



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:53 AM UTC

PDB ID : 1LW0 / pdb_00001lw0
Title : CRYSTAL STRUCTURE OF T215Y MUTANT HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH NEVIRAPINE
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Deposited on : 2002-05-30
Resolution : 2.80 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

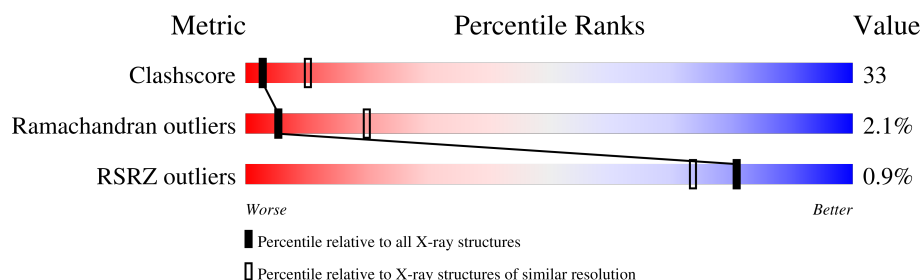
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	1301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7546 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 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			4210	2730	692	780	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	TYR	THR	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	399	Total	C	N	O	S	0	0	0
			3306	2156	546	597	7			

There is a discrepancy between the modelled and reference sequences:

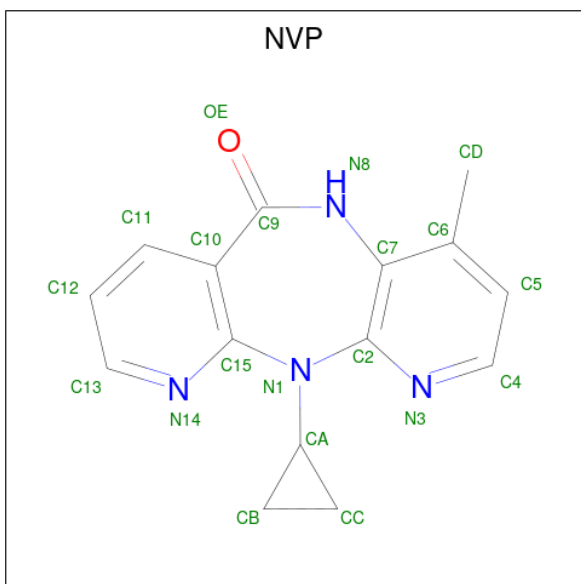
Chain	Residue	Modelled	Actual	Comment	Reference
B	215	TYR	THR	engineered mutation	UNP P04585

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 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: $C_{15}H_{14}N_4O$).

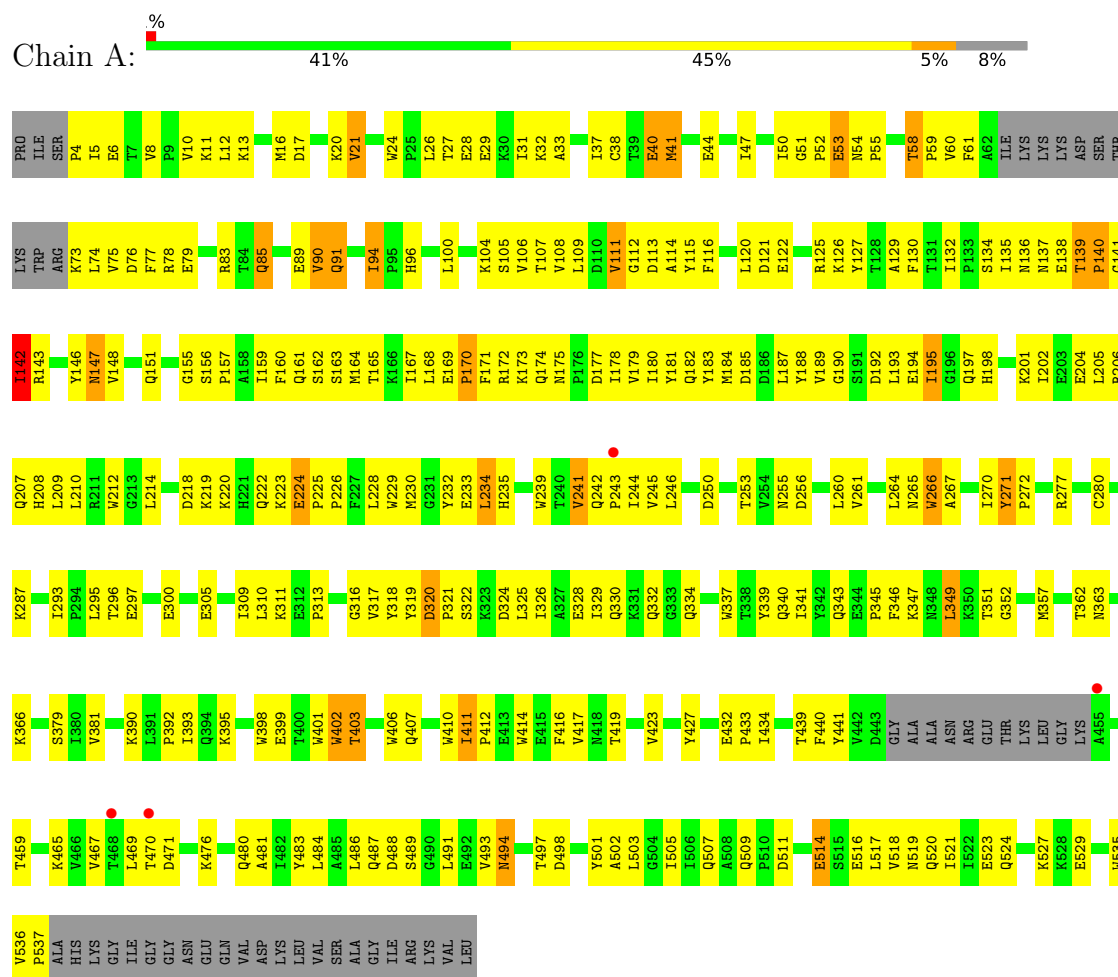


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			20	15	4	1		

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 REVERSE TRANSCRIPTASE



K390	K391	P392	I393	Q394	K395	W401	W402	T403	E404	Y405	T409	W410	I411	E415	F416	W417	N418	T419	P420	P421	L422	V423	K424	L425	W426	Y427	Q428	LEU	GLU	LYS	GLU	PRO	ILE	VAL	GLY	GLY	ALA	GLU	THR	PHE																			
P321	I325	E326	K327	E328	I329	Q330	K331	Q332	G335	Q340	Q343	E344	F345	F346	K347	N348	L349	K350	T351	G352	K353	T354	A355	K356	MET	ARG	GLY	ALA	HIS	T362	N363	D364	V365	K366	Q367	L368	A371	V372	T375	T376	T377	E378	S379	I380	V381	W383	G384	K385	T386	P387	K388	F389							
Q242	P243	E248	K249	D250	S251	W252	T253	V254	W255	D256	T257	Q258	K259	L260	V261	N265	W266	A267	S268	Q269	L270	Y271	I274	K275	V276	R277	Q278	W212	C280	K281	L282	L283	K287	A288	L289	T290	E291	V292	T293	P294	L295	N306	I309	L310	K311	E312	P313	G316	V317	Y318	Y319	D320							
Q182	Y183	M184	D185	D186	L187	Y188	V189	G190	S191	D192	L193	E194	I195	G196	Q197	H198	R199	T200	K201	L202	E203	E204	L205	R206	Q207	L208	L209	L210	R211	W212	C213	LEU	TYR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU	P225	F226	F227	L228	W229	W230	C231	Y232	E233	L234	H235	P236	D237	K238	W239	T240	V241
P85	R86	P87	A88	G89	K102	K103	V106	T107	V108	L109	D110	V111	L120	D121	R125	A126	Y127	T131	I135	E138	I142	R143	Y144	Q145	Y146	N147	P150	Q151	P157	F160	Q161	S162	S163	M164	T165	K166	I167	L168	E169	P170	F171	R172	K173	G174	N175	P176	D177												

