



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:47 AM EDT

PDB ID : 1S1X / pdb_00001s1x
Title : Crystal structure of V108I mutant HIV-1 reverse transcriptase in complex with nevirapine
Authors : Ren, J.; Nichols, C.E.; Chamberlain, P.P.; Stammers, D.K.
Deposited on : 2004-01-07
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

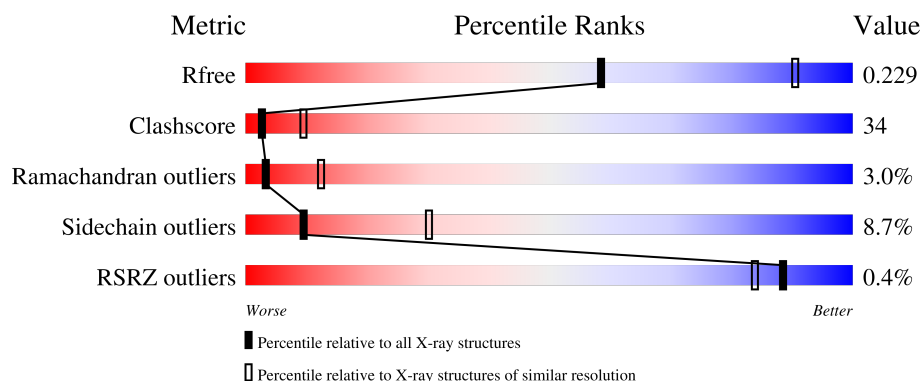
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

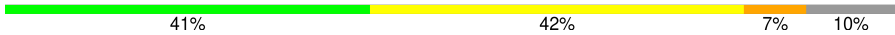
The reported resolution of this entry is 2.80 Å.

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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7790 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	0	0
			4459	2883	743	825	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	ILE	VAL	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

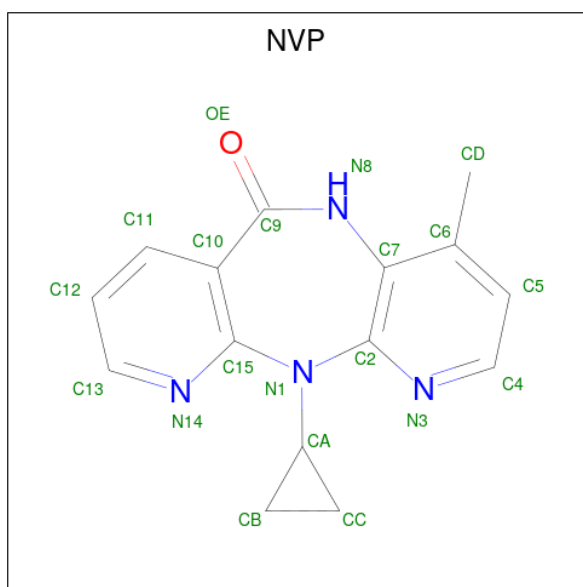
- Molecule 2 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	397	Total	C	N	O	S	0	0	0
			3290	2139	547	597	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	108	ILE	VAL	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		

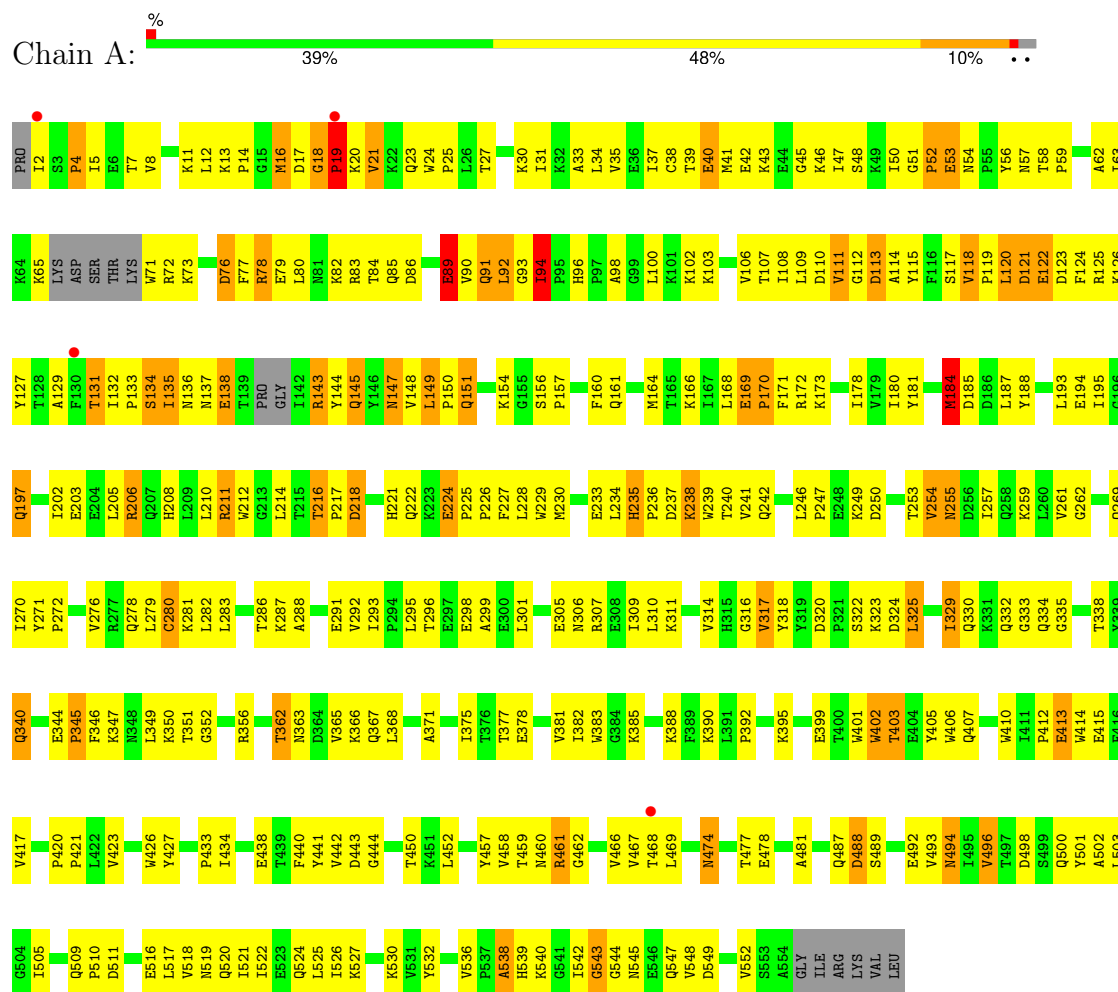
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	7	Total	O	0	0
			7	7		

