



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:31 AM UTC

PDB ID : 1JLF / pdb_00001jlf
Title : CRYSTAL STRUCTURE OF Y188C MUTANT HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH NEVIRAPINE
Authors : Ren, J.; Nichols, C.; Bird, L.; Chamberlain, P.; Weaver, K.; Short, S.; Stuart, D.I.; Stammers, D.K.
Deposited on : 2001-07-16
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

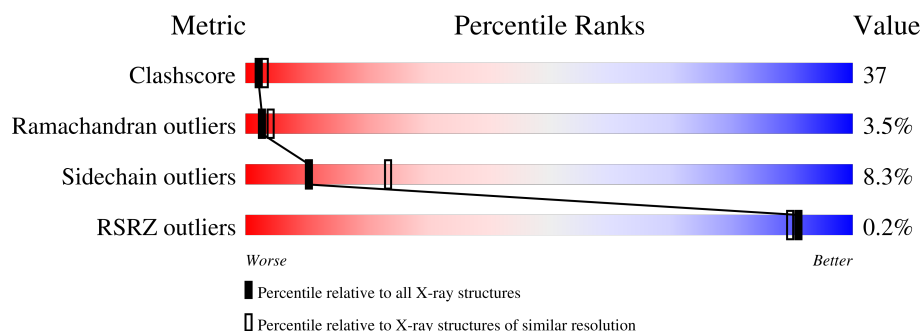
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

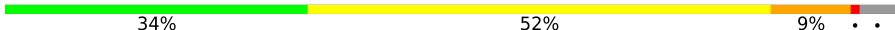
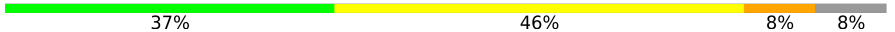
The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	440	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7829 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 HIV-1 RT A-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4404	2847	734	814	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	CYS	TYR	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

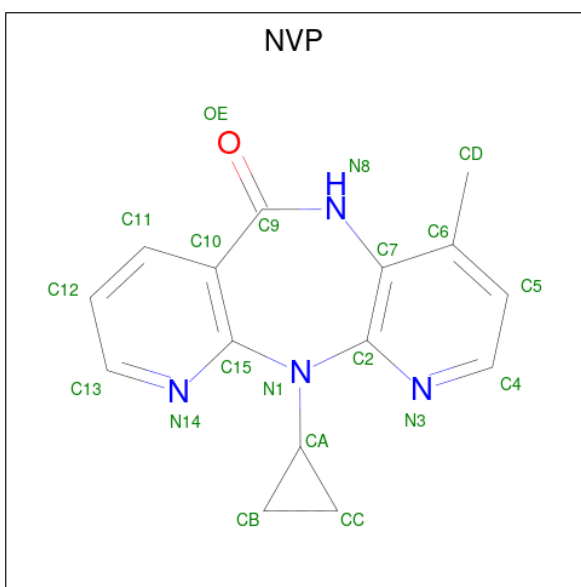
- Molecule 2 is a protein called HIV-1 RT B-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3345	2173	557	607	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	188	CYS	TYR	engineered mutation	UNP P04585

- Molecule 3 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-6-ONE (CCD ID: NVP) (formula: C₁₅H₁₄N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	15	4	1		

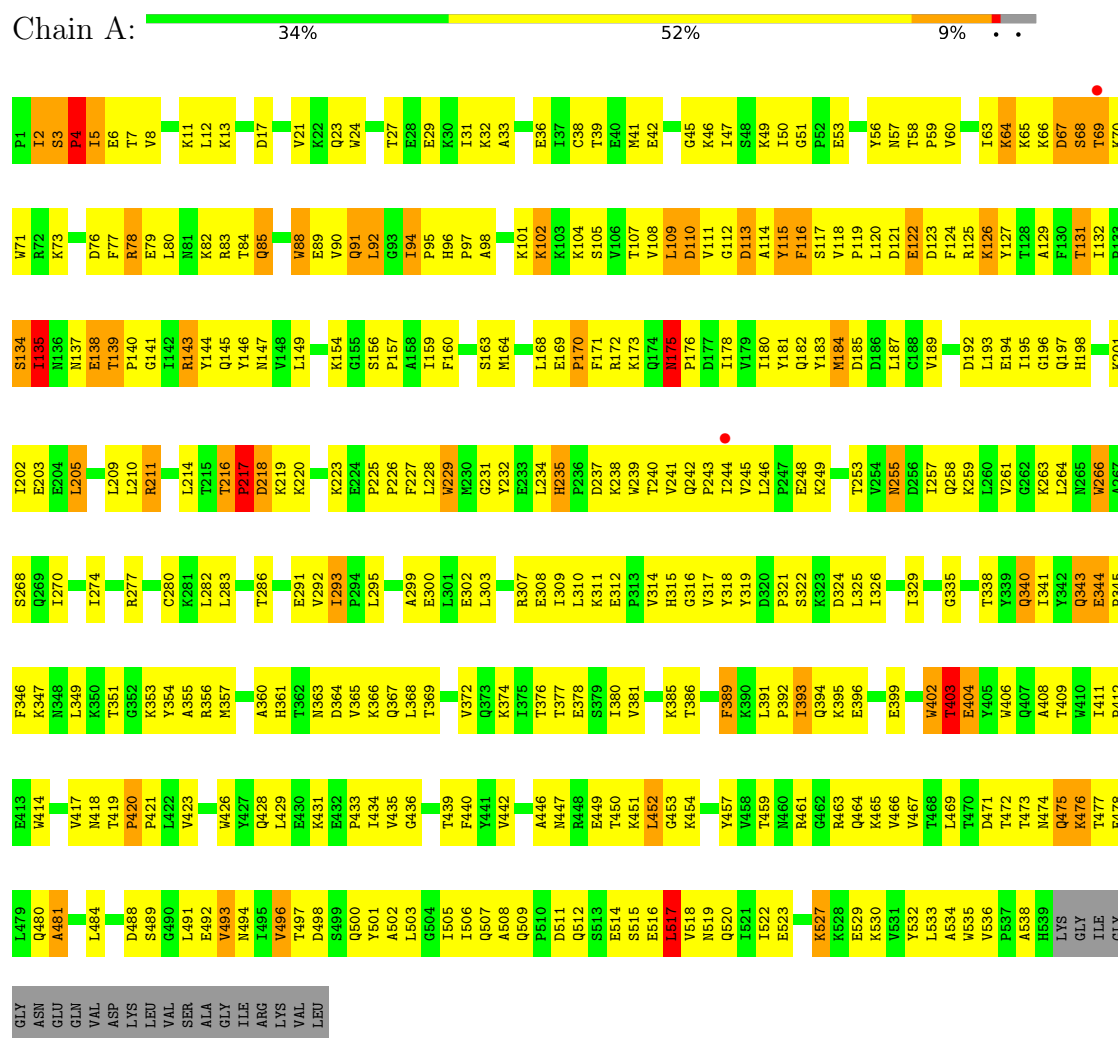
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	26	Total	O	0	0
			26	26		