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.70Å 115.00Å 65.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.85 – 2.80 29.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (29.85-2.80) 93.8 (29.85-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.301 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 88.7	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	0.94	EDS
Total number of atoms	7546	wwPDB-VP
Average B, all atoms (Å ²)	83.0	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, PO4

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	0.69	0/4314	1.17	34/5867 (0.6%)
2	B	0.65	0/3401	1.24	42/4618 (0.9%)
All	All	0.68	0/7715	1.20	76/10485 (0.7%)

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	225	PRO	CA-C-N	21.35	146.53	119.84
2	B	225	PRO	C-N-CA	21.35	146.53	119.84
1	A	349	LEU	N-CA-C	-13.27	96.83	113.55
2	B	226	PRO	CA-C-N	-10.71	106.00	122.81
2	B	226	PRO	C-N-CA	-10.71	106.00	122.81
1	A	419	THR	CA-C-N	-10.62	109.44	120.38
1	A	419	THR	C-N-CA	-10.62	109.44	120.38
2	B	312	GLU	N-CA-C	8.91	116.24	108.22
2	B	234	LEU	N-CA-C	-8.67	97.65	110.48
1	A	234	LEU	N-CA-C	8.08	122.01	108.20
1	A	53	GLU	N-CA-C	-7.91	103.08	112.89
1	A	224	GLU	CA-C-N	7.74	128.36	120.38
1	A	224	GLU	C-N-CA	7.74	128.36	120.38
1	A	58	THR	CA-C-N	7.66	129.41	119.84
1	A	58	THR	C-N-CA	7.66	129.41	119.84
2	B	382	ILE	N-CA-C	7.37	117.46	110.53
1	A	320	ASP	CA-C-N	7.30	128.96	119.84
1	A	320	ASP	C-N-CA	7.30	128.96	119.84
2	B	248	GLU	N-CA-C	-7.20	97.50	109.24
1	A	494	ASN	N-CA-C	-7.11	97.30	108.90
1	A	334	GLN	N-CA-C	-7.05	99.22	109.59
1	A	21	VAL	N-CA-C	6.66	117.43	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	GLU	N-CA-C	-6.53	104.16	111.28
2	B	225	PRO	C-N-CD	-6.53	98.23	125.00
1	A	287	LYS	N-CA-C	6.50	121.36	113.17
2	B	51	GLY	CA-C-N	6.33	126.01	119.56
2	B	51	GLY	C-N-CA	6.33	126.01	119.56
1	A	241	VAL	N-CA-C	-6.27	99.43	108.53
2	B	189	VAL	N-CA-C	6.26	116.40	106.88
2	B	209	LEU	N-CA-C	-6.15	105.93	113.50
1	A	155	GLY	N-CA-C	6.08	122.85	115.31
2	B	177	ASP	N-CA-C	-6.03	105.92	113.28
2	B	229	TRP	N-CA-C	6.01	119.86	111.74
1	A	514	GLU	N-CA-C	-6.01	104.66	112.23
1	A	96	HIS	N-CA-C	-5.89	100.46	109.64
2	B	235	HIS	CA-C-N	5.86	125.72	119.28
2	B	235	HIS	C-N-CA	5.86	125.72	119.28
2	B	316	GLY	N-CA-C	5.85	121.74	114.37
2	B	232	TYR	N-CA-C	5.84	119.23	109.95
2	B	68	SER	N-CA-C	-5.82	100.50	109.52
2	B	343	GLN	N-CA-C	-5.79	106.85	114.04
2	B	294	PRO	N-CA-C	-5.77	102.08	110.80
2	B	293	ILE	CA-C-N	-5.75	113.86	119.90
2	B	293	ILE	C-N-CA	-5.75	113.86	119.90
2	B	186	ASP	N-CA-C	5.71	119.03	109.95
1	A	41	MET	N-CA-C	5.71	117.58	111.36
2	B	147	ASN	N-CA-C	-5.60	107.10	114.04
2	B	389	PHE	N-CA-C	5.53	118.30	110.50
2	B	249	LYS	N-CA-C	5.52	117.66	108.99
2	B	98	ALA	N-CA-C	-5.49	106.66	113.19
1	A	111	VAL	N-CA-C	5.42	115.66	107.75
2	B	24	TRP	CA-C-N	5.41	125.42	119.90
2	B	24	TRP	C-N-CA	5.41	125.42	119.90
1	A	329	ILE	N-CA-C	5.41	117.18	108.85
2	B	391	LEU	N-CA-C	5.41	118.48	110.32
2	B	227	PHE	N-CA-CB	5.41	120.32	111.08
1	A	142	ILE	N-CA-C	5.35	120.46	109.34
2	B	228	LEU	N-CA-C	-5.32	102.87	110.59
1	A	137	ASN	N-CA-C	5.29	122.07	110.80
2	B	58	THR	CA-C-N	5.28	126.10	120.13
2	B	58	THR	C-N-CA	5.28	126.10	120.13
1	A	411	ILE	CA-C-N	5.27	126.43	119.84
1	A	411	ILE	C-N-CA	5.27	126.43	119.84
2	B	348	ASN	N-CA-C	5.22	118.06	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ILE	CA-C-N	5.21	125.14	119.78
1	A	94	ILE	C-N-CA	5.21	125.14	119.78
1	A	147	ASN	N-CA-C	-5.21	105.80	113.61
1	A	4	PRO	N-CA-C	-5.19	99.13	112.10
2	B	184	MET	CB-CA-C	-5.18	110.58	116.54
2	B	31	ILE	N-CA-C	5.16	115.37	110.42
2	B	37	ILE	N-CA-C	5.14	115.58	110.23
2	B	390	LYS	N-CA-C	-5.12	100.06	108.41
2	B	401	TRP	N-CA-C	5.08	120.13	113.88
1	A	174	GLN	N-CA-C	-5.04	107.13	113.28
1	A	271	TYR	CA-C-N	5.02	125.41	119.99
1	A	271	TYR	C-N-CA	5.02	125.41	119.99

There are no chirality outliers.

There are no planarity outliers.

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	4210	0	4230	291	0
2	B	3306	0	3334	209	0
3	A	10	0	0	2	0
4	A	20	0	14	1	0
All	All	7546	0	7578	495	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 33.

