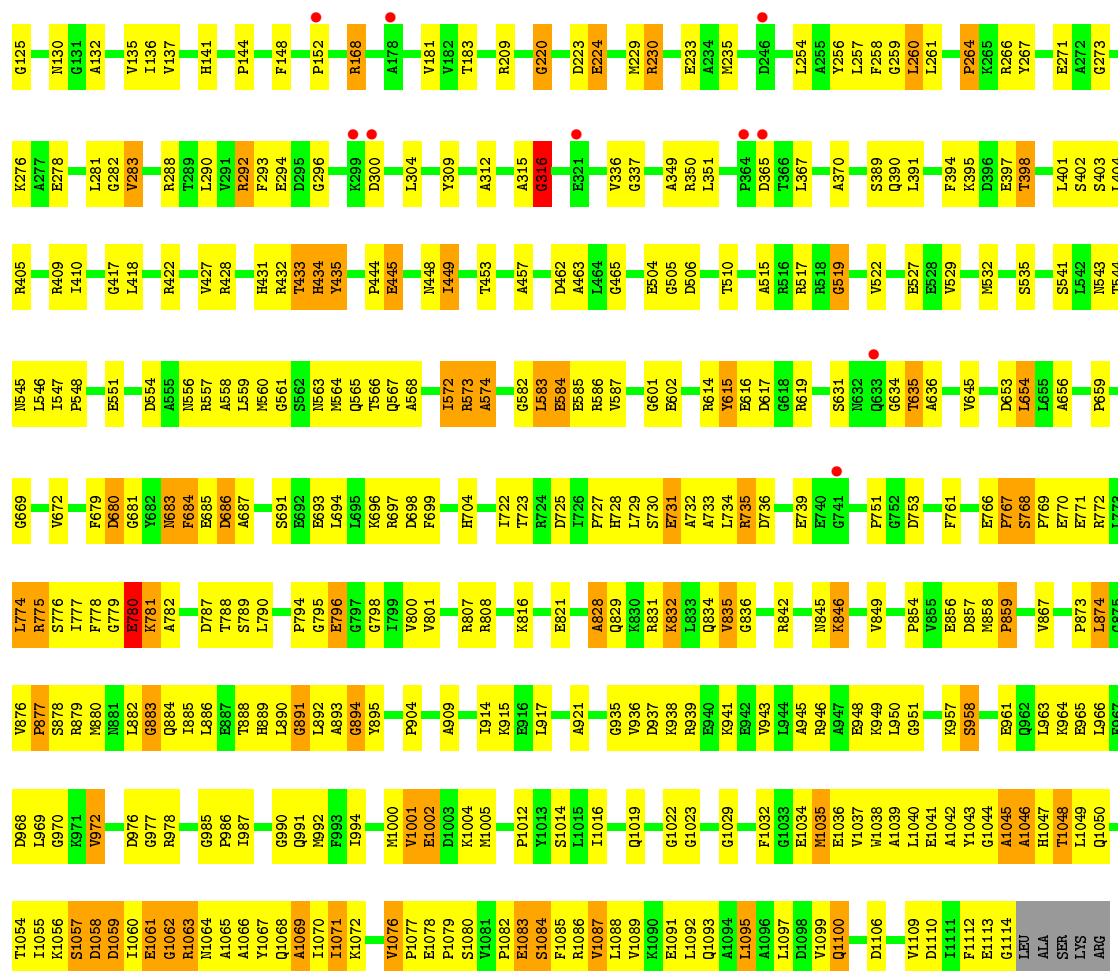
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	1114	Total	C	N	O	0	0	0
			4456	2228	1114	1114			

- Molecule 3 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	1196	Total	C	N	O	0	0	0
			4784	2392	1196	1196			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	159	GLY	-	LINKER	UNP Q9KWU6
D	160	GLY	-	LINKER	UNP Q9KWU6



ARG	A1438	E1345	ILE	E378	F780	D662	V595	M513
GLU	S1439	R1346	T1253	D879	F780	D662	G596	A514
GLN	F1440	Y1347	Q1254	V880	S783	Q670	E597	
PRO	Q1441	L1348	G1255	H881	H784		A598	P518
GLY	N1442	V1349		F882		E674	V599	
LYS	T1443	D1350	R1258	L883	R787		G600	L522
GLY	T1444	E1351	V1259			L680	D601	A523
LEU	H1445	I1352	I1260	A887	G790		E802	A524
	V1446	Q1353	E1261	E888	A791	Q682		Y525
	L1447		L1262	A889	D792		A605	E526
	T1448	L1363	F1263	G890	T793	G690	Q606	A527
	E1449	H1364	E1264		A794		E607	G528
	A1450	D1365	A1265	P800		I702		E529
	A1451	K1366	R1266	L901	A798	Q703	Q610	V530
	I1452	H1367	R1267	T902	D799	L704	M611	A531
	A1453	I1368	P1268	C903	S800		D612	L532
	G1454	E1369	K1269	R906	G801	T713	V613	N533
	K1455	I1370	A1270	Y907	L803	Q714	A534	
		V1371	K1271	G908	T804	A715	E816	P535
		R1372	A1272		R805	F717	K617	I536
		R1373			K806		S619	V538
		Q1374	I1277	C913	L807	F720	L620	A539
		M1375	D1278	Y914	V808		K621	
		L1376	G1279	G915	D809	Y724	D622	S544
		K1377		Y916	V810	P725	L623	T545
		Y1378	G1286	D917		F726	V624	G546
			E1287	L918	A811	N727	Y625	R547
				S919		P728	Q626	L548
			S1296	N920	E813	P729	A627	
					I814	L729	F628	D556
			K1307	Y924	V815	V730	L629	E557
			D1308			M732		A558
			V1313	A929	D820	A733	G632	L559
			K1314	V930	G821	Q734	M633	L560
			D1315	G931			E634	A561
			G1316	V932	N825	S735	K635	V562
			D1317	V933		G736	T636	A563
			Y1318	A934		A737	A637	H564
			E1319	A935	K845	Q742	R638	G565
			A1321	E936	R846	Q743	L639	L566
			G1322	S937	S847	I744	L640	
				I938	D848	R745	D641	D568
					I849	Q746	A642	L569
					E850	L747	L643	Q570
				P941	S851	C748	K644	
				G942	G852	G749	Y645	L578
				T943	L853	M750	G646	G579
				Q944	Y854		G647	B580
							F648	
			P1332	T949	R860	K756	T649	E583
			H1333	PHE	E861		L650	T584
			Q1334	HIS		E760		
			L1335	THR			T652	
			L1336	GLY	A864	G773		G587
			E1337	GLY	L865	L774		
			A1338	VAL	G866		G655	L590
			K1339	ALA		T775		F591
			G1340	VAL	E870	V776		A592
			P1341	VAL		L777	G659	I660
			E1342	GLY	S876	E778	I661	R593
			A1343	THR				
			V1344	ASP	L877	Y779		I594

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	202.80 Å 202.80 Å 326.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 5.00 24.99 – 4.10	Depositor EDS
% Data completeness (in resolution range)	87.1 (25.00-5.00) 80.7 (24.99-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 4.10 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.336 , 0.337 0.377 , 0.366	Depositor DCC
R_{free} test set	1580 reflections (3.64%)	DCC
Wilson B-factor (Å ²)	138.4	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.04 , -9.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 43458 reflections	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	11060	wwPDB-VP
Average B, all atoms (Å ²)	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.35	0/919	0.77	0/1147
1	B	0.40	0/899	0.78	0/1122
2	C	0.55	7/4455 (0.2%)	0.93	9/5567 (0.2%)
3	D	0.56	8/4782 (0.2%)	1.03	22/5974 (0.4%)
All	All	0.53	15/11055 (0.1%)	0.95	31/13810 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	704	HIS	C-N	11.46	1.60	1.34
3	D	943	THR	C-N	-9.94	1.11	1.34
2	C	828	ALA	C-N	7.47	1.51	1.34
3	D	137	PRO	N-CA	-7.25	1.34	1.47
3	D	1435	LEU	C-N	-6.64	1.18	1.34
2	C	1057	SER	C-N	6.22	1.48	1.34
3	D	139	GLY	N-CA	-6.19	1.36	1.46
2	C	141	HIS	C-N	5.86	1.47	1.34
2	C	768	SER	N-CA	5.76	1.57	1.46
2	C	769	PRO	N-CA	5.71	1.56	1.47
3	D	138	LYS	N-CA	-5.69	1.34	1.46
2	C	130	ASN	C-N	-5.45	1.23	1.33
3	D	138	LYS	C-N	-5.20	1.23	1.33
3	D	142	LEU	N-CA	5.19	1.56	1.46
3	D	138	LYS	CA-C	-5.16	1.39	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	137	PRO	CA-C-N	-15.02	84.17	117.20
3	D	137	PRO	O-C-N	10.21	139.04	122.70
2	C	781	LYS	C-N-CA	-9.35	98.32	121.70
3	D	140	ALA	C-N-CA	9.26	144.84	121.70
3	D	151	GLN	CA-C-N	-9.15	97.06	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	141	VAL	N-CA-C	9.04	135.41	111.00
2	C	772	ARG	CA-C-N	-7.93	99.74	117.20
3	D	943	THR	O-C-N	-7.68	110.40	122.70
3	D	137	PRO	C-N-CA	7.40	140.20	121.70
3	D	1459	LEU	O-C-N	-6.88	111.69	122.70
2	C	780	GLU	N-CA-C	-6.88	92.44	111.00
3	D	137	PRO	CA-C-O	6.88	136.70	120.20
3	D	150	ARG	C-N-CA	-6.77	104.78	121.70
3	D	1319	VAL	N-CA-C	6.59	128.79	111.00
3	D	1313	VAL	N-CA-C	-6.54	93.35	111.00
2	C	316	GLY	N-CA-C	6.52	129.40	113.10
3	D	151	GLN	O-C-N	6.04	132.36	122.70
3	D	1321	ALA	N-CA-C	6.04	127.30	111.00
3	D	943	THR	C-N-CA	6.02	136.75	121.70
3	D	138	LYS	C-N-CA	-5.98	109.75	122.30
2	C	772	ARG	O-C-N	5.97	132.25	122.70
3	D	147	VAL	C-N-CA	5.93	136.54	121.70
3	D	446	ASN	N-CA-C	-5.82	95.30	111.00
2	C	828	ALA	O-C-N	-5.78	113.46	122.70
3	D	322	ARG	O-C-N	-5.66	113.65	122.70
2	C	1076	VAL	N-CA-C	5.59	126.09	111.00
3	D	138	LYS	CA-C-N	-5.46	105.29	116.20
3	D	1314	LYS	N-CA-C	5.42	125.64	111.00
2	C	224	GLU	N-CA-C	-5.24	96.85	111.00
3	D	1279	GLY	N-CA-C	5.19	126.08	113.10
2	C	220	GLY	N-CA-C	-5.04	100.51	113.10

There are no chirality outliers.