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: Reverse transcriptase



• Molecule 2: Reverse transcriptase



T376	K287	G213	W153	Q85
T377		L214	K154	D86
E378	E291	T215	G155	F87
S379		THR	S156	W88
I380	T296	PRO	P157	GLU
V381	E297	ASP	A158	VAL
I382	E298	LYS	I159	GLN
W383		LYS	F160	LEU
G384	L301	HIS	Q161	GLY
K385	E302	GLN	S162	ILE
T386	L303	LYS	S163	PRO
P387		GLU	M164	H96
K388	R307	PRO	T165	P97
F389	E308	PRO	K166	A98
K390	I309	PHE	I167	
L391	L310	LEU	L168	K101
P392	K311	TRP	E169	K102
I393	E312	MET	P170	K103
Q394		GLY	F171	
K395	V317	TYR	R172	I108
	Y318	E233	K173	
W401	Y319	L234	Q174	V111
W402	D320	H235	N175	G112
T403	P321	P236	P176	D113
		D237	D177	A114
W406	L325	K238	I178	Y115
Q407	Q332	W239	V179	F116
T409		V241	I180	S117
	T338	Q242	Y181	P119
F416		P243	Y183	L120
V417	Q343	I244	M184	D121
N418	E344		D185	
		E248	D186	
P421	K347	K249	L187	R125
L422	N348		Y188	K126
V423	L349	W252	V189	Y127
K424	K350	T253	G190	T128
L425		V254	S191	A129
W426	Y354		D192	F130
Y427	A355	Q258	L193	T131
Q428	R356	K259	E194	I132
LEU	K357	L260	I195	P133
GLU	R358		G196	S134
LYS	G359	W266	Q197	I135
GLU	ALA	A267	H198	M136
PRO	HIS	S268	R199	M137
ILE	T362	Q269	E138	E138
VAL			T200	T139
GLY	V365	I274	K201	
ALA	K366		L202	I142
GLU	Q367	R277	E203	R143
THR	L368	Q278	E204	Y144
PHE	T369		L205	Q145
	E370	K281	R206	Y146
	A371	L282	Q207	M147
	V372	L283	H208	V148
	Q373	R284	L209	L149
	K374	G285	L210	P150
	I375	T286	R211	Q151
			W212	G152

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	138.40Å 109.00Å 72.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.57 – 2.80 29.57 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.57-2.80) 98.6 (29.57-2.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.235 , 0.295 0.226 , 0.229	Depositor DCC
R_{free} test set	1313 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 82.3	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	0.93	EDS
Total number of atoms	7790	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: CSD, NVP

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	0.61	0/4564	1.10	37/6199 (0.6%)
2	B	0.59	0/3380	1.08	22/4587 (0.5%)
All	All	0.60	0/7944	1.09	59/10786 (0.5%)