All (495) 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:164:MET:SD	1:A:168:LEU:HD21	1.95	1.06
1:A:469:LEU:HD21	1:A:480:GLN:HG3	1.32	1.05
2:B:295:LEU:H	2:B:295:LEU:HD12	1.24	0.99
1:A:395:LYS:H	1:A:395:LYS:HD2	1.25	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HD13	1:A:142:ILE:H	1.30	0.93
2:B:166:LYS:HE3	2:B:166:LYS:HA	1.50	0.92
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.50	0.92
1:A:28:GLU:OE1	1:A:135:ILE:HG23	1.69	0.91
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.53	0.90
1:A:167:ILE:O	1:A:170:PRO:HD2	1.72	0.89
1:A:195:ILE:HD13	1:A:195:ILE:H	1.37	0.89
1:A:503:LEU:HD12	1:A:535:TRP:HB2	1.54	0.88
1:A:89:GLU:C	1:A:91:GLN:H	1.78	0.88
2:B:173:LYS:HA	2:B:176:PRO:HG3	1.58	0.86
2:B:168:LEU:HD21	2:B:172:ARG:HD2	1.58	0.85
2:B:195:ILE:HD11	2:B:233:GLU:CD	2.01	0.85
2:B:206:ARG:NH2	2:B:226:PRO:C	2.35	0.85
1:A:277:ARG:NH1	3:A:1301:PO4:O3	2.10	0.84
1:A:168:LEU:HD22	1:A:168:LEU:N	1.94	0.83
1:A:395:LYS:HD2	1:A:395:LYS:N	1.93	0.83
2:B:295:LEU:H	2:B:295:LEU:CD1	1.92	0.83
1:A:395:LYS:H	1:A:395:LYS:CD	1.91	0.82
2:B:195:ILE:HD11	2:B:233:GLU:OE1	1.78	0.82
1:A:317:VAL:HG12	1:A:349:LEU:HD23	1.60	0.82
2:B:295:LEU:HD12	2:B:295:LEU:N	1.94	0.82
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.59	0.82
1:A:161:GLN:HA	1:A:182:GLN:HE22	1.45	0.81
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.16	0.80
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.63	0.80
1:A:195:ILE:HD13	1:A:195:ILE:N	1.97	0.79
1:A:139:THR:HB	1:A:140:PRO:HD2	1.64	0.79
1:A:5:ILE:HD12	1:A:6:GLU:H	1.45	0.79
1:A:51:GLY:C	1:A:53:GLU:H	1.90	0.78
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.65	0.78
1:A:138:GLU:O	1:A:138:GLU:HG3	1.84	0.78
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.13	0.78
1:A:104:LYS:HB3	1:A:104:LYS:HZ3	1.48	0.78
1:A:182:GLN:HA	1:A:187:LEU:HD12	1.66	0.77
2:B:31:ILE:O	2:B:35:VAL:HG23	1.85	0.76
1:A:168:LEU:HD22	1:A:168:LEU:H	1.49	0.76
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.66	0.76
2:B:395:LYS:HD2	2:B:416:PHE:CE1	2.20	0.76
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.21	0.76
1:A:253:THR:HG22	1:A:256:ASP:H	1.52	0.75
1:A:168:LEU:H	1:A:168:LEU:CD2	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:HD13	1:A:230:MET:HE2	1.69	0.74
1:A:469:LEU:CD2	1:A:480:GLN:HG3	2.16	0.74
2:B:353:LYS:NZ	2:B:428:GLN:HG3	2.02	0.74
1:A:28:GLU:CD	1:A:135:ILE:HG23	2.12	0.73
1:A:503:LEU:CD1	1:A:535:TRP:HB2	2.16	0.73
1:A:89:GLU:OE1	1:A:91:GLN:HA	1.89	0.73
1:A:324:ASP:O	1:A:343:GLN:HG2	1.90	0.71
1:A:27:THR:HG22	1:A:29:GLU:H	1.54	0.71
2:B:66:LYS:HG2	2:B:230:MET:HG2	1.71	0.71
2:B:332:GLN:HB3	2:B:428:GLN:HE22	1.56	0.71
2:B:142:ILE:H	2:B:142:ILE:HD12	1.54	0.70
2:B:206:ARG:NH2	2:B:227:PHE:CD1	2.60	0.70
2:B:28:GLU:CG	2:B:32:LYS:HE3	2.20	0.70
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.55	0.70
1:A:497:THR:O	1:A:535:TRP:HA	1.92	0.70
1:A:61:PHE:CE2	1:A:74:LEU:HB3	2.28	0.69
2:B:203:GLU:O	2:B:206:ARG:HB2	1.92	0.69
1:A:28:GLU:O	1:A:32:LYS:HG3	1.93	0.69
1:A:295:LEU:HD12	1:A:300:GLU:CD	2.18	0.68
1:A:175:ASN:HB3	1:A:178:ILE:HG12	1.74	0.68
2:B:420:PRO:O	2:B:423:VAL:HG12	1.93	0.68
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.08	0.68
2:B:169:GLU:N	2:B:170:PRO:HD2	2.08	0.68
1:A:241:VAL:HB	1:A:266:TRP:HE1	1.58	0.68
2:B:275:LYS:HD2	2:B:277:ARG:HH21	1.58	0.68
2:B:175:ASN:N	2:B:176:PRO:HD3	2.09	0.68
1:A:51:GLY:O	1:A:53:GLU:N	2.27	0.67
1:A:207:GLN:NE2	1:A:207:GLN:HA	2.07	0.67
2:B:275:LYS:CD	2:B:277:ARG:HH21	2.07	0.67
2:B:168:LEU:HD21	2:B:172:ARG:CD	2.24	0.67
2:B:379:SER:OG	2:B:387:PRO:HG3	1.94	0.67
1:A:363:ASN:HA	1:A:511:ASP:OD1	1.95	0.66
2:B:206:ARG:HH22	2:B:226:PRO:C	2.02	0.66
2:B:206:ARG:HH22	2:B:227:PHE:N	1.94	0.66
1:A:104:LYS:HB3	1:A:104:LYS:NZ	2.10	0.66
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.30	0.66
1:A:94:ILE:CD1	1:A:230:MET:HE2	2.26	0.65
1:A:136:ASN:CB	1:A:139:THR:OG1	2.44	0.65
1:A:208:HIS:O	1:A:212:TRP:CD1	2.49	0.65
2:B:228:LEU:HD11	2:B:409:THR:HG23	1.77	0.65
1:A:168:LEU:N	1:A:168:LEU:CD2	2.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LEU:HD11	1:A:480:GLN:HE21	1.62	0.65
1:A:139:THR:CB	1:A:140:PRO:HD2	2.26	0.65
2:B:172:ARG:O	2:B:176:PRO:HG3	1.97	0.65
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.31	0.64
1:A:399:GLU:HG3	1:A:402:TRP:CZ3	2.33	0.64
1:A:136:ASN:HB3	1:A:139:THR:OG1	1.98	0.64
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.80	0.64
1:A:195:ILE:H	1:A:195:ILE:CD1	2.09	0.63
1:A:524:GLN:HA	1:A:524:GLN:OE1	1.97	0.63
1:A:89:GLU:O	1:A:91:GLN:N	2.31	0.63
2:B:266:TRP:O	2:B:269:GLN:HG2	1.99	0.63
1:A:89:GLU:C	1:A:91:GLN:N	2.49	0.62
2:B:167:ILE:HD12	2:B:212:TRP:CB	2.29	0.62
2:B:175:ASN:ND2	2:B:201:LYS:HD3	2.15	0.62
1:A:244:ILE:HD11	1:A:246:LEU:HD23	1.82	0.62
2:B:425:LEU:HD22	2:B:426:TRP:CD1	2.35	0.62
1:A:132:ILE:HB	1:A:142:ILE:HG12	1.81	0.61
1:A:161:GLN:HA	1:A:182:GLN:NE2	2.13	0.61
2:B:330:GLN:OE1	2:B:340:GLN:NE2	2.28	0.61
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.81	0.61
1:A:392:PRO:O	1:A:423:VAL:HG13	2.02	0.60
2:B:380:ILE:O	2:B:384:GLY:N	2.34	0.60
1:A:239:TRP:O	1:A:316:GLY:N	2.31	0.60
2:B:229:TRP:O	2:B:232:TYR:HB2	2.02	0.59
2:B:311:LYS:O	2:B:312:GLU:HG3	2.03	0.59
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.84	0.59
1:A:467:VAL:HG21	1:A:484:LEU:HD11	1.84	0.58
2:B:353:LYS:HZ2	2:B:428:GLN:HG3	1.66	0.58
1:A:245:VAL:HG13	1:A:245:VAL:O	2.03	0.58
1:A:51:GLY:C	1:A:53:GLU:N	2.59	0.58
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.01	0.58
2:B:40:GLU:O	2:B:44:GLU:HG3	2.03	0.58
1:A:5:ILE:HD12	1:A:6:GLU:N	2.15	0.58
1:A:33:ALA:O	1:A:37:ILE:HG13	2.03	0.58
2:B:135:ILE:O	2:B:138:GLU:HG3	2.03	0.58
1:A:134:SER:HB2	1:A:140:PRO:O	2.02	0.58