There are no planarity outliers.

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	920	0	246	39	0
1	B	900	0	242	34	0
2	C	4456	0	1247	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	4784	0	1309	435	0
All	All	11060	0	3044	732	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 52.

All (732) 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)
3:D:145:VAL:O	3:D:146:PRO:O	1.56	1.19
2:C:775:ARG:O	2:C:778:PHE:N	1.88	1.05
3:D:1438:ALA:O	3:D:1440:PHE:N	1.98	0.94
2:C:775:ARG:O	2:C:779:GLY:N	2.00	0.94
3:D:917:ASP:C	3:D:919:SER:H	1.68	0.87
3:D:918:LEU:C	3:D:920:MET:H	1.76	0.86
2:C:554:ASP:N	2:C:880:MET:O	2.09	0.84
3:D:101:HIS:O	3:D:103:TRP:N	2.11	0.84
3:D:1423:GLY:O	3:D:1425:THR:N	2.14	0.81
2:C:52:PHE:C	2:C:54:ILE:H	1.84	0.81
3:D:798:ALA:O	3:D:800:SER:N	2.13	0.80
2:C:74:GLY:HA3	2:C:93:PRO:O	1.80	0.80
3:D:145:VAL:C	3:D:146:PRO:O	2.19	0.80
3:D:22:SER:O	3:D:24:GLY:N	2.12	0.80
2:C:1039:ALA:O	2:C:1042:ALA:N	2.14	0.80
3:D:218:PRO:O	3:D:220:TRP:N	2.14	0.79
3:D:650:LEU:C	3:D:652:THR:H	1.86	0.79
3:D:420:LEU:O	3:D:422:ILE:N	2.15	0.79
3:D:801:GLY:O	3:D:804:THR:N	2.17	0.78
3:D:1270:ALA:O	3:D:1272:ALA:N	2.17	0.78
2:C:734:LEU:O	2:C:736:ASP:N	2.18	0.77
3:D:887:ALA:C	3:D:890:GLY:H	1.90	0.75
2:C:18:LEU:O	2:C:20:GLU:N	2.20	0.74
3:D:917:ASP:C	3:D:919:SER:N	2.39	0.74
3:D:461:SER:C	3:D:463:PHE:N	2.39	0.73
3:D:401:GLU:C	3:D:403:VAL:H	1.89	0.73
2:C:257:LEU:O	2:C:259:GLY:N	2.21	0.73
3:D:26:VAL:C	3:D:28:LYS:H	1.92	0.73
3:D:900:PRO:O	3:D:902:THR:N	2.21	0.73
3:D:887:ALA:O	3:D:890:GLY:N	2.22	0.72
3:D:212:LEU:O	3:D:214:SER:N	2.21	0.72
3:D:318:GLY:C	3:D:321:GLY:H	1.93	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:312:ALA:O	2:C:316:GLY:HA3	1.90	0.71
3:D:1376:LEU:O	3:D:1378:TYR:N	2.23	0.71
2:C:349:ALA:C	2:C:351:LEU:H	1.93	0.71
3:D:84:ILE:O	3:D:86:ARG:N	2.24	0.71
3:D:420:LEU:C	3:D:422:ILE:H	1.93	0.71
3:D:468:ALA:O	3:D:472:MET:N	2.20	0.71
2:C:18:LEU:C	2:C:20:GLU:H	1.95	0.70
3:D:119:SER:O	3:D:121:THR:N	2.24	0.70
2:C:679:PHE:O	2:C:681:GLY:N	2.25	0.70
3:D:650:LEU:O	3:D:652:THR:N	2.24	0.70
1:A:89:PHE:O	1:A:91:ASP:N	2.25	0.69
3:D:495:ILE:O	3:D:496:LEU:C	2.30	0.69
3:D:622:ASP:O	3:D:623:LEU:C	2.30	0.69
3:D:394:ASP:O	3:D:396:VAL:N	2.26	0.69
3:D:418:HIS:O	3:D:421:GLY:N	2.25	0.68
3:D:401:GLU:C	3:D:403:VAL:N	2.47	0.68
2:C:566:THR:C	2:C:568:ALA:H	1.96	0.68
3:D:145:VAL:O	3:D:146:PRO:C	2.29	0.68
3:D:321:GLY:O	3:D:323:PHE:N	2.27	0.68
2:C:774:LEU:O	2:C:776:SER:N	2.27	0.68
3:D:930:VAL:O	3:D:931:GLY:C	2.30	0.68
2:C:52:PHE:O	2:C:54:ILE:N	2.27	0.67
3:D:918:LEU:C	3:D:920:MET:N	2.48	0.67
2:C:775:ARG:C	2:C:778:PHE:H	1.97	0.67
3:D:1372:VAL:O	3:D:1375:MET:N	2.25	0.67
1:B:37:GLY:O	1:B:40:LEU:N	2.27	0.67
2:C:1093:GLN:C	2:C:1095:LEU:H	1.98	0.67
3:D:626:GLN:O	3:D:629:LEU:N	2.28	0.67
3:D:431:GLU:O	3:D:432:GLY:O	2.13	0.67
1:A:121:GLU:O	1:A:123:MET:N	2.28	0.66
3:D:487:LEU:C	3:D:489:LYS:H	1.98	0.66
3:D:231:PRO:C	3:D:233:LEU:H	1.99	0.66
2:C:1039:ALA:O	2:C:1040:LEU:C	2.35	0.66
3:D:526:GLU:O	3:D:529:GLU:N	2.23	0.66
2:C:254:LEU:C	2:C:256:TYR:H	1.99	0.66
2:C:795:GLY:O	2:C:796:GLU:O	2.14	0.65
3:D:605:ALA:O	3:D:607:GLU:N	2.29	0.65
3:D:1443:THR:O	3:D:1444:THR:C	2.34	0.65
2:C:1043:TYR:C	2:C:1045:ALA:H	1.99	0.65
3:D:399:ALA:O	3:D:401:GLU:N	2.29	0.65
2:C:1014:SER:N	2:C:1019:GLN:O	2.20	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:439:PRO:O	3:D:441:VAL:N	2.29	0.65
3:D:847:SER:O	3:D:848:ASP:C	2.36	0.65
2:C:267:TYR:O	2:C:273:GLY:HA3	1.97	0.65
3:D:167:ALA:O	3:D:168:GLU:C	2.35	0.64
3:D:112:ILE:C	3:D:114:THR:H	2.01	0.64
3:D:641:ASP:O	3:D:644:LYS:N	2.29	0.64
3:D:639:LEU:O	3:D:640:LEU:C	2.35	0.64
3:D:642:ALA:O	3:D:643:LEU:C	2.36	0.64
3:D:397:TRP:O	3:D:398:ASP:C	2.35	0.64
1:B:112:GLY:C	1:B:114:PHE:H	2.01	0.64
3:D:1427:SER:O	3:D:1429:LEU:N	2.31	0.64
1:B:172:SER:O	1:B:174:VAL:N	2.31	0.64
2:C:774:LEU:O	2:C:777:ILE:N	2.25	0.63
3:D:1434:TRP:O	3:D:1437:ALA:N	2.31	0.63
3:D:546:GLY:O	3:D:548:LEU:N	2.32	0.63
3:D:934:ALA:O	3:D:935:ALA:C	2.36	0.63
3:D:309:LEU:O	3:D:310:ARG:O	2.17	0.63
3:D:1423:GLY:O	3:D:1424:VAL:C	2.37	0.63
3:D:801:GLY:O	3:D:803:LEU:N	2.31	0.63
3:D:932:VAL:O	3:D:933:VAL:C	2.37	0.63
1:A:75:VAL:O	1:A:79:ILE:N	2.28	0.63
2:C:877:PRO:O	2:C:879:ARG:O	2.16	0.63
3:D:157:GLU:O	3:D:158:TYR:O	2.17	0.63
3:D:363:LYS:O	3:D:364:PRO:O	2.16	0.63
3:D:364:PRO:O	3:D:366:LEU:N	2.32	0.63
3:D:1262:LEU:O	3:D:1263:PHE:C	2.37	0.62
2:C:52:PHE:C	2:C:54:ILE:N	2.50	0.62
3:D:929:ALA:O	3:D:930:VAL:C	2.37	0.62
3:D:702:ILE:C	3:D:704:LEU:H	2.01	0.62
2:C:1047:HIS:O	2:C:1049:LEU:N	2.32	0.62
3:D:730:TYR:O	3:D:731:VAL:C	2.37	0.62
3:D:461:SER:C	3:D:463:PHE:H	2.01	0.62
2:C:16:PRO:C	2:C:18:LEU:H	2.03	0.62
1:A:110:ARG:O	1:A:112:GLY:N	2.32	0.62
2:C:1001:VAL:O	2:C:1004:LYS:N	2.33	0.62
2:C:948:GLU:O	2:C:951:GLY:N	2.21	0.62
3:D:420:LEU:C	3:D:422:ILE:N	2.53	0.62
2:C:582:GLY:O	2:C:584:GLU:N	2.32	0.62
2:C:543:ASN:C	2:C:545:ASN:H	2.03	0.62
3:D:495:ILE:O	3:D:497:GLY:N	2.32	0.61
3:D:1262:LEU:O	3:D:1265:ALA:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1316:GLY:O	3:D:1317:ASP:O	2.19	0.61
3:D:643:LEU:O	3:D:644:LYS:C	2.38	0.61
3:D:620:LEU:O	3:D:621:LYS:C	2.38	0.61
3:D:63:TYR:C	3:D:65:ARG:H	2.03	0.61
2:C:1000:MET:O	2:C:1002:GLU:N	2.33	0.61
3:D:45:PHE:O	3:D:46:ASP:C	2.39	0.61
3:D:623:LEU:O	3:D:627:ALA:N	2.34	0.61
2:C:504:GLU:O	2:C:506:ASP:N	2.34	0.61
3:D:1427:SER:O	3:D:1428:ALA:C	2.38	0.61
3:D:650:LEU:C	3:D:652:THR:N	2.54	0.61
2:C:1058:ASP:O	2:C:1060:ILE:N	2.34	0.61
3:D:935:ALA:O	3:D:936:GLU:C	2.40	0.60
3:D:659:GLY:O	3:D:661:ASP:N	2.34	0.60
3:D:620:LEU:O	3:D:623:LEU:N	2.34	0.60
3:D:801:GLY:O	3:D:802:TYR:C	2.40	0.60
3:D:1261:GLU:O	3:D:1265:ALA:N	2.33	0.60
3:D:324:ARG:O	3:D:326:ASN:N	2.34	0.60
2:C:349:ALA:O	2:C:351:LEU:N	2.34	0.60
2:C:1032:PHE:O	3:D:329:GLY:HA2	2.02	0.60
2:C:845:ASN:O	2:C:846:LYS:C	2.38	0.60
2:C:1034:GLU:O	2:C:1035:MET:C	2.38	0.60
3:D:900:PRO:C	3:D:902:THR:N	2.55	0.59
3:D:592:ALA:O	3:D:595:VAL:N	2.35	0.59
1:A:74:ASP:O	1:A:75:VAL:C	2.41	0.59
3:D:289:ALA:O	3:D:293:ASN:N	2.35	0.59
3:D:508:LYS:O	3:D:510:GLY:N	2.32	0.59
3:D:853:LEU:O	3:D:854:TYR:C	2.40	0.59
3:D:171:GLN:O	3:D:173:LEU:N	2.36	0.59
3:D:1335:LEU:O	3:D:1336:LEU:C	2.41	0.59
3:D:641:ASP:O	3:D:642:ALA:C	2.41	0.59
3:D:511:ALA:O	3:D:513:MET:N	2.36	0.59
3:D:373:LYS:O	3:D:375:PHE:N	2.36	0.59
2:C:1038:TRP:O	2:C:1042:ALA:N	2.35	0.59
3:D:637:ALA:O	3:D:640:LEU:N	2.35	0.59
2:C:798:GLY:HA3	2:C:828:ALA:O	2.02	0.59
3:D:1426:LYS:O	3:D:1427:SER:O	2.20	0.59
3:D:583:GLU:O	3:D:584:THR:O	2.21	0.59
3:D:362:PHE:O	3:D:363:LYS:C	2.41	0.58
2:C:561:GLY:HA3	2:C:842:ARG:O	2.03	0.58
3:D:355:LYS:O	3:D:356:ARG:C	2.41	0.58
3:D:171:GLN:C	3:D:173:LEU:N	2.55	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:683:ASN:O	2:C:687:ALA:N	2.33	0.58
3:D:876:SER:O	3:D:879:ASP:N	2.36	0.58
3:D:941:PRO:C	3:D:943:THR:N	2.55	0.58
3:D:622:ASP:O	3:D:626:GLN:N	2.33	0.58
1:A:44:LEU:O	1:A:46:SER:N	2.35	0.58
3:D:1466:VAL:O	3:D:1469:GLY:N	2.36	0.58
2:C:563:ASN:C	2:C:565:GLN:H	2.06	0.58
2:C:1054:THR:C	2:C:1056:LYS:H	2.07	0.58
3:D:849:ILE:O	3:D:852:GLY:N	2.36	0.58
3:D:219:GLU:O	3:D:221:MET:N	2.36	0.58
3:D:40:GLU:O	3:D:41:ARG:C	2.42	0.58
2:C:1045:ALA:O	2:C:1046:ALA:C	2.42	0.58
3:D:596:GLY:O	3:D:599:VAL:N	2.32	0.58
3:D:26:VAL:C	3:D:28:LYS:N	2.57	0.58
3:D:916:TYR:O	3:D:918:LEU:N	2.37	0.57
2:C:775:ARG:O	2:C:778:PHE:CA	2.51	0.57
3:D:730:TYR:O	3:D:732:MET:N	2.37	0.57
2:C:1093:GLN:C	2:C:1095:LEU:N	2.58	0.57
3:D:231:PRO:O	3:D:233:LEU:N	2.37	0.57
3:D:877:LEU:O	3:D:878:GLU:C	2.42	0.57
2:C:858:MET:O	2:C:859:PRO:C	2.42	0.57
3:D:1471:LEU:O	3:D:1472:ILE:O	2.23	0.57
1:B:224:TYR:C	1:B:226:ALA:H	2.08	0.57