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	356	ARG	N-CA-C	10.59	126.50	109.24
2	B	401	TRP	N-CA-C	8.55	125.42	114.56
2	B	195	ILE	N-CA-C	8.10	118.65	110.23
1	A	18	GLY	CA-C-N	7.74	129.52	119.84
1	A	18	GLY	C-N-CA	7.74	129.52	119.84
1	A	118	VAL	N-CA-C	7.62	115.19	108.63
2	B	202	ILE	N-CA-C	-7.59	103.14	110.42
2	B	366	LYS	N-CA-C	-7.09	103.48	111.14
1	A	235	HIS	N-CA-C	-6.99	101.31	110.39
1	A	539	HIS	N-CA-C	6.90	119.97	109.62
1	A	19	PRO	N-CA-C	6.88	126.65	112.47
2	B	349	LEU	N-CA-C	-6.85	103.93	112.90
1	A	94	ILE	CA-C-N	6.79	127.19	119.93
1	A	94	ILE	C-N-CA	6.79	127.19	119.93
1	A	250	ASP	N-CA-C	-6.71	105.00	113.72
1	A	54	ASN	CA-C-N	6.65	126.35	119.64
1	A	54	ASN	C-N-CA	6.65	126.35	119.64
2	B	391	LEU	N-CA-C	6.63	118.01	109.72
1	A	184	MET	CB-CA-C	-6.56	108.99	116.54
1	A	93	GLY	N-CA-C	-6.51	99.70	111.15
2	B	131	THR	N-CA-C	6.40	120.02	108.69
2	B	343	GLN	N-CA-C	-6.30	105.62	113.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	118	VAL	N-CA-C	6.24	115.41	108.05
1	A	234	LEU	N-CA-C	6.20	118.80	108.20
2	B	235	HIS	CA-C-N	6.17	125.89	119.05
2	B	235	HIS	C-N-CA	6.17	125.89	119.05
2	B	312	GLU	CA-C-N	6.16	125.92	119.76
2	B	312	GLU	C-N-CA	6.16	125.92	119.76
1	A	34	LEU	N-CA-C	-6.14	105.82	113.55
2	B	417	VAL	N-CA-C	6.12	116.29	108.82
2	B	242	GLN	CA-C-N	6.10	126.58	119.99
2	B	242	GLN	C-N-CA	6.10	126.58	119.99
1	A	20	LYS	N-CA-C	6.02	123.62	110.80
1	A	76	ASP	N-CA-C	5.90	118.82	108.56
1	A	494	ASN	N-CA-C	-5.89	98.80	108.76
1	A	211	ARG	N-CA-C	-5.85	105.99	113.01
1	A	538	ALA	N-CA-C	5.72	122.99	110.80
1	A	131	THR	N-CA-C	5.72	117.87	109.24
1	A	180	ILE	N-CA-C	5.71	116.11	108.11
1	A	149	LEU	CA-C-N	5.69	126.56	120.13
1	A	149	LEU	C-N-CA	5.69	126.56	120.13
1	A	325	LEU	N-CA-C	-5.57	100.16	109.24
1	A	333	GLY	CA-C-O	-5.55	118.32	122.37
1	A	92	LEU	N-CA-C	-5.47	106.28	113.17
2	B	312	GLU	N-CA-C	5.45	113.12	108.22
1	A	254	VAL	N-CA-C	-5.36	105.27	110.42
2	B	115	TYR	N-CA-C	5.34	117.85	111.71
2	B	355	ALA	CA-C-N	-5.25	115.48	122.72
2	B	355	ALA	C-N-CA	-5.25	115.48	122.72
1	A	329	ILE	N-CA-C	5.24	116.92	108.85
1	A	147	ASN	N-CA-C	-5.21	106.94	113.72
2	B	173	LYS	N-CA-C	-5.21	106.98	113.55
1	A	333	GLY	N-CA-C	-5.18	106.85	112.08
1	A	349	LEU	N-CA-C	-5.15	104.62	112.04
1	A	134	SER	N-CA-C	-5.12	99.89	110.80
1	A	118	VAL	CA-C-N	5.11	125.04	119.78
1	A	118	VAL	C-N-CA	5.11	125.04	119.78
1	A	388	LYS	N-CA-C	-5.04	100.95	108.96
1	A	440	PHE	N-CA-C	5.02	116.94	108.96

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	4459	0	4501	304	0
2	B	3290	0	3321	228	0
3	A	20	0	14	0	0
4	A	14	0	0	1	0
4	B	7	0	0	1	0
All	All	7790	0	7836	524	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 34.

