



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:44 PM GMT

PDB ID : 1QE1
Title : CRYSTAL STRUCTURE OF 3TC-RESISTANT M184I MUTANT OF HIV-1
REVERSE TRANSCRIPTASE
Authors : Sarafianos, S.G.; Das, K.; Ding, J.; Hughes, S.H.; Arnold, E.
Deposited on : 1999-07-12
Resolution : 2.85 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

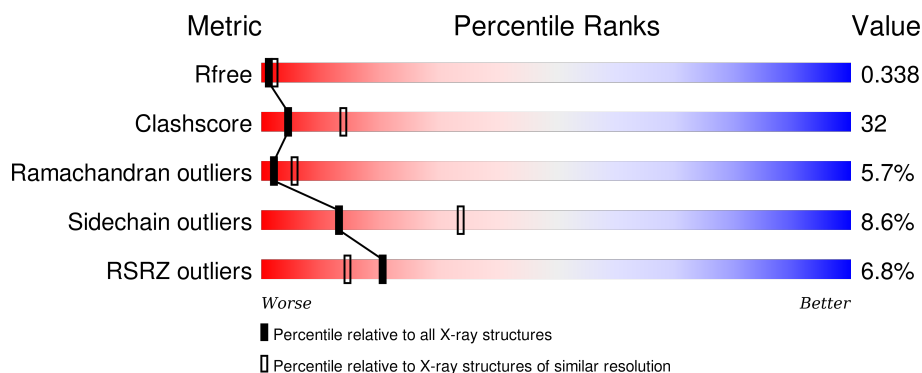
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	558	 7% 46% 44% 9%
2	B	427	 6% 44% 44% 8% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7699 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, SUBUNIT P66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	0	0
			4378	2840	728	805	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	ILE	MET	engineered	UNP P03366
A	280	SER	CYS	engineered	UNP P03366

- Molecule 2 is a protein called REVERSE TRANSCRIPTASE, SUBUNIT P51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	0	0	0
			3321	2164	549	604	4			

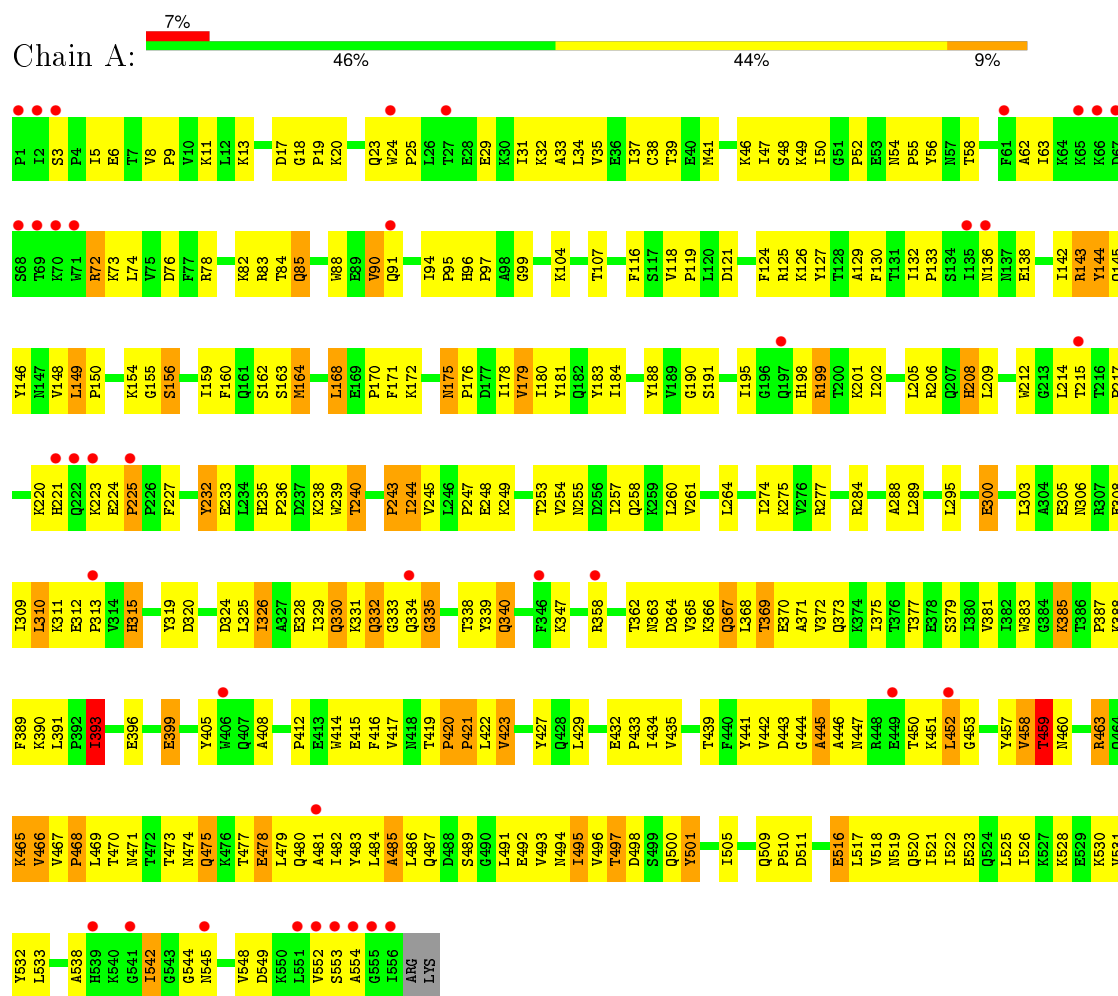
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	184	ILE	MET	engineered	UNP P03366
B	280	SER	CYS	engineered	UNP P03366

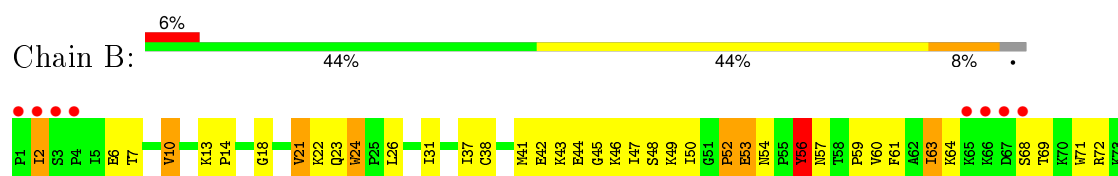
3 Residue-property plots

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, SUBUNIT P66



• Molecule 2: REVERSE TRANSCRIPTASE, SUBUNIT P51





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	238.60 Å 72.70 Å 95.30 Å 90.00° 105.60° 90.00°	Depositor
Resolution (Å)	8.00 – 2.85 20.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.85) 88.9 (20.00-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.83 Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.259 , 0.346 0.256 , 0.338	Depositor DCC
R_{free} test set	1279 reflections (4.09%)	DCC
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 69.6	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 35030 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7699	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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	0.72	0/4494	0.88	3/6130 (0.0%)
2	B	0.75	0/3416	0.92	3/4656 (0.1%)
All	All	0.73	0/7910	0.90	6/10786 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	3
All	All	0	5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	218	ASP	N-CA-C	5.87	126.84	111.00
1	A	168	LEU	CB-CG-CD1	-5.58	101.51	111.00
1	A	149	LEU	CB-CG-CD1	-5.22	102.13	111.00
1	A	143	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	B	82	LYS	CD-CE-NZ	5.13	123.50	111.70
2	B	56	TYR	N-CA-C	5.09	124.75	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	TYR	Sidechain
1	A	232	TYR	Sidechain
2	B	160	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	B	183	TYR	Sidechain
2	B	342	TYR	Sidechain