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.38	0.58
1:A:398:TRP:NE1	1:A:411:ILE:HD12	2.18	0.58
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.34	0.58
2:B:167:ILE:HD12	2:B:212:TRP:HB2	1.86	0.57
2:B:395:LYS:HD2	2:B:416:PHE:HE1	1.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PHE:O	1:A:161:GLN:C	2.46	0.57
1:A:125:ARG:HG2	1:A:146:TYR:O	2.05	0.57
1:A:182:GLN:HA	1:A:187:LEU:CD1	2.34	0.57
1:A:317:VAL:HG12	1:A:349:LEU:CD2	2.34	0.57
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.85	0.57
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.35	0.57
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.70	0.57
1:A:175:ASN:HB3	1:A:178:ILE:CG1	2.34	0.56
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.40	0.56
1:A:76:ASP:OD2	1:A:78:ARG:HG3	2.05	0.56
1:A:107:THR:HG22	1:A:109:LEU:HD13	1.88	0.56
1:A:142:ILE:H	1:A:142:ILE:CD1	2.02	0.56
2:B:206:ARG:CZ	2:B:227:PHE:CD1	2.89	0.56
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.40	0.56
2:B:9:PRO:HA	2:B:121:ASP:OD2	2.06	0.56
2:B:276:VAL:HG12	2:B:276:VAL:O	2.05	0.56
1:A:244:ILE:HD13	1:A:244:ILE:C	2.31	0.56
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.88	0.56
1:A:115:TYR:CD1	1:A:151:GLN:HG2	2.41	0.56
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.87	0.56
2:B:277:ARG:HG3	2:B:278:GLN:H	1.71	0.56
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.41	0.55
1:A:61:PHE:N	1:A:61:PHE:CD2	2.74	0.55
2:B:325:LEU:O	2:B:387:PRO:HA	2.06	0.55
1:A:24:TRP:HZ3	1:A:61:PHE:CG	2.24	0.55
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.88	0.55
1:A:61:PHE:N	1:A:61:PHE:HD2	2.04	0.55
1:A:8:VAL:HG21	1:A:159:ILE:HG23	1.87	0.55
1:A:10:VAL:HG12	1:A:11:LYS:N	2.21	0.55
2:B:28:GLU:HG2	2:B:32:LYS:HE3	1.89	0.55
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.40	0.55
2:B:103:LYS:HE3	2:B:191:SER:HA	1.88	0.55
2:B:161:GLN:O	2:B:164:MET:HB3	2.06	0.55
2:B:366:LYS:HA	2:B:405:TYR:CD1	2.42	0.55
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.20	0.55
1:A:108:VAL:HG11	1:A:223:LYS:HB2	1.88	0.55
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.38	0.54
1:A:16:MET:HE2	1:A:83:ARG:HG2	1.90	0.54
2:B:332:GLN:HB3	2:B:428:GLN:NE2	2.22	0.54
1:A:232:TYR:HA	1:A:241:VAL:HA	1.88	0.54
1:A:270:ILE:HG23	1:A:271:TYR:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:LYS:HA	2:B:176:PRO:CG	2.33	0.54
2:B:206:ARG:NH2	2:B:227:PHE:N	2.54	0.54
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.40	0.53
1:A:139:THR:HB	1:A:140:PRO:CD	2.36	0.53
2:B:65:LYS:HB2	2:B:68:SER:HB3	1.88	0.53
2:B:168:LEU:CD2	2:B:172:ARG:HD2	2.36	0.53
1:A:346:PHE:N	1:A:346:PHE:CD1	2.76	0.53
1:A:104:LYS:NZ	1:A:104:LYS:CB	2.71	0.53
1:A:183:TYR:CZ	1:A:184:MET:HE3	2.42	0.53
1:A:516:GLU:O	1:A:520:GLN:HG3	2.07	0.53
1:A:113:ASP:O	1:A:114:ALA:C	2.52	0.53
1:A:345:PRO:C	1:A:346:PHE:HD1	2.17	0.53
1:A:363:ASN:HB2	1:A:511:ASP:OD2	2.08	0.53
2:B:208:HIS:O	2:B:212:TRP:HE3	1.91	0.53
1:A:208:HIS:O	1:A:212:TRP:HD1	1.90	0.53
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.43	0.53
2:B:234:LEU:HD21	2:B:377:THR:CG2	2.39	0.53
1:A:402:TRP:CG	1:A:403:THR:N	2.77	0.53
1:A:17:ASP:O	1:A:83:ARG:HD3	2.09	0.53
1:A:108:VAL:HG13	1:A:108:VAL:O	2.09	0.53
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.44	0.53
1:A:207:GLN:NE2	1:A:207:GLN:CA	2.72	0.52
1:A:209:LEU:O	1:A:214:LEU:HB2	2.09	0.52
2:B:142:ILE:HD12	2:B:142:ILE:N	2.24	0.52
2:B:237:ASP:OD2	2:B:238:LYS:HG3	2.09	0.52
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.45	0.52
1:A:37:ILE:O	1:A:41:MET:HG3	2.08	0.52
1:A:164:MET:O	1:A:165:THR:C	2.53	0.52
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.90	0.52
2:B:229:TRP:HA	2:B:229:TRP:CE3	2.45	0.52
2:B:106:VAL:O	2:B:233:GLU:HA	2.10	0.52
1:A:113:ASP:HA	1:A:116:PHE:CD2	2.46	0.52
1:A:253:THR:HB	1:A:256:ASP:OD2	2.10	0.52
1:A:139:THR:CB	1:A:140:PRO:CD	2.88	0.51
2:B:371:ALA:O	2:B:375:ILE:HG13	2.08	0.51
1:A:139:THR:HG22	1:A:140:PRO:CD	2.40	0.51
2:B:163:SER:O	2:B:167:ILE:HG22	2.10	0.51
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.92	0.51
1:A:253:THR:HG23	1:A:255:ASN:H	1.75	0.51
2:B:169:GLU:N	2:B:170:PRO:CD	2.73	0.51
2:B:275:LYS:HD2	2:B:277:ARG:NH2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:HE3	1:A:224:GLU:OE1	2.10	0.51
1:A:357:MET:HE1	1:A:514:GLU:HG2	1.93	0.51
2:B:254:VAL:O	2:B:258:GLN:HG3	2.10	0.51
1:A:134:SER:HB2	1:A:140:PRO:C	2.36	0.51
1:A:265:ASN:O	1:A:266:TRP:C	2.52	0.51
1:A:523:GLU:O	1:A:527:LYS:HG2	2.11	0.51
2:B:167:ILE:HD12	2:B:212:TRP:HB3	1.93	0.51
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.41	0.51
2:B:241:VAL:HG11	2:B:313:PRO:HG3	1.93	0.51
2:B:335:GLY:O	2:B:355:ALA:HA	2.10	0.51
2:B:365:VAL:O	2:B:366:LYS:C	2.51	0.51
1:A:100:LEU:HB2	1:A:318:TYR:CD1	2.46	0.50
1:A:8:VAL:HG21	1:A:159:ILE:HG12	1.94	0.50
1:A:326:ILE:O	1:A:341:ILE:HA	2.10	0.50
2:B:28:GLU:HG3	2:B:32:LYS:HE3	1.93	0.50
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.11	0.50
2:B:206:ARG:CZ	2:B:227:PHE:CE1	2.95	0.50
1:A:111:VAL:HG23	1:A:185:ASP:O	2.12	0.50
1:A:363:ASN:ND2	1:A:401:TRP:CH2	2.78	0.50
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.93	0.50
1:A:100:LEU:O	1:A:318:TYR:HB3	2.11	0.50
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.42	0.50
2:B:33:ALA:O	2:B:37:ILE:HG13	2.12	0.50
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.45	0.50
2:B:168:LEU:C	2:B:170:PRO:HD2	2.36	0.50
2:B:227:PHE:CD2	2:B:231:GLY:HA2	2.47	0.50
1:A:188:TYR:CD1	1:A:188:TYR:N	2.80	0.50
2:B:97:PRO:C	2:B:99:GLY:H	2.20	0.50
2:B:199:ARG:HH22	2:B:232:TYR:HE2	1.60	0.50
1:A:225:PRO:HA	1:A:226:PRO:C	2.36	0.50
1:A:77:PHE:O	1:A:78:ARG:C	2.55	0.50
1:A:194:GLU:O	1:A:194:GLU:HG3	2.12	0.50
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.47	0.50
