



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:16 PM GMT

PDB ID : 1SUQ
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE (RT) IN
COMPLEX WITH JANSSEN-R185545
Authors : Das, K.; Arnold, E.
Deposited on : 2004-03-26
Resolution : 3.00 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

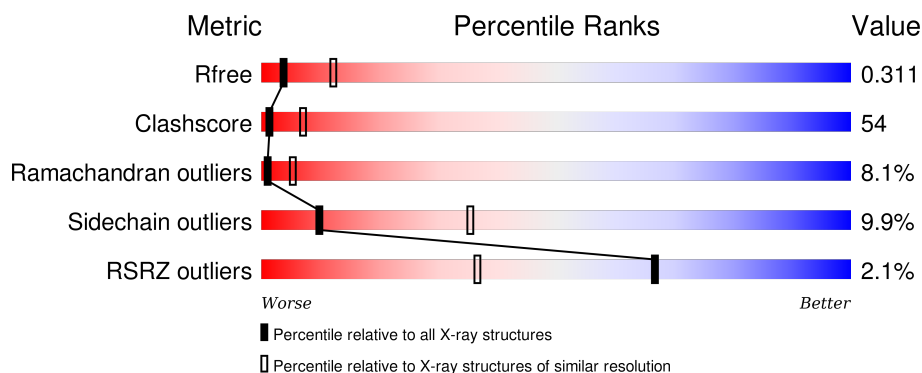
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 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	560	<div> <div></div> <div> <div></div> <div>32%</div> <div>55%</div> <div>10%</div> <div>..</div> </div> </div>
2	B	430	<div> <div>4%</div> <div> <div></div> <div>30%</div> <div>56%</div> <div>12%</div> <div>..</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8053 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 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	121	0	0
			4497	2912	748	830	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	60	0	0
			3526	2297	584	638	7			

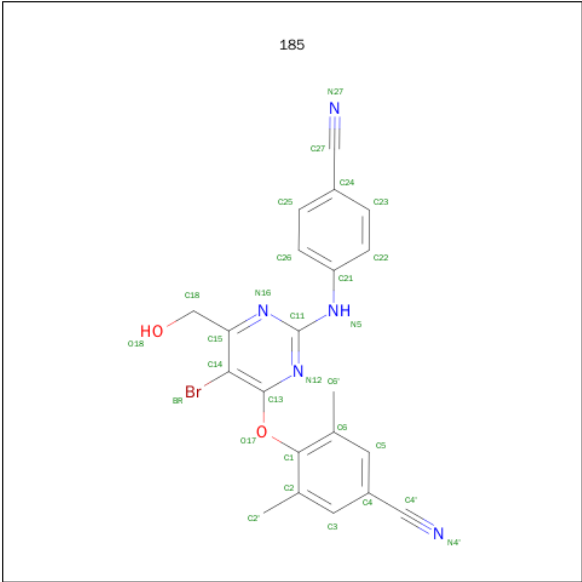
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (6-[4-(AMINOMETHYL)-2,6-DIMETHYLPHENOXY]-2-{[4-(AMINOMETHYL)PHENYL]AMINO}-5-BROMOPYRIMIDIN-4-YL)METHANOL (three-letter code: 185) (formula: C₂₁H₁₆BrN₅O₂).

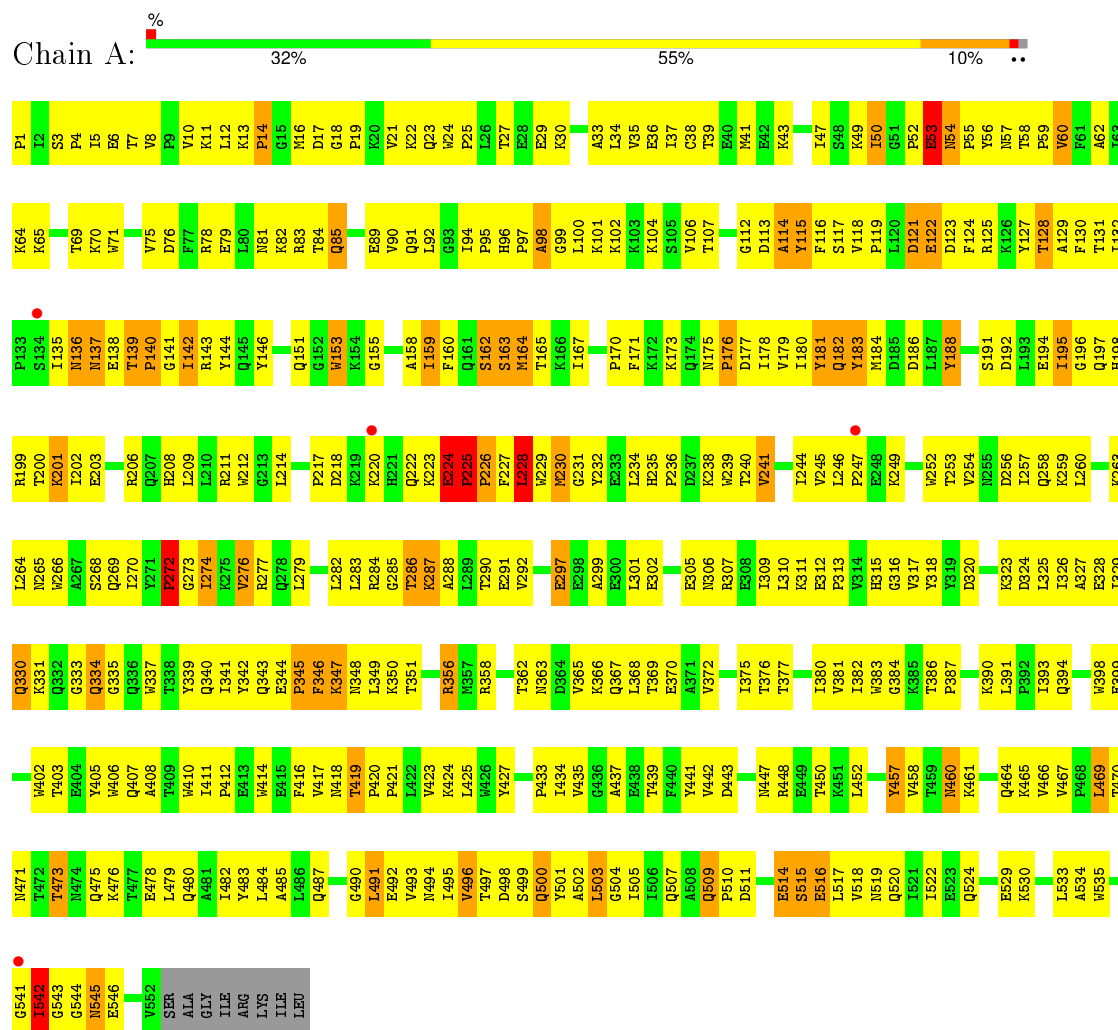


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
4	A	1	29	1	21	5	2	0	0

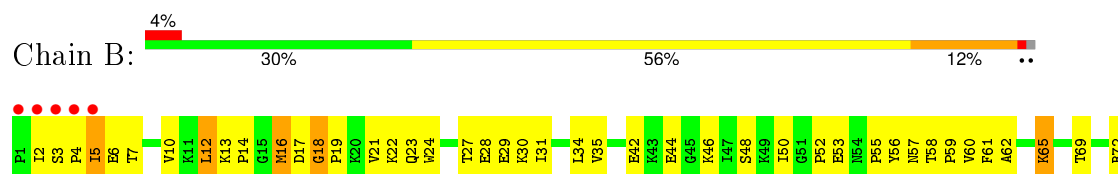
3 Residue-property plots

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

• Molecule 1: REVERSE TRANSCRIPTASE



• Molecule 2: REVERSE TRANSCRIPTASE



K73	M137	T202	L270	W337	T409
L74	E138	E203	Y271	T338	W410
W75	T139	E204	L274	Y339	L411
D76	P140	L205	K275	Q340	P412
F77	R143	R206	V276	I341	E413
R78	Y144	Q207	K277	Y342	W414
E79	Q145	L210	Q278	F346	E415
L80	Y146	R211	L279	L349	F416
T84	N147	W212	S280	K350	W417
Q85	V148	G213	L281	L351	M418
D86	L149	L214	L282	T351	T419
F87	P150	T215	L283	Y354	P420
W88	Q151	T216	K284	A355	P421
E89	W152	P217	K287	R356	L422
V90	W153	D218	A288	M357	L425
Q91	K154	K219	L289	R358	W426
L92	G155	K220	T290	G359	Y427
G93	S156	R221	E291	A360	GLN
I94	P157	Q222	V292	R361	LEU
P95	A158	K223	L293	T362	GLU
H96	I159	E224	P294	N363	
P97	F160	P225	L295	D364	
Q98	Q161	P226	T296	V365	
S162	S162	F227	E297	K366	
L100	S163	G231	E298	Q367	
K101	M164	Y232	A299	L368	
K102	T165	E233	E300	T369	
K103	K166	L234	L301	E370	
K104	I167	E235	E302	A371	
S105	L168	P236	L303	V372	
V106	E169	D237	A304	Q373	
T107	F170	K238	E305	K374	
V108	F171	W239	N306	I375	
L109	K172	L245	R307	T376	
D110	K173	L246	E308	S379	
V111	V111	L246	L309	I380	
G112	D177	P247	L310	V381	
D113	I178	E248	K311	I382	
A114	V179	K249	V314	W383	
Y115	I180	W252	H315	G384	
F116	F116	T253	G316	K385	
S117	Y183	V254	V317	T386	
V118	M184	N255	Y318	P387	
P119	D185	D256	Y319	K388	
L120	L186	I257	P320	P392	
D121	L187	Q258	P321	I393	
E122	Y188	K259	L325	Q394	
D123	V189	V261	I326	R395	
F124	G190	G262	I329	W398	
K125	S191	K263	Q330	E399	
K126	E194	L264	K331	T403	
Y127	I195	N265	Q332	E404	
T128	A129	W266	G335	Y405	
A129	Q197	A267	Q336	W406	
F130	H198	S268			
T131	R199	Q269			
L135	T200				
N136	K201				

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.11Å 69.47Å 104.26Å 90.00° 106.82° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 34.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.1 (19.99-3.00) 93.0 (34.75-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.325 0.255 , 0.311	Depositor DCC
R_{free} test set	1430 reflections (5.16%)	DCC
Wilson B-factor (Å ²)	78.4	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 71.1	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 29227 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8053	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 185

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	0.49	0/4615	0.79	5/6270 (0.1%)
2	B	0.57	1/3631 (0.0%)	0.85	0/4936
All	All	0.53	1/8246 (0.0%)	0.82	5/11206 (0.0%)

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	1	0
2	B	0	1
All	All	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	383	TRP	CB-CG	-5.36	1.40	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	PRO	C-N-CD	-9.69	99.29	120.60
1	A	225	PRO	C-N-CA	6.90	150.99	122.00
1	A	226	PRO	N-CA-C	5.41	126.16	112.10
1	A	228	LEU	CA-CB-CG	5.30	127.48	115.30
1	A	224	GLU	C-N-CD	-5.29	108.95	120.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	31	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	PHE	Sidechain

5.2 Too-close contacts [i](#)

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	4497	0	4555	494	0
2	B	3526	0	3559	375	0
3	A	1	0	0	0	0
4	A	29	0	15	8	0
All	All	8053	0	8129	849	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 54.