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	4378	0	4327	285	0
2	B	3321	0	3296	226	0
All	All	7699	0	7623	497	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 32.

All (497) 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)
2:B:26:LEU:HD12	2:B:133:PRO:HG3	1.34	1.08
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.36	1.03
1:A:446:ALA:HA	1:A:453:GLY:HA3	1.44	0.98
2:B:21:VAL:HG12	2:B:22:LYS:H	1.26	0.97
1:A:171:PHE:HB2	1:A:208:HIS:HD2	1.29	0.96
2:B:57:ASN:HD22	2:B:143:ARG:HH21	1.18	0.87
1:A:240:THR:HG23	1:A:315:HIS:HB3	1.56	0.87
2:B:21:VAL:HG12	2:B:22:LYS:N	1.88	0.86
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.10	0.85
2:B:348:ASN:HD22	2:B:351:THR:HG22	1.41	0.84
1:A:254:VAL:HB	1:A:289:LEU:HA	1.59	0.82
1:A:255:ASN:HD22	1:A:289:LEU:HD13	1.44	0.82
1:A:520:GLN:O	1:A:523:GLU:HG2	1.80	0.82
1:A:72:ARG:HG2	1:A:73:LYS:H	1.46	0.81
1:A:274:ILE:HA	1:A:306:ASN:ND2	1.96	0.81
2:B:195:ILE:HG12	2:B:199:ARG:NE	1.96	0.80
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.63	0.80
1:A:465:LYS:O	1:A:466:VAL:HG23	1.83	0.79
1:A:495:ILE:HD12	1:A:495:ILE:H	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:LEU:HD12	2:B:133:PRO:CG	2.14	0.78
1:A:248:GLU:O	1:A:249:LYS:HG3	1.86	0.75
1:A:441:TYR:O	1:A:548:VAL:HG21	1.87	0.74
1:A:458:VAL:O	1:A:458:VAL:HG12	1.88	0.74
2:B:327:ALA:HA	2:B:340:GLN:O	1.89	0.72
1:A:523:GLU:HA	1:A:526:ILE:HD12	1.72	0.72
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.25	0.72
2:B:115:TYR:OH	2:B:157:PRO:HB3	1.89	0.72
1:A:3:SER:OG	1:A:5:ILE:HG22	1.89	0.72
2:B:264:LEU:HD22	2:B:274:ILE:HD11	1.70	0.71
1:A:47:ILE:HD13	1:A:130:PHE:HZ	1.56	0.71
2:B:343:GLN:HG3	2:B:349:LEU:HD11	1.72	0.71
1:A:208:HIS:HE1	1:A:212:TRP:HE1	1.38	0.71
1:A:420:PRO:HB2	1:A:421:PRO:CD	2.21	0.71
2:B:38:CYS:HB3	2:B:144:TYR:CE1	2.26	0.71
1:A:452:LEU:HD21	1:A:470:THR:HG22	1.73	0.70
2:B:191:SER:OG	2:B:198:HIS:HD2	1.74	0.70
2:B:24:TRP:NE1	2:B:59:PRO:HB3	2.06	0.70
2:B:253:THR:O	2:B:257:ILE:HD12	1.92	0.70
2:B:24:TRP:N	2:B:24:TRP:CD1	2.51	0.69
2:B:257:ILE:O	2:B:261:VAL:HG23	1.91	0.69
1:A:33:ALA:O	1:A:37:ILE:HG13	1.92	0.69
1:A:305:GLU:O	1:A:308:GLU:HB3	1.90	0.69
2:B:184:ILE:HG22	2:B:185:ASP:OD1	1.92	0.69
1:A:544:GLY:O	1:A:548:VAL:HG23	1.92	0.69
1:A:116:PHE:O	1:A:148:VAL:HG11	1.93	0.69
2:B:56:TYR:O	2:B:143:ARG:NH2	2.25	0.69
2:B:21:VAL:CG1	2:B:22:LYS:H	2.05	0.69
1:A:47:ILE:HG23	1:A:145:GLN:O	1.91	0.68
1:A:199:ARG:HE	1:A:220:LYS:HE2	1.58	0.68
1:A:129:ALA:HA	1:A:145:GLN:HA	1.74	0.68
2:B:101:LYS:O	2:B:236:PRO:HB2	1.94	0.68
2:B:111:VAL:HG21	2:B:187:LEU:HD13	1.74	0.68
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.74	0.68
1:A:199:ARG:HD3	1:A:199:ARG:O	1.93	0.67
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.75	0.67
2:B:374:LYS:O	2:B:378:GLU:HG3	1.94	0.67
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.29	0.67
2:B:24:TRP:H	2:B:24:TRP:HD1	1.37	0.67
1:A:20:LYS:HG2	1:A:55:PRO:O	1.95	0.67
1:A:493:VAL:HG22	1:A:495:ILE:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LYS:HE3	1:A:127:TYR:CE2	2.29	0.66
2:B:18:GLY:HA3	2:B:56:TYR:CE2	2.31	0.66
1:A:412:PRO:O	1:A:414:TRP:HD1	1.79	0.66
1:A:442:VAL:CG1	1:A:481:ALA:HB1	2.27	0.65
2:B:195:ILE:HG12	2:B:199:ARG:HE	1.58	0.65
1:A:116:PHE:C	1:A:148:VAL:HG11	2.17	0.65
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.78	0.65
1:A:326:ILE:N	1:A:326:ILE:HD12	2.11	0.65
2:B:41:MET:HG3	2:B:46:LYS:HD2	1.76	0.65
2:B:260:LEU:HD11	2:B:303:LEU:HD21	1.79	0.65
2:B:244:ILE:HB	2:B:310:LEU:HD22	1.77	0.65
2:B:369:THR:HG22	2:B:370:GLU:N	2.11	0.65
1:A:275:LYS:H	1:A:306:ASN:HD21	1.44	0.65
1:A:466:VAL:HG12	1:A:467:VAL:N	2.12	0.65
1:A:439:THR:CG2	1:A:441:TYR:HE1	2.11	0.64
1:A:198:HIS:CE1	1:A:202:ILE:HD11	2.32	0.64
2:B:10:VAL:HG12	2:B:87:PHE:CE2	2.32	0.64
1:A:9:PRO:HA	1:A:121:ASP:OD2	1.96	0.64
1:A:221:HIS:O	1:A:227:PHE:HE2	1.81	0.64
1:A:326:ILE:H	1:A:326:ILE:HD12	1.62	0.64
1:A:442:VAL:HG12	1:A:443:ASP:N	2.13	0.64
1:A:99:GLY:HA3	2:B:136:ASN:ND2	2.14	0.64
1:A:542:ILE:CG2	2:B:283:LEU:HD13	2.28	0.63
1:A:35:VAL:O	1:A:39:THR:HG23	1.98	0.63
1:A:439:THR:HG22	1:A:441:TYR:HE1	1.62	0.63
2:B:115:TYR:CE2	2:B:156:SER:HB3	2.33	0.63
2:B:209:LEU:HD22	2:B:214:LEU:HD12	1.79	0.63
1:A:168:LEU:O	1:A:172:LYS:HG3	1.98	0.63
1:A:419:THR:CG2	1:A:420:PRO:HD2	2.29	0.63
2:B:326:ILE:O	2:B:341:ILE:HA	1.99	0.63
1:A:518:VAL:O	1:A:522:ILE:HG12	1.98	0.63
1:A:458:VAL:HG23	1:A:548:VAL:HG13	1.81	0.63
2:B:10:VAL:HG12	2:B:87:PHE:HE2	1.64	0.63
1:A:74:LEU:HD21	1:A:255:ASN:ND2	2.13	0.62