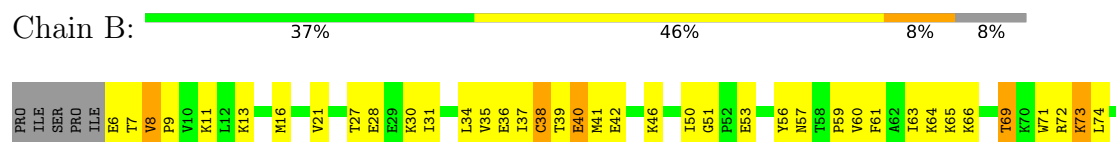
3 Residue-property plots

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

• Molecule 1: HIV-1 RT A-chain



• Molecule 2: HIV-1 RT B-chain



VAL	GLY	ALA	GLU	THR	PHE
K366	Q367	L368	T369	E370	A371
V372	Q373	K374	T377	E378	S379
I380	V381	W382	W383	F387	F388
F389	L391	P392	I393	Q394	K395
E396	T397	W398	W401	E404	T409
E413	W414	E415	F416	W417	N418
T419	P420	P421	L422	W423	K424
L425	W426	Y427	Q428	L429	E430
K431	E432	PRO	ILE		
K287	A288	L289	T290	I293	P294
L295	E298	A299	E300	L301	E302
L303	A304	E305	N306	R307	E308
K311	E312	P313	V314	H315	G316
V317	I326	A327	Q332	G333	Q334
T338	Q343	E344	F345	F346	K347
K348	L349	K350	T351	G352	K353
Y354	A355	R356	M357	R358	R361
T362	N363	D364	V365		
THR	PRO	LEU	GLY	W212	L209
H208	P140	G141	I142	R143	I144
E138	T139	P130	A129	K126	R125
I132	T131	F130	D121	L120	P119
G190	V189	C188	L187	D186	D185
S191	G197	Q197	I195	E194	I178
N175	Q174	P170	E169	L168	I167
K166	T165	M164	S163	Q161	F160
P157	P157	S156	L149	P150	Q151
L148	R147	N147	Y146	Q145	Y144
E143	R143	I142	G141	T139	E138
I135	L135	I132	T131	F130	A129
K126	R125	G196	I195	E194	N195
S117	C188	V189	G190	D186	L187
Y115	F116	S117	P119	L120	D121
V111	V108	Y107	V106	K103	K102
K101	A99	P97	H96	P95	I94
G93	LEU	GLN	VAL	GLU	W88
Q85	T84	R83	N81	K82	R82
L80	E79	L78	A79	L78	ASP
P150	L149	V148	F77		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.30Å 109.20Å 72.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.60 19.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.99-2.60) 99.1 (19.99-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.59Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.303 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 95.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7829	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.56	0/4512	1.06	27/6133 (0.4%)
2	B	0.52	0/3438	1.12	26/4667 (0.6%)
All	All	0.54	0/7950	1.09	53/10800 (0.5%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	LYS	N-CA-C	-12.23	98.46	113.50
2	B	235	HIS	CA-C-N	11.70	131.29	119.82
2	B	235	HIS	C-N-CA	11.70	131.29	119.82
2	B	250	ASP	N-CA-C	-9.27	101.15	111.07
1	A	3	SER	N-CA-C	9.18	118.70	108.14
2	B	241	VAL	N-CA-C	8.96	119.81	110.05
1	A	235	HIS	N-CA-C	-8.52	99.31	110.39
2	B	349	LEU	N-CA-C	-8.48	102.37	112.89
2	B	419	THR	N-CA-C	6.90	118.06	109.57
2	B	69	THR	N-CA-C	-6.85	104.90	113.18
1	A	131	THR	N-CA-C	6.83	119.53	108.34
1	A	216	THR	CA-C-N	6.82	128.37	119.84
1	A	216	THR	C-N-CA	6.82	128.37	119.84
2	B	428	GLN	N-CA-C	-6.76	105.14	113.19
2	B	184	MET	CB-CA-C	-6.76	108.77	116.54
2	B	401	TRP	N-CA-C	6.62	124.35	113.89
1	A	118	VAL	N-CA-C	6.57	115.80	108.05
1	A	481	ALA	N-CA-C	-6.38	104.24	111.07
2	B	369	THR	N-CA-C	-6.31	104.40	111.28
2	B	343	GLN	N-CA-C	-6.27	106.59	114.56
1	A	5	ILE	N-CA-C	6.16	116.80	108.17
1	A	389	PHE	N-CA-C	6.14	118.96	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	THR	N-CA-C	6.13	119.54	108.69
2	B	146	TYR	N-CA-C	6.12	119.13	110.50
1	A	70	LYS	N-CA-C	-6.12	100.59	110.32
1	A	154	LYS	N-CA-C	5.94	118.52	111.33
2	B	417	VAL	N-CA-C	5.85	117.34	108.80
2	B	242	GLN	CA-C-N	5.76	126.22	120.52
2	B	242	GLN	C-N-CA	5.76	126.22	120.52
2	B	420	PRO	N-CA-C	-5.74	103.69	110.70
1	A	88	TRP	N-CA-C	-5.74	102.95	110.53
1	A	527	LYS	N-CA-C	5.56	117.14	111.14
2	B	312	GLU	N-CA-C	5.55	117.22	108.23
2	B	382	ILE	N-CA-C	5.54	115.74	110.53
2	B	96	HIS	N-CA-C	5.53	116.62	109.65
2	B	94	ILE	N-CA-C	5.53	114.57	108.05
1	A	494	ASN	N-CA-C	-5.48	99.96	108.90
1	A	69	THR	N-CA-C	-5.45	105.98	113.56
2	B	391	LEU	N-CA-C	5.41	117.47	109.62
1	A	110	ASP	N-CA-C	-5.40	100.98	109.25
1	A	175	ASN	CA-C-N	5.39	126.58	119.84
1	A	175	ASN	C-N-CA	5.39	126.58	119.84
1	A	92	LEU	N-CA-C	-5.39	106.75	113.38
1	A	134	SER	N-CA-C	-5.29	102.37	110.14
1	A	343	GLN	N-CA-C	-5.23	106.59	113.12
2	B	270	ILE	N-CA-C	-5.23	107.67	111.90
2	B	174	GLN	N-CA-C	-5.21	106.19	112.54
1	A	46	LYS	N-CA-C	5.20	116.76	111.14
1	A	3	SER	CA-C-N	5.19	126.32	119.84
1	A	3	SER	C-N-CA	5.19	126.32	119.84
1	A	234	LEU	N-CA-C	5.04	116.62	108.41
2	B	38	CYS	N-CA-C	5.01	117.12	111.11
1	A	80	LEU	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4404	0	4450	339	0
2	B	3345	0	3373	249	0
3	A	20	0	14	0	0
4	A	34	0	0	5	0
4	B	26	0	0	4	0
All	All	7829	0	7837	577	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 37.