All (849) 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:226:PRO:HG3	1:A:235:HIS:CE1	1.72	1.25
2:B:362:THR:HG22	2:B:367:GLN:HE21	1.16	1.11
1:A:224:GLU:HB3	1:A:225:PRO:HD2	1.21	1.10
2:B:314:VAL:HG22	2:B:315:HIS:H	1.16	1.10
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.27	1.09
1:A:228:LEU:O	1:A:228:LEU:HD13	1.50	1.08
1:A:287:LYS:HG3	1:A:288:ALA:H	1.13	1.08
2:B:422:LEU:HD12	2:B:425:LEU:HD12	1.34	1.07
2:B:206:ARG:HB3	2:B:206:ARG:NH1	1.75	1.01
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.37	1.00
1:A:224:GLU:HB3	1:A:225:PRO:CD	1.92	0.99
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.46	0.97
1:A:244:ILE:HD11	1:A:310:LEU:HD22	1.47	0.97
1:A:460:ASN:HD22	1:A:461:LYS:H	1.01	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:THR:CG2	2:B:367:GLN:HE21	1.78	0.96
2:B:12:LEU:H	2:B:12:LEU:HD12	1.27	0.96
2:B:222:GLN:HG2	2:B:223:LYS:H	1.28	0.96
1:A:337:TRP:HE1	1:A:367:GLN:HE21	0.98	0.95
1:A:545:ASN:HD22	1:A:545:ASN:H	1.15	0.94
1:A:545:ASN:N	1:A:545:ASN:HD22	1.66	0.92
2:B:5:ILE:HG12	2:B:119:PRO:HD2	1.51	0.92
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.33	0.92
2:B:2:ILE:HG13	2:B:4:PRO:HD2	1.50	0.92
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.50	0.92
1:A:318:TYR:HE1	4:A:600:185:H26	1.35	0.92
1:A:53:GLU:C	1:A:55:PRO:HD3	1.91	0.91
1:A:135:ILE:HG22	1:A:137:ASN:H	1.37	0.90
2:B:314:VAL:CG2	2:B:315:HIS:H	1.85	0.90
1:A:69:THR:HG23	1:A:70:LYS:HG3	1.55	0.89
1:A:287:LYS:CG	1:A:288:ALA:H	1.83	0.89
1:A:356:ARG:NH1	1:A:358:ARG:HB2	1.89	0.88
2:B:277:ARG:H	2:B:277:ARG:HD2	1.39	0.88
1:A:460:ASN:ND2	1:A:461:LYS:H	1.71	0.88
1:A:460:ASN:HD22	1:A:461:LYS:N	1.71	0.88
2:B:314:VAL:HG22	2:B:315:HIS:N	1.86	0.88
2:B:206:ARG:HB3	2:B:206:ARG:HH11	1.38	0.86
2:B:5:ILE:HG13	2:B:6:GLU:N	1.87	0.86
1:A:27:THR:HG22	1:A:29:GLU:HG2	1.57	0.86
1:A:434:ILE:H	1:A:494:ASN:HD21	1.23	0.85
1:A:181:TYR:HH	1:A:183:TYR:HD1	1.24	0.85
1:A:224:GLU:CB	1:A:225:PRO:CD	2.54	0.85
1:A:178:ILE:HG12	1:A:201:LYS:HG2	1.59	0.85
1:A:424:LYS:HD3	1:A:425:LEU:N	1.92	0.85
1:A:287:LYS:HG3	1:A:288:ALA:N	1.90	0.84
2:B:296:THR:OG1	2:B:299:ALA:HB2	1.76	0.84
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.57	0.84
2:B:7:THR:HB	2:B:121:ASP:HA	1.58	0.84
2:B:100:LEU:HD11	2:B:106:VAL:HG22	1.60	0.84
2:B:125:ARG:O	2:B:127:TYR:N	2.11	0.83
2:B:361:HIS:H	2:B:361:HIS:CD2	1.95	0.83
1:A:182:GLN:H	1:A:182:GLN:HE21	1.22	0.83
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.43	0.83
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.60	0.83
1:A:317:VAL:HG22	1:A:318:TYR:H	1.44	0.83
2:B:362:THR:HG22	2:B:367:GLN:NE2	1.95	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:ILE:HG23	2:B:145:GLN:HG2	1.61	0.82
2:B:2:ILE:HG21	2:B:119:PRO:HG3	1.61	0.82
1:A:228:LEU:O	1:A:228:LEU:CD1	2.28	0.81
2:B:65:LYS:HA	2:B:72:ARG:HG3	1.60	0.81
1:A:362:THR:HG22	1:A:363:ASN:H	1.43	0.81
1:A:288:ALA:CB	1:A:291:GLU:HB2	2.09	0.81
1:A:382:ILE:HA	2:B:136:ASN:HD22	1.45	0.81
1:A:340:GLN:HA	1:A:351:THR:HA	1.62	0.81
1:A:270:ILE:O	1:A:272:PRO:HD3	1.81	0.81
2:B:31:ILE:O	2:B:35:VAL:HG23	1.81	0.80
2:B:195:ILE:HG23	2:B:196:GLY:H	1.45	0.80
1:A:53:GLU:HG3	1:A:53:GLU:O	1.81	0.79
2:B:104:LYS:HA	2:B:237:ASP:OD2	1.83	0.79
1:A:33:ALA:O	1:A:36:GLU:HB2	1.83	0.79
1:A:224:GLU:HG2	1:A:225:PRO:HD3	1.65	0.78
2:B:195:ILE:HG12	2:B:199:ARG:HE	1.49	0.78
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.65	0.78
1:A:3:SER:HB3	1:A:212:TRP:O	1.83	0.78
1:A:135:ILE:HB	1:A:139:THR:OG1	1.84	0.78
1:A:183:TYR:CD2	1:A:184:MET:HG3	2.18	0.78
1:A:175:ASN:HB3	1:A:178:ILE:HD13	1.64	0.78
2:B:13:LYS:O	2:B:16:MET:HB2	1.84	0.78
1:A:497:THR:HG22	1:A:498:ASP:N	1.97	0.78
1:A:337:TRP:HE1	1:A:367:GLN:NE2	1.79	0.78
2:B:393:ILE:HG21	2:B:398:TRP:HB2	1.65	0.78
1:A:19:PRO:O	1:A:56:TYR:HB3	1.84	0.78
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.15	0.77
1:A:57:ASN:ND2	1:A:58:THR:H	1.82	0.77
2:B:101:LYS:O	2:B:236:PRO:HB2	1.84	0.77
2:B:255:ASN:O	2:B:258:GLN:HB2	1.85	0.76
1:A:1:PRO:O	1:A:117:SER:HA	1.85	0.76
1:A:501:TYR:O	1:A:505:ILE:HG13	1.87	0.75
2:B:274:ILE:HG23	2:B:306:ASN:CG	2.07	0.75
1:A:356:ARG:CZ	1:A:358:ARG:HD2	2.16	0.75
1:A:60:VAL:HG21	1:A:131:THR:O	1.87	0.75
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.20	0.75
1:A:178:ILE:N	1:A:178:ILE:HD12	2.02	0.75
2:B:257:ILE:O	2:B:261:VAL:HG23	1.86	0.75
1:A:545:ASN:ND2	1:A:545:ASN:H	1.83	0.75
2:B:361:HIS:H	2:B:361:HIS:HD2	1.34	0.74
2:B:27:THR:O	2:B:31:ILE:HD12	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.68	0.74
1:A:244:ILE:CD1	1:A:310:LEU:HD22	2.17	0.74
2:B:195:ILE:HG23	2:B:196:GLY:N	2.01	0.74
1:A:188:TYR:N	1:A:188:TYR:CD1	2.56	0.73
1:A:497:THR:HG22	1:A:499:SER:H	1.51	0.73
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.23	0.73
1:A:317:VAL:HG22	1:A:318:TYR:N	2.02	0.73
1:A:188:TYR:H	1:A:188:TYR:HD1	1.35	0.73
2:B:128:THR:OG1	2:B:146:TYR:HB2	1.88	0.73
1:A:136:ASN:C	1:A:138:GLU:H	1.91	0.73
1:A:417:VAL:O	1:A:419:THR:HG23	1.89	0.72
2:B:231:GLY:O	2:B:233:GLU:HG3	1.89	0.72
2:B:369:THR:O	2:B:373:GLN:HG3	1.88	0.72
2:B:118:VAL:HB	2:B:149:LEU:HG	1.71	0.72
1:A:181:TYR:HE2	1:A:183:TYR:HB2	1.54	0.72
2:B:223:LYS:O	2:B:225:PRO:HD3	1.88	0.72
1:A:542:ILE:HD13	1:A:543:GLY:H	1.53	0.72
1:A:288:ALA:HB1	1:A:291:GLU:HB2	1.70	0.72
1:A:427:TYR:OH	1:A:509:GLN:HA	1.89	0.72
1:A:253:THR:HG22	1:A:256:ASP:OD1	1.90	0.71
2:B:156:SER:N	2:B:157:PRO:HD2	2.04	0.71
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.72	0.71
1:A:500:GLN:HE21	1:A:500:GLN:H	1.38	0.71
1:A:132:ILE:HG22	1:A:142:ILE:O	1.91	0.71
2:B:222:GLN:HG2	2:B:223:LYS:N	2.05	0.70
2:B:274:ILE:HA	2:B:306:ASN:HD21	1.56	0.70
1:A:104:LYS:HG2	1:A:192:ASP:OD1	1.91	0.70
1:A:97:PRO:HA	1:A:100:LEU:HD12	1.73	0.70
2:B:365:VAL:O	2:B:365:VAL:HG12	1.92	0.70
2:B:253:THR:O	2:B:257:ILE:HG22	1.91	0.70
1:A:542:ILE:HD13	1:A:544:GLY:N	2.07	0.70
1:A:326:ILE:N	1:A:326:ILE:HD12	2.07	0.70
1:A:259:LYS:O	1:A:263:LYS:HG3	1.91	0.69
1:A:317:VAL:HG12	1:A:348:ASN:O	1.93	0.69
2:B:5:ILE:HD13	2:B:118:VAL:HG13	1.74	0.69
1:A:5:ILE:HD11	1:A:167:ILE:HD11	1.75	0.69
2:B:252:TRP:O	2:B:292:VAL:HG13	1.92	0.69
1:A:288:ALA:CB	1:A:291:GLU:CB	2.70	0.69
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.22	0.69
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.23	0.69
1:A:226:PRO:CG	1:A:235:HIS:CE1	2.66	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.28	0.68