1:A:181:TYR:CE2	2:B:138:GLU:HB2	2.33	0.62
2:B:257:ILE:HD12	2:B:257:ILE:H	1.64	0.62
1:A:442:VAL:HG13	1:A:481:ALA:HB1	1.82	0.62
1:A:58:THR:HG23	1:A:76:ASP:O	1.99	0.62
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.34	0.62
2:B:52:PRO:O	2:B:54:ASN:N	2.32	0.62
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ARG:HE	2:B:409:THR:HG22	1.62	0.62
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.81	0.61
2:B:38:CYS:HB3	2:B:144:TYR:HE1	1.65	0.61
1:A:247:PRO:HD2	1:A:260:LEU:HD13	1.83	0.61
1:A:435:VAL:HG13	2:B:290:THR:CG2	2.20	0.61
2:B:244:ILE:O	2:B:310:LEU:HD13	1.99	0.61
1:A:362:THR:HG22	1:A:363:ASN:N	2.14	0.61
1:A:199:ARG:HH22	1:A:206:ARG:HD3	1.66	0.61
2:B:63:ILE:HG13	2:B:64:LYS:N	2.16	0.61
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.18	0.61
1:A:221:HIS:HB3	1:A:227:PHE:CD2	2.35	0.61
1:A:447:ASN:HB3	1:A:450:THR:OG1	1.99	0.61
2:B:251:SER:HA	2:B:257:ILE:HG13	1.83	0.60
1:A:221:HIS:HD2	1:A:227:PHE:HA	1.64	0.60
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.84	0.60
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.37	0.60
1:A:452:LEU:HA	1:A:469:LEU:O	2.01	0.60
2:B:284:ARG:O	2:B:287:LYS:NZ	2.35	0.60
1:A:17:ASP:O	1:A:83:ARG:HD3	2.02	0.60
1:A:50:ILE:HG21	1:A:145:GLN:HE21	1.67	0.59
1:A:372:VAL:HG13	1:A:389:PHE:CE1	2.37	0.59
1:A:330:GLN:HE22	1:A:340:GLN:NE2	2.00	0.59
1:A:126:LYS:HG3	1:A:127:TYR:CD2	2.36	0.59
2:B:64:LYS:NZ	2:B:68:SER:HA	2.18	0.59
1:A:253:THR:O	1:A:257:ILE:HG13	2.02	0.59
1:A:480:GLN:O	1:A:483:TYR:HB3	2.02	0.59
1:A:375:ILE:HB	1:A:389:PHE:HZ	1.66	0.59
2:B:286:THR:O	2:B:286:THR:HG22	2.02	0.59
1:A:531:VAL:HG12	1:A:532:TYR:N	2.18	0.59
1:A:389:PHE:O	1:A:414:TRP:HA	2.02	0.59
1:A:47:ILE:CG2	1:A:144:TYR:HB3	2.32	0.59
1:A:445:ALA:O	1:A:477:THR:HG21	2.03	0.59
2:B:43:LYS:C	2:B:45:GLY:H	2.06	0.58
2:B:160:PHE:HD2	2:B:160:PHE:O	1.84	0.58
1:A:72:ARG:CG	1:A:73:LYS:H	2.15	0.58
2:B:52:PRO:HD2	2:B:53:GLU:OE1	2.03	0.58
1:A:215:THR:O	1:A:217:PRO:HD3	2.03	0.58
1:A:74:LEU:HD21	1:A:255:ASN:HD21	1.66	0.58
1:A:420:PRO:O	1:A:422:LEU:N	2.36	0.58
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.85	0.58
2:B:85:GLN:O	2:B:85:GLN:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:LYS:O	2:B:104:LYS:HD3	2.03	0.58
1:A:363:ASN:HB3	1:A:366:LYS:HB3	1.85	0.58
2:B:63:ILE:CG2	2:B:74:LEU:HD23	2.34	0.58
2:B:43:LYS:O	2:B:45:GLY:N	2.37	0.58
1:A:377:THR:O	1:A:381:VAL:HG23	2.04	0.57
2:B:82:LYS:HE2	2:B:413:GLU:OE2	2.04	0.57
2:B:195:ILE:HG12	2:B:199:ARG:CZ	2.33	0.57
1:A:319:TYR:CD1	1:A:320:ASP:N	2.72	0.57
1:A:175:ASN:O	1:A:178:ILE:HG22	2.05	0.57
2:B:126:LYS:HE3	2:B:127:TYR:CE2	2.39	0.57
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.85	0.57
2:B:254:VAL:HB	2:B:289:LEU:O	2.04	0.57
2:B:49:LYS:HG2	2:B:144:TYR:CE2	2.39	0.57
2:B:246:LEU:HD12	2:B:307:ARG:HA	1.87	0.57
1:A:164:MET:SD	1:A:214:LEU:CD1	2.93	0.57
2:B:54:ASN:HD21	2:B:129:ALA:HB2	1.69	0.56
1:A:473:THR:O	1:A:477:THR:HG23	2.06	0.56
2:B:191:SER:OG	2:B:198:HIS:CD2	2.57	0.56
2:B:96:HIS:CD2	2:B:384:GLY:HA3	2.41	0.56
1:A:47:ILE:HG22	1:A:48:SER:N	2.21	0.56
1:A:221:HIS:CD2	1:A:227:PHE:HA	2.40	0.56
2:B:331:LYS:O	2:B:332:GLN:HG2	2.06	0.56
2:B:348:ASN:ND2	2:B:351:THR:HG22	2.17	0.55
1:A:442:VAL:CG1	1:A:443:ASP:N	2.70	0.55
2:B:94:ILE:H	2:B:94:ILE:HD13	1.70	0.55
1:A:47:ILE:HG21	1:A:144:TYR:HB3	1.86	0.55
2:B:24:TRP:HZ3	2:B:403:THR:HG21	1.68	0.55
1:A:369:THR:HG22	1:A:370:GLU:N	2.22	0.55
1:A:434:ILE:HD12	1:A:434:ILE:H	1.72	0.55
2:B:56:TYR:N	2:B:56:TYR:CD1	2.75	0.55
2:B:260:LEU:HD21	2:B:303:LEU:HD11	1.88	0.55
1:A:221:HIS:HB3	1:A:227:PHE:CE2	2.41	0.55
2:B:293:ILE:HG23	2:B:294:PRO:HD2	1.89	0.55
1:A:78:ARG:O	1:A:82:LYS:HG3	2.06	0.55
2:B:49:LYS:HG2	2:B:144:TYR:HE2	1.71	0.55
1:A:525:LEU:HD23	1:A:531:VAL:HG21	1.88	0.55
2:B:410:TRP:HE3	2:B:410:TRP:O	1.89	0.55
2:B:366:LYS:O	2:B:370:GLU:HG3	2.07	0.54
2:B:63:ILE:HG21	2:B:74:LEU:HD23	1.88	0.54
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.87	0.54
2:B:258:GLN:HG2	2:B:283:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:PHE:CD2	2:B:160:PHE:O	2.59	0.54
1:A:178:ILE:HA	1:A:191:SER:HB3	1.89	0.54
1:A:125:ARG:HB3	1:A:145:GLN:OE1	2.08	0.54
1:A:56:TYR:O	1:A:143:ARG:NH2	2.39	0.54
1:A:368:LEU:O	1:A:371:ALA:HB3	2.07	0.54
1:A:47:ILE:HG22	1:A:48:SER:H	1.72	0.54
2:B:87:PHE:CE1	2:B:155:GLY:HA2	2.42	0.54
2:B:72:ARG:HH21	2:B:409:THR:HB	1.73	0.54
1:A:516:GLU:O	1:A:519:ASN:HB2	2.07	0.54
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.90	0.54
1:A:415:GLU:HG2	1:A:416:PHE:N	2.21	0.54
2:B:271:TYR:CD1	2:B:271:TYR:N	2.76	0.54