All (577) 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:502:ALA:HA	1:A:505:ILE:HD12	1.42	1.01
2:B:195:ILE:HG23	2:B:196:GLY:H	1.30	0.94
1:A:2:ILE:HG22	1:A:3:SER:H	1.33	0.91
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.52	0.89
1:A:238:LYS:HB2	1:A:316:GLY:O	1.72	0.88
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.54	0.88
1:A:335:GLY:HA2	1:A:367:GLN:OE1	1.72	0.88
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.56	0.85
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.58	0.85
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.59	0.84
1:A:475:GLN:HE21	1:A:475:GLN:N	1.76	0.84
2:B:164:MET:O	2:B:167:ILE:HG12	1.77	0.83
1:A:226:PRO:HB3	1:A:235:HIS:ND1	1.93	0.83
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.58	0.82
2:B:31:ILE:O	2:B:35:VAL:HG23	1.80	0.82
1:A:503:LEU:HA	1:A:506:ILE:HD12	1.60	0.81
2:B:195:ILE:HG23	2:B:196:GLY:N	1.96	0.81
1:A:195:ILE:HG13	1:A:196:GLY:N	1.96	0.81
2:B:79:GLU:O	2:B:83:ARG:HG3	1.81	0.81
1:A:17:ASP:O	1:A:83:ARG:HD3	1.79	0.80
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.64	0.80
1:A:164:MET:HE1	1:A:214:LEU:HD13	1.64	0.78
1:A:516:GLU:O	1:A:520:GLN:HG3	1.83	0.78
2:B:241:VAL:CG1	2:B:350:LYS:HA	2.14	0.77
2:B:366:LYS:O	2:B:370:GLU:HB2	1.83	0.77
1:A:141:GLY:HA2	4:A:1035:HOH:O	1.84	0.77
1:A:65:LYS:HG2	1:A:66:LYS:H	1.50	0.77
1:A:2:ILE:HG22	1:A:3:SER:N	1.99	0.76
1:A:66:LYS:H	1:A:66:LYS:HD2	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:SER:OG	1:A:518:VAL:HG23	1.86	0.76
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.69	0.75
1:A:516:GLU:O	1:A:519:ASN:HB2	1.85	0.75
1:A:94:ILE:HD13	1:A:94:ILE:H	1.50	0.75
1:A:110:ASP:O	1:A:217:PRO:HD2	1.87	0.75
2:B:241:VAL:HG12	2:B:350:LYS:HA	1.67	0.74
2:B:206:ARG:HB3	2:B:206:ARG:NH1	2.01	0.74
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.21	0.74
1:A:211:ARG:NH1	1:A:211:ARG:HB3	2.01	0.74
2:B:245:VAL:HG11	2:B:431:LYS:HB2	1.71	0.73
1:A:64:LYS:H	1:A:64:LYS:HD2	1.51	0.73
1:A:116:PHE:HE1	1:A:146:TYR:HE1	1.36	0.73
1:A:446:ALA:HB2	1:A:453:GLY:HA3	1.71	0.73
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.18	0.72
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.69	0.72
1:A:2:ILE:HD11	1:A:45:GLY:HA3	1.71	0.72
1:A:27:THR:O	1:A:31:ILE:HG13	1.90	0.72
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.71	0.72
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.05	0.71
1:A:23:GLN:HG2	1:A:131:THR:O	1.89	0.71
2:B:420:PRO:HG3	4:B:1024:HOH:O	1.90	0.71
1:A:480:GLN:HE21	1:A:484:LEU:HG	1.54	0.71
2:B:107:THR:HA	2:B:232:TYR:O	1.91	0.71
2:B:365:VAL:O	2:B:369:THR:HG23	1.91	0.71
2:B:61:PHE:CE1	2:B:74:LEU:HD23	2.25	0.71
1:A:175:ASN:HB2	1:A:178:ILE:HD13	1.71	0.70
1:A:523:GLU:O	1:A:527:LYS:HG3	1.91	0.70
1:A:96:HIS:HD2	1:A:98:ALA:H	1.40	0.70
2:B:426:TRP:O	2:B:429:LEU:HB2	1.90	0.70
2:B:78:ARG:O	2:B:82:LYS:HG3	1.92	0.70
2:B:98:ALA:O	2:B:101:LYS:HG2	1.92	0.69
2:B:191:SER:HG	2:B:198:HIS:HD1	1.37	0.69
1:A:109:LEU:HG	1:A:216:THR:HG21	1.74	0.69
2:B:379:SER:CB	2:B:387:PRO:HD3	2.23	0.69
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.74	0.68
1:A:135:ILE:O	1:A:138:GLU:HG3	1.93	0.68
2:B:88:TRP:HE3	2:B:88:TRP:C	2.02	0.68
2:B:139:THR:HG22	2:B:140:PRO:O	1.93	0.68
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.29	0.67
2:B:108:VAL:HA	2:B:187:LEU:O	1.93	0.67
2:B:160:PHE:O	2:B:160:PHE:CD1	2.47	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:HD3	1:A:67:ASP:OD2	1.92	0.67
2:B:205:LEU:O	2:B:208:HIS:HB2	1.95	0.67
1:A:211:ARG:HB3	1:A:211:ARG:HH11	1.57	0.67
2:B:281:LYS:NZ	2:B:284:ARG:HH22	1.93	0.67
1:A:418:ASN:C	1:A:420:PRO:HD3	2.20	0.67
1:A:180:ILE:HG23	1:A:189:VAL:HG22	1.76	0.66
2:B:195:ILE:HG13	2:B:199:ARG:NE	2.10	0.66
2:B:239:TRP:CZ2	2:B:378:GLU:HG2	2.30	0.66
2:B:254:VAL:O	2:B:258:GLN:HG3	1.95	0.66
2:B:195:ILE:CG2	2:B:196:GLY:H	2.06	0.66
2:B:427:TYR:C	2:B:429:LEU:H	2.03	0.66
1:A:2:ILE:HD11	1:A:45:GLY:C	2.21	0.66
1:A:171:PHE:O	1:A:175:ASN:ND2	2.29	0.65
2:B:161:GLN:O	2:B:165:THR:HG22	1.97	0.65
1:A:94:ILE:HB	1:A:229:TRP:HH2	1.60	0.65
1:A:110:ASP:OD1	1:A:217:PRO:HG2	1.97	0.65
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.79	0.65
1:A:357:MET:HB3	1:A:367:GLN:NE2	2.12	0.65
1:A:492:GLU:HA	1:A:530:LYS:O	1.97	0.65
1:A:3:SER:HB3	1:A:4:PRO:HD2	1.78	0.65
1:A:64:LYS:HE3	1:A:71:TRP:CZ3	2.31	0.65
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.32	0.64
2:B:118:VAL:HG13	2:B:119:PRO:HD2	1.79	0.64
2:B:161:GLN:HB3	4:B:1052:HOH:O	1.97	0.64
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.63	0.64
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.80	0.64
2:B:131:THR:OG1	2:B:143:ARG:HD2	1.98	0.64
1:A:164:MET:O	1:A:168:LEU:HG	1.97	0.64
2:B:125:ARG:HB3	2:B:145:GLN:HE21	1.61	0.64
1:A:255:ASN:O	1:A:259:LYS:HG2	1.97	0.64
1:A:31:ILE:HD12	1:A:135:ILE:HD12	1.79	0.64
1:A:135:ILE:O	1:A:135:ILE:HG22	1.98	0.64
1:A:377:THR:O	1:A:381:VAL:HG23	1.99	0.63
2:B:163:SER:O	2:B:167:ILE:HG23	1.98	0.63
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.80	0.62
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.62	0.62
1:A:293:ILE:N	1:A:293:ILE:HD12	2.14	0.62
1:A:95:PRO:O	1:A:229:TRP:HZ3	1.80	0.62
1:A:63:ILE:C	1:A:63:ILE:HD12	2.25	0.62
1:A:164:MET:HE1	1:A:214:LEU:CD1	2.28	0.62
1:A:248:GLU:O	1:A:249:LYS:HD3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ILE:CG2	1:A:3:SER:H	2.11	0.61
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.81	0.61
1:A:2:ILE:HD11	1:A:45:GLY:CA	2.30	0.61
1:A:175:ASN:HB2	1:A:178:ILE:CD1	2.30	0.61
1:A:261:VAL:HA	1:A:264:LEU:HD12	1.80	0.61
1:A:408:ALA:HB2	2:B:368:LEU:HD12	1.81	0.61
2:B:380:ILE:O	2:B:384:GLY:HA2	2.00	0.61
1:A:268:SER:HB3	1:A:353:LYS:HE2	1.82	0.61
1:A:246:LEU:HD12	1:A:307:ARG:HA	1.83	0.61
2:B:41:MET:HB3	2:B:46:LYS:HB2	1.83	0.61
1:A:418:ASN:O	1:A:420:PRO:HD3	2.01	0.61
1:A:3:SER:CB	1:A:5:ILE:HG13	2.31	0.60
1:A:108:VAL:HG11	1:A:223:LYS:HB2	1.83	0.60
2:B:332:GLN:NE2	2:B:428:GLN:HB2	2.16	0.60
2:B:94:ILE:HD11	2:B:182:GLN:H	1.67	0.60
2:B:194:GLU:OE2	2:B:195:ILE:HG22	2.01	0.60
1:A:122:GLU:H	1:A:122:GLU:CD	2.09	0.60
1:A:257:ILE:O	1:A:261:VAL:HG23	2.02	0.60
2:B:88:TRP:C	2:B:88:TRP:CE3	2.80	0.60
1:A:108:VAL:HG13	1:A:108:VAL:O	2.01	0.60
1:A:396:GLU:H	1:A:396:GLU:CD	2.10	0.60
1:A:451:LYS:O	1:A:472:THR:N	2.35	0.60
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.36	0.59
2:B:35:VAL:O	2:B:39:THR:HG23	2.02	0.59
1:A:66:LYS:HD2	1:A:66:LYS:N	2.16	0.59
1:A:195:ILE:HG13	1:A:196:GLY:H	1.65	0.59
1:A:17:ASP:OD1	1:A:56:TYR:HE1	1.85	0.59
2:B:108:VAL:H	2:B:232:TYR:N	2.00	0.59
1:A:122:GLU:C	1:A:124:PHE:H	2.10	0.59
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.83	0.59