1:A:458:VAL:HG22	1:A:464:GLN:CG	2.16	0.68
1:A:301:LEU:O	1:A:305:GLU:HG3	1.93	0.68
1:A:460:ASN:ND2	1:A:461:LYS:N	2.37	0.68
2:B:422:LEU:HD12	2:B:425:LEU:CD1	2.17	0.67
2:B:217:PRO:O	2:B:219:LYS:N	2.27	0.67
1:A:244:ILE:HD12	1:A:310:LEU:HD13	1.75	0.67
1:A:183:TYR:HE2	1:A:184:MET:SD	2.17	0.67
1:A:497:THR:CG2	1:A:498:ASP:N	2.57	0.67
1:A:542:ILE:CG1	1:A:543:GLY:H	2.06	0.67
1:A:465:LYS:HG3	1:A:466:VAL:N	2.09	0.67
1:A:478:GLU:OE2	1:A:497:THR:HG23	1.95	0.67
2:B:376:THR:HG21	2:B:410:TRP:CH2	2.30	0.66
1:A:318:TYR:CE1	4:A:600:185:H26	2.25	0.66
2:B:100:LEU:HD11	2:B:106:VAL:CG2	2.25	0.66
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.30	0.66
2:B:94:ILE:HG12	2:B:161:GLN:CD	2.16	0.66
2:B:274:ILE:HA	2:B:306:ASN:ND2	2.10	0.66
2:B:350:LYS:HG2	2:B:351:THR:N	2.10	0.66
1:A:465:LYS:HG3	1:A:466:VAL:H	1.60	0.66
1:A:181:TYR:C	1:A:181:TYR:CD2	2.69	0.66
2:B:332:GLN:HB2	2:B:336:GLN:O	1.95	0.66
2:B:94:ILE:HG12	2:B:161:GLN:OE1	1.95	0.66
1:A:542:ILE:CD1	1:A:543:GLY:H	2.07	0.66
2:B:24:TRP:HE1	2:B:399:GLU:HG2	1.61	0.66
2:B:198:HIS:O	2:B:201:LYS:N	2.29	0.65
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.26	0.65
2:B:350:LYS:HG2	2:B:351:THR:H	1.62	0.65
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.25	0.65
1:A:3:SER:OG	1:A:5:ILE:HG13	1.96	0.65
2:B:257:ILE:HG12	2:B:283:LEU:HD11	1.78	0.65
1:A:424:LYS:HD3	1:A:425:LEU:H	1.62	0.65
1:A:21:VAL:O	1:A:57:ASN:HB3	1.97	0.65
1:A:131:THR:OG1	1:A:143:ARG:HG3	1.96	0.65
1:A:55:PRO:HB2	1:A:143:ARG:CZ	2.27	0.64
2:B:278:GLN:O	2:B:281:LYS:HG2	1.97	0.64
1:A:98:ALA:CB	1:A:350:LYS:HB2	2.27	0.64
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.32	0.64
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.78	0.64
1:A:245:VAL:O	1:A:247:PRO:HD3	1.98	0.64
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:ALA:O	2:B:375:ILE:HG13	1.97	0.64
1:A:244:ILE:CD1	1:A:310:LEU:HD13	2.27	0.64
1:A:342:TYR:HA	1:A:349:LEU:HB2	1.80	0.64
1:A:478:GLU:HG2	1:A:499:SER:HB3	1.80	0.64
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.32	0.64
2:B:395:LYS:HG2	2:B:399:GLU:OE1	1.97	0.64
1:A:518:VAL:O	1:A:522:ILE:HG13	1.97	0.63
2:B:195:ILE:CG1	2:B:199:ARG:HE	2.11	0.63
2:B:361:HIS:N	2:B:361:HIS:CD2	2.66	0.63
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.80	0.63
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.34	0.63
2:B:249:LYS:HB2	2:B:252:TRP:CZ3	2.33	0.63
1:A:328:GLU:HG2	1:A:390:LYS:CB	2.28	0.63
1:A:276:VAL:O	1:A:276:VAL:HG12	1.98	0.63
1:A:188:TYR:N	1:A:188:TYR:HD1	1.95	0.63
1:A:492:GLU:OE1	1:A:530:LYS:HD2	1.99	0.63
1:A:112:GLY:C	1:A:114:ALA:H	2.00	0.63
1:A:514:GLU:HA	1:A:514:GLU:OE1	1.98	0.63
1:A:95:PRO:HG3	1:A:181:TYR:CE1	2.34	0.62
1:A:497:THR:HG22	1:A:499:SER:N	2.13	0.62
1:A:543:GLY:HA3	2:B:284:ARG:HH11	1.64	0.62
1:A:341:ILE:O	1:A:349:LEU:HB3	2.00	0.62
1:A:195:ILE:O	1:A:199:ARG:HG3	2.00	0.62
1:A:64:LYS:HG3	1:A:64:LYS:O	1.99	0.62
1:A:173:LYS:O	1:A:176:PRO:HD3	1.99	0.62
2:B:7:THR:CB	2:B:121:ASP:HA	2.28	0.62
1:A:362:THR:HG22	1:A:363:ASN:N	2.13	0.62
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.32	0.62
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.34	0.62
2:B:131:THR:OG1	2:B:143:ARG:HG2	1.99	0.62
1:A:258:GLN:HE21	1:A:283:LEU:HD21	1.63	0.62
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.82	0.62
2:B:115:TYR:OH	2:B:184:MET:O	2.17	0.61
2:B:44:GLU:OE1	2:B:46:LYS:HE3	2.00	0.61
1:A:90:VAL:HG12	1:A:91:GLN:N	2.15	0.61
2:B:278:GLN:HE21	2:B:296:THR:CB	2.13	0.61
2:B:5:ILE:CG1	2:B:6:GLU:N	2.54	0.61
1:A:50:ILE:HD11	1:A:55:PRO:HG3	1.83	0.61
2:B:78:ARG:HD3	2:B:412:PRO:O	2.00	0.61
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.81	0.61
2:B:198:HIS:O	2:B:199:ARG:C	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:GLN:HG2	2:B:298:GLU:C	2.21	0.61
1:A:420:PRO:HA	1:A:421:PRO:O	2.01	0.61
2:B:308:GLU:C	2:B:310:LEU:H	2.04	0.61
2:B:50:ILE:HG13	2:B:143:ARG:HB3	1.82	0.61
1:A:95:PRO:HG2	1:A:229:TRP:CH2	2.35	0.61
1:A:288:ALA:HB3	1:A:291:GLU:HB3	1.83	0.60
1:A:460:ASN:HD21	1:A:461:LYS:HD3	1.66	0.60
2:B:5:ILE:CG1	2:B:6:GLU:H	2.14	0.60
1:A:112:GLY:C	1:A:114:ALA:N	2.55	0.60
1:A:408:ALA:O	2:B:393:ILE:HG13	2.01	0.60
1:A:287:LYS:CG	1:A:288:ALA:N	2.55	0.60
1:A:138:GLU:OE1	1:A:138:GLU:HA	2.01	0.60
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.36	0.60
1:A:224:GLU:CG	1:A:225:PRO:HD3	2.31	0.60
1:A:54:ASN:N	1:A:55:PRO:HD3	2.16	0.60
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.17	0.60
1:A:543:GLY:CA	2:B:284:ARG:HH11	2.15	0.59
1:A:183:TYR:HD2	1:A:184:MET:HG3	1.64	0.59
2:B:357:MET:HB3	2:B:361:HIS:CE1	2.37	0.59
2:B:56:TYR:O	2:B:143:ARG:NH2	2.35	0.59
2:B:100:LEU:HD12	2:B:100:LEU:O	2.02	0.59
2:B:266:TRP:C	2:B:268:SER:N	2.52	0.59
1:A:220:LYS:HB3	1:A:222:GLN:HE22	1.68	0.59
2:B:277:ARG:HA	2:B:280:SER:OG	2.02	0.59
2:B:305:GLU:O	2:B:308:GLU:HB3	2.03	0.59
1:A:194:GLU:O	1:A:196:GLY:N	2.35	0.59
1:A:491:LEU:O	1:A:529:GLU:HB3	2.02	0.59
1:A:433:PRO:HB3	2:B:255:ASN:HD22	1.68	0.59
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.38	0.59
1:A:478:GLU:HG2	1:A:499:SER:CB	2.33	0.59
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.37	0.59
1:A:326:ILE:CD1	1:A:343:GLN:HA	2.33	0.59
1:A:115:TYR:OH	1:A:151:GLN:HG3	2.03	0.59
2:B:363:ASN:HD21	2:B:366:LYS:HB2	1.67	0.59
1:A:191:SER:OG	1:A:198:HIS:ND1	2.36	0.59
2:B:308:GLU:O	2:B:310:LEU:N	2.35	0.58
1:A:182:GLN:N	1:A:182:GLN:HE21	1.99	0.58
2:B:267:ALA:HA	2:B:426:TRP:CZ2	2.38	0.58
1:A:178:ILE:CG1	1:A:201:LYS:HG2	2.32	0.58
1:A:545:ASN:N	1:A:545:ASN:ND2	2.39	0.58
2:B:298:GLU:HB3	2:B:301:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:O	1:A:226:PRO:O	2.21	0.58
2:B:265:ASN:O	2:B:268:SER:HB3	2.03	0.58
2:B:266:TRP:CZ3	2:B:346:PHE:CE2	2.91	0.58
2:B:267:ALA:HA	2:B:426:TRP:CH2	2.39	0.58
1:A:510:PRO:O	1:A:522:ILE:HD13	2.04	0.58
1:A:408:ALA:HB1	2:B:364:ASP:CB	2.33	0.58
1:A:53:GLU:H	1:A:55:PRO:HD3	1.68	0.58
1:A:417:VAL:HG12	1:A:419:THR:CG2	2.34	0.58
2:B:287:LYS:HZ2	2:B:287:LYS:HB3	1.69	0.57
2:B:12:LEU:N	2:B:12:LEU:HD12	2.10	0.57
2:B:27:THR:HG22	2:B:29:GLU:H	1.70	0.57
2:B:419:THR:H	2:B:420:PRO:HD3	1.68	0.57
2:B:278:GLN:HG3	2:B:296:THR:OG1	2.03	0.57
2:B:100:LEU:CD1	2:B:106:VAL:HG22	2.33	0.57
2:B:232:TYR:CE1	2:B:234:LEU:HD21	2.40	0.57
1:A:460:ASN:N	1:A:460:ASN:HD22	2.03	0.57
1:A:229:TRP:HB2	1:A:234:LEU:HD12	1.87	0.57
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.87	0.57