All (524) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:ARG:H	2:B:358:ARG:HD2	1.16	1.07
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.38	1.04
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.45	0.96
1:A:50:ILE:HG13	1:A:51:GLY:H	1.30	0.96
1:A:57:ASN:HB2	1:A:143:ARG:HH22	1.32	0.95
2:B:113:ASP:HB2	2:B:214:LEU:HD23	1.50	0.92
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.49	0.91
1:A:206:ARG:NH1	1:A:216:THR:HG23	1.88	0.89
2:B:358:ARG:H	2:B:358:ARG:CD	1.86	0.88
1:A:48:SER:HB2	1:A:147:ASN:HD21	1.39	0.88
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.09	0.87
2:B:358:ARG:HD2	2:B:358:ARG:N	1.87	0.86
2:B:65:LYS:HE2	2:B:72:ARG:CD	2.06	0.86
2:B:135:ILE:O	2:B:138:GLU:HG3	1.76	0.85
2:B:278:GLN:HE21	2:B:298:GLU:CB	1.90	0.84
2:B:111:VAL:HA	2:B:214:LEU:HD22	1.60	0.84
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.76	0.84
1:A:206:ARG:HH11	1:A:216:THR:HG23	1.39	0.83
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.44	0.83
2:B:278:GLN:HE21	2:B:298:GLU:HB3	1.44	0.82
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.41	0.82
2:B:98:ALA:HB1	2:B:101:LYS:HE3	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HD12	1:A:52:PRO:HD2	1.63	0.81
1:A:206:ARG:NH1	1:A:206:ARG:HB3	1.96	0.80
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.16	0.80
2:B:154:LYS:HA	2:B:184:MET:HE1	1.63	0.80
1:A:206:ARG:O	1:A:210:LEU:HD23	1.82	0.79
1:A:106:VAL:HG23	1:A:236:PRO:HB3	1.64	0.79
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.63	0.79
1:A:52:PRO:C	1:A:53:GLU:HG3	2.07	0.79
1:A:254:VAL:HG13	1:A:283:LEU:HD12	1.64	0.79
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.18	0.79
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.18	0.78
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.46	0.78
1:A:94:ILE:HD13	1:A:94:ILE:H	1.47	0.78
2:B:163:SER:O	2:B:167:ILE:HG23	1.84	0.77
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.67	0.77
1:A:96:HIS:HB2	4:A:1004:HOH:O	1.85	0.76
1:A:31:ILE:HG12	1:A:133:PRO:HB2	1.68	0.76
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.68	0.76
2:B:98:ALA:O	2:B:101:LYS:HG2	1.86	0.76
2:B:249:LYS:HB2	2:B:249:LYS:HZ3	1.51	0.75
2:B:136:ASN:HB3	2:B:138:GLU:HG3	1.69	0.75
1:A:58:THR:HG23	1:A:76:ASP:O	1.85	0.75
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.22	0.75
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.69	0.74
2:B:350:LYS:NZ	2:B:382:ILE:HD12	2.02	0.74
1:A:23:GLN:O	1:A:25:PRO:HD3	1.88	0.74
2:B:84:THR:HB	2:B:154:LYS:HE2	1.70	0.73
1:A:50:ILE:CG1	1:A:51:GLY:H	2.01	0.72
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.69	0.72
1:A:94:ILE:H	1:A:94:ILE:CD1	2.03	0.72
2:B:350:LYS:HZ1	2:B:382:ILE:HD12	1.55	0.72
1:A:31:ILE:O	1:A:35:VAL:HG23	1.90	0.72
1:A:77:PHE:HD2	1:A:80:LEU:HD23	1.52	0.72
1:A:385:LYS:NZ	1:A:385:LYS:HB3	2.04	0.71
1:A:50:ILE:HG13	1:A:51:GLY:N	2.05	0.71
1:A:50:ILE:HB	1:A:145:GLN:HG2	1.73	0.71
1:A:399:GLU:O	1:A:403:THR:HB	1.90	0.71
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.21	0.70
2:B:195:ILE:HG23	2:B:196:GLY:N	2.06	0.70
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.26	0.70
1:A:143:ARG:HG2	1:A:143:ARG:NH1	2.06	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.74	0.69
2:B:319:TYR:HE1	2:B:321:PRO:HG3	1.57	0.69
2:B:65:LYS:HE2	2:B:72:ARG:HD2	1.73	0.69
1:A:110:ASP:O	1:A:217:PRO:HD3	1.92	0.69
2:B:31:ILE:O	2:B:35:VAL:HG23	1.93	0.69
2:B:136:ASN:HB3	2:B:138:GLU:CG	2.23	0.68
2:B:344:GLU:HB2	2:B:347:LYS:HE3	1.75	0.68
1:A:12:LEU:HD13	1:A:17:ASP:HA	1.76	0.68
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.27	0.68
2:B:56:TYR:CE2	2:B:126:LYS:HE2	2.28	0.68
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.75	0.67
1:A:335:GLY:HA3	1:A:356:ARG:HD3	1.76	0.67