3:D:205:LEU:O	3:D:208:VAL:N	2.37	0.57
2:C:410:ILE:N	2:C:453:THR:O	2.37	0.57
2:C:1066:ALA:O	2:C:1067:TYR:C	2.42	0.57
2:C:563:ASN:O	2:C:565:GLN:N	2.28	0.57
2:C:723:THR:C	2:C:725:ASP:H	2.08	0.57
3:D:357:MET:O	3:D:359:LEU:N	2.38	0.57
3:D:860:ARG:O	3:D:861:GLU:O	2.22	0.57
2:C:1041:GLU:O	2:C:1042:ALA:C	2.43	0.56
3:D:401:GLU:O	3:D:403:VAL:N	2.38	0.56
1:B:37:GLY:O	1:B:38:ASN:C	2.43	0.56
3:D:55:ASP:O	3:D:57:GLU:N	2.38	0.56
3:D:620:LEU:O	3:D:624:VAL:N	2.38	0.56
3:D:1450:ALA:O	3:D:1451:ALA:C	2.43	0.56
3:D:647:GLY:O	3:D:651:SER:N	2.22	0.56
3:D:1344:VAL:O	3:D:1345:GLU:C	2.43	0.56
1:A:208:LEU:O	1:A:211:LEU:N	2.39	0.56
1:A:74:ASP:O	1:A:77:GLU:N	2.39	0.56
2:C:1047:HIS:C	2:C:1049:LEU:N	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:25:GLU:O	3:D:27:GLU:N	2.34	0.56
2:C:292:ARG:O	2:C:294:GLU:N	2.38	0.56
1:B:209:GLU:O	1:B:210:ALA:C	2.42	0.56
3:D:635:LYS:O	3:D:636:THR:C	2.42	0.56
3:D:493:ASP:O	3:D:494:ILE:C	2.44	0.56
3:D:441:VAL:O	3:D:443:GLU:N	2.39	0.56
2:C:941:LYS:O	2:C:945:ALA:N	2.36	0.56
3:D:805:ARG:O	3:D:806:LYS:C	2.43	0.56
3:D:396:VAL:O	3:D:399:ALA:N	2.38	0.56
3:D:119:SER:O	3:D:121:THR:O	2.24	0.56
1:A:171:PHE:O	1:A:172:SER:C	2.44	0.56
3:D:623:LEU:O	3:D:624:VAL:C	2.44	0.56
2:C:558:ALA:O	2:C:561:GLY:N	2.38	0.56
1:A:208:LEU:O	1:A:209:GLU:C	2.44	0.56
3:D:1390:LEU:O	3:D:1391:GLU:C	2.43	0.56
2:C:882:LEU:O	2:C:884:GLN:N	2.38	0.56
2:C:431:HIS:O	2:C:433:THR:N	2.39	0.56
2:C:1093:GLN:O	2:C:1095:LEU:N	2.30	0.56
1:A:209:GLU:O	1:A:210:ALA:C	2.45	0.56
1:A:74:ASP:O	1:A:76:VAL:N	2.39	0.56
2:C:527:GLU:C	2:C:529:VAL:H	2.09	0.56
3:D:102:ILE:C	3:D:104:PHE:H	2.09	0.55
3:D:499:TYR:O	3:D:502:THR:N	2.29	0.55
3:D:876:SER:O	3:D:877:LEU:C	2.44	0.55
3:D:743:GLN:O	3:D:744:ILE:C	2.45	0.55
3:D:1365:ASP:O	3:D:1366:LYS:C	2.44	0.55
3:D:441:VAL:O	3:D:442:CYS:C	2.44	0.55
3:D:371:GLU:C	3:D:373:LYS:H	2.08	0.55
2:C:561:GLY:O	2:C:563:ASN:O	2.24	0.55
2:C:882:LEU:O	2:C:885:ILE:N	2.36	0.55
1:A:218:LEU:O	1:A:219:LYS:C	2.44	0.55
3:D:171:GLN:C	3:D:173:LEU:H	2.09	0.55
3:D:1466:VAL:C	3:D:1468:LEU:N	2.57	0.55
3:D:1395:LEU:O	3:D:1398:TRP:N	2.39	0.55
2:C:82:GLU:O	2:C:84:ARG:N	2.39	0.55
2:C:1070:ILE:O	2:C:1072:LYS:N	2.40	0.55
3:D:1425:THR:O	3:D:1426:LYS:C	2.44	0.55
3:D:637:ALA:O	3:D:638:ARG:C	2.44	0.55
3:D:284:GLN:O	3:D:286:ALA:N	2.40	0.55
3:D:626:GLN:O	3:D:627:ALA:C	2.44	0.55
3:D:648:PHE:O	3:D:649:THR:C	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:174:LEU:O	3:D:175:LYS:C	2.46	0.55
3:D:1350:ASP:O	3:D:1351:GLU:C	2.45	0.55
2:C:966:LEU:O	2:C:969:LEU:N	2.40	0.55
3:D:102:ILE:O	3:D:104:PHE:N	2.40	0.55
3:D:645:TYR:O	3:D:648:PHE:N	2.40	0.55
3:D:1342:GLU:O	3:D:1345:GLU:N	2.40	0.55
2:C:891:GLY:O	2:C:892:LEU:C	2.45	0.55
3:D:259:ARG:O	3:D:261:ASN:N	2.40	0.55
3:D:932:VAL:O	3:D:935:ALA:N	2.40	0.54
3:D:592:ALA:O	3:D:593:ARG:C	2.46	0.54
2:C:1054:THR:O	2:C:1056:LYS:N	2.41	0.54
3:D:1349:VAL:O	3:D:1350:ASP:C	2.45	0.54
3:D:799:ASP:O	3:D:800:SER:C	2.46	0.54
3:D:292:ASP:O	3:D:293:ASN:C	2.46	0.54
3:D:1341:PRO:O	3:D:1342:GLU:C	2.45	0.54
2:C:1047:HIS:O	2:C:1050:GLN:N	2.40	0.54
1:B:112:GLY:O	1:B:114:PHE:N	2.41	0.54
3:D:364:PRO:O	3:D:367:LEU:N	2.39	0.54
2:C:948:GLU:C	2:C:950:LEU:N	2.59	0.54
3:D:367:LEU:O	3:D:370:MET:N	2.40	0.54
3:D:129:PHE:O	3:D:131:LYS:N	2.41	0.54
3:D:252:LEU:C	3:D:254:ARG:N	2.57	0.54
2:C:543:ASN:C	2:C:545:ASN:N	2.60	0.54
2:C:556:ASN:C	2:C:558:ALA:H	2.10	0.54
3:D:564:HIS:O	3:D:566:LEU:N	2.40	0.54
3:D:1447:LEU:O	3:D:1448:THR:C	2.46	0.53
3:D:941:PRO:O	3:D:943:THR:N	2.40	0.53
3:D:275:ILE:O	3:D:276:ILE:C	2.47	0.53
1:A:209:GLU:O	1:A:212:ASN:N	2.41	0.53
3:D:743:GLN:O	3:D:745:ARG:N	2.41	0.53
3:D:348:LEU:O	3:D:350:GLN:N	2.41	0.53
3:D:815:VAL:H	3:D:908:GLY:HA2	1.72	0.53
3:D:792:ASP:O	3:D:794:ALA:N	2.42	0.53
3:D:933:VAL:O	3:D:934:ALA:C	2.46	0.53
3:D:742:GLN:O	3:D:743:GLN:C	2.46	0.53
2:C:876:VAL:O	2:C:879:ARG:O	2.26	0.53
3:D:1266:ARG:O	3:D:1268:PRO:N	2.42	0.53
3:D:559:LEU:O	3:D:561:ALA:N	2.42	0.53
3:D:318:GLY:CA	3:D:321:GLY:H	2.21	0.53
3:D:1448:THR:O	3:D:1449:GLU:C	2.47	0.53
2:C:517:ARG:O	2:C:519:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:33:ASN:O	3:D:35:ARG:N	2.42	0.53
3:D:702:ILE:C	3:D:704:LEU:N	2.61	0.53
3:D:811:ALA:O	3:D:931:GLY:HA3	2.09	0.53
2:C:82:GLU:C	2:C:84:ARG:H	2.09	0.53
2:C:731:GLU:C	2:C:733:ALA:N	2.61	0.53
3:D:205:LEU:O	3:D:207:VAL:N	2.42	0.53
3:D:1399:ASP:C	3:D:1401:GLU:H	2.12	0.53
2:C:968:ASP:C	2:C:970:GLY:H	2.11	0.53
1:B:34:VAL:O	1:B:35:THR:C	2.47	0.53
2:C:775:ARG:C	2:C:777:ILE:N	2.59	0.52
2:C:680:ASP:O	2:C:681:GLY:C	2.47	0.52
2:C:1047:HIS:O	2:C:1048:THR:C	2.45	0.52
2:C:13:ILE:O	2:C:14:PRO:O	2.27	0.52
2:C:1088:LEU:O	2:C:1089:VAL:C	2.47	0.52
3:D:121:THR:C	3:D:123:LEU:H	2.12	0.52
2:C:1068:GLN:O	2:C:1071:ILE:N	2.43	0.52
3:D:118:LEU:O	3:D:119:SER:C	2.48	0.52
3:D:1371:VAL:O	3:D:1372:VAL:C	2.47	0.52
2:C:433:THR:O	2:C:435:TYR:N	2.43	0.52
2:C:1070:ILE:C	2:C:1072:LYS:N	2.61	0.52
3:D:633:MET:O	3:D:634:GLU:C	2.48	0.52
3:D:1425:THR:O	3:D:1427:SER:N	2.43	0.52
2:C:74:GLY:CA	2:C:93:PRO:O	2.57	0.52
2:C:18:LEU:C	2:C:20:GLU:N	2.59	0.52
3:D:397:TRP:O	3:D:400:LEU:N	2.43	0.52
2:C:551:GLU:O	3:D:773:GLY:HA2	2.10	0.52
3:D:805:ARG:O	3:D:808:VAL:N	2.43	0.52
1:A:156:HIS:O	1:A:157:GLY:O	2.28	0.52
3:D:1462:LEU:C	3:D:1464:GLU:N	2.63	0.52
2:C:1000:MET:O	2:C:1001:VAL:C	2.48	0.52
3:D:1466:VAL:O	3:D:1467:ILE:C	2.48	0.52
3:D:287:VAL:O	3:D:288:ASP:C	2.48	0.52
2:C:780:GLU:O	2:C:782:ALA:N	2.43	0.52
3:D:524:ALA:O	3:D:525:TYR:C	2.46	0.52
2:C:751:PRO:C	2:C:753:ASP:H	2.13	0.52
1:B:37:GLY:O	1:B:39:PRO:N	2.43	0.52
2:C:349:ALA:C	2:C:351:LEU:N	2.62	0.52
3:D:546:GLY:C	3:D:548:LEU:N	2.62	0.52
2:C:82:GLU:C	2:C:84:ARG:N	2.63	0.52
2:C:684:PHE:O	2:C:686:ASP:N	2.37	0.52
3:D:728:PRO:O	3:D:729:LEU:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1336:LEU:O	3:D:1337:GLU:C	2.48	0.51
2:C:634:GLY:O	2:C:635:THR:C	2.48	0.51
2:C:16:PRO:O	2:C:18:LEU:N	2.42	0.51
2:C:566:THR:C	2:C:568:ALA:N	2.64	0.51
1:A:164:ALA:O	1:A:165:ILE:C	2.48	0.51
3:D:729:LEU:O	3:D:730:TYR:C	2.48	0.51
2:C:1062:GLY:O	2:C:1066:ALA:N	2.38	0.51
2:C:948:GLU:O	2:C:950:LEU:N	2.44	0.51
3:D:745:ARG:O	3:D:747:LEU:N	2.44	0.51
3:D:136:ASP:O	3:D:137:PRO:O	2.29	0.51
3:D:736:GLY:O	3:D:737:ALA:C	2.47	0.51
2:C:582:GLY:C	2:C:584:GLU:N	2.64	0.51
3:D:474:SER:O	3:D:477:ASN:O	2.28	0.51
3:D:379:VAL:O	3:D:382:ALA:N	2.42	0.51
2:C:563:ASN:C	2:C:565:GLN:N	2.64	0.51
3:D:916:TYR:H	3:D:924:VAL:H	1.58	0.51
3:D:399:ALA:O	3:D:400:LEU:C	2.49	0.51
3:D:597:GLU:O	3:D:600:GLY:N	2.44	0.51
3:D:371:GLU:C	3:D:373:LYS:N	2.64	0.51
1:B:225:PHE:O	1:B:226:ALA:O	2.29	0.51
3:D:1367:HIS:O	3:D:1368:ILE:C	2.49	0.51
3:D:792:ASP:C	3:D:794:ALA:N	2.61	0.51
3:D:929:ALA:O	3:D:932:VAL:N	2.44	0.51
3:D:364:PRO:O	3:D:365:PHE:C	2.48	0.51
3:D:366:LEU:O	3:D:367:LEU:C	2.49	0.51
2:C:964:LYS:O	2:C:965:GLU:C	2.49	0.51
3:D:637:ALA:O	3:D:639:LEU:N	2.43	0.51
3:D:124:GLU:O	3:D:127:LEU:N	2.36	0.51
3:D:444:ALA:C	3:D:446:ASN:H	2.14	0.51
2:C:1037:VAL:O	2:C:1041:GLU:N	2.30	0.50
3:D:396:VAL:O	3:D:397:TRP:C	2.50	0.50
3:D:231:PRO:C	3:D:233:LEU:N	2.65	0.50
2:C:582:GLY:O	2:C:583:LEU:C	2.50	0.50
3:D:617:LYS:O	3:D:618:ASN:C	2.49	0.50
3:D:491:SER:O	3:D:493:ASP:N	2.44	0.50
2:C:1044:GLY:C	2:C:1046:ALA:H	2.14	0.50
3:D:148:GLU:O	3:D:150:ARG:N	2.44	0.50
3:D:318:GLY:O	3:D:321:GLY:N	2.44	0.50
3:D:259:ARG:C	3:D:261:ASN:H	2.14	0.50
3:D:559:LEU:C	3:D:561:ALA:N	2.62	0.50
2:C:888:THR:O	2:C:990:GLY:HA3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:834:GLN:O	2:C:835:VAL:C	2.49	0.50
3:D:461:SER:O	3:D:463:PHE:N	2.43	0.50
3:D:440:LEU:O	3:D:441:VAL:C	2.50	0.50
2:C:402:SER:O	2:C:403:SER:C	2.50	0.50
3:D:777:LEU:O	3:D:780:PHE:N	2.45	0.50