1:A:328:GLU:O	1:A:339:TYR:HA	2.08	0.54
1:A:480:GLN:HE22	1:A:483:TYR:HD2	1.56	0.54
2:B:2:ILE:HG22	2:B:117:SER:O	2.07	0.54
2:B:419:THR:HG21	2:B:423:VAL:HG23	1.89	0.54
2:B:24:TRP:CH2	2:B:61:PHE:CD2	2.96	0.53
1:A:148:VAL:HG12	1:A:149:LEU:H	1.73	0.53
2:B:54:ASN:ND2	2:B:129:ALA:HB2	2.23	0.53
1:A:275:LYS:N	1:A:306:ASN:HD21	2.06	0.53
1:A:466:VAL:CG1	1:A:467:VAL:N	2.71	0.53
1:A:493:VAL:CG2	1:A:494:ASN:N	2.71	0.53
2:B:49:LYS:CG	2:B:144:TYR:HE2	2.21	0.53
1:A:362:THR:CG2	1:A:363:ASN:N	2.72	0.53
1:A:319:TYR:HD1	1:A:320:ASP:H	1.55	0.53
2:B:282:LEU:HD22	2:B:293:ILE:HG23	1.90	0.53
2:B:10:VAL:HG21	2:B:153:TRP:HH2	1.74	0.53
2:B:50:ILE:HG23	2:B:145:GLN:HG2	1.91	0.53
1:A:90:VAL:HG23	1:A:91:GLN:N	2.24	0.53
2:B:60:VAL:HG11	2:B:130:PHE:CD1	2.44	0.53
2:B:94:ILE:N	2:B:94:ILE:HD13	2.24	0.53
2:B:78:ARG:NH1	2:B:412:PRO:O	2.38	0.53
1:A:363:ASN:OD1	1:A:364:ASP:N	2.42	0.53
2:B:42:GLU:O	2:B:42:GLU:HG2	2.09	0.53
2:B:255:ASN:O	2:B:258:GLN:HB2	2.09	0.52
2:B:94:ILE:HB	2:B:95:PRO:HD2	1.90	0.52
2:B:314:VAL:HG12	2:B:315:HIS:N	2.25	0.52
2:B:195:ILE:HG23	2:B:196:GLY:N	2.25	0.52
1:A:50:ILE:HD13	1:A:144:TYR:O	2.09	0.52
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.90	0.52
1:A:501:TYR:CE2	1:A:505:ILE:HD11	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:GLU:O	1:A:309:ILE:HG13	2.08	0.52
1:A:365:VAL:C	1:A:367:GLN:H	2.13	0.52
2:B:293:ILE:HG23	2:B:294:PRO:CD	2.40	0.52
1:A:363:ASN:O	1:A:367:GLN:HG3	2.10	0.52
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.92	0.52
1:A:333:GLY:O	1:A:335:GLY:N	2.42	0.52
1:A:159:ILE:HG22	1:A:160:PHE:N	2.24	0.52
1:A:17:ASP:OD1	1:A:18:GLY:N	2.41	0.52
1:A:146:TYR:CE2	1:A:150:PRO:HA	2.44	0.52
1:A:171:PHE:CE2	1:A:205:LEU:HA	2.44	0.52
1:A:542:ILE:O	2:B:283:LEU:HB3	2.08	0.52
2:B:125:ARG:NH2	2:B:147:ASN:O	2.43	0.52
1:A:417:VAL:HG22	1:A:419:THR:OG1	2.10	0.52
2:B:266:TRP:O	2:B:269:GLN:HG3	2.10	0.52
2:B:264:LEU:CD2	2:B:274:ILE:HD11	2.39	0.51
1:A:331:LYS:HG2	1:A:332:GLN:H	1.75	0.51
1:A:459:THR:HG23	1:A:463:ARG:HB3	1.92	0.51
1:A:132:ILE:HB	1:A:142:ILE:HB	1.92	0.51
1:A:255:ASN:ND2	1:A:289:LEU:HD13	2.20	0.51
2:B:24:TRP:HE1	2:B:59:PRO:HB3	1.75	0.51
1:A:8:VAL:O	1:A:121:ASP:HB2	2.10	0.51
2:B:353:LYS:HG3	2:B:353:LYS:O	2.11	0.51
2:B:319:TYR:CD1	2:B:383:TRP:CD1	2.98	0.51
1:A:495:ILE:HG22	1:A:496:VAL:N	2.24	0.51
2:B:152:GLY:O	2:B:153:TRP:O	2.29	0.51
2:B:52:PRO:HG2	2:B:53:GLU:H	1.76	0.51
2:B:63:ILE:O	2:B:71:TRP:CE3	2.64	0.51
1:A:497:THR:HG22	1:A:498:ASP:H	1.75	0.51
1:A:235:HIS:HB2	1:A:238:LYS:O	2.10	0.51
1:A:149:LEU:HD21	1:A:159:ILE:HG21	1.91	0.50
1:A:484:LEU:O	1:A:486:LEU:N	2.44	0.50
1:A:427:TYR:CD1	1:A:429:LEU:HD21	2.46	0.50
1:A:466:VAL:CG1	1:A:467:VAL:H	2.25	0.50
1:A:385:LYS:HB2	1:A:385:LYS:NZ	2.26	0.50
1:A:549:ASP:O	1:A:553:SER:N	2.41	0.50
1:A:420:PRO:HB2	1:A:421:PRO:HD3	1.92	0.50
2:B:50:ILE:HG21	2:B:145:GLN:HE21	1.77	0.50
2:B:208:HIS:ND1	2:B:208:HIS:C	2.65	0.50
2:B:216:THR:HG22	2:B:217:PRO:O	2.11	0.50
2:B:282:LEU:HD22	2:B:293:ILE:CG2	2.42	0.50
2:B:396:GLU:O	2:B:400:THR:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PHE:HA	1:A:148:VAL:HG11	1.94	0.50
1:A:208:HIS:O	1:A:212:TRP:HD1	1.94	0.50
1:A:107:THR:HG21	1:A:220:LYS:HZ3	1.77	0.50
1:A:18:GLY:HA3	1:A:56:TYR:CE2	2.46	0.50
1:A:148:VAL:HG12	1:A:149:LEU:N	2.27	0.49
1:A:479:LEU:HB3	1:A:517:LEU:HD21	1.93	0.49
1:A:3:SER:HB3	1:A:119:PRO:HD3	1.94	0.49
2:B:72:ARG:HH11	2:B:72:ARG:HG3	1.76	0.49
2:B:130:PHE:CZ	2:B:144:TYR:CB	2.95	0.49
1:A:199:ARG:NH2	1:A:206:ARG:HD3	2.27	0.49
2:B:63:ILE:O	2:B:71:TRP:HE3	1.95	0.49
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.93	0.49
2:B:21:VAL:CG1	2:B:22:LYS:N	2.61	0.49
1:A:245:VAL:HG12	1:A:245:VAL:O	2.12	0.49
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.94	0.49
1:A:491:LEU:O	1:A:492:GLU:HG2	2.13	0.49
2:B:113:ASP:OD1	2:B:113:ASP:N	2.45	0.49
2:B:13:LYS:HB3	2:B:14:PRO:HD2	1.94	0.49
1:A:458:VAL:O	1:A:458:VAL:CG1	2.59	0.49
1:A:434:ILE:HD12	1:A:434:ILE:N	2.28	0.48
2:B:271:TYR:HD1	2:B:271:TYR:H	1.57	0.48
1:A:480:GLN:NE2	1:A:483:TYR:HD2	2.10	0.48
2:B:118:VAL:HG12	2:B:119:PRO:O	2.13	0.48
1:A:427:TYR:O	1:A:427:TYR:CD1	2.66	0.48
2:B:235:HIS:C	2:B:237:ASP:H	2.17	0.48
1:A:72:ARG:HG2	1:A:73:LYS:N	2.22	0.48
1:A:466:VAL:HG12	1:A:467:VAL:H	1.79	0.48
1:A:358:ARG:CB	1:A:362:THR:HG23	2.42	0.48
2:B:64:LYS:HZ3	2:B:68:SER:HA	1.78	0.48
1:A:5:ILE:CG1	1:A:6:GLU:N	2.77	0.48
2:B:60:VAL:HG13	2:B:130:PHE:HB2	1.94	0.48
1:A:365:VAL:HG23	1:A:366:LYS:N	2.29	0.48
1:A:485:ALA:O	1:A:489:SER:HB2	2.13	0.48
2:B:277:ARG:C	2:B:279:LEU:H	2.16	0.48