2:B:254:VAL:O	2:B:258:GLN:HG3	1.94	0.67
1:A:293:ILE:N	1:A:293:ILE:HD12	2.10	0.66
2:B:13:LYS:HE3	2:B:84:THR:O	1.94	0.66
1:A:57:ASN:HA	1:A:129:ALA:O	1.96	0.66
1:A:270:ILE:HG22	1:A:314:VAL:HG21	1.77	0.65
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.31	0.65
2:B:118:VAL:HB	2:B:149:LEU:HG	1.77	0.65
1:A:135:ILE:HG22	1:A:136:ASN:N	2.10	0.65
2:B:376:THR:CG2	2:B:386:THR:HG22	2.26	0.65
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.32	0.65
2:B:195:ILE:CD1	2:B:199:ARG:HE	2.10	0.65
1:A:100:LEU:O	1:A:318:TYR:HB3	1.96	0.64
1:A:441:TYR:O	1:A:548:VAL:HG11	1.97	0.64
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.32	0.64
2:B:163:SER:HA	2:B:166:LYS:HD3	1.78	0.64
1:A:282:LEU:HD11	1:A:296:THR:HG23	1.79	0.64
2:B:87:PHE:O	2:B:88:TRP:HB2	1.97	0.64
1:A:17:ASP:C	1:A:19:PRO:HD3	2.22	0.64
2:B:389:PHE:HB3	2:B:391:LEU:HD21	1.78	0.64
1:A:84:THR:O	1:A:154:LYS:NZ	2.31	0.64
1:A:138:GLU:O	1:A:138:GLU:HG2	1.96	0.64
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.79	0.64
2:B:380:ILE:O	2:B:384:GLY:HA2	1.98	0.64
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.33	0.63
2:B:65:LYS:O	2:B:407:GLN:NE2	2.31	0.63
2:B:191:SER:CB	2:B:193:LEU:HD13	2.23	0.63
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.80	0.63
1:A:122:GLU:HG2	1:A:123:ASP:H	1.62	0.63
1:A:5:ILE:HD11	1:A:166:LYS:NZ	2.13	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:CD1	1:A:94:ILE:N	2.61	0.63
1:A:306:ASN:O	1:A:310:LEU:HG	1.98	0.63
2:B:236:PRO:C	2:B:238:LYS:H	2.07	0.63
2:B:298:GLU:OE1	2:B:298:GLU:N	2.31	0.62
1:A:206:ARG:HB3	1:A:206:ARG:CZ	2.26	0.62
2:B:31:ILE:HA	2:B:34:LEU:HD12	1.80	0.62
2:B:421:PRO:O	2:B:425:LEU:HD13	1.98	0.62
1:A:8:VAL:O	1:A:121:ASP:HB2	1.99	0.62
1:A:37:ILE:O	1:A:40:GLU:HB3	1.99	0.62
2:B:195:ILE:HG23	2:B:196:GLY:H	1.63	0.62
1:A:129:ALA:HA	1:A:144:TYR:O	2.00	0.61
2:B:195:ILE:CD1	2:B:199:ARG:HG3	2.30	0.61
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.82	0.61
1:A:91:GLN:OE1	1:A:91:GLN:HA	2.00	0.61
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.01	0.61
1:A:118:VAL:HB	1:A:149:LEU:HD22	1.83	0.61
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.36	0.61
1:A:59:PRO:HG2	1:A:76:ASP:HB2	1.82	0.60
1:A:458:VAL:HG23	1:A:548:VAL:HG12	1.83	0.60
2:B:173:LYS:O	2:B:176:PRO:HD3	2.01	0.60
1:A:246:LEU:O	1:A:307:ARG:NH1	2.26	0.60
2:B:201:LYS:O	2:B:204:GLU:HB3	2.01	0.60
1:A:122:GLU:N	1:A:122:GLU:OE1	2.34	0.60
1:A:170:PRO:HA	1:A:173:LYS:HD3	1.82	0.60
2:B:160:PHE:HE1	2:B:164:MET:HE2	1.66	0.60
2:B:240:THR:O	2:B:350:LYS:HG2	2.02	0.60
1:A:378:GLU:O	1:A:382:ILE:HG12	2.02	0.59
1:A:307:ARG:O	1:A:311:LYS:HG3	2.03	0.59
1:A:450:THR:OG1	1:A:452:LEU:HB2	2.02	0.59
1:A:228:LEU:HD22	1:A:242:GLN:OE1	2.03	0.59
1:A:522:ILE:O	1:A:526:ILE:HG13	2.03	0.59
2:B:57:ASN:HB2	2:B:143:ARG:HH12	1.67	0.59
2:B:65:LYS:NZ	2:B:409:THR:HG22	2.18	0.59
1:A:72:ARG:HD3	1:A:73:LYS:H	1.68	0.58
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.84	0.58
1:A:12:LEU:O	1:A:13:LYS:C	2.46	0.58
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.84	0.58
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.37	0.58
2:B:422:LEU:O	2:B:424:LYS:N	2.36	0.58
2:B:195:ILE:HA	2:B:198:HIS:HB3	1.85	0.58
2:B:57:ASN:ND2	2:B:143:ARG:NH1	2.50	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:HD12	1:A:135:ILE:HD12	1.85	0.58
1:A:108:ILE:C	1:A:109:LEU:HD12	2.29	0.58
1:A:111:VAL:HG21	1:A:114:ALA:HB2	1.86	0.57
2:B:113:ASP:O	2:B:116:PHE:HD2	1.87	0.57
1:A:493:VAL:HG12	1:A:494:ASN:N	2.19	0.57
2:B:162:SER:O	2:B:165:THR:HG23	2.04	0.57
2:B:179:VAL:O	2:B:189:VAL:HA	2.05	0.57
2:B:182:GLN:HB2	2:B:187:LEU:HD12	1.86	0.57
2:B:376:THR:O	2:B:380:ILE:HG13	2.05	0.57
1:A:31:ILE:CG1	1:A:133:PRO:HB2	2.33	0.57
1:A:111:VAL:HG22	1:A:185:ASP:HB3	1.87	0.57
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.53	0.57