1:A:509:GLN:N	1:A:510:PRO:HD3	2.20	0.57
2:B:210:LEU:C	2:B:212:TRP:H	2.07	0.57
1:A:202:ILE:O	1:A:206:ARG:HB2	2.04	0.57
2:B:34:LEU:HD21	2:B:61:PHE:O	2.04	0.57
2:B:335:GLY:O	2:B:355:ALA:HA	2.05	0.57
1:A:277:ARG:HD2	1:A:334:GLN:HB3	1.85	0.57
1:A:417:VAL:HG12	1:A:417:VAL:O	2.05	0.57
2:B:84:THR:O	2:B:86:ASP:N	2.38	0.57
1:A:178:ILE:HG12	1:A:201:LYS:CG	2.31	0.57
2:B:308:GLU:C	2:B:310:LEU:N	2.57	0.57
1:A:22:LYS:HG2	1:A:24:TRP:CZ2	2.40	0.57
2:B:183:TYR:O	2:B:184:MET:HB2	2.05	0.56
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.70	0.56
1:A:164:MET:O	1:A:167:ILE:N	2.33	0.56
1:A:307:ARG:O	1:A:311:LYS:HB2	2.05	0.56
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.70	0.56
1:A:407:GLN:HG2	2:B:392:PRO:O	2.06	0.56
1:A:124:PHE:CE2	1:A:153:TRP:CZ2	2.94	0.56
2:B:210:LEU:HA	2:B:214:LEU:O	2.04	0.56
1:A:200:THR:O	1:A:203:GLU:N	2.39	0.56
2:B:91:GLN:O	2:B:92:LEU:HD23	2.05	0.56
1:A:241:VAL:CG1	1:A:266:TRP:HE1	2.18	0.56
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:LEU:HD12	2:B:385:LYS:HG3	1.87	0.56
1:A:35:VAL:O	1:A:39:THR:HG23	2.04	0.56
1:A:33:ALA:HA	1:A:36:GLU:OE1	2.05	0.56
2:B:303:LEU:O	2:B:307:ARG:HB2	2.06	0.56
2:B:314:VAL:HG13	2:B:317:VAL:HG21	1.86	0.56
1:A:97:PRO:HA	1:A:100:LEU:CD1	2.35	0.56
2:B:50:ILE:CG1	2:B:143:ARG:HB3	2.36	0.56
2:B:376:THR:HG22	2:B:380:ILE:HD11	1.87	0.56
2:B:376:THR:O	2:B:380:ILE:HG13	2.06	0.56
1:A:288:ALA:HB3	1:A:291:GLU:CB	2.35	0.56
1:A:238:LYS:HA	1:A:316:GLY:O	2.07	0.55
1:A:183:TYR:CE2	1:A:184:MET:SD	2.99	0.55
1:A:125:ARG:HG2	1:A:146:TYR:O	2.06	0.55
2:B:4:PRO:HG3	2:B:117:SER:O	2.07	0.55
2:B:275:LYS:HB2	2:B:302:GLU:OE1	2.06	0.55
1:A:96:HIS:CD2	1:A:98:ALA:HB3	2.41	0.55
2:B:261:VAL:HG21	2:B:283:LEU:HD12	1.87	0.55
2:B:53:GLU:O	2:B:55:PRO:HD3	2.06	0.55
2:B:366:LYS:O	2:B:370:GLU:HG3	2.07	0.55
2:B:139:THR:CG2	2:B:140:PRO:HD2	2.30	0.55
1:A:96:HIS:HE1	1:A:269:GLN:NE2	2.05	0.55
1:A:226:PRO:HG3	1:A:235:HIS:NE2	2.18	0.55
1:A:232:TYR:HE2	1:A:269:GLN:HE22	1.51	0.55
1:A:69:THR:CG2	1:A:70:LYS:HE2	2.37	0.55
1:A:181:TYR:OH	1:A:183:TYR:HD1	1.85	0.55
2:B:206:ARG:CZ	2:B:206:ARG:HB3	2.33	0.55
1:A:317:VAL:CG2	1:A:318:TYR:H	2.17	0.55
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.89	0.55
2:B:271:TYR:HD2	2:B:274:ILE:HD11	1.71	0.55
1:A:84:THR:HG22	1:A:124:PHE:CZ	2.33	0.55
1:A:95:PRO:O	1:A:229:TRP:HH2	1.88	0.55
2:B:278:GLN:HA	2:B:281:LYS:HE3	1.89	0.55
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.88	0.55
1:A:402:TRP:O	1:A:402:TRP:HE3	1.89	0.55
1:A:342:TYR:CD1	1:A:342:TYR:C	2.80	0.55
1:A:247:PRO:O	1:A:252:TRP:HH2	1.90	0.55
1:A:94:ILE:HG12	1:A:183:TYR:HE1	1.72	0.55
2:B:254:VAL:O	2:B:258:GLN:HG3	2.06	0.55
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.72	0.54
2:B:195:ILE:CG2	2:B:196:GLY:H	2.16	0.54
1:A:34:LEU:HB3	1:A:132:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASP:OD2	1:A:56:TYR:HE2	1.90	0.54
1:A:365:VAL:O	1:A:368:LEU:HB3	2.07	0.54
1:A:460:ASN:ND2	1:A:461:LYS:HD3	2.22	0.54
2:B:77:PHE:CD1	2:B:80:LEU:HD23	2.42	0.54
1:A:96:HIS:CE1	1:A:350:LYS:HE2	2.42	0.54
2:B:359:GLY:O	2:B:361:HIS:N	2.41	0.54
1:A:330:GLN:OE1	1:A:340:GLN:NE2	2.39	0.54
1:A:79:GLU:HG3	1:A:83:ARG:HH12	1.72	0.54
2:B:369:THR:HG23	2:B:406:TRP:HE3	1.73	0.54
1:A:377:THR:O	1:A:381:VAL:HG23	2.08	0.54
1:A:467:VAL:HG23	1:A:484:LEU:HD21	1.90	0.54
1:A:424:LYS:CD	1:A:425:LEU:H	2.20	0.54
2:B:168:LEU:C	2:B:170:PRO:HD2	2.28	0.54
1:A:390:LYS:O	1:A:391:LEU:HD23	2.07	0.54
2:B:376:THR:O	2:B:379:SER:HB3	2.07	0.54
1:A:457:TYR:CD2	1:A:457:TYR:C	2.81	0.54
2:B:129:ALA:HA	2:B:145:GLN:HA	1.89	0.54
1:A:208:HIS:HA	1:A:211:ARG:NH1	2.22	0.54
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.43	0.54
1:A:198:HIS:O	1:A:202:ILE:HG12	2.08	0.54
2:B:282:LEU:HG	2:B:293:ILE:HD12	1.90	0.54
2:B:339:TYR:C	2:B:340:GLN:OE1	2.47	0.54
2:B:103:LYS:HD2	2:B:191:SER:CA	2.39	0.53
2:B:195:ILE:CD1	2:B:199:ARG:HE	2.22	0.53
1:A:95:PRO:HG3	1:A:181:TYR:HE1	1.73	0.53
2:B:332:GLN:HA	2:B:332:GLN:OE1	2.09	0.53
2:B:341:ILE:HD11	2:B:375:ILE:HG23	1.90	0.53
1:A:155:GLY:O	1:A:159:ILE:HG13	2.08	0.53
2:B:131:THR:OG1	2:B:143:ARG:NH1	2.41	0.53
1:A:228:LEU:H	1:A:228:LEU:HD12	1.74	0.53
1:A:465:LYS:CG	1:A:466:VAL:N	2.71	0.53
2:B:266:TRP:O	2:B:267:ALA:C	2.46	0.53
1:A:457:TYR:C	1:A:457:TYR:HD2	2.12	0.53
1:A:434:ILE:HB	1:A:494:ASN:OD1	2.08	0.53
2:B:202:ILE:O	2:B:205:LEU:HB3	2.08	0.53
1:A:223:LYS:HE2	1:A:228:LEU:HG	1.89	0.53
1:A:135:ILE:HG22	1:A:137:ASN:N	2.15	0.53
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.90	0.53
1:A:178:ILE:N	1:A:178:ILE:CD1	2.70	0.53
1:A:106:VAL:HG12	1:A:107:THR:N	2.24	0.53
1:A:10:VAL:HG12	1:A:11:LYS:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LYS:HB2	1:A:337:TRP:CZ3	2.44	0.53
2:B:21:VAL:O	2:B:57:ASN:ND2	2.41	0.53
1:A:254:VAL:O	1:A:257:ILE:HG22	2.08	0.53
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.91	0.53
1:A:114:ALA:O	1:A:116:PHE:N	2.42	0.53
1:A:239:TRP:O	1:A:240:THR:HB	2.08	0.53
2:B:326:ILE:O	2:B:341:ILE:HA	2.09	0.52
2:B:363:ASN:HD22	2:B:363:ASN:C	2.10	0.52
2:B:300:GLU:OE1	2:B:300:GLU:HA	2.10	0.52
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.38	0.52
1:A:290:THR:HG22	1:A:290:THR:O	2.08	0.52
1:A:312:GLU:O	1:A:312:GLU:HG2	2.09	0.52
2:B:164:MET:O	2:B:167:ILE:N	2.42	0.52
1:A:49:LYS:HA	1:A:143:ARG:O	2.10	0.52
2:B:266:TRP:CZ3	2:B:269:GLN:HB2	2.44	0.52
2:B:107:THR:HA	2:B:232:TYR:O	2.09	0.52
1:A:382:ILE:CA	2:B:136:ASN:HD22	2.20	0.52
2:B:219:LYS:O	2:B:221:HIS:N	2.43	0.52
2:B:341:ILE:HD11	2:B:375:ILE:CG2	2.38	0.52
2:B:72:ARG:NH2	2:B:409:THR:HG22	2.25	0.52
1:A:277:ARG:HD2	1:A:334:GLN:CB	2.40	0.52
2:B:111:VAL:O	2:B:113:ASP:N	2.43	0.52
1:A:479:LEU:O	1:A:482:ILE:N	2.43	0.52
1:A:447:ASN:CG	1:A:450:THR:HG23	2.29	0.52
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.44	0.52
1:A:54:ASN:N	1:A:55:PRO:CD	2.73	0.52
1:A:317:VAL:CG2	1:A:318:TYR:N	2.73	0.52
1:A:417:VAL:HG12	1:A:419:THR:HG23	1.92	0.52
1:A:324:ASP:O	1:A:343:GLN:HG2	2.10	0.52
1:A:398:TRP:CZ2	1:A:411:ILE:HG12	2.45	0.52
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.43	0.52
2:B:255:ASN:OD1	2:B:259:LYS:HE3	2.10	0.52
2:B:252:TRP:CE3	2:B:252:TRP:HA	2.45	0.52
2:B:337:TRP:NE1	2:B:367:GLN:HB3	2.24	0.51
2:B:354:TYR:OH	2:B:370:GLU:OE1	2.27	0.51
2:B:149:LEU:N	2:B:149:LEU:HD23	2.24	0.51
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.46	0.51