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.84	0.59
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.84	0.59
2:B:248:GLU:HG2	2:B:307:ARG:NH2	2.17	0.59
1:A:57:ASN:HA	1:A:129:ALA:O	2.03	0.59
1:A:475:GLN:HA	1:A:478:GLU:OE2	2.03	0.58
2:B:175:ASN:ND2	2:B:201:LYS:HD2	2.18	0.58
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.21	0.58
1:A:474:ASN:O	1:A:478:GLU:HG3	2.02	0.58
1:A:64:LYS:H	1:A:64:LYS:CD	2.16	0.58
1:A:111:VAL:HG22	1:A:185:ASP:HB3	1.86	0.58
1:A:112:GLY:O	1:A:114:ALA:N	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ILE:HG22	2:B:65:LYS:H	1.68	0.58
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.38	0.58
1:A:465:LYS:HG2	1:A:466:VAL:N	2.17	0.58
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.85	0.58
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.39	0.58
2:B:379:SER:OG	2:B:387:PRO:HD3	2.03	0.58
1:A:307:ARG:O	1:A:311:LYS:HG3	2.03	0.58
1:A:475:GLN:HE21	1:A:475:GLN:H	1.49	0.57
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.39	0.57
1:A:42:GLU:HA	1:A:47:ILE:HG13	1.87	0.57
1:A:94:ILE:H	1:A:94:ILE:CD1	2.16	0.57
1:A:376:THR:O	1:A:380:ILE:HG12	2.04	0.57
2:B:350:LYS:HE2	2:B:378:GLU:OE1	2.05	0.57
1:A:360:ALA:HA	1:A:514:GLU:OE2	2.03	0.57
1:A:380:ILE:CD1	1:A:386:THR:HG22	2.30	0.57
2:B:64:LYS:HG2	2:B:71:TRP:CE3	2.40	0.57
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.86	0.57
2:B:281:LYS:HZ3	2:B:284:ARG:HH22	1.53	0.57
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.33	0.57
2:B:239:TRP:HH2	2:B:378:GLU:HA	1.69	0.57
1:A:49:LYS:HB2	1:A:144:TYR:CE2	2.40	0.57
1:A:102:LYS:HB2	1:A:102:LYS:NZ	2.18	0.57
1:A:295:LEU:HB2	1:A:300:GLU:OE1	2.04	0.57
2:B:178:ILE:HG12	2:B:191:SER:CB	2.31	0.57
1:A:302:GLU:HA	4:A:1006:HOH:O	2.05	0.56
2:B:236:PRO:O	2:B:239:TRP:HB2	2.05	0.56
2:B:332:GLN:HE22	2:B:428:GLN:HB2	1.69	0.56
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.87	0.56
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.03	0.56
2:B:427:TYR:C	2:B:429:LEU:N	2.63	0.56
1:A:21:VAL:HG11	1:A:59:PRO:HD3	1.87	0.56
1:A:108:VAL:HG11	1:A:227:PHE:CE1	2.40	0.56
2:B:27:THR:O	2:B:31:ILE:HG13	2.06	0.56
2:B:98:ALA:C	2:B:101:LYS:HZ3	2.13	0.56
2:B:245:VAL:O	2:B:245:VAL:HG23	2.04	0.56
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.40	0.56
2:B:393:ILE:HG12	2:B:394:GLN:N	2.20	0.56
1:A:41:MET:SD	1:A:73:LYS:HE3	2.46	0.56
1:A:228:LEU:HD22	1:A:242:GLN:OE1	2.05	0.56
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.05	0.56
2:B:206:ARG:HB3	2:B:206:ARG:CZ	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:HE22	2:B:424:LYS:HD3	1.69	0.56
2:B:9:PRO:HA	2:B:121:ASP:OD2	2.06	0.56
2:B:241:VAL:HG12	2:B:351:THR:H	1.71	0.56
1:A:169:GLU:CB	1:A:170:PRO:HD3	2.34	0.56
2:B:97:PRO:O	2:B:98:ALA:C	2.48	0.56
1:A:241:VAL:O	1:A:243:PRO:HD3	2.05	0.56
1:A:402:TRP:CH2	2:B:362:THR:HA	2.41	0.56
2:B:373:GLN:O	2:B:377:THR:HG23	2.06	0.55
1:A:110:ASP:O	1:A:216:THR:HG23	2.07	0.55
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.46	0.55
2:B:125:ARG:CB	2:B:145:GLN:HE21	2.19	0.55
1:A:33:ALA:O	1:A:36:GLU:HB3	2.07	0.55
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.41	0.55
2:B:197:GLN:O	2:B:201:LYS:HB2	2.05	0.55
2:B:301:LEU:O	2:B:304:ALA:N	2.39	0.55
1:A:134:SER:OG	1:A:138:GLU:HB2	2.06	0.55
1:A:65:LYS:HG2	1:A:66:LYS:N	2.21	0.55
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.41	0.55
1:A:497:THR:O	1:A:535:TRP:HA	2.07	0.55
2:B:235:HIS:N	2:B:236:PRO:HD3	2.21	0.55
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.89	0.55
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.42	0.55
1:A:475:GLN:N	1:A:475:GLN:NE2	2.52	0.55
1:A:517:LEU:O	1:A:518:VAL:C	2.49	0.55
1:A:317:VAL:HG12	1:A:318:TYR:N	2.22	0.55
1:A:474:ASN:O	1:A:477:THR:OG1	2.24	0.55
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.89	0.54
1:A:102:LYS:HB3	1:A:318:TYR:HB2	1.88	0.54
1:A:111:VAL:HG22	1:A:185:ASP:CA	2.38	0.54
2:B:245:VAL:CG1	2:B:431:LYS:HB2	2.37	0.54
1:A:125:ARG:NE	1:A:147:ASN:HA	2.23	0.54
1:A:139:THR:HB	1:A:140:PRO:CD	2.38	0.54
2:B:255:ASN:OD1	2:B:259:LYS:HE2	2.07	0.54
1:A:111:VAL:HG23	1:A:114:ALA:HB2	1.90	0.54
2:B:308:GLU:OE1	2:B:311:LYS:HD2	2.07	0.54
1:A:418:ASN:OD1	1:A:420:PRO:HD3	2.07	0.53
1:A:436:GLY:O	1:A:461:ARG:NH2	2.40	0.53
1:A:168:LEU:O	1:A:172:ARG:HB2	2.09	0.53
1:A:389:PHE:HB2	1:A:414:TRP:HB3	1.91	0.53
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.89	0.53
2:B:125:ARG:CB	2:B:145:GLN:NE2	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:CG	1:A:66:LYS:H	2.19	0.53
1:A:125:ARG:HG2	1:A:146:TYR:O	2.08	0.53
2:B:39:THR:O	2:B:42:GLU:HB3	2.08	0.53
2:B:57:ASN:HB2	2:B:143:ARG:HH12	1.72	0.53
2:B:57:ASN:HA	2:B:129:ALA:O	2.09	0.53
2:B:244:ILE:HG23	2:B:429:LEU:HB3	1.90	0.53
1:A:419:THR:HG22	1:A:419:THR:O	2.07	0.53
1:A:143:ARG:HG2	1:A:143:ARG:NH1	2.23	0.53
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.44	0.53
1:A:473:THR:CG2	1:A:476:LYS:HG3	2.39	0.53
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.91	0.53
2:B:161:GLN:HA	2:B:161:GLN:HE21	1.72	0.53
2:B:27:THR:HG22	2:B:28:GLU:N	2.24	0.53
2:B:63:ILE:HG22	2:B:65:LYS:N	2.23	0.53
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.43	0.53
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.44	0.53
1:A:228:LEU:HA	1:A:232:TYR:O	2.09	0.53
2:B:115:TYR:O	2:B:117:SER:N	2.42	0.53
1:A:454:LYS:HA	1:A:467:VAL:O	2.08	0.52
1:A:451:LYS:HD3	1:A:471:ASP:OD2	2.08	0.52
2:B:106:VAL:HA	2:B:189:VAL:O	2.09	0.52
2:B:374:LYS:O	2:B:378:GLU:HG3	2.09	0.52
1:A:508:ALA:O	1:A:509:GLN:C	2.52	0.52
1:A:11:LYS:O	1:A:85:GLN:HB3	2.10	0.52
1:A:248:GLU:HB2	1:A:307:ARG:NH2	2.25	0.52
2:B:156:SER:HB2	2:B:157:PRO:CD	2.40	0.52
1:A:408:ALA:HB3	2:B:393:ILE:HB	1.92	0.52
2:B:315:HIS:O	2:B:317:VAL:HG23	2.10	0.52
1:A:160:PHE:C	1:A:160:PHE:CD2	2.88	0.52
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.91	0.52
2:B:169:GLU:HB2	2:B:170:PRO:CD	2.37	0.52
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.10	0.51
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.92	0.51
2:B:53:GLU:OE1	2:B:53:GLU:N	2.42	0.51
2:B:259:LYS:O	2:B:260:LEU:C	2.51	0.51
2:B:344:GLU:HB3	2:B:347:LYS:NZ	2.25	0.51
1:A:501:TYR:C	1:A:501:TYR:CD2	2.89	0.51
2:B:303:LEU:O	2:B:307:ARG:HG3	2.11	0.51
2:B:428:GLN:HG2	2:B:428:GLN:O	2.10	0.51
1:A:240:THR:HG22	1:A:241:VAL:N	2.26	0.51
1:A:446:ALA:CB	1:A:453:GLY:HA3	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:O	1:A:195:ILE:C	2.54	0.51
1:A:465:LYS:HG2	1:A:466:VAL:H	1.76	0.51
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.93	0.51
2:B:232:TYR:HB3	2:B:234:LEU:HD11	1.92	0.51
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.93	0.51