1:A:419:THR:HG22	1:A:420:PRO:HD2	1.96	0.48
2:B:43:LYS:C	2:B:45:GLY:N	2.67	0.48
2:B:78:ARG:HD3	2:B:411:ILE:O	2.14	0.48
2:B:183:TYR:CD2	2:B:380:ILE:HD13	2.49	0.48
2:B:85:GLN:NE2	2:B:87:PHE:CD2	2.81	0.47
2:B:293:ILE:HG23	2:B:294:PRO:N	2.29	0.47
1:A:224:GLU:HA	1:A:225:PRO:HD2	1.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PRO:HG2	1:A:232:TYR:CE2	2.48	0.47
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.44	0.47
2:B:2:ILE:HA	2:B:117:SER:O	2.13	0.47
2:B:56:TYR:H	2:B:56:TYR:HD1	1.59	0.47
1:A:379:SER:OG	1:A:387:PRO:HG3	2.14	0.47
2:B:250:ASP:OD2	2:B:303:LEU:HD13	2.14	0.47
1:A:257:ILE:O	1:A:261:VAL:HG23	2.15	0.47
1:A:331:LYS:HG2	1:A:332:GLN:N	2.30	0.47
2:B:100:LEU:HD12	2:B:100:LEU:O	2.14	0.47
2:B:18:GLY:HA3	2:B:56:TYR:HE2	1.75	0.47
1:A:31:ILE:HD11	1:A:133:PRO:C	2.35	0.47
1:A:363:ASN:HB3	1:A:366:LYS:CB	2.45	0.47
2:B:253:THR:O	2:B:256:ASP:HB2	2.15	0.47
2:B:92:LEU:HD13	2:B:184:ILE:HD11	1.97	0.47
1:A:94:ILE:HG23	1:A:95:PRO:CD	2.45	0.47
2:B:132:ILE:HG23	2:B:133:PRO:HD2	1.97	0.47
1:A:435:VAL:CG1	2:B:290:THR:HG21	2.26	0.47
2:B:343:GLN:CG	2:B:349:LEU:HD11	2.44	0.47
2:B:24:TRP:HE1	2:B:59:PRO:CB	2.28	0.47
1:A:295:LEU:HD12	1:A:300:GLU:OE2	2.15	0.46
1:A:84:THR:HG22	1:A:154:LYS:HD3	1.97	0.46
1:A:63:ILE:HD11	1:A:74:LEU:HD13	1.97	0.46
1:A:443:ASP:O	1:A:481:ALA:CB	2.63	0.46
2:B:254:VAL:HB	2:B:289:LEU:HA	1.97	0.46
1:A:260:LEU:HG	1:A:264:LEU:HD12	1.97	0.46
2:B:326:ILE:N	2:B:326:ILE:HD12	2.30	0.46
1:A:369:THR:O	1:A:372:VAL:N	2.48	0.46
2:B:124:PHE:CE2	2:B:153:TRP:CZ2	3.03	0.46
1:A:363:ASN:OD1	1:A:365:VAL:HG22	2.16	0.46
1:A:443:ASP:OD1	1:A:444:GLY:N	2.39	0.46
1:A:168:LEU:HD13	1:A:180:ILE:HG21	1.98	0.46
1:A:54:ASN:HA	1:A:55:PRO:HD3	1.64	0.46
1:A:243:PRO:HG2	1:A:243:PRO:O	2.16	0.46
2:B:139:THR:HA	2:B:140:PRO:HD3	1.80	0.46
1:A:466:VAL:O	1:A:467:VAL:HG23	2.16	0.46
1:A:452:LEU:HG	1:A:470:THR:HA	1.98	0.46
1:A:319:TYR:CD2	1:A:383:TRP:HD1	2.33	0.46
1:A:460:ASN:HA	2:B:286:THR:HG22	1.97	0.46
1:A:11:LYS:O	1:A:85:GLN:HB3	2.16	0.46
1:A:309:ILE:C	1:A:311:LYS:H	2.20	0.46
2:B:331:LYS:C	2:B:332:GLN:HG2	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:VAL:CG1	2:B:130:PHE:HB2	2.47	0.45
2:B:277:ARG:O	2:B:279:LEU:N	2.46	0.45
1:A:458:VAL:HB	1:A:548:VAL:HG22	1.97	0.45
1:A:373:GLN:NE2	2:B:397:THR:HG23	2.30	0.45
1:A:255:ASN:O	1:A:258:GLN:HB3	2.17	0.45
1:A:458:VAL:CG2	1:A:548:VAL:HG22	2.46	0.45
1:A:427:TYR:CE1	1:A:429:LEU:HD21	2.51	0.45
1:A:451:LYS:O	1:A:471:ASN:N	2.49	0.45
1:A:330:GLN:HB2	1:A:330:GLN:HE21	1.42	0.45
2:B:202:ILE:O	2:B:205:LEU:N	2.50	0.45
1:A:457:TYR:O	1:A:458:VAL:HG23	2.16	0.45
2:B:185:ASP:N	2:B:185:ASP:OD1	2.50	0.45
2:B:52:PRO:C	2:B:54:ASN:H	2.20	0.45
1:A:474:ASN:OD1	1:A:474:ASN:O	2.35	0.45
2:B:369:THR:CG2	2:B:370:GLU:N	2.79	0.45
1:A:442:VAL:CG1	1:A:443:ASP:H	2.29	0.45
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.82	0.45
1:A:509:GLN:N	1:A:510:PRO:HD3	2.32	0.45
2:B:350:LYS:HE2	2:B:378:GLU:OE1	2.17	0.45
2:B:260:LEU:HD21	2:B:303:LEU:HD21	1.98	0.45
1:A:531:VAL:CG1	1:A:532:TYR:N	2.80	0.45
2:B:320:ASP:OD1	2:B:322:SER:OG	2.33	0.45
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.17	0.45
2:B:419:THR:HA	2:B:420:PRO:HD3	1.65	0.45
1:A:94:ILE:HG23	1:A:95:PRO:HD2	1.98	0.45
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.75	0.45
1:A:493:VAL:HG22	1:A:494:ASN:N	2.30	0.44
1:A:542:ILE:HG22	2:B:283:LEU:HD13	1.96	0.44
2:B:103:LYS:HD3	2:B:103:LYS:HA	1.73	0.44
2:B:18:GLY:CA	2:B:56:TYR:HE2	2.30	0.44
2:B:402:TRP:CG	2:B:403:THR:N	2.85	0.44
1:A:480:GLN:O	1:A:483:TYR:CB	2.63	0.44
2:B:145:GLN:HG3	2:B:145:GLN:O	2.17	0.44
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.52	0.44
1:A:179:VAL:HG23	1:A:190:GLY:O	2.16	0.44
2:B:391:LEU:HA	2:B:392:PRO:HD2	1.61	0.44
2:B:87:PHE:HE1	2:B:155:GLY:HA2	1.82	0.44
1:A:362:THR:HG22	1:A:363:ASN:O	2.17	0.44
1:A:368:LEU:HD11	1:A:391:LEU:HD22	1.99	0.44
2:B:314:VAL:HG12	2:B:315:HIS:H	1.82	0.44
2:B:64:LYS:HE2	2:B:69:THR:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:TRP:CZ3	2:B:368:LEU:HD13	2.52	0.44
2:B:203:GLU:HA	2:B:206:ARG:HB2	2.00	0.44
2:B:280:SER:O	2:B:283:LEU:HB2	2.18	0.44
1:A:479:LEU:HD22	1:A:521:ILE:HD12	2.00	0.43
2:B:118:VAL:HG13	2:B:119:PRO:HD2	2.00	0.43
1:A:465:LYS:CG	1:A:466:VAL:N	2.80	0.43
2:B:52:PRO:HG2	2:B:53:GLU:N	2.32	0.43
1:A:171:PHE:CD1	1:A:171:PHE:O	2.72	0.43
1:A:379:SER:HA	1:A:383:TRP:CZ3	2.53	0.43
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.53	0.43
1:A:221:HIS:CD2	1:A:227:PHE:HD2	2.35	0.43
1:A:31:ILE:HG23	1:A:32:LYS:N	2.34	0.43