1:A:318:TYR:HE1	4:A:600:185:C26	2.17	0.51
1:A:188:TYR:HD2	4:A:600:185:C4'	2.23	0.51
2:B:296:THR:H	2:B:299:ALA:HB3	1.75	0.51
2:B:17:ASP:O	2:B:18:GLY:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:SER:O	1:A:163:SER:C	2.47	0.51
1:A:5:ILE:CD1	1:A:167:ILE:HD11	2.40	0.51
2:B:96:HIS:HE1	2:B:381:VAL:O	1.92	0.51
1:A:382:ILE:HG23	2:B:136:ASN:ND2	2.24	0.51
2:B:99:GLY:O	2:B:102:LYS:HB2	2.10	0.51
2:B:419:THR:H	2:B:420:PRO:CD	2.24	0.51
2:B:266:TRP:HZ3	2:B:346:PHE:CE2	2.29	0.51
2:B:130:PHE:CE2	2:B:144:TYR:HB2	2.46	0.51
1:A:341:ILE:O	1:A:349:LEU:CB	2.59	0.51
1:A:496:VAL:CG2	1:A:534:ALA:HB3	2.41	0.51
2:B:419:THR:O	2:B:420:PRO:C	2.49	0.51
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.76	0.51
2:B:357:MET:CB	2:B:361:HIS:CE1	2.93	0.51
2:B:198:HIS:O	2:B:200:THR:N	2.44	0.51
2:B:252:TRP:HE3	2:B:252:TRP:HA	1.75	0.51
2:B:30:LYS:HD2	2:B:62:ALA:HB3	1.91	0.51
1:A:424:LYS:CD	1:A:425:LEU:N	2.70	0.51
2:B:125:ARG:O	2:B:126:LYS:C	2.50	0.51
1:A:276:VAL:CG1	1:A:276:VAL:O	2.58	0.51
1:A:460:ASN:ND2	1:A:461:LYS:CD	2.74	0.50
2:B:278:GLN:HE21	2:B:296:THR:HB	1.75	0.50
2:B:278:GLN:NE2	2:B:296:THR:OG1	2.43	0.50
1:A:323:LYS:NZ	1:A:344:GLU:OE2	2.41	0.50
2:B:314:VAL:HG13	2:B:317:VAL:CG2	2.42	0.50
1:A:288:ALA:HB1	1:A:291:GLU:CB	2.35	0.50
2:B:4:PRO:CG	2:B:117:SER:O	2.60	0.50
1:A:542:ILE:CG1	1:A:543:GLY:N	2.75	0.50
2:B:271:TYR:CE2	2:B:310:LEU:HA	2.47	0.50
1:A:95:PRO:HG2	1:A:229:TRP:HH2	1.76	0.50
1:A:132:ILE:O	1:A:132:ILE:HG23	2.12	0.50
1:A:34:LEU:HB2	1:A:132:ILE:HD11	1.92	0.50
2:B:301:LEU:O	2:B:305:GLU:HB3	2.11	0.50
1:A:325:LEU:HD23	1:A:387:PRO:HB3	1.93	0.50
2:B:203:GLU:HG3	2:B:207:GLN:HE22	1.77	0.49
1:A:182:GLN:H	1:A:182:GLN:NE2	2.00	0.49
2:B:85:GLN:NE2	2:B:89:GLU:HB2	2.27	0.49
1:A:362:THR:CG2	1:A:363:ASN:H	2.21	0.49
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.46	0.49
1:A:59:PRO:O	1:A:75:VAL:HG13	2.11	0.49
1:A:136:ASN:OD1	1:A:136:ASN:N	2.37	0.49
1:A:515:SER:O	1:A:517:LEU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:HE	1:A:370:GLU:CD	2.15	0.49
1:A:84:THR:CG2	1:A:124:PHE:HZ	2.20	0.49
1:A:37:ILE:O	1:A:41:MET:HB2	2.12	0.49
1:A:286:THR:HG22	1:A:286:THR:O	2.13	0.49
2:B:346:PHE:CD1	2:B:346:PHE:N	2.80	0.49
2:B:304:ALA:HA	2:B:307:ARG:HB2	1.93	0.49
2:B:5:ILE:HD13	2:B:118:VAL:CG1	2.40	0.49
2:B:195:ILE:CD1	2:B:199:ARG:NE	2.75	0.49
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.48	0.49
1:A:326:ILE:HB	1:A:342:TYR:CE1	2.47	0.49
2:B:2:ILE:HG13	2:B:4:PRO:CD	2.33	0.49
2:B:94:ILE:HA	2:B:161:GLN:OE1	2.13	0.49
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.48	0.49
2:B:253:THR:HG22	2:B:292:VAL:HG22	1.93	0.49
1:A:136:ASN:C	1:A:138:GLU:N	2.59	0.49
1:A:442:VAL:HG13	1:A:485:ALA:HB2	1.95	0.49
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.48	0.49
1:A:96:HIS:HD2	1:A:98:ALA:HB3	1.77	0.49
1:A:260:LEU:HD21	1:A:279:LEU:HD13	1.95	0.49
1:A:115:TYR:CE2	1:A:151:GLN:HA	2.48	0.49
2:B:296:THR:H	2:B:299:ALA:CB	2.25	0.48
2:B:416:PHE:CD2	2:B:416:PHE:N	2.80	0.48
1:A:460:ASN:N	1:A:460:ASN:ND2	2.60	0.48
1:A:102:LYS:HG3	1:A:102:LYS:O	2.13	0.48
4:A:600:185:N12	4:A:600:185:H22	2.29	0.48
2:B:276:VAL:O	2:B:279:LEU:N	2.33	0.48
2:B:7:THR:CG2	2:B:121:ASP:HA	2.43	0.48
2:B:308:GLU:O	2:B:311:LYS:N	2.45	0.48
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.48	0.48
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.31	0.48
2:B:379:SER:OG	2:B:387:PRO:HD3	2.14	0.48
1:A:284:ARG:HG3	1:A:285:GLY:N	2.29	0.48
1:A:236:PRO:HA	4:A:600:185:H25	1.94	0.48
2:B:305:GLU:HG3	2:B:306:ASN:N	2.29	0.48
2:B:363:ASN:ND2	2:B:363:ASN:C	2.67	0.48
1:A:53:GLU:O	1:A:54:ASN:HB3	2.13	0.48
2:B:31:ILE:HG22	2:B:35:VAL:CG2	2.43	0.48
1:A:341:ILE:HG21	1:A:383:TRP:CZ3	2.49	0.48
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.95	0.48
1:A:90:VAL:HG12	1:A:91:GLN:H	1.79	0.48
1:A:81:ASN:C	1:A:83:ARG:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ILE:HG23	2:B:283:LEU:HD21	1.95	0.48
1:A:339:TYR:HE2	1:A:341:ILE:HD11	1.77	0.48
2:B:364:ASP:O	2:B:366:LYS:N	2.47	0.48
1:A:81:ASN:O	1:A:83:ARG:N	2.47	0.48
1:A:473:THR:HG23	1:A:476:LYS:H	1.77	0.48
1:A:98:ALA:HB2	1:A:350:LYS:HB2	1.94	0.48
1:A:57:ASN:ND2	1:A:58:THR:N	2.58	0.48
1:A:482:ILE:HD12	1:A:502:ALA:HB1	1.95	0.48
1:A:503:LEU:HD12	1:A:533:LEU:HD13	1.96	0.47
1:A:95:PRO:CD	1:A:181:TYR:HE1	2.27	0.47
1:A:170:PRO:HG2	1:A:171:PHE:H	1.79	0.47
2:B:114:ALA:CB	2:B:214:LEU:HD22	2.43	0.47
1:A:514:GLU:O	1:A:516:GLU:N	2.47	0.47
1:A:96:HIS:CD2	1:A:98:ALA:H	2.32	0.47
2:B:314:VAL:CG1	2:B:317:VAL:HG11	2.43	0.47
2:B:222:GLN:CG	2:B:223:LYS:H	2.15	0.47
2:B:18:GLY:HA3	2:B:56:TYR:CE1	2.49	0.47
2:B:195:ILE:O	2:B:198:HIS:N	2.48	0.47
1:A:41:MET:HG2	1:A:47:ILE:HG23	1.95	0.47
2:B:13:LYS:O	2:B:16:MET:CB	2.58	0.47
2:B:376:THR:CG2	2:B:410:TRP:CH2	2.97	0.47
1:A:282:LEU:HD11	1:A:299:ALA:HB2	1.95	0.47
2:B:326:ILE:HB	2:B:342:TYR:CE1	2.50	0.47
1:A:434:ILE:HG21	1:A:492:GLU:OE2	2.15	0.47
1:A:57:ASN:HD22	1:A:58:THR:H	1.58	0.47
2:B:207:GLN:HE21	2:B:207:GLN:HB2	1.52	0.47
1:A:244:ILE:HD11	1:A:310:LEU:CD2	2.31	0.47
2:B:195:ILE:O	2:B:196:GLY:C	2.53	0.47
1:A:8:VAL:O	1:A:10:VAL:HG23	2.15	0.47
1:A:333:GLY:C	1:A:335:GLY:H	2.18	0.47
2:B:279:LEU:C	2:B:281:LYS:H	2.17	0.47
2:B:125:ARG:C	2:B:127:TYR:N	2.68	0.47
2:B:50:ILE:HD13	2:B:129:ALA:HB1	1.97	0.47
2:B:178:ILE:HG23	2:B:190:GLY:O	2.15	0.47
1:A:541:GLY:O	1:A:542:ILE:O	2.31	0.47
1:A:542:ILE:HG12	1:A:543:GLY:H	1.80	0.47
1:A:320:ASP:OD2	1:A:323:LYS:HG3	2.14	0.47
1:A:264:LEU:CD1	1:A:279:LEU:HD12	2.44	0.47
2:B:178:ILE:CG2	2:B:189:VAL:HG12	2.44	0.47
1:A:208:HIS:HE1	1:A:212:TRP:HE1	1.61	0.47
1:A:17:ASP:O	1:A:83:ARG:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:TYR:CG	1:A:375:ILE:HD11	2.50	0.47
1:A:344:GLU:HA	1:A:345:PRO:HD3	1.65	0.47
1:A:235:HIS:HB2	1:A:238:LYS:HG3	1.97	0.47
2:B:329:ILE:HD11	2:B:375:ILE:HD12	1.96	0.47
1:A:100:LEU:O	1:A:318:TYR:HB3	2.15	0.47
1:A:241:VAL:CG1	1:A:266:TRP:NE1	2.78	0.47
1:A:98:ALA:HB1	1:A:350:LYS:HB2	1.95	0.47
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.80	0.47
1:A:326:ILE:CD1	1:A:342:TYR:O	2.63	0.47
1:A:279:LEU:CD2	1:A:299:ALA:HB1	2.45	0.47
1:A:102:LYS:HA	1:A:318:TYR:HD1	1.81	0.46
2:B:48:SER:O	2:B:144:TYR:HA	2.14	0.46
2:B:145:GLN:HG3	2:B:145:GLN:O	2.15	0.46
1:A:497:THR:CG2	1:A:498:ASP:H	2.26	0.46
1:A:206:ARG:HH22	1:A:217:PRO:C	2.18	0.46
1:A:11:LYS:O	1:A:85:GLN:HG2	2.15	0.46