1:A:104:LYS:NZ	1:A:193:LEU:O	2.42	0.49
2:B:28:GLU:CA	2:B:135:ILE:HD11	2.42	0.49
2:B:206:ARG:NH2	2:B:227:PHE:CG	2.79	0.49
1:A:40:GLU:O	1:A:44:GLU:HG3	2.12	0.49
1:A:201:LYS:HD3	1:A:204:GLU:CD	2.38	0.49
1:A:489:SER:HB2	1:A:493:VAL:HG13	1.94	0.49
2:B:173:LYS:CA	2:B:176:PRO:HG3	2.35	0.49
2:B:249:LYS:HG3	2:B:252:TRP:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:SER:HB2	1:A:198:HIS:CD2	2.47	0.49
1:A:277:ARG:NH1	3:A:1301:PO4:P	2.85	0.49
1:A:114:ALA:CB	1:A:185:ASP:OD2	2.61	0.49
1:A:120:LEU:HB2	1:A:148:VAL:O	2.13	0.49
1:A:228:LEU:HD21	1:A:233:GLU:HG3	1.95	0.49
2:B:99:GLY:HA2	2:B:102:LYS:HE2	1.95	0.49
2:B:385:LYS:HG2	2:B:386:THR:N	2.28	0.49
1:A:218:ASP:O	1:A:222:GLN:HG3	2.13	0.48
2:B:316:GLY:O	2:B:318:TYR:CD2	2.65	0.48
2:B:205:LEU:CD2	2:B:209:LEU:HG	2.43	0.48
1:A:340:GLN:HA	1:A:351:THR:HA	1.94	0.48
1:A:104:LYS:HD3	1:A:192:ASP:O	2.14	0.48
1:A:126:LYS:HG3	1:A:127:TYR:N	2.28	0.48
1:A:164:MET:O	1:A:168:LEU:HD23	2.14	0.48
2:B:195:ILE:O	2:B:199:ARG:HG3	2.14	0.48
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.79	0.48
1:A:164:MET:SD	1:A:168:LEU:CD2	2.87	0.48
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.13	0.48
2:B:173:LYS:C	2:B:176:PRO:HD3	2.38	0.47
2:B:208:HIS:CD2	2:B:212:TRP:HZ3	2.32	0.47
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.96	0.47
1:A:228:LEU:HA	1:A:232:TYR:O	2.14	0.47
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.66	0.47
1:A:317:VAL:CG1	1:A:349:LEU:HD23	2.38	0.47
1:A:345:PRO:C	1:A:347:LYS:H	2.21	0.47
2:B:209:LEU:O	2:B:213:GLY:N	2.47	0.47
1:A:481:ALA:O	1:A:484:LEU:HB2	2.13	0.47
1:A:503:LEU:HD21	1:A:507:GLN:CD	2.39	0.47
2:B:249:LYS:HD3	2:B:251:SER:O	2.13	0.47
1:A:100:LEU:O	1:A:319:TYR:N	2.45	0.47
1:A:427:TYR:OH	1:A:509:GLN:HA	2.14	0.47
1:A:265:ASN:O	1:A:267:ALA:N	2.47	0.47
1:A:8:VAL:CG2	1:A:159:ILE:HG23	2.45	0.47
1:A:21:VAL:HG22	1:A:59:PRO:CD	2.44	0.47
1:A:160:PHE:C	1:A:160:PHE:CD2	2.91	0.47
1:A:253:THR:CG2	1:A:255:ASN:H	2.27	0.47
1:A:305:GLU:O	1:A:309:ILE:HG13	2.15	0.47
1:A:325:LEU:HD22	1:A:341:ILE:CG2	2.45	0.47
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.15	0.47
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.45	0.47
1:A:5:ILE:HG13	1:A:6:GLU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ALA:O	2:B:389:PHE:HA	2.15	0.47
2:B:423:VAL:HG13	2:B:424:LYS:N	2.29	0.47
1:A:169:GLU:O	1:A:172:ARG:HB2	2.15	0.47
2:B:195:ILE:HD11	2:B:233:GLU:CG	2.45	0.47
1:A:270:ILE:CG2	1:A:271:TYR:N	2.77	0.47
1:A:163:SER:O	1:A:164:MET:C	2.58	0.46
1:A:393:ILE:O	1:A:414:TRP:CZ3	2.67	0.46
2:B:28:GLU:O	2:B:32:LYS:HG3	2.15	0.46
1:A:177:ASP:OD1	1:A:177:ASP:N	2.42	0.46
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.50	0.46
2:B:40:GLU:O	2:B:40:GLU:HG3	2.15	0.46
2:B:170:PRO:HG2	2:B:208:HIS:CE1	2.49	0.46
2:B:306:ASN:O	2:B:310:LEU:HG	2.16	0.46
1:A:54:ASN:OD1	1:A:54:ASN:C	2.56	0.46
1:A:21:VAL:HG22	1:A:59:PRO:CG	2.45	0.46
2:B:330:GLN:CD	2:B:340:GLN:HE22	2.18	0.46
1:A:195:ILE:N	1:A:195:ILE:CD1	2.66	0.46
2:B:271:TYR:OH	2:B:312:GLU:O	2.30	0.46
1:A:229:TRP:HB3	1:A:234:LEU:HD12	1.98	0.46
2:B:24:TRP:CD1	2:B:25:PRO:HD2	2.50	0.46
2:B:27:THR:OG1	2:B:30:LYS:HG2	2.16	0.46
2:B:175:ASN:N	2:B:176:PRO:CD	2.79	0.46
2:B:345:PRO:O	2:B:346:PHE:HB2	2.15	0.46
1:A:58:THR:HG21	1:A:77:PHE:CD2	2.50	0.46
1:A:260:LEU:O	1:A:261:VAL:C	2.57	0.46
1:A:205:LEU:C	1:A:207:GLN:N	2.74	0.46
1:A:20:LYS:HG3	1:A:55:PRO:O	2.16	0.45
1:A:136:ASN:HB2	1:A:139:THR:OG1	2.16	0.45
2:B:428:GLN:HG2	2:B:428:GLN:O	2.16	0.45
1:A:439:THR:O	1:A:459:THR:HA	2.15	0.45
1:A:201:LYS:O	1:A:204:GLU:HB2	2.17	0.45
1:A:207:GLN:CA	1:A:207:GLN:HE21	2.30	0.45
1:A:229:TRP:HB3	1:A:234:LEU:CD1	2.47	0.45
1:A:106:VAL:HA	1:A:190:GLY:HA2	1.98	0.45
1:A:250:ASP:OD2	1:A:250:ASP:N	2.50	0.45
2:B:34:LEU:CD2	2:B:73:LYS:HG3	2.46	0.45
2:B:206:ARG:NH2	2:B:226:PRO:O	2.48	0.45
2:B:401:TRP:O	2:B:402:TRP:C	2.59	0.45
1:A:332:GLN:O	1:A:332:GLN:HG2	2.16	0.45
2:B:260:LEU:HD23	2:B:279:LEU:HD22	1.98	0.45
2:B:380:ILE:O	2:B:384:GLY:HA2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASP:OD2	1:A:322:SER:OG	2.30	0.45
2:B:111:VAL:CG1	2:B:187:LEU:HD22	2.34	0.45
2:B:317:VAL:HG23	2:B:317:VAL:O	2.16	0.45
1:A:417:VAL:O	1:A:417:VAL:HG13	2.17	0.45
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.52	0.45
1:A:167:ILE:C	1:A:170:PRO:HD2	2.40	0.45
2:B:103:LYS:HG2	2:B:191:SER:N	2.32	0.45
2:B:168:LEU:C	2:B:168:LEU:HD23	2.41	0.45
1:A:11:LYS:O	1:A:85:GLN:HG2	2.17	0.45
1:A:363:ASN:ND2	1:A:401:TRP:CZ3	2.85	0.45
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.52	0.45
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.52	0.45
2:B:274:ILE:CD1	2:B:310:LEU:HD21	2.41	0.44
2:B:353:LYS:HZ3	2:B:428:GLN:HG3	1.80	0.44
2:B:389:PHE:HB3	2:B:391:LEU:HD21	1.99	0.44
2:B:379:SER:HA	2:B:383:TRP:CE3	2.52	0.44
2:B:228:LEU:HD23	2:B:228:LEU:HA	1.52	0.44
1:A:13:LYS:O	1:A:16:MET:HB2	2.18	0.44
1:A:401:TRP:O	1:A:402:TRP:C	2.60	0.44
2:B:368:LEU:O	2:B:372:VAL:HG23	2.17	0.44
1:A:61:PHE:CZ	1:A:74:LEU:HD23	2.53	0.44
2:B:319:TYR:O	2:B:321:PRO:HD3	2.18	0.44
2:B:379:SER:HB3	2:B:385:LYS:O	2.17	0.44
1:A:398:TRP:O	1:A:399:GLU:C	2.61	0.44
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.52	0.44
1:A:476:LYS:HD2	1:A:476:LYS:O	2.17	0.44
2:B:34:LEU:HD21	2:B:73:LYS:HG3	1.99	0.44
2:B:78:ARG:NH2	2:B:411:ILE:HG21	2.33	0.44
2:B:241:VAL:HG13	2:B:351:THR:OG1	2.17	0.44
2:B:276:VAL:O	2:B:277:ARG:C	2.60	0.44
1:A:467:VAL:CG2	1:A:484:LEU:HD11	2.48	0.44
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.98	0.44
2:B:163:SER:O	2:B:167:ILE:CG2	2.66	0.44
1:A:345:PRO:C	1:A:346:PHE:CD1	2.95	0.44
2:B:276:VAL:O	2:B:276:VAL:CG1	2.65	0.44
1:A:518:VAL:O	1:A:519:ASN:C	2.59	0.43
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.53	0.43
2:B:372:VAL:HA	2:B:389:PHE:CE2	2.53	0.43