2:B:63:ILE:HG13	2:B:64:LYS:H	1.80	0.43
1:A:420:PRO:CB	1:A:421:PRO:CD	2.92	0.43
2:B:156:SER:HB2	2:B:157:PRO:CD	2.48	0.43
2:B:376:THR:CG2	2:B:386:THR:HG22	2.49	0.43
2:B:24:TRP:NE1	2:B:59:PRO:CB	2.80	0.43
1:A:199:ARG:HH22	1:A:206:ARG:CD	2.30	0.43
1:A:118:VAL:O	1:A:148:VAL:HG13	2.18	0.43
1:A:181:TYR:CE2	2:B:138:GLU:CB	3.02	0.43
2:B:410:TRP:HE3	2:B:410:TRP:C	2.22	0.43
1:A:390:LYS:HE2	1:A:415:GLU:OE1	2.19	0.43
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.49	0.42
1:A:501:TYR:C	1:A:501:TYR:CD2	2.92	0.42
1:A:484:LEU:O	1:A:487:GLN:N	2.51	0.42
1:A:24:TRP:HA	1:A:25:PRO:HD2	1.88	0.42
1:A:49:LYS:HA	1:A:143:ARG:O	2.19	0.42
1:A:233:GLU:O	1:A:239:TRP:HA	2.20	0.42
1:A:434:ILE:HG12	1:A:530:LYS:HB3	2.00	0.42
2:B:146:TYR:CE2	2:B:150:PRO:HB3	2.54	0.42
1:A:84:THR:HG22	1:A:84:THR:O	2.19	0.42
2:B:47:ILE:HG22	2:B:146:TYR:HA	2.02	0.42
1:A:155:GLY:O	1:A:156:SER:C	2.57	0.42
1:A:419:THR:HG23	1:A:420:PRO:HD2	2.01	0.42
1:A:31:ILE:O	1:A:35:VAL:HG23	2.19	0.42
1:A:365:VAL:C	1:A:367:GLN:N	2.73	0.42
1:A:84:THR:HG21	1:A:154:LYS:HB3	2.00	0.42
1:A:34:LEU:HD21	1:A:62:ALA:HB2	2.01	0.42
1:A:274:ILE:HA	1:A:306:ASN:HD21	1.79	0.42
1:A:19:PRO:O	1:A:56:TYR:HB3	2.20	0.42
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:THR:HG22	2:B:119:PRO:HG2	2.01	0.42
1:A:451:LYS:CB	1:A:471:ASN:HA	2.49	0.42
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.55	0.42
2:B:181:TYR:HB3	2:B:188:TYR:HB2	2.01	0.42
1:A:396:GLU:HA	1:A:399:GLU:HB2	2.02	0.42
2:B:56:TYR:O	2:B:57:ASN:HB2	2.19	0.42
2:B:59:PRO:HD2	2:B:76:ASP:HB3	2.01	0.42
1:A:221:HIS:HB3	1:A:227:PHE:HD2	1.81	0.42
1:A:88:TRP:CD1	1:A:90:VAL:HA	2.55	0.42
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.51	0.42
1:A:466:VAL:O	1:A:467:VAL:CG2	2.68	0.42
2:B:326:ILE:HG22	2:B:327:ALA:N	2.35	0.42
1:A:136:ASN:C	1:A:138:GLU:H	2.21	0.42
1:A:325:LEU:O	1:A:388:LYS:N	2.47	0.42
1:A:47:ILE:HD13	1:A:130:PHE:CZ	2.45	0.42
1:A:116:PHE:CA	1:A:148:VAL:HG11	2.49	0.42
1:A:480:GLN:O	1:A:483:TYR:N	2.51	0.42
1:A:479:LEU:HB3	1:A:517:LEU:CD2	2.49	0.42
2:B:336:GLN:HG3	2:B:355:ALA:HB2	2.01	0.42
2:B:323:LYS:HE3	2:B:344:GLU:OE1	2.20	0.42
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.91	0.42
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.59	0.42
1:A:94:ILE:HD11	1:A:183:TYR:OH	2.19	0.42
1:A:473:THR:C	1:A:475:GLN:N	2.74	0.41
2:B:57:ASN:ND2	2:B:143:ARG:HH21	2.00	0.41
1:A:465:LYS:HG3	1:A:466:VAL:H	1.85	0.41
1:A:457:TYR:HB2	1:A:458:VAL:H	1.66	0.41
1:A:13:LYS:N	1:A:83:ARG:O	2.48	0.41
1:A:178:ILE:HD13	1:A:178:ILE:HG21	1.80	0.41
2:B:257:ILE:HD12	2:B:257:ILE:N	2.32	0.41
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.79	0.41
2:B:194:GLU:O	2:B:198:HIS:N	2.54	0.41
2:B:310:LEU:HD23	2:B:310:LEU:HA	1.89	0.41
1:A:332:GLN:HB3	1:A:333:GLY:H	1.48	0.41
2:B:320:ASP:HA	2:B:321:PRO:HD3	1.89	0.41
2:B:328:GLU:O	2:B:339:TYR:HA	2.20	0.41
2:B:31:ILE:HG12	2:B:133:PRO:HG2	2.02	0.41
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.56	0.41
2:B:182:GLN:HA	2:B:186:ASP:O	2.21	0.41
1:A:275:LYS:NZ	1:A:277:ARG:HH11	2.19	0.41
1:A:37:ILE:HG22	1:A:41:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ILE:HD12	2:B:407:GLN:O	2.20	0.41
1:A:199:ARG:HH21	1:A:220:LYS:CD	2.33	0.41
2:B:170:PRO:O	2:B:173:LYS:N	2.54	0.41
1:A:244:ILE:HD12	1:A:310:LEU:HD22	2.03	0.41
2:B:290:THR:HG22	2:B:290:THR:O	2.21	0.41
1:A:315:HIS:ND1	1:A:315:HIS:N	2.68	0.41
1:A:465:LYS:O	1:A:466:VAL:CG2	2.62	0.41
2:B:115:TYR:CE2	2:B:157:PRO:N	2.89	0.41
2:B:251:SER:HA	2:B:257:ILE:CG1	2.49	0.41
2:B:283:LEU:HD23	2:B:283:LEU:HA	1.81	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.86	0.41
1:A:46:LYS:HD3	1:A:46:LYS:HA	1.90	0.41
2:B:132:ILE:CG2	2:B:133:PRO:HD2	2.51	0.41
1:A:501:TYR:CE2	1:A:505:ILE:CD1	3.04	0.41
2:B:242:GLN:NE2	2:B:353:LYS:HD2	2.37	0.41
1:A:482:ILE:O	1:A:486:LEU:HG	2.21	0.40
1:A:373:GLN:NE2	2:B:397:THR:OG1	2.54	0.40
1:A:475:GLN:O	1:A:478:GLU:HB2	2.21	0.40
1:A:205:LEU:O	1:A:209:LEU:HG	2.22	0.40
1:A:465:LYS:CG	1:A:466:VAL:H	2.35	0.40
1:A:467:VAL:HG12	1:A:468:PRO:N	2.36	0.40
2:B:207:GLN:HA	2:B:207:GLN:OE1	2.22	0.40
1:A:432:GLU:HB3	1:A:433:PRO:HD2	2.03	0.40
1:A:162:SER:O	1:A:163:SER:C	2.60	0.40
2:B:250:ASP:CG	2:B:303:LEU:HD13	2.42	0.40
1:A:339:TYR:CD1	1:A:339:TYR:C	2.95	0.40
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.78	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	554/558 (99%)	453 (82%)	69 (12%)	32 (6%)	2	5
2	B	413/427 (97%)	330 (80%)	60 (14%)	23 (6%)	2	6
All	All	967/985 (98%)	783 (81%)	129 (13%)	55 (6%)	2	5