2:B:179:VAL:HG23	2:B:179:VAL:O	2.15	0.46
2:B:362:THR:HG21	2:B:367:GLN:HG3	1.97	0.46
1:A:55:PRO:HB2	1:A:143:ARG:NH2	2.30	0.46
2:B:23:GLN:HG3	2:B:24:TRP:O	2.15	0.46
1:A:27:THR:CG2	1:A:29:GLU:HG2	2.37	0.46
1:A:229:TRP:O	1:A:231:GLY:N	2.49	0.46
1:A:424:LYS:HD3	1:A:425:LEU:C	2.36	0.46
1:A:542:ILE:O	2:B:284:ARG:HD2	2.16	0.46
1:A:326:ILE:N	1:A:326:ILE:CD1	2.77	0.46
1:A:328:GLU:HG2	1:A:390:LYS:HB3	1.97	0.46
2:B:332:GLN:HE21	2:B:338:THR:CG2	2.27	0.46
1:A:101:LYS:HB3	4:A:600:185:H181	1.98	0.46
2:B:277:ARG:CD	2:B:277:ARG:H	2.11	0.46
1:A:34:LEU:HD12	1:A:132:ILE:HG13	1.97	0.46
1:A:158:ALA:O	1:A:160:PHE:N	2.48	0.46
2:B:332:GLN:CG	2:B:338:THR:HG23	2.45	0.46
1:A:247:PRO:O	1:A:252:TRP:CH2	2.69	0.46
1:A:306:ASN:HA	1:A:309:ILE:HD12	1.98	0.46
1:A:416:PHE:CD1	1:A:417:VAL:N	2.84	0.46
1:A:328:GLU:CG	1:A:390:LYS:HB2	2.44	0.46
2:B:326:ILE:HB	2:B:342:TYR:CD1	2.51	0.46
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.98	0.46
2:B:194:GLU:O	2:B:195:ILE:C	2.53	0.46
1:A:158:ALA:C	1:A:160:PHE:N	2.69	0.46
2:B:364:ASP:C	2:B:366:LYS:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ASP:OD2	1:A:545:ASN:HB3	2.16	0.46
1:A:328:GLU:O	1:A:339:TYR:HB2	2.15	0.46
1:A:442:VAL:O	1:A:443:ASP:HB2	2.16	0.46
1:A:186:ASP:HB2	1:A:188:TYR:HE1	1.80	0.46
1:A:97:PRO:HG2	1:A:232:TYR:CG	2.51	0.46
1:A:135:ILE:HG22	1:A:137:ASN:CB	2.45	0.46
2:B:120:LEU:HD21	2:B:124:PHE:HD2	1.81	0.46
2:B:80:LEU:HD11	2:B:124:PHE:HZ	1.81	0.46
1:A:78:ARG:CG	1:A:79:GLU:N	2.78	0.46
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.50	0.46
1:A:406:TRP:CZ3	2:B:420:PRO:HD2	2.51	0.46
1:A:34:LEU:HB2	1:A:132:ILE:CD1	2.46	0.46
1:A:101:LYS:H	4:A:600:185:H181	1.81	0.46
1:A:33:ALA:O	1:A:37:ILE:HG12	2.16	0.46
1:A:339:TYR:CD1	1:A:375:ILE:HD11	2.51	0.46
2:B:259:LYS:O	2:B:262:GLY:N	2.46	0.45
2:B:109:LEU:O	2:B:186:ASP:HB3	2.16	0.45
1:A:181:TYR:HD2	1:A:181:TYR:C	2.17	0.45
1:A:163:SER:O	1:A:167:ILE:HG13	2.15	0.45
2:B:395:LYS:CG	2:B:399:GLU:OE1	2.64	0.45
1:A:376:THR:O	1:A:380:ILE:HG13	2.17	0.45
2:B:187:LEU:HA	2:B:187:LEU:HD12	1.82	0.45
1:A:186:ASP:HB2	1:A:188:TYR:CE1	2.51	0.45
1:A:356:ARG:NE	1:A:358:ARG:HD2	2.31	0.45
2:B:278:GLN:HG3	2:B:296:THR:HG1	1.80	0.45
2:B:80:LEU:HD11	2:B:124:PHE:CZ	2.51	0.45
2:B:197:GLN:O	2:B:200:THR:HB	2.17	0.45
1:A:315:HIS:CD2	1:A:347:LYS:HD3	2.51	0.45
1:A:393:ILE:HD12	1:A:423:VAL:CG1	2.47	0.45
1:A:497:THR:CG2	1:A:499:SER:H	2.24	0.45
2:B:261:VAL:HG21	2:B:283:LEU:CD1	2.47	0.45
2:B:53:GLU:OE1	2:B:53:GLU:N	2.44	0.45
1:A:410:TRP:CG	1:A:410:TRP:O	2.70	0.45
2:B:388:LYS:NZ	2:B:415:GLU:OE1	2.41	0.45
2:B:363:ASN:HD22	2:B:363:ASN:H	1.63	0.45
1:A:503:LEU:O	1:A:504:GLY:C	2.54	0.45
2:B:124:PHE:O	2:B:125:ARG:C	2.54	0.45
2:B:60:VAL:HG13	2:B:130:PHE:HB2	1.99	0.45
2:B:85:GLN:O	2:B:89:GLU:N	2.50	0.45
2:B:10:VAL:HA	2:B:88:TRP:CZ2	2.51	0.45
1:A:490:GLY:C	1:A:492:GLU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:HD11	1:A:201:LYS:HZ2	1.81	0.45
2:B:302:GLU:HA	2:B:305:GLU:HB3	1.99	0.45
1:A:56:TYR:N	1:A:56:TYR:CD1	2.84	0.45
2:B:370:GLU:O	2:B:371:ALA:C	2.54	0.45
2:B:262:GLY:O	2:B:263:LYS:C	2.54	0.45
1:A:439:THR:CG2	1:A:441:TYR:CE1	3.00	0.45
1:A:183:TYR:O	1:A:184:MET:HB2	2.17	0.45
1:A:501:TYR:CD1	1:A:505:ILE:HD11	2.52	0.45
1:A:326:ILE:HD13	1:A:343:GLN:HA	1.98	0.45
1:A:252:TRP:O	1:A:292:VAL:HG13	2.17	0.45
2:B:58:THR:HA	2:B:59:PRO:HD3	1.87	0.45
2:B:245:VAL:HG12	2:B:246:LEU:O	2.17	0.45
1:A:273:GLY:O	1:A:274:ILE:C	2.54	0.45
1:A:235:HIS:HB2	1:A:238:LYS:CG	2.48	0.44
2:B:203:GLU:HA	2:B:206:ARG:HG3	1.99	0.44
2:B:203:GLU:HG3	2:B:207:GLN:NE2	2.32	0.44
2:B:10:VAL:HA	2:B:88:TRP:HZ2	1.83	0.44
1:A:34:LEU:CB	1:A:132:ILE:HD12	2.47	0.44
1:A:3:SER:HB2	1:A:4:PRO:HD2	1.98	0.44
1:A:22:LYS:O	1:A:23:GLN:CD	2.55	0.44
2:B:319:TYR:O	2:B:321:PRO:HD3	2.18	0.44
2:B:326:ILE:CG2	2:B:342:TYR:CE1	3.01	0.44
1:A:241:VAL:HG11	1:A:266:TRP:CD1	2.51	0.44
1:A:356:ARG:HH11	1:A:356:ARG:CG	2.31	0.44
2:B:332:GLN:HG2	2:B:338:THR:HG23	1.99	0.44
1:A:13:LYS:CB	1:A:14:PRO:HD2	2.17	0.44
2:B:103:LYS:HD2	2:B:191:SER:HA	1.98	0.44
2:B:168:LEU:CD1	2:B:180:ILE:HG21	2.47	0.44
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.16	0.44
1:A:542:ILE:HD13	1:A:543:GLY:N	2.27	0.44
1:A:125:ARG:O	1:A:128:THR:OG1	2.31	0.44
1:A:470:THR:O	1:A:471:ASN:HB3	2.17	0.44
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.47	0.44
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.82	0.44
1:A:136:ASN:O	1:A:138:GLU:N	2.51	0.44
2:B:349:LEU:HB3	2:B:383:TRP:HZ2	1.83	0.44
1:A:487:GLN:HA	1:A:524:GLN:OE1	2.18	0.44
2:B:419:THR:N	2:B:420:PRO:CD	2.80	0.44
1:A:96:HIS:CE1	1:A:269:GLN:NE2	2.86	0.44
1:A:117:SER:HB2	1:A:214:LEU:HD23	2.00	0.44
2:B:96:HIS:CE1	2:B:381:VAL:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:ASN:O	2:B:258:GLN:N	2.50	0.44
1:A:411:ILE:HA	1:A:412:PRO:HD3	1.70	0.44
1:A:411:ILE:HD12	1:A:414:TRP:CD1	2.52	0.44
2:B:153:TRP:O	2:B:155:GLY:N	2.39	0.44
2:B:153:TRP:C	2:B:155:GLY:H	2.20	0.44
1:A:39:THR:O	1:A:43:LYS:HB2	2.18	0.44
1:A:483:TYR:O	1:A:487:GLN:HG3	2.17	0.44
1:A:503:LEU:HG	1:A:507:GLN:NE2	2.33	0.43
2:B:115:TYR:C	2:B:117:SER:H	2.21	0.43
1:A:493:VAL:HG22	1:A:494:ASN:N	2.32	0.43
2:B:191:SER:OG	2:B:198:HIS:ND1	2.31	0.43
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.47	0.43
1:A:158:ALA:C	1:A:160:PHE:H	2.21	0.43
2:B:156:SER:N	2:B:157:PRO:CD	2.76	0.43
1:A:283:LEU:C	1:A:285:GLY:N	2.68	0.43
1:A:484:LEU:O	1:A:485:ALA:C	2.55	0.43
1:A:232:TYR:HE2	1:A:269:GLN:NE2	2.15	0.43
1:A:178:ILE:HD11	1:A:201:LYS:NZ	2.33	0.43
1:A:10:VAL:CG1	1:A:11:LYS:N	2.81	0.43
2:B:331:LYS:HA	2:B:337:TRP:CE3	2.53	0.43
1:A:384:GLY:O	2:B:27:THR:HG23	2.18	0.43
2:B:266:TRP:O	2:B:268:SER:N	2.52	0.43
2:B:90:VAL:HG12	2:B:91:GLN:N	2.32	0.43
1:A:452:LEU:HD22	1:A:470:THR:HG22	2.00	0.43
1:A:285:GLY:O	1:A:287:LYS:N	2.50	0.43
2:B:125:ARG:HD3	2:B:147:ASN:OD1	2.18	0.43
1:A:5:ILE:HG22	1:A:6:GLU:O	2.17	0.43
2:B:13:LYS:HG3	2:B:14:PRO:HD2	2.00	0.43
1:A:325:LEU:C	1:A:326:ILE:HD12	2.39	0.43
2:B:363:ASN:ND2	2:B:363:ASN:H	2.17	0.43
2:B:362:THR:CG2	2:B:363:ASN:N	2.81	0.43
2:B:363:ASN:ND2	2:B:363:ASN:O	2.49	0.43
2:B:393:ILE:CG2	2:B:398:TRP:HB2	2.41	0.43
2:B:315:HIS:C	2:B:317:VAL:HG22	2.39	0.43
1:A:162:SER:HB2	2:B:52:PRO:CG	2.48	0.43
1:A:279:LEU:HG	1:A:302:GLU:OE1	2.18	0.43
1:A:50:ILE:CD1	1:A:55:PRO:HG3	2.48	0.43
1:A:356:ARG:NH2	1:A:358:ARG:HD2	2.34	0.43
2:B:279:LEU:C	2:B:281:LYS:N	2.72	0.43