2:B:11:LYS:N	2:B:85:GLN:OE1	2.32	0.50
2:B:281:LYS:HG2	2:B:284:ARG:NH2	2.25	0.50
1:A:183:TYR:CD1	1:A:184:MET:HB2	2.45	0.50
1:A:283:LEU:O	1:A:286:THR:HG23	2.10	0.50
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.41	0.50
1:A:98:ALA:HB2	1:A:349:LEU:O	2.10	0.50
1:A:181:TYR:HB2	2:B:138:GLU:OE1	2.11	0.50
2:B:37:ILE:O	2:B:40:GLU:HB2	2.12	0.50
1:A:319:TYR:OH	1:A:385:LYS:HD3	2.10	0.50
1:A:346:PHE:N	1:A:346:PHE:CD2	2.77	0.50
2:B:6:GLU:HG2	2:B:7:THR:H	1.77	0.50
2:B:98:ALA:HA	2:B:101:LYS:NZ	2.27	0.50
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.93	0.50
1:A:96:HIS:CD2	1:A:97:PRO:HD2	2.47	0.50
1:A:2:ILE:CD1	1:A:45:GLY:HA3	2.39	0.50
1:A:357:MET:HE2	4:A:1041:HOH:O	2.12	0.50
1:A:496:VAL:HA	1:A:534:ALA:O	2.12	0.50
2:B:195:ILE:O	2:B:198:HIS:HB3	2.12	0.50
1:A:39:THR:O	1:A:42:GLU:HB3	2.12	0.50
1:A:268:SER:CB	1:A:353:LYS:HE2	2.42	0.50
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.47	0.50
2:B:118:VAL:CG1	2:B:119:PRO:HD2	2.41	0.50
1:A:357:MET:HB3	1:A:367:GLN:HE22	1.76	0.49
1:A:94:ILE:HB	1:A:229:TRP:CH2	2.45	0.49
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.94	0.49
2:B:46:LYS:HE2	2:B:116:PHE:HD1	1.77	0.49
2:B:125:ARG:HB2	2:B:145:GLN:NE2	2.27	0.49
1:A:402:TRP:CD1	1:A:402:TRP:C	2.89	0.49
2:B:266:TRP:CZ3	2:B:426:TRP:CG	3.00	0.49
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.41	0.49
2:B:107:THR:O	2:B:188:CYS:HA	2.12	0.49
1:A:465:LYS:NZ	1:A:488:ASP:OD1	2.43	0.49
2:B:115:TYR:C	2:B:117:SER:N	2.69	0.49
1:A:50:ILE:HG23	1:A:145:GLN:HG2	1.93	0.49
2:B:234:LEU:C	2:B:236:PRO:HD3	2.38	0.49
2:B:184:MET:HE3	2:B:184:MET:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ALA:HA	1:A:144:TYR:O	2.13	0.48
1:A:402:TRP:CG	1:A:403:THR:N	2.80	0.48
1:A:498:ASP:HA	1:A:536:VAL:O	2.13	0.48
2:B:244:ILE:CG2	2:B:429:LEU:HD23	2.42	0.48
1:A:90:VAL:O	1:A:91:GLN:C	2.55	0.48
1:A:107:THR:HG22	1:A:108:VAL:N	2.29	0.48
1:A:457:TYR:CD1	1:A:457:TYR:C	2.91	0.48
2:B:77:PHE:HD2	2:B:80:LEU:HD23	1.78	0.48
1:A:340:GLN:CB	1:A:351:THR:HG22	2.43	0.48
1:A:77:PHE:O	1:A:79:GLU:N	2.47	0.48
2:B:357:MET:O	2:B:358:ARG:C	2.56	0.48
1:A:218:ASP:HB3	1:A:220:LYS:H	1.78	0.48
1:A:344:GLU:O	1:A:345:PRO:C	2.57	0.48
2:B:206:ARG:HH11	2:B:206:ARG:CB	2.27	0.48
2:B:170:PRO:O	2:B:174:GLN:HG3	2.14	0.48
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.14	0.48
1:A:244:ILE:HD11	1:A:263:LYS:HB3	1.96	0.48
2:B:165:THR:HG23	2:B:166:LYS:H	1.77	0.48
1:A:66:LYS:C	1:A:68:SER:H	2.22	0.48
1:A:95:PRO:O	1:A:229:TRP:CZ3	2.65	0.48
1:A:108:VAL:CG1	1:A:223:LYS:HB2	2.42	0.48
2:B:64:LYS:HG2	2:B:71:TRP:CZ3	2.49	0.48
2:B:344:GLU:CB	2:B:347:LYS:HE3	2.44	0.48
2:B:356:ARG:HG3	2:B:356:ARG:HH11	1.78	0.48
2:B:423:VAL:O	2:B:427:TYR:CD2	2.67	0.48
1:A:394:GLN:HB3	1:A:396:GLU:OE1	2.13	0.47
1:A:426:TRP:H	1:A:426:TRP:CD1	2.31	0.47
2:B:175:ASN:HD21	2:B:201:LYS:HD2	1.77	0.47
1:A:77:PHE:C	1:A:79:GLU:N	2.72	0.47
2:B:160:PHE:O	2:B:160:PHE:HD1	1.95	0.47
2:B:191:SER:OG	2:B:198:HIS:ND1	2.38	0.47
2:B:195:ILE:HG13	2:B:199:ARG:HE	1.79	0.47
2:B:395:LYS:NZ	4:B:1060:HOH:O	2.47	0.47
2:B:56:TYR:O	2:B:57:ASN:HB2	2.14	0.47
2:B:301:LEU:HD11	2:B:305:GLU:HG3	1.97	0.47
1:A:102:LYS:NZ	1:A:237:ASP:HA	2.29	0.47
1:A:198:HIS:O	1:A:201:LYS:N	2.47	0.47
1:A:135:ILE:O	1:A:135:ILE:CG2	2.63	0.47
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.80	0.47
1:A:170:PRO:O	1:A:171:PHE:C	2.57	0.47
2:B:202:ILE:O	2:B:205:LEU:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:TYR:HB3	2:B:234:LEU:CD1	2.45	0.47
1:A:17:ASP:OD1	1:A:56:TYR:CE1	2.67	0.47
1:A:308:GLU:O	1:A:309:ILE:C	2.57	0.47
1:A:439:THR:O	1:A:459:THR:HA	2.15	0.47
1:A:475:GLN:NE2	1:A:475:GLN:CA	2.78	0.47
1:A:225:PRO:HA	1:A:226:PRO:C	2.40	0.47
1:A:402:TRP:C	1:A:404:GLU:H	2.22	0.47
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.14	0.47
1:A:463:ARG:HG2	1:A:464:GLN:N	2.30	0.46
1:A:102:LYS:HZ3	1:A:237:ASP:HA	1.80	0.46
1:A:108:VAL:O	1:A:108:VAL:CG1	2.64	0.46
1:A:163:SER:O	1:A:164:MET:C	2.57	0.46
1:A:258:GLN:O	1:A:259:LYS:C	2.57	0.46
1:A:308:GLU:O	1:A:311:LYS:N	2.46	0.46
1:A:345:PRO:O	1:A:346:PHE:HB2	2.14	0.46
1:A:419:THR:O	1:A:420:PRO:C	2.56	0.46
2:B:282:LEU:HD13	2:B:295:LEU:CD2	2.45	0.46
1:A:66:LYS:O	1:A:68:SER:N	2.48	0.46
1:A:518:VAL:O	1:A:522:ILE:HG13	2.15	0.46
2:B:94:ILE:HG13	2:B:181:TYR:HE2	1.80	0.46
1:A:473:THR:HG23	1:A:476:LYS:H	1.79	0.46
1:A:2:ILE:CG2	1:A:3:SER:N	2.71	0.46
1:A:231:GLY:C	1:A:242:GLN:HB3	2.41	0.46
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.31	0.46
2:B:206:ARG:O	2:B:207:GLN:C	2.59	0.46
2:B:308:GLU:OE1	2:B:308:GLU:HA	2.15	0.46
1:A:111:VAL:HG22	1:A:185:ASP:CB	2.46	0.46
1:A:363:ASN:O	1:A:366:LYS:HB3	2.16	0.46
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.51	0.46
2:B:198:HIS:O	2:B:201:LYS:HB3	2.16	0.46
2:B:422:LEU:C	2:B:424:LYS:N	2.71	0.46
2:B:80:LEU:O	2:B:81:ASN:C	2.58	0.46
1:A:253:THR:HA	1:A:291:GLU:O	2.16	0.46
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.46	0.46
2:B:121:ASP:N	4:B:1049:HOH:O	2.35	0.46
2:B:333:GLY:O	2:B:334:GLN:HB2	2.16	0.46
1:A:238:LYS:HG3	1:A:239:TRP:N	2.30	0.45
1:A:498:ASP:CG	1:A:538:ALA:HB2	2.41	0.45
2:B:165:THR:HG23	2:B:166:LYS:N	2.30	0.45
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.51	0.45
1:A:53:GLU:HG3	1:A:53:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:HB3	1:A:185:ASP:H	1.43	0.45
1:A:241:VAL:CG2	1:A:314:VAL:HG23	2.47	0.45
1:A:411:ILE:HG22	1:A:412:PRO:O	2.16	0.45
1:A:507:GLN:OE1	2:B:421:PRO:HG3	2.14	0.45
2:B:63:ILE:HG22	2:B:64:LYS:N	2.31	0.45
2:B:268:SER:HA	2:B:271:TYR:O	2.17	0.45
2:B:422:LEU:O	2:B:423:VAL:C	2.59	0.45
1:A:59:PRO:HG2	1:A:76:ASP:CB	2.45	0.45
1:A:408:ALA:CB	2:B:368:LEU:HD12	2.44	0.45
1:A:475:GLN:HE21	1:A:475:GLN:CA	2.25	0.45
2:B:130:PHE:CD1	2:B:130:PHE:C	2.94	0.45
1:A:399:GLU:O	1:A:403:THR:HG22	2.17	0.45
2:B:94:ILE:HG13	2:B:94:ILE:O	2.16	0.45
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.99	0.45
1:A:299:ALA:O	1:A:303:LEU:HB3	2.16	0.45
1:A:409:THR:O	2:B:364:ASP:HB2	2.16	0.45
1:A:452:LEU:HD23	1:A:469:LEU:O	2.16	0.45
2:B:195:ILE:CG1	2:B:199:ARG:NE	2.79	0.45
1:A:115:TYR:OH	1:A:157:PRO:HG3	2.16	0.45
1:A:501:TYR:CD2	1:A:501:TYR:O	2.70	0.45
2:B:195:ILE:O	2:B:196:GLY:C	2.60	0.45
1:A:402:TRP:C	1:A:404:GLU:N	2.75	0.45
2:B:356:ARG:NH2	2:B:361:HIS:HB3	2.32	0.45
2:B:125:ARG:HB3	2:B:145:GLN:NE2	2.29	0.45
2:B:249:LYS:HD2	2:B:251:SER:O	2.17	0.45
2:B:338:THR:CG2	2:B:353:LYS:HE2	2.47	0.45
1:A:69:THR:O	1:A:69:THR:HG22	2.17	0.44
1:A:277:ARG:HD2	4:A:1038:HOH:O	2.18	0.44
1:A:447:ASN:CG	1:A:450:THR:HG23	2.42	0.44
2:B:377:THR:O	2:B:381:VAL:HG23	2.16	0.44
1:A:109:LEU:HG	1:A:216:THR:CG2	2.44	0.44
1:A:149:LEU:HD11	1:A:159:ILE:HG21	1.99	0.44