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	104	LYS
1	A	195	ILE
1	A	223	LYS
1	A	334	GLN
1	A	420	PRO
1	A	458	VAL
1	A	528	LYS
1	A	554	ALA
2	B	53	GLU
2	B	88	TRP
2	B	153	TRP
2	B	277	ARG
1	A	176	PRO
1	A	288	ALA
1	A	310	LEU
1	A	459	THR
1	A	463	ARG
1	A	485	ALA
1	A	542	ILE
2	B	44	GLU
2	B	63	ILE
2	B	112	GLY
2	B	140	PRO
1	A	124	PHE
1	A	225	PRO
1	A	421	PRO
2	B	21	VAL
2	B	97	PRO
2	B	156	SER
2	B	212	TRP
2	B	278	GLN
2	B	290	THR
2	B	420	PRO
1	A	184	ILE

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Mol	Chain	Res	Type
1	A	369	THR
1	A	393	ILE
2	B	95	PRO
2	B	184	ILE
1	A	445	ALA
1	A	465	LYS
1	A	466	VAL
2	B	160	PHE
2	B	270	ILE
2	B	286	THR
1	A	90	VAL
1	A	156	SER
1	A	170	PRO
1	A	335	GLY
1	A	468	PRO
2	B	52	PRO
2	B	37	ILE
1	A	52	PRO
2	B	2	ILE
1	A	495	ILE