1:A:127:LEU:O	1:A:128:HIS:C	2.50	0.50
3:D:397:TRP:O	3:D:399:ALA:N	2.45	0.50
3:D:849:ILE:O	3:D:850:GLU:C	2.48	0.50
1:B:152:PRO:C	1:B:154:GLU:H	2.15	0.50
3:D:590:LEU:O	3:D:591:PHE:C	2.49	0.50
3:D:715:ALA:C	3:D:717:PHE:N	2.64	0.50
3:D:916:TYR:N	3:D:924:VAL:H	2.10	0.50
3:D:483:SER:O	3:D:485:GLU:N	2.45	0.50
3:D:439:PRO:O	3:D:440:LEU:C	2.51	0.49
2:C:1060:ILE:O	2:C:1061:GLU:C	2.51	0.49
3:D:632:GLY:O	3:D:633:MET:C	2.51	0.49
3:D:1449:GLU:O	3:D:1450:ALA:C	2.49	0.49
3:D:1348:LEU:O	3:D:1349:VAL:C	2.51	0.49
2:C:515:ALA:O	2:C:522:VAL:O	2.30	0.49
2:C:653:ASP:O	2:C:654:LEU:C	2.51	0.49
3:D:811:ALA:C	3:D:813:GLU:H	2.14	0.49
3:D:730:TYR:O	3:D:733:ALA:N	2.45	0.49
2:C:556:ASN:O	2:C:558:ALA:N	2.46	0.49
3:D:219:GLU:C	3:D:221:MET:N	2.65	0.49
3:D:557:GLU:O	3:D:558:ALA:C	2.51	0.49
2:C:697:ARG:O	2:C:698:ASP:C	2.51	0.49
3:D:1336:LEU:O	3:D:1339:LYS:N	2.46	0.49
3:D:1466:VAL:O	3:D:1468:LEU:N	2.45	0.49
1:A:219:LYS:O	1:A:222:LEU:N	2.45	0.49
2:C:766:GLU:O	2:C:767:PRO:O	2.29	0.49
1:B:116:PRO:O	1:B:117:SER:O	2.31	0.49
2:C:389:SER:O	2:C:391:LEU:N	2.46	0.49
2:C:572:ILE:C	2:C:574:ALA:H	2.15	0.49
3:D:418:HIS:O	3:D:419:ARG:C	2.51	0.49
2:C:543:ASN:O	2:C:545:ASN:N	2.45	0.49
2:C:1088:LEU:O	2:C:1091:GLU:N	2.46	0.49
2:C:694:LEU:O	2:C:698:ASP:N	2.45	0.49
2:C:1043:TYR:C	2:C:1045:ALA:N	2.66	0.49
3:D:808:VAL:O	3:D:810:VAL:N	2.46	0.49
3:D:154:THR:O	3:D:157:GLU:N	2.44	0.49
3:D:487:LEU:C	3:D:489:LYS:N	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:254:LEU:C	2:C:256:TYR:N	2.67	0.49
2:C:572:ILE:O	2:C:574:ALA:N	2.37	0.49
2:C:282:GLY:O	2:C:283:VAL:O	2.31	0.49
2:C:92:ALA:O	2:C:93:PRO:C	2.51	0.48
3:D:813:GLU:O	3:D:814:ILE:C	2.51	0.48
2:C:89:THR:O	2:C:90:TYR:C	2.50	0.48
3:D:480:SER:O	3:D:481:PRO:C	2.51	0.48
2:C:831:ARG:O	2:C:832:LYS:O	2.31	0.48
2:C:1035:MET:O	2:C:1036:GLU:C	2.50	0.48
2:C:731:GLU:O	2:C:733:ALA:N	2.46	0.48
3:D:399:ALA:C	3:D:401:GLU:N	2.65	0.48
3:D:811:ALA:C	3:D:813:GLU:N	2.66	0.48
3:D:880:VAL:O	3:D:881:HIS:C	2.52	0.48
1:B:41:ARG:C	1:B:43:ILE:H	2.16	0.48
2:C:1044:GLY:O	2:C:1046:ALA:N	2.42	0.48
3:D:934:ALA:O	3:D:935:ALA:O	2.31	0.48
2:C:831:ARG:O	2:C:832:LYS:C	2.52	0.48
2:C:787:ASP:O	2:C:789:SER:N	2.46	0.48
3:D:569:LEU:O	3:D:587:GLY:N	2.42	0.48
3:D:1434:TRP:O	3:D:1435:LEU:C	2.51	0.48
3:D:1444:THR:O	3:D:1445:HIS:C	2.52	0.48
3:D:642:ALA:O	3:D:646:TYR:N	2.45	0.48
3:D:84:ILE:C	3:D:86:ARG:H	2.17	0.48
3:D:493:ASP:C	3:D:495:ILE:N	2.62	0.48
3:D:480:SER:C	3:D:482:ALA:N	2.65	0.48
3:D:680:LEU:C	3:D:682:GLN:H	2.17	0.48
2:C:462:ASP:O	2:C:463:ALA:C	2.51	0.48
3:D:1347:TYR:O	3:D:1348:LEU:C	2.52	0.48
2:C:448:ASN:O	2:C:449:ILE:C	2.51	0.48
3:D:461:SER:O	3:D:462:SER:C	2.50	0.48
3:D:1445:HIS:O	3:D:1446:VAL:C	2.51	0.48
1:B:105:GLY:HA2	1:B:135:GLY:HA2	1.96	0.48
2:C:775:ARG:O	2:C:778:PHE:C	2.52	0.48
3:D:1424:VAL:O	3:D:1425:THR:O	2.32	0.48
3:D:592:ALA:O	3:D:596:GLY:N	2.46	0.48
2:C:1066:ALA:O	2:C:1069:ALA:N	2.47	0.48
2:C:1083:GLU:O	2:C:1085:PHE:N	2.47	0.48
2:C:1043:TYR:O	2:C:1045:ALA:N	2.45	0.47
3:D:605:ALA:C	3:D:607:GLU:N	2.66	0.47
2:C:775:ARG:C	2:C:778:PHE:N	2.59	0.47
3:D:900:PRO:C	3:D:902:THR:H	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:948:GLU:C	2:C:950:LEU:H	2.16	0.47
3:D:792:ASP:C	3:D:794:ALA:H	2.17	0.47
2:C:168:ARG:O	2:C:264:PRO:O	2.32	0.47
1:B:114:PHE:O	1:B:115:THR:C	2.52	0.47
3:D:1369:GLU:O	3:D:1370:ILE:C	2.52	0.47
2:C:961:GLU:C	2:C:963:LEU:N	2.66	0.47
3:D:557:GLU:O	3:D:560:LEU:N	2.47	0.47
3:D:1462:LEU:O	3:D:1464:GLU:N	2.47	0.47
2:C:135:VAL:O	2:C:137:VAL:N	2.47	0.47
3:D:318:GLY:HA2	3:D:321:GLY:H	1.79	0.47
3:D:430:VAL:O	3:D:431:GLU:O	2.32	0.47
2:C:1064:ASN:O	2:C:1065:ALA:C	2.52	0.47
3:D:605:ALA:O	3:D:606:GLN:C	2.52	0.47
3:D:112:ILE:C	3:D:114:THR:N	2.68	0.47
3:D:596:GLY:O	3:D:597:GLU:C	2.53	0.47
3:D:371:GLU:O	3:D:373:LYS:N	2.48	0.47
3:D:56:TYR:O	3:D:57:GLU:O	2.33	0.47
1:B:152:PRO:C	1:B:154:GLU:N	2.67	0.47
3:D:680:LEU:C	3:D:682:GLN:N	2.68	0.47
3:D:787:ARG:C	3:D:790:GLY:H	2.18	0.47
3:D:431:GLU:C	3:D:432:GLY:O	2.53	0.47
3:D:642:ALA:O	3:D:645:TYR:N	2.47	0.47
3:D:648:PHE:O	3:D:651:SER:N	2.48	0.47
2:C:448:ASN:O	2:C:449:ILE:O	2.33	0.47
3:D:21:TRP:C	3:D:23:TYR:H	2.17	0.47
3:D:783:SER:O	3:D:784:HIS:C	2.50	0.47
3:D:318:GLY:C	3:D:320:GLN:N	2.66	0.47
2:C:545:ASN:O	2:C:547:ILE:N	2.47	0.47
3:D:557:GLU:O	3:D:559:LEU:N	2.48	0.47
3:D:715:ALA:C	3:D:717:PHE:H	2.18	0.47
3:D:21:TRP:O	3:D:23:TYR:N	2.48	0.47
2:C:614:ARG:O	2:C:615:TYR:O	2.33	0.47
3:D:368:LYS:O	3:D:369:LYS:C	2.52	0.47
3:D:900:PRO:O	3:D:901:LEU:C	2.53	0.46
2:C:891:GLY:O	2:C:893:ALA:N	2.48	0.46
3:D:773:GLY:O	3:D:774:LEU:C	2.53	0.46
1:A:229:GLU:O	1:A:230:ALA:C	2.53	0.46
3:D:805:ARG:O	3:D:807:LEU:N	2.48	0.46
2:C:1062:GLY:O	2:C:1065:ALA:N	2.48	0.46
1:A:219:LYS:O	1:A:220:GLU:C	2.52	0.46
3:D:347:LYS:O	3:D:348:LEU:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1261:GLU:O	3:D:1265:ALA:CA	2.63	0.46
3:D:1434:TRP:O	3:D:1438:ALA:N	2.45	0.46
3:D:635:LYS:O	3:D:637:ALA:N	2.49	0.46
3:D:941:PRO:O	3:D:942:GLY:C	2.52	0.46
3:D:736:GLY:O	3:D:737:ALA:O	2.34	0.46
2:C:836:GLY:N	2:C:849:VAL:O	2.49	0.46
3:D:1369:GLU:O	3:D:1372:VAL:N	2.48	0.46
3:D:559:LEU:O	3:D:560:LEU:C	2.52	0.46
3:D:1258:ARG:O	3:D:1259:VAL:C	2.54	0.46
2:C:733:ALA:O	2:C:734:LEU:C	2.52	0.46
3:D:593:ARG:O	3:D:594:ILE:C	2.53	0.46
3:D:887:ALA:C	3:D:890:GLY:N	2.65	0.46
2:C:601:GLY:HA3	2:C:615:TYR:CA	2.46	0.46
2:C:1100:GLN:N	3:D:9:ARG:O	2.49	0.46
2:C:730:SER:O	2:C:733:ALA:N	2.36	0.46
1:B:112:GLY:C	1:B:114:PHE:N	2.66	0.46
3:D:148:GLU:O	3:D:149:LYS:C	2.54	0.46
3:D:906:ARG:O	3:D:908:GLY:N	2.44	0.45
3:D:45:PHE:O	3:D:47:GLU:N	2.49	0.45
3:D:745:ARG:O	3:D:746:GLN:C	2.54	0.45
2:C:13:ILE:C	2:C:14:PRO:O	2.54	0.45
3:D:1451:ALA:O	3:D:1452:ILE:C	2.54	0.45
1:B:172:SER:O	1:B:173:PRO:C	2.54	0.45
2:C:917:LEU:O	2:C:921:ALA:N	2.49	0.45
3:D:628:PHE:O	3:D:629:LEU:C	2.55	0.45
1:A:110:ARG:O	1:A:111:ALA:C	2.55	0.45
2:C:1086:ARG:O	2:C:1087:VAL:C	2.55	0.45
3:D:625:TYR:O	3:D:626:GLN:C	2.54	0.45
3:D:702:ILE:O	3:D:704:LEU:N	2.50	0.45
3:D:777:LEU:O	3:D:779:TYR:N	2.50	0.45
2:C:972:VAL:O	2:C:987:ILE:N	2.43	0.45
3:D:807:LEU:O	3:D:808:VAL:C	2.54	0.45
2:C:545:ASN:C	2:C:547:ILE:N	2.69	0.45
3:D:63:TYR:C	3:D:65:ARG:N	2.69	0.45
2:C:669:GLY:HA3	2:C:994:ILE:O	2.16	0.45
2:C:727:PRO:C	2:C:729:LEU:H	2.20	0.45
3:D:641:ASP:O	3:D:643:LEU:N	2.49	0.45
3:D:284:GLN:C	3:D:286:ALA:N	2.69	0.45
2:C:976:ASP:O	2:C:978:ARG:N	2.50	0.45
3:D:117:ASP:O	3:D:118:LEU:C	2.54	0.45
2:C:566:THR:O	2:C:568:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LEU:O	1:B:212:ASN:C	2.55	0.45
3:D:394:ASP:O	3:D:395:GLU:C	2.55	0.45
3:D:493:ASP:O	3:D:495:ILE:N	2.50	0.45
3:D:1260:ILE:O	3:D:1261:GLU:C	2.54	0.45
3:D:1399:ASP:C	3:D:1401:GLU:N	2.70	0.45
3:D:263:LEU:C	3:D:265:LYS:N	2.70	0.45
3:D:820:ASP:C	3:D:822:GLY:N	2.69	0.45
2:C:733:ALA:C	2:C:735:ARG:N	2.69	0.45
1:A:34:VAL:C	1:A:36:LEU:N	2.68	0.45
2:C:1041:GLU:O	2:C:1043:TYR:O	2.35	0.44
3:D:1369:GLU:O	3:D:1371:VAL:N	2.50	0.44
3:D:1446:VAL:O	3:D:1447:LEU:C	2.55	0.44
3:D:114:THR:C	3:D:116:LEU:N	2.71	0.44
3:D:259:ARG:C	3:D:261:ASN:N	2.71	0.44
2:C:401:LEU:O	2:C:404:LEU:N	2.49	0.44
2:C:397:GLU:O	2:C:398:THR:C	2.55	0.44
3:D:317:SER:O	3:D:318:GLY:C	2.56	0.44
3:D:438:HIS:O	3:D:439:PRO:O	2.35	0.44
3:D:1345:GLU:O	3:D:1346:ARG:C	2.55	0.44
1:A:26:GLU:O	1:A:193:ASP:O	2.35	0.44
1:B:83:LYS:C	1:B:85:LEU:N	2.70	0.44
1:A:217:ILE:O	1:A:218:LEU:C	2.54	0.44
1:B:105:GLY:HA2	1:B:136:GLY:H	1.82	0.44
2:C:672:VAL:O	2:C:992:MET:N	2.46	0.44
3:D:1462:LEU:O	3:D:1463:LYS:C	2.55	0.44
3:D:535:PRO:O	3:D:536:ILE:C	2.56	0.44
3:D:913:CYS:O	3:D:915:GLY:N	2.51	0.44
2:C:1034:GLU:O	2:C:1037:VAL:N	2.50	0.44
3:D:889:ALA:O	3:D:890:GLY:O	2.34	0.44