1:A:168:LEU:O	1:A:172:ARG:HG3	2.17	0.43
2:B:12:LEU:HD11	2:B:127:TYR:CZ	2.53	0.43
1:A:260:LEU:HG	1:A:264:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:PRO:C	2:B:99:GLY:N	2.74	0.43
2:B:183:TYR:CD1	2:B:184:MET:HG2	2.53	0.43
2:B:205:LEU:HD22	2:B:209:LEU:CD1	2.48	0.43
2:B:208:HIS:NE2	2:B:212:TRP:CZ3	2.87	0.43
1:A:54:ASN:O	1:A:143:ARG:NH2	2.51	0.43
1:A:325:LEU:HD22	1:A:341:ILE:HG22	1.99	0.43
1:A:406:TRP:CH2	1:A:407:GLN:NE2	2.87	0.43
2:B:66:LYS:CG	2:B:230:MET:HG2	2.45	0.43
1:A:161:GLN:O	1:A:162:SER:C	2.61	0.43
2:B:277:ARG:HG3	2:B:278:GLN:N	2.32	0.43
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.33	0.43
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.74	0.43
1:A:5:ILE:CD1	1:A:6:GLU:N	2.81	0.43
1:A:210:LEU:HD12	1:A:210:LEU:HA	1.64	0.43
2:B:161:GLN:O	2:B:162:SER:C	2.61	0.43
2:B:372:VAL:HA	2:B:389:PHE:HE2	1.83	0.43
1:A:379:SER:C	1:A:381:VAL:N	2.71	0.43
1:A:465:LYS:HD3	1:A:488:ASP:OD1	2.18	0.43
2:B:103:LYS:O	2:B:236:PRO:HG2	2.19	0.43
1:A:38:CYS:O	1:A:47:ILE:HD11	2.19	0.43
1:A:193:LEU:HD13	1:A:197:GLN:HG3	2.01	0.43
2:B:287:LYS:HD3	2:B:291:GLU:OE2	2.19	0.43
1:A:476:LYS:CD	1:A:517:LEU:HD12	2.48	0.43
1:A:28:GLU:OE1	1:A:31:ILE:HD12	2.19	0.42
1:A:393:ILE:O	1:A:414:TRP:HZ3	2.01	0.42
2:B:188:TYR:CZ	2:B:380:ILE:HG21	2.54	0.42
1:A:125:ARG:NE	1:A:147:ASN:HA	2.34	0.42
1:A:311:LYS:O	1:A:313:PRO:HD3	2.20	0.42
2:B:103:LYS:CG	2:B:191:SER:N	2.83	0.42
2:B:350:LYS:HG3	2:B:351:THR:N	2.34	0.42
2:B:30:LYS:HE2	2:B:404:GLU:OE2	2.19	0.42
1:A:224:GLU:HA	1:A:225:PRO:HD3	1.82	0.42
1:A:483:TYR:O	1:A:484:LEU:C	2.60	0.42
2:B:24:TRP:HA	2:B:25:PRO:HD3	1.89	0.42
2:B:212:TRP:O	2:B:213:GLY:C	2.62	0.42
1:A:220:LYS:NZ	1:A:220:LYS:HB3	2.34	0.42
1:A:293:ILE:N	1:A:293:ILE:HD12	2.35	0.42
2:B:257:ILE:O	2:B:260:LEU:HB3	2.20	0.42
1:A:107:THR:HB	1:A:202:ILE:HD12	2.00	0.42
1:A:433:PRO:HB2	2:B:290:THR:HG23	2.02	0.42
1:A:26:LEU:HB3	1:A:27:THR:H	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:GLN:NE2	2:B:161:GLN:HA	2.35	0.42
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.49	0.42
1:A:470:THR:O	1:A:471:ASP:HB2	2.20	0.42
2:B:234:LEU:HD21	2:B:377:THR:HG22	2.01	0.42
1:A:60:VAL:HG13	1:A:75:VAL:HG22	2.00	0.42
1:A:194:GLU:O	1:A:195:ILE:C	2.63	0.42
1:A:491:LEU:O	1:A:529:GLU:HB2	2.19	0.42
2:B:207:GLN:HA	2:B:210:LEU:HB2	2.01	0.42
1:A:58:THR:HG23	1:A:76:ASP:O	2.20	0.42
1:A:120:LEU:O	1:A:121:ASP:C	2.63	0.42
1:A:184:MET:HB3	1:A:185:ASP:H	1.66	0.42
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.78	0.42
1:A:296:THR:HG22	1:A:297:GLU:H	1.85	0.42
2:B:58:THR:HA	2:B:59:PRO:HD3	1.76	0.42
2:B:225:PRO:HA	2:B:226:PRO:HD3	1.31	0.42
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.78	0.41
1:A:469:LEU:HD21	1:A:480:GLN:CB	2.49	0.41
1:A:434:ILE:HD12	1:A:493:VAL:O	2.20	0.41
2:B:65:LYS:CB	2:B:68:SER:HB3	2.49	0.41
2:B:160:PHE:O	2:B:161:GLN:C	2.63	0.41
2:B:265:ASN:O	2:B:268:SER:OG	2.28	0.41
2:B:281:LYS:C	2:B:283:LEU:H	2.29	0.41
1:A:170:PRO:O	1:A:173:LYS:N	2.50	0.41
1:A:271:TYR:OH	1:A:313:PRO:HA	2.21	0.41
2:B:27:THR:O	2:B:28:GLU:C	2.63	0.41
2:B:241:VAL:O	2:B:243:PRO:HD3	2.21	0.41
1:A:241:VAL:O	1:A:242:GLN:C	2.63	0.41
1:A:494:ASN:HB3	2:B:289:LEU:HD22	2.03	0.41
2:B:282:LEU:HB3	2:B:293:ILE:HG21	2.01	0.41
1:A:339:TYR:CE2	1:A:352:GLY:HA3	2.56	0.41
1:A:399:GLU:O	1:A:403:THR:HB	2.20	0.41
1:A:27:THR:O	1:A:31:ILE:HG13	2.21	0.41
1:A:197:GLN:HA	1:A:197:GLN:NE2	2.35	0.41
1:A:205:LEU:O	1:A:206:ARG:C	2.62	0.41
1:A:265:ASN:C	1:A:267:ALA:N	2.78	0.41
2:B:108:VAL:C	2:B:109:LEU:HD12	2.46	0.41
2:B:380:ILE:O	2:B:384:GLY:CA	2.69	0.41
1:A:90:VAL:O	1:A:91:GLN:O	2.38	0.41
1:A:393:ILE:O	1:A:416:PHE:HD1	2.03	0.41
1:A:393:ILE:HD12	1:A:423:VAL:CG2	2.50	0.41
1:A:433:PRO:HB3	2:B:289:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:GLU:HA	2:B:135:ILE:HD11	2.02	0.41
2:B:67:ASP:HB2	2:B:230:MET:HE1	2.02	0.41
2:B:120:LEU:O	2:B:121:ASP:C	2.64	0.41
2:B:185:ASP:OD2	2:B:185:ASP:N	2.53	0.41
1:A:5:ILE:CG1	1:A:6:GLU:N	2.84	0.41
1:A:112:GLY:C	1:A:114:ALA:N	2.79	0.41
1:A:132:ILE:HB	1:A:142:ILE:CG1	2.50	0.41
1:A:164:MET:O	1:A:168:LEU:CD2	2.69	0.41
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.43	0.41
1:A:310:LEU:O	1:A:311:LYS:C	2.64	0.41
1:A:498:ASP:HA	1:A:536:VAL:O	2.21	0.41
1:A:536:VAL:HA	1:A:537:PRO:HD3	1.90	0.41
2:B:193:LEU:N	2:B:193:LEU:HD12	2.36	0.41
1:A:244:ILE:HD13	1:A:244:ILE:O	2.21	0.41
1:A:503:LEU:HD23	1:A:503:LEU:C	2.46	0.41
2:B:157:PRO:O	2:B:161:GLN:N	2.53	0.41
2:B:193:LEU:CD1	2:B:193:LEU:H	2.34	0.41
2:B:253:THR:HG23	2:B:256:ASP:OD1	2.21	0.41
1:A:54:ASN:ND2	1:A:129:ALA:HB2	2.36	0.40
1:A:226:PRO:HB3	1:A:235:HIS:NE2	2.36	0.40
1:A:330:GLN:O	1:A:337:TRP:HA	2.21	0.40
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.51	0.40
2:B:102:LYS:HE3	2:B:102:LYS:HB2	1.85	0.40
1:A:362:THR:HG22	1:A:366:LYS:HD3	2.03	0.40
1:A:487:GLN:HA	1:A:524:GLN:NE2	2.36	0.40
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.56	0.40
1:A:502:ALA:O	1:A:503:LEU:C	2.64	0.40
2:B:390:LYS:NZ	2:B:415:GLU:OE1	2.53	0.40
1:A:168:LEU:O	1:A:169:GLU:C	2.65	0.40
1:A:201:LYS:HA	1:A:204:GLU:HG3	2.03	0.40
1:A:223:LYS:HB2	1:A:223:LYS:HE3	1.86	0.40
1:A:432:GLU:HB2	1:A:433:PRO:HD2	2.02	0.40
1:A:115:TYR:CD1	1:A:156:SER:HB3	2.56	0.40
1:A:363:ASN:HA	1:A:511:ASP:CG	2.46	0.40
2:B:205:LEU:HD22	2:B:209:LEU:HG	2.03	0.40
1:A:179:VAL:HG12	4:A:999:NVP:HCB2	2.04	0.40
2:B:193:LEU:HD23	2:B:197:GLN:HB3	2.02	0.40
2:B:227:PHE:CD2	2:B:231:GLY:CA	3.05	0.40
2:B:375:ILE:O	2:B:375:ILE:HG22	2.21	0.40
2:B:393:ILE:HG12	2:B:394:GLN:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	506/560 (90%)	447 (88%)	43 (8%)	16 (3%)	3	11
2	B	391/440 (89%)	344 (88%)	44 (11%)	3 (1%)	16	44
All	All	897/1000 (90%)	791 (88%)	87 (10%)	19 (2%)	5	20