1:A:98:ALA:CB	1:A:350:LYS:HB2	2.35	0.57
1:A:16:MET:HE1	1:A:82:LYS:NZ	2.19	0.57
1:A:269:GLN:HB3	1:A:352:GLY:HA2	1.86	0.57
1:A:402:TRP:CD1	1:A:402:TRP:C	2.83	0.57
2:B:136:ASN:C	2:B:138:GLU:N	2.62	0.57
2:B:350:LYS:NZ	2:B:382:ILE:CD1	2.67	0.57
1:A:65:LYS:HB2	1:A:71:TRP:N	2.20	0.56
1:A:122:GLU:HG2	1:A:123:ASP:N	2.20	0.56
2:B:283:LEU:O	2:B:284:ARG:C	2.49	0.56
1:A:121:ASP:O	1:A:122:GLU:C	2.47	0.56
1:A:181:TYR:HB3	1:A:188:TYR:HB2	1.88	0.56
1:A:335:GLY:HA2	1:A:367:GLN:HE21	1.70	0.56
2:B:425:LEU:HD13	2:B:425:LEU:H	1.69	0.56
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.88	0.56
1:A:210:LEU:HD22	1:A:214:LEU:O	2.04	0.56
2:B:53:GLU:O	2:B:55:PRO:HD3	2.06	0.56
1:A:518:VAL:O	1:A:522:ILE:HG13	2.04	0.56
1:A:413:GLU:HA	1:A:413:GLU:OE1	2.06	0.56
2:B:27:THR:O	2:B:31:ILE:HG13	2.05	0.56
1:A:51:GLY:N	1:A:52:PRO:CD	2.69	0.56
2:B:317:VAL:HG11	2:B:348:ASN:O	2.05	0.56
1:A:134:SER:O	1:A:135:ILE:C	2.47	0.55
1:A:11:LYS:O	1:A:85:GLN:HB3	2.07	0.55
1:A:168:LEU:HD13	1:A:172:ARG:HH21	1.71	0.55
1:A:122:GLU:HA	1:A:125:ARG:NE	2.22	0.55
1:A:278:GLN:O	1:A:282:LEU:HD13	2.07	0.55
1:A:426:TRP:O	1:A:526:ILE:HG23	2.07	0.55
2:B:205:LEU:HD13	2:B:205:LEU:C	2.30	0.55
1:A:37:ILE:HG22	1:A:41:MET:HE3	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:GLN:O	2:B:165:THR:HG22	2.05	0.55
1:A:134:SER:O	1:A:135:ILE:O	2.25	0.55
2:B:156:SER:N	2:B:157:PRO:HD2	2.21	0.55
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.46	0.55
2:B:114:ALA:H	2:B:214:LEU:HD21	1.72	0.55
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.42	0.55
2:B:8:VAL:HG11	2:B:159:ILE:HG23	1.89	0.55
2:B:65:LYS:HZ3	2:B:409:THR:HG22	1.70	0.55
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.16	0.55
2:B:308:GLU:HA	2:B:311:LYS:HD2	1.88	0.55
1:A:241:VAL:HG21	1:A:270:ILE:CG2	2.36	0.54
1:A:114:ALA:HB1	1:A:160:PHE:HE2	1.70	0.54
2:B:103:LYS:HE2	2:B:190:GLY:O	2.07	0.54
1:A:39:THR:O	1:A:42:GLU:HB3	2.06	0.54
1:A:224:GLU:HG3	1:A:225:PRO:HD2	1.89	0.54
1:A:335:GLY:HA3	1:A:356:ARG:CD	2.37	0.54
2:B:366:LYS:O	2:B:370:GLU:HG3	2.06	0.54
2:B:29:GLU:HG2	2:B:71:TRP:CZ2	2.42	0.54
2:B:136:ASN:C	2:B:138:GLU:H	2.15	0.54
2:B:87:PHE:O	2:B:88:TRP:CB	2.56	0.54
1:A:31:ILE:HD13	1:A:134:SER:N	2.23	0.54
1:A:292:VAL:C	1:A:293:ILE:HD12	2.32	0.54
1:A:30:LYS:HE2	1:A:71:TRP:CZ3	2.43	0.54
1:A:500:GLN:OE1	2:B:422:LEU:HD22	2.08	0.53
2:B:64:LYS:HE3	2:B:71:TRP:CD2	2.43	0.53
1:A:63:ILE:N	1:A:63:ILE:HD12	2.23	0.53
2:B:178:ILE:CG2	2:B:189:VAL:HG12	2.38	0.53
1:A:287:LYS:HG2	1:A:291:GLU:OE2	2.09	0.53
2:B:153:TRP:O	2:B:157:PRO:HD2	2.08	0.53
2:B:195:ILE:HD11	2:B:199:ARG:HG3	1.89	0.53
1:A:350:LYS:HE2	1:A:378:GLU:CD	2.34	0.53
1:A:77:PHE:O	1:A:80:LEU:N	2.41	0.53
1:A:322:SER:O	1:A:323:LYS:HG2	2.08	0.53
2:B:402:TRP:HZ3	2:B:406:TRP:CG	2.26	0.53
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.38	0.53
1:A:522:ILE:O	1:A:525:LEU:HB2	2.09	0.52
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.90	0.52
1:A:119:PRO:HA	1:A:148:VAL:HG12	1.91	0.52
2:B:180:ILE:HG12	2:B:189:VAL:CG1	2.30	0.52
2:B:266:TRP:O	2:B:269:GLN:HG3	2.09	0.52
1:A:38:CYS:O	1:A:47:ILE:HD11	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.92	0.52
2:B:205:LEU:HD13	2:B:205:LEU:O	2.09	0.52
1:A:31:ILE:HD13	1:A:134:SER:CA	2.40	0.52
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.75	0.51
1:A:237:ASP:OD1	1:A:237:ASP:C	2.52	0.51
1:A:305:GLU:O	1:A:309:ILE:HG13	2.10	0.51
1:A:377:THR:O	1:A:381:VAL:HG23	2.11	0.51
2:B:132:ILE:HB	2:B:142:ILE:HB	1.92	0.51
2:B:376:THR:HG23	2:B:386:THR:HG22	1.92	0.51
1:A:385:LYS:HB3	1:A:385:LYS:HZ3	1.76	0.51
1:A:17:ASP:O	1:A:83:ARG:HD3	2.11	0.51
1:A:18:GLY:HA2	1:A:83:ARG:HD2	1.92	0.51
1:A:218:ASP:O	1:A:222:GLN:HG3	2.10	0.51
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.92	0.51