1:A:112:GLY:O	1:A:114:ALA:N	2.52	0.43
2:B:22:LYS:HG2	2:B:23:GLN:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:VAL:HG23	2:B:417:VAL:O	2.19	0.43
1:A:95:PRO:CG	1:A:181:TYR:HE1	2.32	0.43
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.99	0.43
1:A:406:TRP:HH2	2:B:418:ASN:CA	2.18	0.43
1:A:81:ASN:C	1:A:83:ARG:N	2.72	0.43
1:A:17:ASP:O	1:A:83:ARG:CD	2.67	0.43
2:B:46:LYS:HZ3	2:B:116:PHE:HD1	1.64	0.43
2:B:295:LEU:H	2:B:295:LEU:HD23	1.83	0.43
2:B:342:TYR:C	2:B:342:TYR:CD1	2.92	0.43
2:B:306:ASN:HA	2:B:309:ILE:HG22	2.00	0.43
1:A:226:PRO:HG3	1:A:235:HIS:HE1	1.62	0.43
2:B:314:VAL:HG13	2:B:317:VAL:HG11	2.00	0.43
1:A:232:TYR:CE2	1:A:269:GLN:NE2	2.78	0.43
1:A:162:SER:O	1:A:164:MET:N	2.52	0.43
2:B:157:PRO:HG2	2:B:158:ALA:H	1.83	0.43
2:B:46:LYS:HD3	2:B:116:PHE:CD1	2.54	0.43
2:B:76:ASP:O	2:B:78:ARG:N	2.49	0.43
1:A:495:ILE:HB	1:A:533:LEU:HD23	2.01	0.42
2:B:85:GLN:HE21	2:B:89:GLU:HB2	1.84	0.42
1:A:469:LEU:HD21	1:A:480:GLN:HG2	2.01	0.42
1:A:249:LYS:NZ	1:A:249:LYS:HB2	2.34	0.42
1:A:490:GLY:O	1:A:492:GLU:N	2.52	0.42
1:A:180:ILE:HG22	1:A:181:TYR:N	2.34	0.42
2:B:31:ILE:C	2:B:35:VAL:HG23	2.38	0.42
2:B:249:LYS:HB2	2:B:252:TRP:CE3	2.54	0.42
2:B:164:MET:O	2:B:165:THR:C	2.56	0.42
2:B:393:ILE:HG22	2:B:416:PHE:HD1	1.84	0.42
1:A:56:TYR:O	1:A:129:ALA:HB3	2.18	0.42
1:A:57:ASN:HD22	1:A:58:THR:N	2.15	0.42
1:A:418:ASN:O	1:A:419:THR:HG22	2.18	0.42
1:A:323:LYS:HB2	1:A:343:GLN:NE2	2.35	0.42
1:A:197:GLN:O	1:A:200:THR:HB	2.20	0.42
2:B:248:GLU:HA	2:B:307:ARG:HH22	1.84	0.42
1:A:496:VAL:HG12	1:A:496:VAL:O	2.19	0.42
1:A:424:LYS:CG	1:A:425:LEU:H	2.33	0.42
2:B:278:GLN:CD	2:B:298:GLU:H	2.22	0.42
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.77	0.42
2:B:325:LEU:HD12	2:B:385:LYS:CG	2.50	0.42
1:A:398:TRP:CE2	1:A:411:ILE:HG12	2.54	0.42
1:A:97:PRO:O	1:A:99:GLY:N	2.52	0.42
2:B:50:ILE:CD1	2:B:129:ALA:HB1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:GLU:HG2	1:A:499:SER:OG	2.19	0.42
1:A:90:VAL:CG1	1:A:91:GLN:N	2.81	0.42
1:A:220:LYS:CB	1:A:222:GLN:HE22	2.32	0.42
1:A:35:VAL:O	1:A:35:VAL:HG12	2.19	0.42
1:A:121:ASP:O	1:A:123:ASP:N	2.52	0.42
1:A:238:LYS:HG2	1:A:238:LYS:HZ3	1.60	0.42
1:A:331:LYS:HB2	1:A:337:TRP:CH2	2.55	0.42
2:B:278:GLN:NE2	2:B:296:THR:HB	2.35	0.42
2:B:19:PRO:HG3	2:B:80:LEU:HB2	2.00	0.42
2:B:358:ARG:O	2:B:361:HIS:NE2	2.53	0.42
1:A:153:TRP:HZ3	1:A:159:ILE:HD12	1.84	0.42
1:A:160:PHE:C	1:A:162:SER:N	2.72	0.42
1:A:399:GLU:HA	1:A:402:TRP:NE1	2.33	0.42
1:A:342:TYR:HD1	1:A:342:TYR:C	2.22	0.42
2:B:161:GLN:O	2:B:162:SER:C	2.58	0.42
2:B:76:ASP:C	2:B:78:ARG:H	2.23	0.42
2:B:363:ASN:HD22	2:B:363:ASN:N	2.17	0.42
1:A:246:LEU:CD1	1:A:310:LEU:HD12	2.49	0.42
2:B:148:VAL:O	2:B:149:LEU:C	2.57	0.42
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.87	0.42
1:A:340:GLN:CB	1:A:351:THR:HG22	2.49	0.42
1:A:326:ILE:HG22	1:A:327:ALA:N	2.35	0.42
1:A:254:VAL:HA	1:A:257:ILE:HG22	2.01	0.42
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.60	0.42
2:B:210:LEU:C	2:B:212:TRP:N	2.72	0.42
1:A:325:LEU:HD23	1:A:387:PRO:HD3	2.01	0.42
2:B:395:LYS:NZ	2:B:399:GLU:OE1	2.52	0.42
1:A:91:GLN:O	1:A:92:LEU:C	2.57	0.42
2:B:393:ILE:HG22	2:B:416:PHE:CD1	2.55	0.42
2:B:3:SER:HB2	2:B:4:PRO:CD	2.49	0.42
2:B:120:LEU:O	2:B:121:ASP:C	2.58	0.42
2:B:27:THR:HG22	2:B:28:GLU:N	2.35	0.42
1:A:419:THR:O	1:A:419:THR:OG1	2.37	0.42
2:B:395:LYS:NZ	2:B:399:GLU:OE2	2.52	0.42
1:A:245:VAL:HG12	1:A:245:VAL:O	2.19	0.42
2:B:224:GLU:O	2:B:226:PRO:HD3	2.20	0.42
1:A:139:THR:O	1:A:141:GLY:N	2.53	0.41
2:B:130:PHE:CZ	2:B:144:TYR:CB	3.01	0.41
1:A:402:TRP:O	1:A:402:TRP:CE3	2.72	0.41
2:B:282:LEU:HA	2:B:282:LEU:HD12	1.83	0.41
2:B:197:GLN:O	2:B:198:HIS:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ILE:O	1:A:341:ILE:HG23	2.20	0.41
1:A:339:TYR:CE2	1:A:341:ILE:HD11	2.55	0.41
2:B:266:TRP:O	2:B:266:TRP:CE3	2.73	0.41
1:A:240:THR:HB	1:A:315:HIS:HA	2.02	0.41
1:A:369:THR:HG1	1:A:398:TRP:HZ3	1.65	0.41
1:A:266:TRP:O	1:A:269:GLN:HG3	2.19	0.41
1:A:309:ILE:O	1:A:312:GLU:CD	2.58	0.41
1:A:519:ASN:O	1:A:520:GLN:C	2.57	0.41
1:A:503:LEU:HG	1:A:507:GLN:HE21	1.86	0.41
1:A:95:PRO:O	1:A:229:TRP:CH2	2.71	0.41
2:B:103:LYS:HG3	2:B:190:GLY:HA3	2.02	0.41
2:B:404:GLU:HB3	2:B:405:TYR:CE1	2.55	0.41
2:B:315:HIS:C	2:B:317:VAL:N	2.72	0.41
1:A:529:GLU:C	1:A:530:LYS:HG3	2.40	0.41
2:B:369:THR:HG22	2:B:373:GLN:NE2	2.35	0.41
2:B:76:ASP:O	2:B:76:ASP:CG	2.58	0.41
1:A:420:PRO:HA	1:A:421:PRO:C	2.39	0.41
2:B:382:ILE:HB	2:B:383:TRP:CE3	2.56	0.41
2:B:3:SER:HB2	2:B:4:PRO:HD3	2.02	0.41
1:A:53:GLU:N	1:A:55:PRO:HD3	2.32	0.41
1:A:178:ILE:H	1:A:178:ILE:HD12	1.83	0.41
1:A:162:SER:HB2	2:B:52:PRO:HG3	2.03	0.41
1:A:24:TRP:N	1:A:25:PRO:CD	2.83	0.41
1:A:393:ILE:HG23	1:A:393:ILE:O	2.20	0.41
1:A:434:ILE:HG21	1:A:437:ALA:HB2	2.03	0.41
1:A:515:SER:O	1:A:518:VAL:N	2.53	0.41
1:A:265:ASN:O	1:A:268:SER:N	2.49	0.41
2:B:326:ILE:HG21	2:B:342:TYR:CE1	2.56	0.41
2:B:123:ASP:O	2:B:126:LYS:HG2	2.20	0.41
2:B:195:ILE:HD13	2:B:199:ARG:HH21	1.85	0.41
1:A:209:LEU:O	1:A:212:TRP:N	2.50	0.41
1:A:509:GLN:N	1:A:510:PRO:CD	2.84	0.41
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.55	0.41
2:B:365:VAL:CG1	2:B:365:VAL:O	2.63	0.41
2:B:380:ILE:O	2:B:384:GLY:HA2	2.21	0.41
1:A:106:VAL:HG12	1:A:107:THR:H	1.85	0.41
2:B:319:TYR:CD2	2:B:383:TRP:HD1	2.39	0.41
2:B:171:PHE:C	2:B:173:LYS:N	2.73	0.41
1:A:533:LEU:HA	1:A:533:LEU:HD23	1.82	0.41
2:B:306:ASN:HA	2:B:306:ASN:HD22	1.74	0.41
1:A:386:THR:HA	1:A:387:PRO:HD2	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:C	1:A:36:GLU:N	2.74	0.40
1:A:344:GLU:O	1:A:346:PHE:N	2.54	0.40
2:B:278:GLN:NE2	2:B:296:THR:CB	2.84	0.40
2:B:60:VAL:HG12	2:B:75:VAL:HG22	2.03	0.40
2:B:369:THR:HG23	2:B:406:TRP:CE3	2.56	0.40
1:A:121:ASP:O	1:A:122:GLU:C	2.58	0.40
1:A:177:ASP:HB3	1:A:178:ILE:HD12	2.03	0.40
1:A:457:TYR:O	1:A:457:TYR:HD2	2.05	0.40
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.56	0.40
1:A:476:LYS:HD3	1:A:517:LEU:CD2	2.52	0.40
2:B:410:TRP:O	2:B:410:TRP:CE3	2.74	0.40
2:B:223:LYS:HA	2:B:223:LYS:HD3	1.90	0.40
2:B:149:LEU:H	2:B:149:LEU:HD23	1.87	0.40
2:B:279:LEU:HA	2:B:279:LEU:HD23	1.96	0.40
1:A:366:LYS:O	1:A:369:THR:HB	2.22	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	550/560 (98%)	400 (73%)	110 (20%)	40 (7%)	1	6
2	B	425/430 (99%)	319 (75%)	67 (16%)	39 (9%)	1	4
All	All	975/990 (98%)	719 (74%)	177 (18%)	79 (8%)	1	5