2:C:564:MET:C	2:C:566:THR:N	2.69	0.44
3:D:850:GLU:O	3:D:854:TYR:N	2.40	0.44
3:D:546:GLY:C	3:D:548:LEU:H	2.20	0.44
2:C:694:LEU:O	2:C:699:PHE:N	2.47	0.44
1:B:219:LYS:O	1:B:220:GLU:C	2.56	0.44
3:D:1437:ALA:O	3:D:1438:ALA:O	2.35	0.44
1:B:105:GLY:HA2	1:B:135:GLY:CA	2.47	0.44
2:C:427:VAL:O	2:C:428:ARG:C	2.55	0.44
1:B:32:PHE:O	1:B:33:GLY:C	2.55	0.44
3:D:1440:PHE:O	3:D:1441:GLN:C	2.56	0.44
3:D:729:LEU:O	3:D:730:TYR:O	2.36	0.44
2:C:1054:THR:C	2:C:1056:LYS:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:473:LEU:O	3:D:474:SER:C	2.56	0.44
3:D:715:ALA:O	3:D:717:PHE:N	2.51	0.44
3:D:864:ALA:O	3:D:866:GLY:N	2.51	0.44
3:D:314:ASP:O	3:D:317:SER:N	2.51	0.43
1:A:122:ILE:O	1:A:123:MET:C	2.56	0.43
3:D:850:GLU:C	3:D:852:GLY:H	2.20	0.43
2:C:684:PHE:C	2:C:686:ASP:H	2.20	0.43
1:A:109:VAL:N	1:A:130:ALA:O	2.44	0.43
2:C:1070:ILE:C	2:C:1072:LYS:H	2.21	0.43
3:D:22:SER:O	3:D:90:MET:O	2.36	0.43
3:D:659:GLY:O	3:D:660:ILE:C	2.56	0.43
2:C:401:LEU:O	2:C:402:SER:C	2.56	0.43
2:C:691:SER:C	2:C:693:GLU:N	2.71	0.43
2:C:731:GLU:O	2:C:732:ALA:C	2.55	0.43
3:D:627:ALA:O	3:D:628:PHE:C	2.57	0.43
2:C:583:LEU:O	2:C:586:ARG:N	2.52	0.43
2:C:845:ASN:O	2:C:846:LYS:O	2.37	0.43
1:A:202:ASP:O	1:A:204:SER:N	2.52	0.43
3:D:941:PRO:C	3:D:943:THR:H	2.21	0.43
2:C:891:GLY:HA3	2:C:991:GLN:H	1.84	0.43
3:D:670:GLN:O	3:D:674:GLU:N	2.50	0.43
3:D:119:SER:O	3:D:120:ALA:C	2.57	0.43
2:C:1092:LEU:O	2:C:1095:LEU:N	2.52	0.43
3:D:112:ILE:O	3:D:114:THR:N	2.50	0.43
3:D:544:SER:O	3:D:547:ARG:N	2.52	0.43
1:A:44:LEU:C	1:A:46:SER:H	2.22	0.43
1:B:211:LEU:O	1:B:214:ALA:N	2.51	0.43
3:D:444:ALA:O	3:D:446:ASN:N	2.51	0.43
2:C:229:MET:O	2:C:230:ARG:O	2.37	0.43
2:C:1112:PHE:O	2:C:1114:GLY:N	2.52	0.43
3:D:624:VAL:O	3:D:625:TYR:C	2.56	0.43
3:D:362:PHE:O	3:D:364:PRO:N	2.52	0.43
3:D:289:ALA:O	3:D:290:VAL:C	2.57	0.43
3:D:1474:ALA:O	3:D:1477:GLY:N	2.48	0.43
2:C:404:LEU:O	2:C:405:ARG:C	2.54	0.43
1:A:34:VAL:C	1:A:36:LEU:H	2.22	0.43
3:D:341:VAL:N	3:D:435:ILE:O	2.51	0.43
2:C:545:ASN:C	2:C:547:ILE:H	2.21	0.43
2:C:891:GLY:O	2:C:894:GLY:N	2.52	0.43
3:D:645:TYR:O	3:D:646:TYR:C	2.57	0.42
3:D:444:ALA:C	3:D:446:ASN:N	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLU:O	1:A:105:GLY:C	2.57	0.42
2:C:1037:VAL:O	2:C:1038:TRP:C	2.55	0.42
3:D:167:ALA:C	3:D:169:ALA:N	2.71	0.42
3:D:1351:GLU:O	3:D:1352:ILE:C	2.56	0.42
3:D:175:LYS:O	3:D:177:LEU:N	2.53	0.42
3:D:557:GLU:C	3:D:559:LEU:N	2.72	0.42
3:D:724:TYR:C	3:D:726:PHE:H	2.21	0.42
3:D:526:GLU:C	3:D:528:GLY:N	2.73	0.42
2:C:1040:LEU:O	2:C:1043:TYR:O	2.37	0.42
2:C:914:ILE:O	2:C:915:LYS:C	2.57	0.42
2:C:775:ARG:C	2:C:777:ILE:H	2.21	0.42
3:D:917:ASP:O	3:D:919:SER:N	2.51	0.42
3:D:101:HIS:O	3:D:102:ILE:C	2.58	0.42
3:D:252:LEU:O	3:D:253:TYR:C	2.57	0.42
1:A:76:VAL:O	1:A:77:GLU:C	2.56	0.42
2:C:1058:ASP:O	2:C:1059:ASP:C	2.58	0.42
3:D:252:LEU:O	3:D:254:ARG:N	2.52	0.42
1:A:164:ALA:O	1:A:166:PRO:N	2.52	0.42
2:C:365:ASP:C	2:C:367:LEU:H	2.22	0.42
2:C:276:LYS:C	2:C:278:GLU:H	2.23	0.42
1:A:82:LEU:O	1:A:83:LYS:C	2.58	0.42
3:D:811:ALA:O	3:D:813:GLU:N	2.52	0.42
1:B:224:TYR:C	1:B:226:ALA:N	2.71	0.42
2:C:1082:PRO:O	2:C:1083:GLU:O	2.38	0.42
3:D:756:LYS:N	3:D:760:GLU:O	2.36	0.42
3:D:93:ILE:O	3:D:95:LEU:N	2.52	0.42
3:D:247:SER:C	3:D:249:LEU:H	2.23	0.42
3:D:102:ILE:C	3:D:104:PHE:N	2.72	0.42
2:C:16:PRO:C	2:C:18:LEU:N	2.71	0.42
3:D:814:ILE:CA	3:D:908:GLY:HA2	2.50	0.42
3:D:1262:LEU:O	3:D:1264:GLU:N	2.51	0.42
2:C:943:VAL:O	2:C:946:ARG:N	2.50	0.42
3:D:717:PHE:O	3:D:720:PHE:N	2.53	0.42
2:C:233:GLU:C	2:C:235:MET:H	2.22	0.42
3:D:568:ASP:O	3:D:570:GLN:N	2.41	0.42
2:C:259:GLY:O	2:C:260:LEU:O	2.37	0.42
3:D:1372:VAL:O	3:D:1373:ARG:C	2.58	0.42
3:D:640:LEU:O	3:D:641:ASP:O	2.37	0.42
3:D:616:GLU:O	3:D:617:LYS:O	2.38	0.42
3:D:845:LYS:O	3:D:846:ARG:C	2.57	0.42
1:A:206:THR:O	1:A:207:PRO:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:528:GLY:O	3:D:532:LEU:O	2.38	0.42
3:D:208:VAL:C	3:D:210:ALA:N	2.72	0.42
3:D:1342:GLU:O	3:D:1343:ALA:C	2.58	0.42
3:D:1344:VAL:O	3:D:1347:TYR:N	2.52	0.42
3:D:378:ASN:O	3:D:379:VAL:C	2.59	0.42
3:D:610:GLN:O	3:D:612:ASP:N	2.53	0.42
2:C:731:GLU:C	2:C:733:ALA:H	2.21	0.41
1:A:75:VAL:O	1:A:76:VAL:C	2.58	0.41
3:D:1395:LEU:O	3:D:1396:GLU:C	2.58	0.41
3:D:522:LEU:C	3:D:524:ALA:N	2.72	0.41
2:C:696:LYS:C	2:C:698:ASP:H	2.23	0.41
3:D:806:LYS:O	3:D:807:LEU:C	2.58	0.41
2:C:556:ASN:C	2:C:558:ALA:N	2.73	0.41
3:D:1366:LYS:O	3:D:1367:HIS:C	2.57	0.41
3:D:286:ALA:O	3:D:287:VAL:C	2.58	0.41
3:D:480:SER:O	3:D:482:ALA:N	2.53	0.41
2:C:873:PRO:O	2:C:874:LEU:C	2.59	0.41
3:D:343:GLY:O	3:D:344:PRO:C	2.58	0.41
3:D:84:ILE:C	3:D:86:ARG:N	2.70	0.41
2:C:583:LEU:O	2:C:585:GLU:N	2.53	0.41
1:A:34:VAL:O	1:A:36:LEU:N	2.54	0.41
1:B:215:VAL:O	1:B:219:LYS:N	2.41	0.41
2:C:957:LYS:O	2:C:958:SER:O	2.39	0.41
1:B:128:HIS:O	1:B:130:ALA:N	2.53	0.41
2:C:730:SER:O	2:C:732:ALA:N	2.53	0.41
3:D:354:PRO:O	3:D:355:LYS:C	2.58	0.41
2:C:434:HIS:O	2:C:435:TYR:C	2.57	0.41
2:C:937:ASP:O	2:C:938:LYS:C	2.59	0.41
3:D:808:VAL:O	3:D:809:ASP:C	2.57	0.41
3:D:1472:ILE:C	3:D:1474:ALA:H	2.24	0.41
2:C:963:LEU:O	2:C:966:LEU:N	2.54	0.41
1:B:207:PRO:O	1:B:208:LEU:C	2.59	0.41
2:C:56:GLU:O	2:C:57:GLY:C	2.59	0.41
3:D:1428:ALA:O	3:D:1429:LEU:C	2.58	0.41
3:D:659:GLY:O	3:D:662:ASP:N	2.41	0.41
3:D:1347:TYR:O	3:D:1348:LEU:O	2.38	0.41
2:C:1070:ILE:O	2:C:1071:ILE:C	2.59	0.41
3:D:347:LYS:O	3:D:348:LEU:O	2.38	0.41
3:D:313:THR:O	3:D:314:ASP:C	2.59	0.41
2:C:1062:GLY:O	2:C:1063:ARG:C	2.58	0.41
1:B:104:GLU:O	1:B:136:GLY:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:889:HIS:O	2:C:890:LEU:C	2.59	0.41
3:D:933:VAL:O	3:D:934:ALA:O	2.39	0.41
3:D:529:GLU:C	3:D:531:ALA:H	2.23	0.41
2:C:586:ARG:O	2:C:587:VAL:C	2.57	0.41
3:D:878:GLU:O	3:D:879:ASP:C	2.59	0.41
3:D:25:GLU:C	3:D:27:GLU:H	2.19	0.41
1:B:215:VAL:O	1:B:216:ALA:C	2.59	0.41
3:D:882:PHE:O	3:D:883:LEU:C	2.57	0.41
2:C:444:PRO:O	2:C:445:GLU:C	2.59	0.41
3:D:345:GLN:O	3:D:346:LEU:C	2.59	0.41
3:D:804:THR:O	3:D:805:ARG:O	2.39	0.41
3:D:847:SER:O	3:D:850:GLU:N	2.54	0.41
3:D:1349:VAL:O	3:D:1352:ILE:N	2.54	0.41
3:D:93:ILE:O	3:D:94:GLU:C	2.59	0.41
2:C:938:LYS:O	2:C:939:ARG:C	2.60	0.41
2:C:985:GLY:O	2:C:986:PRO:C	2.58	0.41
1:A:224:TYR:C	1:A:226:ALA:H	2.24	0.41
3:D:460:LEU:O	3:D:461:SER:C	2.59	0.41
3:D:493:ASP:O	3:D:496:LEU:N	2.55	0.41
3:D:546:GLY:O	3:D:547:ARG:C	2.60	0.41
3:D:1350:ASP:O	3:D:1353:GLN:N	2.54	0.41
2:C:883:GLY:O	2:C:886:LEU:N	2.53	0.41
2:C:558:ALA:O	2:C:559:LEU:C	2.59	0.40
2:C:943:VAL:C	2:C:945:ALA:N	2.72	0.40
3:D:559:LEU:O	3:D:562:VAL:N	2.54	0.40
3:D:280:LYS:C	3:D:282:MET:N	2.75	0.40
3:D:889:ALA:O	3:D:890:GLY:C	2.59	0.40
2:C:560:MET:O	2:C:563:ASN:O	2.40	0.40
3:D:219:GLU:C	3:D:221:MET:H	2.23	0.40
2:C:15:LEU:O	2:C:16:PRO:O	2.39	0.40
3:D:645:TYR:O	3:D:647:GLY:N	2.54	0.40
1:A:171:PHE:O	1:A:173:PRO:N	2.55	0.40
2:C:1083:GLU:O	2:C:1084:SER:C	2.60	0.40
1:B:83:LYS:O	1:B:84:GLU:C	2.60	0.40
2:C:854:PRO:C	2:C:856:GLU:H	2.25	0.40
1:A:40:LEU:O	1:A:41:ARG:C	2.60	0.40
1:B:58:ILE:O	1:B:59:GLU:C	2.59	0.40
3:D:1453:ALA:O	3:D:1454:GLY:C	2.59	0.40
3:D:497:GLY:O	3:D:499:TYR:N	2.54	0.40
2:C:696:LYS:C	2:C:698:ASP:N	2.75	0.40
2:C:573:ARG:O	2:C:574:ALA:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LYS:O	1:B:222:LEU:N	2.50	0.40
3:D:845:LYS:O	3:D:846:ARG:O	2.38	0.40
3:D:397:TRP:C	3:D:399:ALA:N	2.73	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	228/314 (73%)	138 (60%)	48 (21%)	42 (18%)	0	3
1	B	223/314 (71%)	133 (60%)	58 (26%)	32 (14%)	0	6
2	C	1112/1119 (99%)	640 (58%)	275 (25%)	197 (18%)	0	4
3	D	1192/1233 (97%)	536 (45%)	339 (28%)	317 (27%)	0	1
All	All	2755/2980 (92%)	1447 (52%)	720 (26%)	588 (21%)	0	2