2:B:281:LYS:C	2:B:283:LEU:N	2.68	0.51
2:B:344:GLU:CB	2:B:347:LYS:HE3	2.39	0.51
1:A:332:GLN:O	1:A:332:GLN:HG2	2.11	0.51
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.46	0.51
1:A:23:GLN:NE2	1:A:24:TRP:H	2.09	0.51
1:A:77:PHE:HD2	1:A:80:LEU:CD2	2.20	0.51
1:A:325:LEU:HD11	1:A:383:TRP:CD2	2.45	0.51
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.93	0.51
2:B:236:PRO:C	2:B:238:LYS:N	2.69	0.50
1:A:270:ILE:HG23	1:A:314:VAL:HG11	1.93	0.50
1:A:487:GLN:C	1:A:489:SER:H	2.19	0.50
2:B:134:SER:HB3	2:B:139:THR:HG22	1.94	0.50
2:B:177:ASP:OD1	2:B:178:ILE:HG13	2.11	0.50
1:A:438:GLU:CD	1:A:461:ARG:HD2	2.36	0.50
1:A:131:THR:HG22	1:A:132:ILE:N	2.26	0.50
1:A:253:THR:O	1:A:257:ILE:HG13	2.10	0.50
1:A:254:VAL:HG22	1:A:286:THR:HG21	1.94	0.50
1:A:545:ASN:O	1:A:549:ASP:HB2	2.12	0.50
1:A:246:LEU:HB2	1:A:307:ARG:NH1	2.27	0.50
1:A:334:GLN:O	1:A:356:ARG:HD3	2.12	0.50
1:A:441:TYR:HA	1:A:496:VAL:HG22	1.94	0.50
1:A:474:ASN:O	1:A:478:GLU:HG2	2.12	0.50
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.92	0.50
1:A:18:GLY:N	1:A:19:PRO:HD3	2.27	0.50
1:A:402:TRP:CZ2	2:B:362:THR:HA	2.47	0.50
2:B:195:ILE:CG2	2:B:196:GLY:N	2.74	0.50
1:A:229:TRP:O	1:A:230:MET:C	2.53	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:TRP:CD1	1:A:230:MET:HG2	2.47	0.50
2:B:266:TRP:CH2	2:B:426:TRP:HB3	2.47	0.50
1:A:62:ALA:C	1:A:63:ILE:HD12	2.37	0.49
1:A:108:ILE:HD12	1:A:188:TYR:CZ	2.47	0.49
2:B:278:GLN:HA	2:B:278:GLN:OE1	2.10	0.49
1:A:254:VAL:HG13	1:A:283:LEU:CD1	2.38	0.49
1:A:460:ASN:C	1:A:462:GLY:H	2.20	0.49
2:B:379:SER:CB	2:B:387:PRO:HD3	2.42	0.49
1:A:329:ILE:O	1:A:392:PRO:HD3	2.12	0.49
1:A:317:VAL:HG12	1:A:318:TYR:H	1.77	0.49
1:A:31:ILE:CD1	1:A:133:PRO:HB2	2.42	0.49
1:A:5:ILE:HD11	1:A:166:LYS:HZ3	1.77	0.49
1:A:50:ILE:CD1	1:A:52:PRO:HD2	2.37	0.49
2:B:108:ILE:HG12	2:B:188:TYR:CE2	2.47	0.49
2:B:277:ARG:H	2:B:277:ARG:HD2	1.78	0.49
1:A:235:HIS:HB2	1:A:238:LYS:O	2.12	0.49
1:A:329:ILE:HG22	1:A:330:GLN:N	2.27	0.49
2:B:61:PHE:CE1	2:B:403:THR:HG22	2.48	0.49
2:B:248:GLU:HG2	2:B:307:ARG:NH2	2.28	0.49
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.93	0.49
2:B:425:LEU:N	2:B:425:LEU:CD1	2.76	0.49
2:B:356:ARG:CZ	2:B:362:THR:N	2.76	0.49
2:B:389:PHE:HB3	2:B:391:LEU:CD2	2.42	0.49
1:A:202:ILE:HG22	1:A:203:GLU:N	2.27	0.49
1:A:443:ASP:OD1	1:A:444:GLY:N	2.45	0.49
1:A:458:VAL:HG23	1:A:548:VAL:CG1	2.43	0.49
2:B:402:TRP:CE2	2:B:403:THR:HG23	2.48	0.49
1:A:124:PHE:O	1:A:127:TYR:HD2	1.94	0.48
1:A:211:ARG:HG2	1:A:211:ARG:NH1	2.27	0.48
2:B:365:VAL:O	2:B:369:THR:HG23	2.12	0.48
1:A:90:VAL:HG23	1:A:90:VAL:O	2.11	0.48
1:A:298:GLU:O	1:A:301:LEU:HB3	2.13	0.48
2:B:160:PHE:CE1	2:B:164:MET:HE2	2.47	0.48
2:B:178:ILE:HG22	2:B:179:VAL:N	2.27	0.48
1:A:420:PRO:HA	1:A:421:PRO:C	2.38	0.48
1:A:115:TYR:OH	1:A:157:PRO:HG3	2.13	0.48
2:B:195:ILE:HD11	2:B:199:ARG:CG	2.44	0.48
2:B:356:ARG:NH2	2:B:362:THR:N	2.61	0.48
1:A:206:ARG:HH11	1:A:206:ARG:HB3	1.75	0.48
2:B:12:LEU:HD11	2:B:127:TYR:CZ	2.48	0.48
2:B:168:LEU:O	2:B:169:GLU:C	2.55	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLU:H	1:A:298:GLU:CD	2.21	0.48
1:A:524:GLN:HA	1:A:524:GLN:OE1	2.14	0.48
2:B:426:TRP:HE3	2:B:426:TRP:HA	1.78	0.48
1:A:466:VAL:O	1:A:467:VAL:HG23	2.14	0.48
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.49	0.48
1:A:48:SER:HB2	1:A:147:ASN:ND2	2.18	0.48
1:A:94:ILE:HD13	1:A:94:ILE:N	2.17	0.48
1:A:121:ASP:O	1:A:123:ASP:N	2.47	0.48
2:B:132:ILE:HB	2:B:142:ILE:HD12	1.96	0.48
1:A:33:ALA:HB1	1:A:71:TRP:HB2	1.95	0.47
1:A:85:GLN:C	1:A:154:LYS:HZ3	2.21	0.47
1:A:52:PRO:O	1:A:53:GLU:HG3	2.12	0.47
2:B:11:LYS:N	2:B:85:GLN:OE1	2.44	0.47
2:B:356:ARG:CG	2:B:367:GLN:HG2	2.45	0.47
1:A:346:PHE:N	1:A:346:PHE:CD2	2.81	0.47
1:A:407:GLN:CG	2:B:393:ILE:HA	2.44	0.47