2:B:196:GLY:O	2:B:200:THR:HG23	2.18	0.44
2:B:254:VAL:HG21	2:B:287:LYS:HG2	1.99	0.44
1:A:193:LEU:HD13	1:A:197:GLN:HB3	2.00	0.44
2:B:211:ARG:HG3	2:B:211:ARG:O	2.18	0.44
1:A:511:ASP:O	1:A:512:GLN:HB3	2.17	0.44
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.52	0.44
1:A:101:LYS:HA	1:A:319:TYR:O	2.17	0.44
2:B:164:MET:HG2	2:B:182:GLN:NE2	2.33	0.44
2:B:303:LEU:HD22	2:B:307:ARG:NE	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:TYR:HE2	1:A:239:TRP:CZ3	2.36	0.44
1:A:96:HIS:O	1:A:97:PRO:C	2.60	0.44
2:B:195:ILE:HD11	2:B:199:ARG:HD3	1.99	0.44
2:B:255:ASN:HB2	2:B:289:LEU:HG	1.99	0.44
2:B:279:LEU:O	2:B:282:LEU:HB2	2.17	0.44
1:A:122:GLU:OE1	1:A:122:GLU:N	2.46	0.44
1:A:266:TRP:CD1	1:A:266:TRP:C	2.93	0.44
2:B:30:LYS:NZ	2:B:404:GLU:OE2	2.46	0.44
2:B:34:LEU:CD2	2:B:73:LYS:HG2	2.48	0.44
2:B:125:ARG:O	2:B:126:LYS:C	2.60	0.44
2:B:257:ILE:O	2:B:261:VAL:HG23	2.17	0.44
2:B:279:LEU:HD23	2:B:299:ALA:HB1	2.00	0.44
2:B:308:GLU:O	2:B:311:LYS:HB2	2.18	0.44
2:B:314:VAL:HG13	2:B:317:VAL:CG2	2.47	0.44
1:A:310:LEU:C	1:A:312:GLU:H	2.26	0.44
1:A:364:ASP:O	1:A:365:VAL:C	2.61	0.44
1:A:402:TRP:O	1:A:404:GLU:N	2.51	0.44
1:A:515:SER:O	1:A:516:GLU:C	2.60	0.44
2:B:115:TYR:CD1	2:B:156:SER:HB3	2.52	0.44
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	3.04	0.44
1:A:196:GLY:O	1:A:197:GLN:C	2.59	0.43
1:A:517:LEU:O	1:A:520:GLN:N	2.51	0.43
1:A:489:SER:HB2	1:A:493:VAL:HG22	2.00	0.43
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.00	0.43
2:B:72:ARG:CZ	2:B:409:THR:HG22	2.48	0.43
1:A:60:VAL:O	1:A:60:VAL:HG13	2.17	0.43
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.50	0.43
2:B:367:GLN:O	2:B:371:ALA:N	2.46	0.43
1:A:38:CYS:O	1:A:42:GLU:HB2	2.18	0.43
1:A:64:LYS:CD	1:A:64:LYS:N	2.82	0.43
1:A:426:TRP:CD1	1:A:426:TRP:N	2.87	0.43
2:B:60:VAL:O	2:B:61:PHE:HB3	2.18	0.43
2:B:132:ILE:HB	2:B:142:ILE:HD12	2.00	0.43
1:A:314:VAL:HG23	1:A:314:VAL:O	2.18	0.43
1:A:338:THR:HG22	1:A:353:LYS:HB3	2.01	0.43
2:B:203:GLU:OE2	2:B:206:ARG:NH1	2.52	0.43
1:A:125:ARG:O	1:A:126:LYS:C	2.62	0.43
1:A:149:LEU:HG	1:A:156:SER:HA	2.01	0.43
1:A:402:TRP:CZ2	2:B:362:THR:HA	2.54	0.43
2:B:8:VAL:HG23	2:B:9:PRO:HD2	2.01	0.43
2:B:115:TYR:C	2:B:117:SER:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:ILE:HB	2:B:383:TRP:CE3	2.54	0.43
1:A:319:TYR:O	1:A:321:PRO:HD3	2.18	0.43
1:A:3:SER:HB3	1:A:4:PRO:CD	2.48	0.42
1:A:102:LYS:HB2	1:A:102:LYS:HZ1	1.84	0.42
1:A:516:GLU:C	1:A:519:ASN:HB2	2.43	0.42
2:B:195:ILE:CG2	2:B:196:GLY:N	2.67	0.42
2:B:282:LEU:HD22	2:B:293:ILE:CG2	2.49	0.42
1:A:211:ARG:HH11	1:A:211:ARG:CB	2.31	0.42
1:A:420:PRO:HA	1:A:421:PRO:C	2.43	0.42
1:A:84:THR:O	1:A:85:GLN:O	2.36	0.42
1:A:132:ILE:O	1:A:141:GLY:HA3	2.18	0.42
2:B:182:GLN:HB2	2:B:187:LEU:HD12	1.99	0.42
2:B:301:LEU:HG	2:B:302:GLU:N	2.32	0.42
1:A:65:LYS:CG	1:A:66:LYS:N	2.82	0.42
1:A:111:VAL:HG22	1:A:185:ASP:HA	2.02	0.42
1:A:132:ILE:O	1:A:132:ILE:HG22	2.19	0.42
1:A:465:LYS:C	1:A:466:VAL:CG2	2.92	0.42
2:B:210:LEU:C	2:B:212:TRP:H	2.26	0.42
2:B:239:TRP:CH2	2:B:378:GLU:HA	2.51	0.42
1:A:51:GLY:C	1:A:53:GLU:H	2.27	0.42
1:A:169:GLU:O	1:A:173:LYS:HD3	2.20	0.42
2:B:279:LEU:HG	2:B:302:GLU:OE2	2.19	0.42
1:A:428:GLN:O	1:A:429:LEU:C	2.62	0.42
2:B:211:ARG:O	2:B:211:ARG:CG	2.67	0.42
1:A:84:THR:C	1:A:85:GLN:O	2.61	0.42
1:A:293:ILE:N	1:A:293:ILE:CD1	2.81	0.42
1:A:396:GLU:CD	1:A:396:GLU:N	2.75	0.42
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.53	0.42
1:A:33:ALA:HB2	1:A:71:TRP:CD1	2.55	0.42
1:A:137:ASN:OD1	1:A:137:ASN:O	2.38	0.42
1:A:202:ILE:HG22	1:A:203:GLU:N	2.35	0.42
1:A:225:PRO:HG3	1:A:227:PHE:CZ	2.55	0.42
2:B:41:MET:HG2	2:B:46:LYS:HD2	2.02	0.42
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.50	0.42
2:B:206:ARG:NH1	2:B:206:ARG:CB	2.74	0.42
2:B:356:ARG:HG3	2:B:356:ARG:NH1	2.34	0.42
1:A:205:LEU:O	1:A:209:LEU:HG	2.19	0.42
1:A:484:LEU:HA	1:A:484:LEU:HD23	1.84	0.42
1:A:338:THR:HG22	1:A:353:LYS:CB	2.49	0.41
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.20	0.41
2:B:98:ALA:CA	2:B:101:LYS:HZ3	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:PRO:HG3	2:B:184:MET:HA	2.02	0.41
2:B:388:LYS:HE2	2:B:415:GLU:HB3	2.02	0.41
1:A:235:HIS:O	1:A:238:LYS:O	2.38	0.41
1:A:274:ILE:HD13	1:A:309:ILE:HD12	2.02	0.41
1:A:465:LYS:C	1:A:466:VAL:HG23	2.45	0.41
1:A:29:GLU:HG2	1:A:71:TRP:HE1	1.85	0.41
1:A:149:LEU:HD21	1:A:160:PHE:N	2.35	0.41
1:A:245:VAL:O	1:A:245:VAL:HG23	2.19	0.41
1:A:255:ASN:HD22	1:A:255:ASN:HA	1.58	0.41
2:B:197:GLN:H	2:B:197:GLN:HG3	1.72	0.41
1:A:13:LYS:HG2	1:A:85:GLN:HA	2.03	0.41
2:B:61:PHE:HE1	2:B:63:ILE:HD11	1.85	0.41
2:B:82:LYS:HD3	2:B:413:GLU:OE1	2.20	0.41
2:B:278:GLN:HA	2:B:278:GLN:NE2	2.35	0.41
1:A:8:VAL:O	1:A:121:ASP:HB2	2.19	0.41
1:A:134:SER:CB	1:A:138:GLU:HB2	2.49	0.41
1:A:368:LEU:O	1:A:372:VAL:HG23	2.20	0.41
2:B:332:GLN:NE2	2:B:424:LYS:HE2	2.36	0.41
1:A:41:MET:HB2	1:A:47:ILE:CD1	2.51	0.41
1:A:324:ASP:O	1:A:343:GLN:HG2	2.19	0.41
1:A:58:THR:CG2	1:A:76:ASP:O	2.69	0.41
2:B:393:ILE:HD11	2:B:397:THR:HG22	2.03	0.41
1:A:31:ILE:O	1:A:32:LYS:C	2.64	0.41
1:A:64:LYS:HE3	1:A:71:TRP:HZ3	1.81	0.41
1:A:168:LEU:O	1:A:169:GLU:C	2.64	0.41
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.56	0.41
1:A:378:GLU:HG3	4:A:1010:HOH:O	2.20	0.41
1:A:96:HIS:CD2	1:A:98:ALA:H	2.29	0.41
1:A:164:MET:CE	1:A:214:LEU:HD13	2.44	0.41
1:A:183:TYR:O	1:A:184:MET:C	2.62	0.41
1:A:326:ILE:O	1:A:341:ILE:HA	2.21	0.41
2:B:28:GLU:CG	2:B:135:ILE:HD11	2.50	0.41
2:B:51:GLY:HA3	2:B:53:GLU:OE1	2.21	0.41
2:B:281:LYS:C	2:B:283:LEU:N	2.76	0.41
1:A:78:ARG:O	1:A:82:LYS:HG2	2.20	0.41
1:A:270:ILE:CG2	1:A:314:VAL:HG21	2.51	0.41
2:B:35:VAL:O	2:B:36:GLU:C	2.64	0.41
2:B:281:LYS:HZ2	2:B:284:ARG:HH22	1.68	0.41
2:B:314:VAL:HG13	2:B:317:VAL:HG21	2.03	0.41
2:B:393:ILE:HG12	2:B:394:GLN:H	1.86	0.41
2:B:111:VAL:HG22	2:B:185:ASP:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.80	0.40
2:B:361:HIS:CD2	2:B:361:HIS:N	2.88	0.40
1:A:12:LEU:O	1:A:13:LYS:C	2.65	0.40
2:B:344:GLU:HB3	2:B:347:LYS:HE3	2.03	0.40
1:A:124:PHE:O	1:A:127:TYR:CD2	2.74	0.40
1:A:329:ILE:O	1:A:392:PRO:HD3	2.21	0.40
1:A:354:TYR:O	1:A:355:ALA:C	2.64	0.40
1:A:491:LEU:HB3	1:A:529:GLU:HB2	2.02	0.40
1:A:84:THR:HG22	1:A:85:GLN:O	2.21	0.40
1:A:115:TYR:C	1:A:117:SER:H	2.29	0.40
1:A:175:ASN:CB	1:A:178:ILE:HD13	2.46	0.40
2:B:13:LYS:HE3	2:B:84:THR:O	2.20	0.40
2:B:116:PHE:HA	2:B:148:VAL:HG21	2.03	0.40
2:B:326:ILE:HG22	2:B:327:ALA:N	2.35	0.40
1:A:408:ALA:HB3	2:B:393:ILE:CB	2.51	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	536/560 (96%)	439 (82%)	72 (13%)	25 (5%)	2	2
2	B	398/440 (90%)	343 (86%)	47 (12%)	8 (2%)	6	12
All	All	934/1000 (93%)	782 (84%)	119 (13%)	33 (4%)	3	4