All (588) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	45	LEU
1	A	59	GLU
1	A	74	ASP
1	A	75	VAL
1	A	90	LEU
1	A	94	MET
1	A	111	ALA
1	A	118	ALA
1	A	138	LEU
1	A	188	GLN
1	A	191	ASP

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Mol	Chain	Res	Type
1	A	198	ARG
1	A	203	GLY
1	A	226	ALA
1	A	230	ALA
1	B	36	LEU
1	B	38	ASN
1	B	63	HIS
1	B	113	ASP
1	B	116	PRO
1	B	117	SER
1	B	133	GLU
1	B	173	PRO
1	B	226	ALA
2	C	19	THR
2	C	42	VAL
2	C	55	GLU
2	C	61	LYS
2	C	63	GLY
2	C	111	ASP
2	C	124	ASP
2	C	132	ALA
2	C	183	THR
2	C	230	ARG
2	C	258	PHE
2	C	260	LEU
2	C	261	LEU
2	C	264	PRO
2	C	266	ARG
2	C	283	VAL
2	C	293	PHE
2	C	300	ASP
2	C	309	TYR
2	C	315	ALA
2	C	316	GLY
2	C	394	PHE
2	C	395	LYS
2	C	422	ARG
2	C	434	HIS
2	C	449	ILE
2	C	510	THR
2	C	574	ALA
2	C	615	TYR