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	460/498 (92%)	420 (91%)	40 (9%)	13	33
2	B	353/389 (91%)	323 (92%)	30 (8%)	13	34
All	All	813/887 (92%)	743 (91%)	70 (9%)	13	34

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	29	GLU
1	A	72	ARG

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Mol	Chain	Res	Type
1	A	164	MET
1	A	175	ASN
1	A	179	VAL
1	A	199	ARG
1	A	208	HIS
1	A	240	THR
1	A	243	PRO
1	A	244	ILE
1	A	284	ARG
1	A	300	GLU
1	A	303	LEU
1	A	315	HIS
1	A	324	ASP
1	A	326	ILE
1	A	330	GLN
1	A	332	GLN
1	A	338	THR
1	A	340	GLN
1	A	347	LYS
1	A	367	GLN
1	A	385	LYS
1	A	393	ILE
1	A	399	GLU
1	A	405	TYR
1	A	423	VAL
1	A	452	LEU
1	A	459	THR
1	A	475	GLN
1	A	478	GLU
1	A	497	THR
1	A	500	GLN
1	A	501	TYR
1	A	511	ASP
1	A	516	GLU
1	A	533	LEU
1	A	545	ASN
1	A	552	VAL
2	B	6	GLU
2	B	10	VAL
2	B	24	TRP
2	B	48	SER
2	B	56	TYR

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Mol	Chain	Res	Type
2	B	85	GLN
2	B	94	ILE
2	B	113	ASP
2	B	169	GLU
2	B	194	GLU
2	B	206	ARG
2	B	208	HIS
2	B	215	THR
2	B	234	LEU
2	B	237	ASP
2	B	245	VAL
2	B	248	GLU
2	B	255	ASN
2	B	269	GLN
2	B	271	TYR
2	B	274	ILE
2	B	276	VAL
2	B	293	ILE
2	B	302	GLU
2	B	315	HIS
2	B	369	THR
2	B	394	GLN
2	B	410	TRP
2	B	413	GLU
2	B	414	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	175	ASN
1	A	198	HIS
1	A	208	HIS
1	A	255	ASN
1	A	306	ASN
1	A	330	GLN
1	A	340	GLN
1	A	361	HIS
1	A	373	GLN
1	A	480	GLN
2	B	54	ASN
2	B	57	ASN

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Mol	Chain	Res	Type
2	B	145	GLN
2	B	198	HIS
2	B	235	HIS
2	B	242	GLN
2	B	278	GLN
2	B	334	GLN
2	B	348	ASN
2	B	373	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	556/558 (99%)	0.12	39 (7%)	19 13	14, 68, 87, 95	0
2	B	415/427 (97%)	0.01	27 (6%)	22 16	5, 59, 88, 91	0
All	All	971/985 (98%)	0.07	66 (6%)	20 14	5, 65, 87, 95	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	10.3
1	A	68	SER	9.9
1	A	70	LYS	8.7
2	B	92	LEU	7.3
1	A	69	THR	7.2
2	B	4	PRO	7.1
2	B	218	ASP	6.8
1	A	223	LYS	6.6
2	B	1	PRO	6.2
2	B	251	SER	5.9
2	B	3	SER	5.9
1	A	67	ASP	5.4
2	B	241	VAL	5.1
2	B	93	GLY	5.0
1	A	554	ALA	4.9
2	B	231	GLY	4.5
2	B	357	MET	4.1
1	A	555	GLY	4.1
2	B	250	ASP	4.0
1	A	71	TRP	3.9
1	A	552	VAL	3.9
2	B	423	VAL	3.9
1	A	136	ASN	3.9
1	A	551	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	553	SER	3.7
1	A	358	ARG	3.6
1	A	3	SER	3.3
1	A	1	PRO	3.1
2	B	67	ASP	3.0
1	A	541	GLY	2.9
2	B	68	SER	2.9
1	A	334	GLN	2.9
2	B	94	ILE	2.9
1	A	225	PRO	2.8
1	A	449	GLU	2.8
2	B	65	LYS	2.8
2	B	318	TYR	2.8
2	B	303	LEU	2.7
1	A	27	THR	2.7
2	B	2	ILE	2.7
1	A	61	PHE	2.7
2	B	232	TYR	2.7
1	A	135	ILE	2.7
1	A	24	TRP	2.6
1	A	221	HIS	2.6
1	A	197	GLN	2.6
2	B	311	LYS	2.6
2	B	362	THR	2.5
1	A	66	LYS	2.5
1	A	545	ASN	2.5
1	A	556	ILE	2.5
2	B	189	VAL	2.5
1	A	215	THR	2.5
1	A	481	ALA	2.4
2	B	195	ILE	2.4
1	A	91	GLN	2.4
2	B	419	THR	2.4
1	A	539	HIS	2.3
1	A	406	TRP	2.3
1	A	313	PRO	2.2
2	B	360	ALA	2.2
2	B	66	LYS	2.2
1	A	452	LEU	2.1
1	A	222	GLN	2.0
1	A	65	LYS	2.0
1	A	346	PHE	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.