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	412	PRO
2	B	226	PRO
1	A	90	VAL
1	A	139	THR
1	A	403	THR
1	A	85	GLN
1	A	140	PRO
1	A	141	GLY
1	A	170	PRO
1	A	195	ILE
1	A	243	PRO
1	A	266	TRP
2	B	193	LEU
1	A	52	PRO
1	A	402	TRP
2	B	67	ASP
1	A	321	PRO
1	A	142	ILE

5.3.2 Protein sidechains

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.99	1 (25%)	1,8,10	6.67	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	3.69	1.51	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	6.67	117.88	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

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Mol	Chain	Res	Type	Atoms
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 [i](#)

3 ligands are 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	PO4	A	1300	-	4,4,4	1.45	0	6,6,6	0.43	0
4	NVP	A	999	-	23,23,23	1.36	2 (8%)	34,34,34	1.70	5 (14%)
3	PO4	A	1301	-	4,4,4	1.63	1 (25%)	6,6,6	0.49	0

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	NVP	C10-C9	4.29	1.54	1.49
4	A	999	NVP	C15-N1	-2.14	1.40	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1301	PO4	P-O3	-2.04	1.48	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	NVP	C7-C2-N1	-5.21	118.14	120.14
4	A	999	NVP	C7-N8-C9	4.87	132.31	128.29
4	A	999	NVP	N3-C2-N1	3.29	119.15	116.67
4	A	999	NVP	N14-C15-N1	2.43	118.50	116.67
4	A	999	NVP	C2-N1-CA	-2.26	114.55	116.34

There are no chirality outliers.