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Mol	Chain	Res	Type
2	C	619	ARG
2	C	635	THR
2	C	636	ALA
2	C	656	ALA
2	C	680	ASP
2	C	686	ASP
2	C	731	GLU
2	C	735	ARG
2	C	767	PRO
2	C	768	SER
2	C	770	GLU
2	C	775	ARG
2	C	780	GLU
2	C	788	THR
2	C	790	LEU
2	C	796	GLU
2	C	800	VAL
2	C	801	VAL
2	C	816	LYS
2	C	832	LYS
2	C	972	VAL
2	C	1001	VAL
2	C	1045	ALA
2	C	1046	ALA
2	C	1055	ILE
2	C	1059	ASP
2	C	1069	ALA
2	C	1076	VAL
2	C	1077	PRO
2	C	1078	GLU
2	C	1083	GLU
2	C	1084	SER
2	C	1095	LEU
2	C	1113	GLU
3	D	23	TYR
3	D	25	GLU
3	D	29	PRO
3	D	32	ILE
3	D	34	TYR
3	D	40	GLU
3	D	41	ARG
3	D	57	GLU

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Mol	Chain	Res	Type
3	D	82	ARG
3	D	85	VAL
3	D	102	ILE
3	D	103	TRP
3	D	120	ALA
3	D	130	ASN
3	D	137	PRO
3	D	146	PRO
3	D	147	VAL
3	D	149	LYS
3	D	158	TYR
3	D	164	ARG
3	D	208	VAL
3	D	212	LEU
3	D	219	GLU
3	D	232	ASP
3	D	239	VAL
3	D	254	ARG
3	D	295	ARG
3	D	310	ARG
3	D	322	ARG
3	D	325	GLN
3	D	348	LEU
3	D	349	HIS
3	D	356	ARG
3	D	358	ALA
3	D	364	PRO
3	D	365	PHE
3	D	367	LEU
3	D	374	ALA
3	D	379	VAL
3	D	395	GLU
3	D	396	VAL
3	D	421	GLY
3	D	426	GLN
3	D	431	GLU
3	D	439	PRO
3	D	440	LEU
3	D	442	CYS
3	D	444	ALA
3	D	468	ALA
3	D	492	ARG

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Mol	Chain	Res	Type
3	D	493	ASP
3	D	495	ILE
3	D	496	LEU
3	D	504	VAL
3	D	514	ALA
3	D	532	LEU
3	D	533	ASN
3	D	536	ILE
3	D	584	THR
3	D	606	GLN
3	D	611	MET
3	D	613	VAL
3	D	617	LYS
3	D	619	SER
3	D	624	VAL
3	D	641	ASP
3	D	645	TYR
3	D	648	PHE
3	D	651	SER
3	D	655	GLY
3	D	660	ILE
3	D	713	THR
3	D	730	TYR
3	D	731	VAL
3	D	737	ALA
3	D	742	GLN
3	D	743	GLN
3	D	799	ASP
3	D	800	SER
3	D	802	TYR
3	D	805	ARG
3	D	808	VAL
3	D	846	ARG
3	D	861	GLU
3	D	865	LEU
3	D	890	GLY
3	D	901	LEU
3	D	903	CYS
3	D	917	ASP
3	D	933	VAL
3	D	936	GLU
3	D	943	THR

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Mol	Chain	Res	Type
3	D	1255	GLY
3	D	1262	LEU
3	D	1271	LYS
3	D	1296	SER
3	D	1313	VAL
3	D	1314	LYS
3	D	1317	ASP
3	D	1327	ARG
3	D	1335	LEU
3	D	1336	LEU
3	D	1339	LYS
3	D	1348	LEU
3	D	1349	VAL
3	D	1377	LYS
3	D	1424	VAL
3	D	1425	THR
3	D	1427	SER
3	D	1428	ALA
3	D	1438	ALA
3	D	1439	SER
3	D	1441	GLN
3	D	1448	THR
3	D	1450	ALA
3	D	1452	ILE
3	D	1472	ILE
1	A	73	GLU
1	A	105	GLY
1	A	122	ILE
1	A	128	HIS
1	A	152	PRO
1	A	157	GLY
1	A	166	PRO
1	A	199	ILE
1	A	232	LEU
1	B	30	ARG
1	B	37	GLY
1	B	42	ARG
1	B	60	ASP
1	B	105	GLY
1	B	119	ASP
1	B	129	ILE
1	B	204	SER