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	217	PRO
1	A	218	ASP

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Mol	Chain	Res	Type
2	B	98	ALA
2	B	195	ILE
2	B	361	HIS
1	A	67	ASP
1	A	85	GLN
1	A	91	GLN
1	A	113	ASP
1	A	138	GLU
2	B	66	LYS
2	B	116	PHE
2	B	208	HIS
1	A	68	SER
1	A	78	ARG
1	A	126	LYS
1	A	170	PRO
1	A	315	HIS
1	A	361	HIS
1	A	517	LEU
1	A	115	TYR
1	A	116	PHE
1	A	403	THR
1	A	4	PRO
1	A	135	ILE
1	A	476	LYS
2	B	85	GLN
1	A	123	ASP
2	B	421	PRO
1	A	139	THR
1	A	176	PRO
1	A	420	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	483/499 (97%)	435 (90%)	48 (10%)	7 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	368/400 (92%)	345 (94%)	23 (6%)	16	36
All	All	851/899 (95%)	780 (92%)	71 (8%)	10	23

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	6	GLU
1	A	24	TRP
1	A	64	LYS
1	A	89	GLU
1	A	92	LEU
1	A	94	ILE
1	A	102	LYS
1	A	105	SER
1	A	109	LEU
1	A	113	ASP
1	A	120	LEU
1	A	122	GLU
1	A	135	ILE
1	A	143	ARG
1	A	175	ASN
1	A	182	GLN
1	A	184	MET
1	A	187	LEU
1	A	205	LEU
1	A	210	LEU
1	A	211	ARG
1	A	217	PRO
1	A	229	TRP
1	A	255	ASN
1	A	266	TRP
1	A	282	LEU
1	A	293	ILE
1	A	322	SER
1	A	325	LEU
1	A	340	GLN
1	A	344	GLU
1	A	369	THR
1	A	374	LYS
1	A	393	ILE
1	A	402	TRP

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Mol	Chain	Res	Type
1	A	403	THR
1	A	404	GLU
1	A	417	VAL
1	A	431	LYS
1	A	449	GLU
1	A	452	LEU
1	A	475	GLN
1	A	493	VAL
1	A	496	VAL
1	A	500	GLN
1	A	517	LEU
1	A	533	LEU
2	B	8	VAL
2	B	40	GLU
2	B	69	THR
2	B	73	LYS
2	B	82	LYS
2	B	88	TRP
2	B	138	GLU
2	B	163	SER
2	B	165	THR
2	B	179	VAL
2	B	209	LEU
2	B	211	ARG
2	B	238	LYS
2	B	239	TRP
2	B	243	PRO
2	B	249	LYS
2	B	283	LEU
2	B	284	ARG
2	B	287	LYS
2	B	290	THR
2	B	361	HIS
2	B	368	LEU
2	B	388	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	96	HIS
1	A	136	ASN

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	161	GLN
1	A	174	GLN
1	A	175	ASN
1	A	255	ASN
1	A	278	GLN
1	A	306	ASN
1	A	315	HIS
1	A	332	GLN
1	A	336	GLN
1	A	428	GLN
1	A	475	GLN
1	A	480	GLN
1	A	500	GLN
1	A	512	GLN
1	A	519	ASN
2	B	54	ASN
2	B	57	ASN
2	B	145	GLN
2	B	147	ASN
2	B	161	GLN
2	B	182	GLN
2	B	197	GLN
2	B	278	GLN
2	B	332	GLN
2	B	348	ASN
2	B	394	GLN
2	B	418	ASN
2	B	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSD	A	280	1	4,7,8	1.60	1 (25%)	1,8,10	4.74	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	OD1-SG	2.59	1.50	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	4.74	114.34	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NVP	A	999	-	23,23,23	1.94	5 (21%)	34,34,34	2.05	6 (17%)

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
3	NVP	A	999	-	-	2/4/6/6	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	NVP	C15-N1	5.16	1.47	1.42
3	A	999	NVP	C10-C9	4.15	1.54	1.49
3	A	999	NVP	C2-N1	3.47	1.45	1.42
3	A	999	NVP	C5-C4	2.32	1.43	1.38
3	A	999	NVP	C7-N8	2.06	1.44	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	NVP	C7-N8-C9	6.80	133.90	128.29
3	A	999	NVP	C7-C2-N1	-5.18	118.15	120.14
3	A	999	NVP	N3-C2-N1	4.04	119.72	116.67
3	A	999	NVP	CC-CA-N1	3.21	117.99	116.09
3	A	999	NVP	N14-C15-N1	3.15	119.05	116.67
3	A	999	NVP	C2-N1-CA	-2.34	114.49	116.34

There are no chirality outliers.