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	54	ASN
1	A	114	ALA

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Mol	Chain	Res	Type
1	A	122	GLU
1	A	195	ILE
1	A	297	GLU
1	A	542	ILE
2	B	18	GLY
2	B	85	GLN
2	B	116	PHE
2	B	126	LYS
2	B	218	ASP
2	B	220	LYS
2	B	231	GLY
2	B	288	ALA
2	B	360	ALA
2	B	365	VAL
2	B	419	THR
1	A	14	PRO
1	A	115	TYR
1	A	121	ASP
1	A	225	PRO
1	A	345	PRO
1	A	516	GLU
2	B	5	ILE
2	B	77	PHE
2	B	112	GLY
2	B	154	LYS
2	B	198	HIS
2	B	277	ARG
2	B	420	PRO
2	B	421	PRO
1	A	82	LYS
1	A	140	PRO
1	A	164	MET
1	A	272	PRO
1	A	287	LYS
1	A	334	GLN
1	A	491	LEU
1	A	515	SER
2	B	137	ASN
2	B	162	SER
2	B	223	LYS
2	B	297	GLU
2	B	309	ILE

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Mol	Chain	Res	Type
2	B	426	TRP
1	A	18	GLY
1	A	65	LYS
1	A	98	ALA
1	A	137	ASN
1	A	162	SER
1	A	230	MET
1	A	286	THR
2	B	65	LYS
2	B	169	GLU
2	B	199	ARG
2	B	294	PRO
2	B	314	VAL
2	B	395	LYS
1	A	53	GLU
1	A	153	TRP
1	A	165	THR
1	A	372	VAL
1	A	503	LEU
2	B	184	MET
2	B	268	SER
2	B	280	SER
2	B	404	GLU
1	A	163	SER
1	A	274	ILE
2	B	195	ILE
2	B	196	GLY
1	A	159	ILE
1	A	176	PRO
1	A	224	GLU
1	A	276	VAL
2	B	225	PRO
2	B	359	GLY
1	A	52	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	493/500 (99%)	445 (90%)	48 (10%)	10	37
2	B	388/392 (99%)	349 (90%)	39 (10%)	9	34
All	All	881/892 (99%)	794 (90%)	87 (10%)	10	35

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	53	GLU
1	A	60	VAL
1	A	71	TRP
1	A	76	ASP
1	A	85	GLN
1	A	89	GLU
1	A	113	ASP
1	A	128	THR
1	A	136	ASN
1	A	139	THR
1	A	142	ILE
1	A	179	VAL
1	A	181	TYR
1	A	182	GLN
1	A	183	TYR
1	A	188	TYR
1	A	201	LYS
1	A	218	ASP
1	A	224	GLU
1	A	225	PRO
1	A	228	LEU
1	A	230	MET
1	A	241	VAL
1	A	272	PRO
1	A	297	GLU
1	A	313	PRO
1	A	330	GLN
1	A	346	PHE
1	A	347	LYS
1	A	356	ARG
1	A	394	GLN
1	A	403	THR
1	A	405	TYR
1	A	419	THR

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Mol	Chain	Res	Type
1	A	448	ARG
1	A	457	TYR
1	A	460	ASN
1	A	469	LEU
1	A	473	THR
1	A	496	VAL
1	A	500	GLN
1	A	509	GLN
1	A	511	ASP
1	A	514	GLU
1	A	542	ILE
1	A	545	ASN
1	A	546	GLU
2	B	12	LEU
2	B	16	MET
2	B	42	GLU
2	B	69	THR
2	B	91	GLN
2	B	113	ASP
2	B	135	ILE
2	B	136	ASN
2	B	139	THR
2	B	149	LEU
2	B	162	SER
2	B	169	GLU
2	B	177	ASP
2	B	186	ASP
2	B	189	VAL
2	B	206	ARG
2	B	207	GLN
2	B	212	TRP
2	B	215	THR
2	B	218	ASP
2	B	232	TYR
2	B	239	TRP
2	B	252	TRP
2	B	266	TRP
2	B	269	GLN
2	B	271	TYR
2	B	277	ARG
2	B	317	VAL
2	B	318	TYR

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Mol	Chain	Res	Type
2	B	330	GLN
2	B	342	TYR
2	B	361	HIS
2	B	363	ASN
2	B	374	LYS
2	B	399	GLU
2	B	403	THR
2	B	414	TRP
2	B	418	ASN
2	B	419	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	151	GLN
1	A	182	GLN
1	A	222	GLN
1	A	258	GLN
1	A	269	GLN
1	A	315	HIS
1	A	332	GLN
1	A	334	GLN
1	A	367	GLN
1	A	460	ASN
1	A	475	GLN
1	A	487	GLN
1	A	500	GLN
1	A	507	GLN
1	A	509	GLN
1	A	519	ASN
2	B	136	ASN
2	B	174	GLN
2	B	207	GLN
2	B	258	GLN
2	B	330	GLN
2	B	363	ASN
2	B	367	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
4	185	A	600	-	30,31,31	1.67	5 (16%)	37,43,43	1.87	6 (16%)

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
4	185	A	600	-	-	0/14/14/14	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	185	BR-C14	-3.66	1.80	1.89
4	A	600	185	O18-C18	-3.23	1.27	1.41
4	A	600	185	C23-C22	2.82	1.43	1.38
4	A	600	185	C13-N12	3.40	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	185	C22-C21	3.80	1.45	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	185	N16-C11-N12	-4.83	118.80	126.22
4	A	600	185	C14-C13-N12	-4.19	119.52	124.00
4	A	600	185	BR-C14-C13	-2.45	117.36	121.48
4	A	600	185	C11-N16-C15	2.19	121.80	116.00
4	A	600	185	C11-N12-C13	4.32	121.60	115.31
4	A	600	185	O18-C18-C15	5.46	123.60	112.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	185	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	545/560 (97%)	-0.25	4 (0%) 89 70	38, 92, 113, 121	18 (3%)
2	B	427/430 (99%)	-0.18	16 (3%) 45 19	22, 75, 115, 121	15 (3%)
All	All	972/990 (98%)	-0.22	20 (2%) 67 36	22, 86, 114, 121	33 (3%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	226	PRO	4.4
2	B	225	PRO	3.9
2	B	5	ILE	3.9
2	B	2	ILE	3.6
2	B	3	SER	3.5
2	B	223	LYS	3.2
1	A	247	PRO	3.2
2	B	4	PRO	3.1
2	B	310	LEU	3.0
2	B	1	PRO	2.9
2	B	227	PHE	2.8
2	B	224	GLU	2.7
2	B	222	GLN	2.4
1	A	134	SER	2.4
1	A	541	GLY	2.3
1	A	220	LYS	2.3
2	B	231	GLY	2.3
2	B	358	ARG	2.3
2	B	276	VAL	2.3
2	B	360	ALA	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	185	A	600	29/29	0.91	0.35	1.97	80,94,97,119	0
3	MG	A	601	1/1	0.81	0.09	-2.76	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.