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Mol	Chain	Res	Type
2	C	7	GLY
2	C	11	GLU
2	C	14	PRO
2	C	18	LEU
2	C	38	LYS
2	C	41	ASN
2	C	66	LEU
2	C	83	CYS
2	C	90	TYR
2	C	148	PHE
2	C	288	ARG
2	C	290	LEU
2	C	336	VAL
2	C	337	GLY
2	C	350	ARG
2	C	390	GLN
2	C	409	ARG
2	C	432	ARG
2	C	433	THR
2	C	435	TYR
2	C	445	GLU
2	C	457	ALA
2	C	465	GLY
2	C	505	GLY
2	C	541	SER
2	C	557	ARG
2	C	572	ILE
2	C	573	ARG
2	C	583	LEU
2	C	584	GLU
2	C	602	GLU
2	C	616	GLU
2	C	654	LEU
2	C	659	PRO
2	C	684	PHE
2	C	685	GLU
2	C	722	ILE
2	C	771	GLU
2	C	774	LEU
2	C	808	ARG
2	C	821	GLU
2	C	867	VAL

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Mol	Chain	Res	Type
2	C	874	LEU
2	C	877	PRO
2	C	883	GLY
2	C	909	ALA
2	C	936	VAL
2	C	977	GLY
2	C	1016	ILE
2	C	1022	GLY
2	C	1048	THR
2	C	1057	SER
2	C	1080	SER
3	D	5	VAL
3	D	26	VAL
3	D	33	ASN
3	D	39	PRO
3	D	58	CYS
3	D	68	PHE
3	D	97	THR
3	D	111	LYS
3	D	136	ASP
3	D	148	GLU
3	D	150	ARG
3	D	155	ASP
3	D	195	ARG
3	D	206	GLU
3	D	213	ASP
3	D	218	PRO
3	D	220	TRP
3	D	235	PRO
3	D	260	ASN
3	D	285	GLU
3	D	293	ASN
3	D	294	GLY
3	D	305	SER
3	D	309	LEU
3	D	318	GLY
3	D	338	SER
3	D	352	GLY
3	D	400	LEU
3	D	432	GLY
3	D	441	VAL
3	D	484	GLY

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Mol	Chain	Res	Type
3	D	497	GLY
3	D	512	GLY
3	D	538	VAL
3	D	539	ALA
3	D	547	ARG
3	D	565	GLY
3	D	592	ALA
3	D	596	GLY
3	D	607	GLU
3	D	626	GLN
3	D	637	ALA
3	D	728	PRO
3	D	729	LEU
3	D	735	SER
3	D	744	ILE
3	D	778	GLU
3	D	798	ALA
3	D	807	LEU
3	D	814	ILE
3	D	848	ASP
3	D	849	ILE
3	D	870	GLU
3	D	907	TYR
3	D	915	GLY
3	D	930	VAL
3	D	934	ALA
3	D	935	ALA
3	D	938	ILE
3	D	944	GLN
3	D	1265	ALA
3	D	1322	GLY
3	D	1328	GLY
3	D	1332	PRO
3	D	1337	GLU
3	D	1363	LEU
3	D	1367	HIS
3	D	1370	ILE
3	D	1371	VAL
3	D	1372	VAL
3	D	1391	GLU
3	D	1444	THR
3	D	1446	VAL

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Mol	Chain	Res	Type
3	D	1455	LYS
3	D	1464	GLU
3	D	1465	ASN
3	D	1475	GLY
3	D	1489	GLN
1	A	15	THR
1	A	44	LEU
1	A	204	SER
1	A	209	GLU
1	A	234	PRO
1	B	32	PHE
1	B	61	VAL
1	B	75	VAL
1	B	96	SER
1	B	157	GLY
1	B	193	ASP
2	C	16	PRO
2	C	54	ILE
2	C	58	ASP
2	C	64	LEU
2	C	112	GLU
2	C	144	PRO
2	C	168	ARG
2	C	209	ARG
2	C	271	GLU
2	C	281	LEU
2	C	304	LEU
2	C	370	ALA
2	C	398	THR
2	C	532	MET
2	C	567	GLN
2	C	617	ASP
2	C	683	ASN
2	C	728	HIS
2	C	739	GLU
2	C	781	LYS
2	C	794	PRO
2	C	846	LYS
2	C	857	ASP
2	C	859	PRO
2	C	1058	ASP
2	C	1061	GLU

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Mol	Chain	Res	Type
2	C	1063	ARG
2	C	1087	VAL
2	C	1110	ASP
3	D	6	ARG
3	D	7	LYS
3	D	22	SER
3	D	56	TYR
3	D	72	VAL
3	D	108	VAL
3	D	132	TYR
3	D	152	LEU
3	D	153	LEU
3	D	169	ALA
3	D	172	GLU
3	D	175	LYS
3	D	227	PRO
3	D	273	GLU
3	D	332	VAL
3	D	353	LEU
3	D	377	PRO
3	D	391	ASP
3	D	483	SER
3	D	491	SER
3	D	498	LEU
3	D	509	LYS
3	D	556	ASP
3	D	597	GLU
3	D	602	GLU
3	D	605	ALA
3	D	634	GLU
3	D	638	ARG
3	D	642	ALA
3	D	646	TYR
3	D	732	MET
3	D	746	GLN
3	D	793	THR
3	D	806	LYS
3	D	809	ASP
3	D	847	SER
3	D	1277	ILE
3	D	1287	GLU
3	D	1333	HIS

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Mol	Chain	Res	Type
3	D	1343	ALA
3	D	1366	LYS
3	D	1369	GLU
3	D	1373	ARG
3	D	1406	ARG
3	D	1413	VAL
3	D	1451	ALA
1	A	26	GLU
1	A	126	ASP
1	A	139	TYR
1	A	171	PHE
1	A	223	ASN
1	B	5	LYS
1	B	138	LEU
2	C	39	ARG
2	C	76	PRO
2	C	223	ASP
2	C	224	GLU
2	C	519	GLY
2	C	829	GLN
2	C	878	SER
2	C	891	GLY
2	C	958	SER
2	C	1002	GLU
2	C	1079	PRO
2	C	1099	VAL
3	D	21	TRP
3	D	42	ASP
3	D	69	GLU
3	D	119	SER
3	D	161	ILE
3	D	171	GLN
3	D	193	PRO
3	D	271	ALA
3	D	290	VAL
3	D	296	ARG
3	D	297	GLY
3	D	363	LYS
3	D	372	GLU
3	D	376	ALA
3	D	394	ASP
3	D	580	ARG

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Mol	Chain	Res	Type
3	D	629	LEU
3	D	636	THR
3	D	639	LEU
3	D	644	LYS
3	D	670	GLN
3	D	724	TYR
3	D	745	ARG
3	D	750	MET
3	D	794	ALA
3	D	804	THR
3	D	810	VAL
3	D	852	GLY
3	D	914	TYR
3	D	1267	ARG
3	D	1307	LYS
3	D	1334	GLN
3	D	1395	LEU
3	D	1410	GLU
3	D	1426	LYS
1	A	165	ILE
1	A	172	SER
1	B	6	LEU
1	B	26	GLU
1	B	35	THR
2	C	91	GLN
2	C	93	PRO
2	C	105	THR
2	C	181	VAL
2	C	220	GLY
2	C	418	LEU
2	C	544	THR
2	C	546	LEU
2	C	895	TYR
2	C	904	PRO
2	C	949	LYS
2	C	1005	MET
2	C	1012	PRO
2	C	1035	MET
2	C	1097	LEU
2	C	1100	GLN
2	C	1106	ASP
2	C	1109	VAL

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Mol	Chain	Res	Type
3	D	110	SER
3	D	141	VAL
3	D	176	GLU
3	D	286	ALA
3	D	289	ALA
3	D	303	PRO
3	D	317	SER
3	D	346	LEU
3	D	389	GLN
3	D	445	PHE
3	D	557	GLU
3	D	558	ALA
3	D	578	LEU
3	D	621	LYS
3	D	627	ALA
3	D	690	GLY
3	D	703	GLN
3	D	825	ASN
3	D	931	GLY
3	D	1272	ALA
3	D	1350	ASP
3	D	1386	ASP
3	D	1449	GLU
1	A	16	GLN
1	A	217	ILE
1	B	227	ASN
2	C	65	VAL
2	C	152	PRO
2	C	292	ARG
2	C	631	SER
2	C	761	PHE
2	C	807	ARG
2	C	835	VAL
2	C	935	GLY
2	C	1062	GLY
2	C	1071	ILE
3	D	98	PRO
3	D	118	LEU
3	D	144	GLY
3	D	494	ILE
3	D	932	VAL
3	D	1263	PHE

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Mol	Chain	Res	Type
3	D	1268	PRO
3	D	1345	GLU
1	A	76	VAL
1	B	115	THR
1	B	135	GLY
2	C	9	ILE
2	C	52	PHE
2	C	417	GLY
2	C	535	SER
2	C	548	PRO
3	D	562	VAL
3	D	1415	VAL
1	A	228	PRO
2	C	1029	GLY
3	D	274	ILE
3	D	518	PRO
3	D	776	VAL
3	D	900	PRO
1	A	49	PRO
1	B	215	VAL
2	C	296	GLY
2	C	1023	GLY
3	D	595	VAL
3	D	725	PRO
2	C	125	GLY
2	C	136	ILE
2	C	894	GLY
3	D	594	ILE
2	C	645	VAL
3	D	1259	VAL

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	230/314 (73%)	-0.58	2 (0%) 85 80	194, 194, 194, 194	0
1	B	225/314 (71%)	-0.60	1 (0%) 93 90	194, 194, 194, 194	0
2	C	1114/1119 (99%)	-0.44	11 (0%) 84 78	194, 194, 194, 194	0
3	D	1196/1233 (96%)	-0.60	16 (1%) 79 72	194, 194, 194, 194	0
All	All	2765/2980 (92%)	-0.53	30 (1%) 82 76	194, 194, 194, 194	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	241	GLY	7.9
3	D	242	GLY	6.7
3	D	1315	ASP	6.2
2	C	321	GLU	3.3
3	D	1501	GLU	3.2
3	D	51	GLY	2.9
3	D	1287	GLU	2.9
3	D	1308	ASP	2.6
3	D	1489	GLN	2.6
3	D	1488	ASP	2.6
3	D	749	GLY	2.5
1	A	50	GLY	2.5
3	D	1496	GLU	2.5
1	B	160	ASP	2.5
3	D	1307	LYS	2.5
2	C	152	PRO	2.5
3	D	240	ASP	2.4
3	D	1286	GLY	2.3
2	C	364	PRO	2.3
2	C	741	GLY	2.3
2	C	178	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	1500	LYS	2.2
2	C	246	ASP	2.1
2	C	116	GLY	2.1
2	C	633	GLN	2.1
1	A	51	THR	2.1
2	C	365	ASP	2.1
3	D	1314	LYS	2.0
2	C	300	ASP	2.0
2	C	299	LYS	2.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.