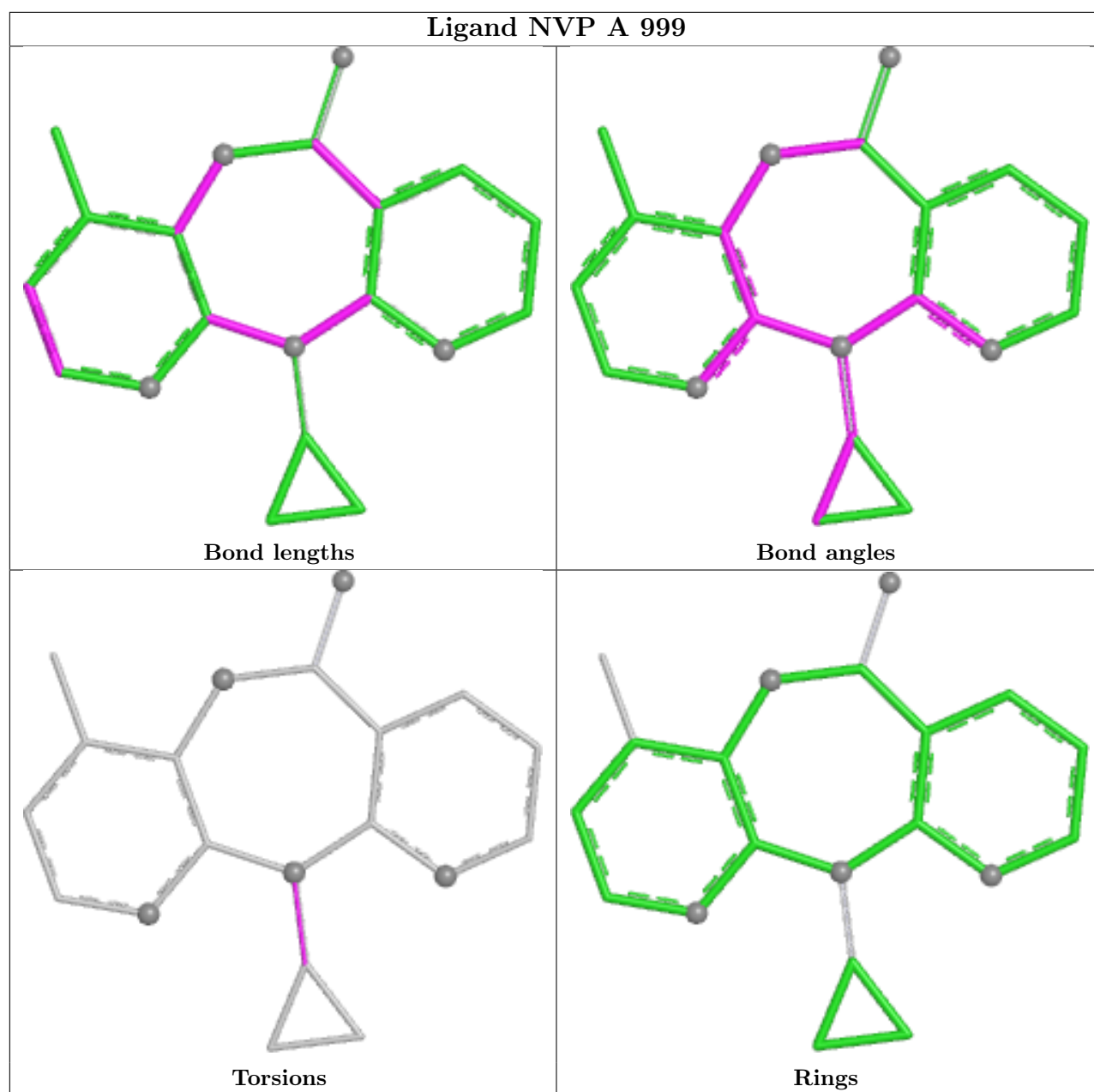
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	NVP	CC-CA-N1-C2
3	A	999	NVP	CB-CA-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	538/560 (96%)	-0.34	2 (0%) 88 86	18, 79, 126, 150	0
2	B	404/440 (91%)	-0.42	0 100 100	29, 73, 119, 150	0
All	All	942/1000 (94%)	-0.37	2 (0%) 91 90	18, 76, 123, 150	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	2.2
1	A	244	ILE	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSD	A	280	8/9	0.91	0.08	76,87,108,126	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

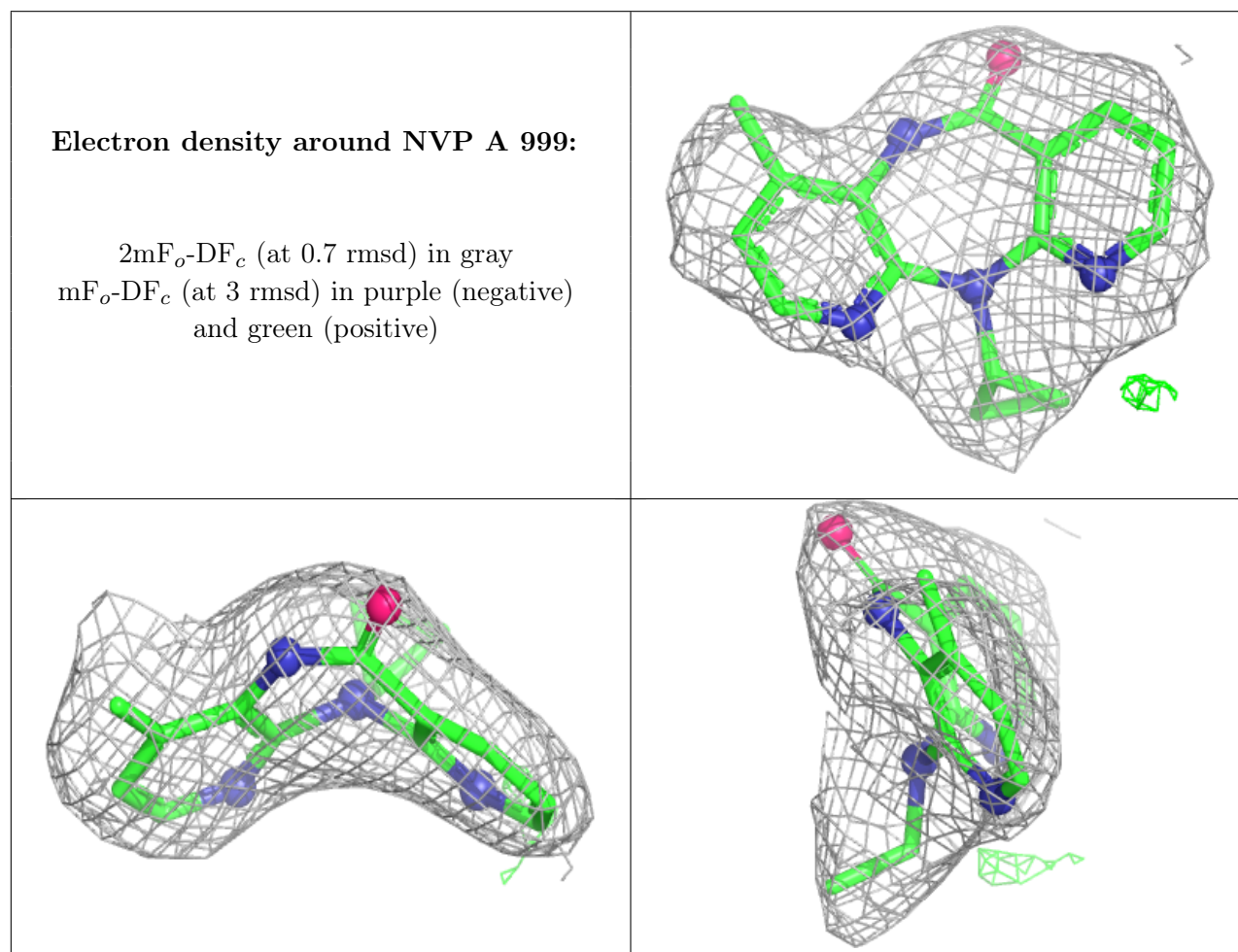
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NVP	A	999	20/20	0.87	0.11	80,99,112,116	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.