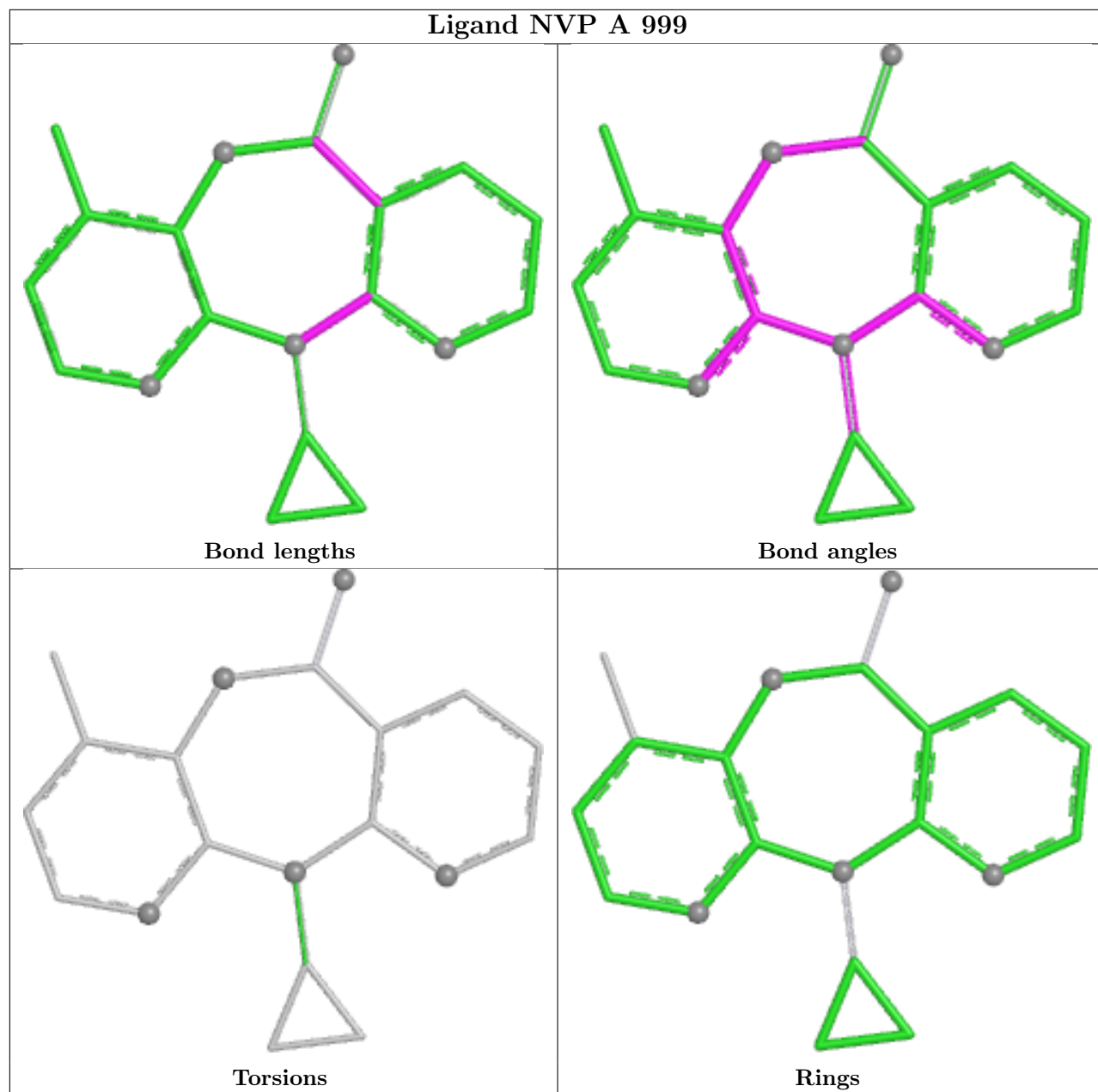
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	NVP	1	0
3	A	1301	PO4	2	0

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	512/560 (91%)	-0.22	4 (0%) 82 75	36, 78, 128, 150	0
2	B	399/440 (90%)	-0.20	4 (1%) 79 72	37, 81, 128, 149	0
All	All	911/1000 (91%)	-0.21	8 (0%) 81 74	36, 79, 128, 150	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	190	GLY	2.9
1	A	468	THR	2.6
1	A	470	THR	2.4
2	B	421	PRO	2.2
1	A	455	ALA	2.2
1	A	243	PRO	2.2
2	B	97	PRO	2.1
2	B	225	PRO	2.0

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	0.93	0.08	69,76,99,105	0

6.3 Carbohydrates [i](#)

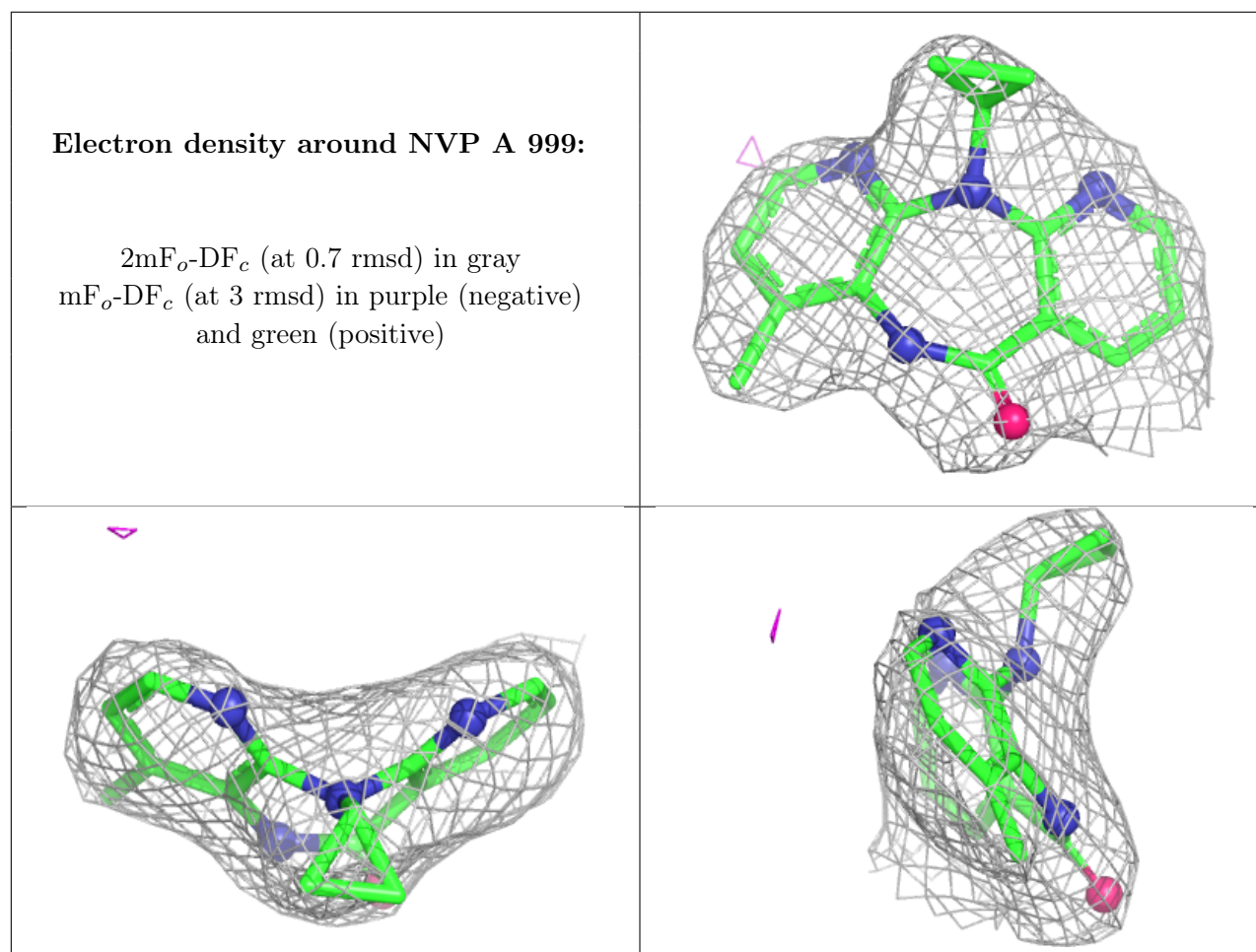
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	PO4	A	1301	5/5	0.69	0.11	130,140,142,146	0
3	PO4	A	1300	5/5	0.70	0.11	149,149,149,149	0
4	NVP	A	999	20/20	0.96	0.08	46,59,73,77	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.