1:A:110:ASP:O	1:A:217:PRO:CD	2.62	0.47
1:A:41:MET:HB2	1:A:47:ILE:CD1	2.44	0.47
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.97	0.47
2:B:320:ASP:O	2:B:343:GLN:NE2	2.45	0.47
1:A:111:VAL:CG2	1:A:114:ALA:HB2	2.44	0.47
2:B:162:SER:O	2:B:165:THR:CG2	2.63	0.47
2:B:428:GLN:HE21	2:B:428:GLN:HB3	1.54	0.47
1:A:77:PHE:O	1:A:78:ARG:C	2.57	0.47
1:A:270:ILE:CG2	1:A:314:VAL:HG21	2.43	0.47
2:B:426:TRP:HA	2:B:426:TRP:CE3	2.49	0.47
1:A:210:LEU:C	1:A:212:TRP:H	2.22	0.47
1:A:270:ILE:CG2	1:A:314:VAL:HG11	2.45	0.47
1:A:282:LEU:HD21	1:A:295:LEU:HA	1.97	0.47
2:B:136:ASN:O	2:B:138:GLU:N	2.48	0.47
1:A:19:PRO:O	1:A:56:TYR:HA	2.15	0.46
1:A:540:LYS:C	1:A:542:ILE:H	2.23	0.46
2:B:129:ALA:HA	2:B:144:TYR:O	2.16	0.46
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.51	0.46
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.97	0.46
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.97	0.46
1:A:468:THR:O	1:A:469:LEU:HD23	2.14	0.46
2:B:191:SER:C	2:B:193:LEU:H	2.24	0.46
2:B:241:VAL:HG22	2:B:350:LYS:HA	1.97	0.46
2:B:64:LYS:HE2	2:B:69:THR:O	2.16	0.46
2:B:278:GLN:NE2	2:B:298:GLU:HB3	2.22	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLY:O	1:A:56:TYR:HD1	1.97	0.46
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.46	0.46
2:B:422:LEU:HD23	2:B:426:TRP:HE1	1.81	0.46
1:A:43:LYS:C	1:A:45:GLY:N	2.71	0.46
1:A:43:LYS:C	1:A:45:GLY:H	2.24	0.46
1:A:161:GLN:O	1:A:164:MET:HB3	2.15	0.46
1:A:208:HIS:O	1:A:212:TRP:HD1	1.99	0.46
2:B:356:ARG:HG3	2:B:367:GLN:CD	2.41	0.46
1:A:210:LEU:C	1:A:212:TRP:N	2.73	0.46
1:A:335:GLY:HA2	1:A:367:GLN:NE2	2.30	0.46
1:A:111:VAL:CG2	1:A:112:GLY:N	2.78	0.45
1:A:168:LEU:O	1:A:169:GLU:C	2.59	0.45
1:A:390:LYS:HA	1:A:415:GLU:O	2.16	0.45
2:B:195:ILE:CG1	2:B:199:ARG:HE	2.30	0.45
2:B:374:LYS:O	2:B:377:THR:OG1	2.34	0.45
1:A:114:ALA:O	1:A:117:SER:HB2	2.16	0.45
1:A:259:LYS:N	1:A:259:LYS:HD3	2.31	0.45
2:B:125:ARG:HB3	2:B:145:GLN:NE2	2.31	0.45
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.16	0.45
2:B:356:ARG:HG3	2:B:367:GLN:HG2	1.98	0.45
2:B:393:ILE:HG12	2:B:394:GLN:N	2.32	0.45
1:A:51:GLY:N	1:A:52:PRO:HD2	2.31	0.45
1:A:261:VAL:O	1:A:262:GLY:C	2.58	0.45
1:A:427:TYR:OH	1:A:509:GLN:HA	2.16	0.45
1:A:237:ASP:OD1	1:A:238:LYS:HB3	2.17	0.45
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.98	0.45
2:B:203:GLU:O	2:B:207:GLN:HG2	2.16	0.45
1:A:98:ALA:HB2	1:A:350:LYS:HB2	1.98	0.45
1:A:365:VAL:HG11	1:A:401:TRP:CG	2.52	0.45
1:A:524:GLN:HA	1:A:527:LYS:HD2	1.98	0.45
1:A:247:PRO:O	1:A:307:ARG:NH2	2.49	0.45
2:B:207:GLN:HA	2:B:207:GLN:OE1	2.17	0.45
1:A:548:VAL:O	1:A:552:VAL:HG22	2.16	0.45
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.52	0.45
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.79	0.45
1:A:241:VAL:O	1:A:242:GLN:C	2.59	0.44
2:B:70:LYS:H	2:B:70:LYS:HG3	1.59	0.44
2:B:98:ALA:CB	2:B:101:LYS:HE3	2.40	0.44
1:A:340:GLN:CB	1:A:351:THR:HG22	2.46	0.44
1:A:509:GLN:N	1:A:510:PRO:HD3	2.32	0.44
1:A:542:ILE:O	1:A:543:GLY:C	2.60	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:HA	1:A:226:PRO:C	2.42	0.44
1:A:233:GLU:O	1:A:239:TRP:HA	2.17	0.44
1:A:382:ILE:O	2:B:135:ILE:CG2	2.65	0.44
2:B:23:GLN:NE2	2:B:24:TRP:O	2.27	0.44
1:A:178:ILE:N	1:A:178:ILE:HD12	2.32	0.44
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.98	0.44
1:A:371:ALA:O	1:A:375:ILE:HG13	2.18	0.44
1:A:498:ASP:HA	1:A:536:VAL:O	2.17	0.44
2:B:281:LYS:C	2:B:283:LEU:H	2.26	0.44
1:A:77:PHE:C	1:A:79:GLU:N	2.72	0.44
1:A:193:LEU:HB3	1:A:197:GLN:HB3	1.99	0.44
1:A:501:TYR:O	1:A:502:ALA:C	2.61	0.44
2:B:65:LYS:HE2	2:B:72:ARG:NE	2.33	0.44
2:B:422:LEU:HG	2:B:426:TRP:CZ2	2.53	0.44
2:B:425:LEU:H	2:B:425:LEU:CD1	2.31	0.44
1:A:320:ASP:CG	1:A:323:LYS:HG3	2.42	0.44
1:A:329:ILE:CG2	1:A:330:GLN:N	2.81	0.44
2:B:332:GLN:NE2	2:B:428:GLN:HG2	2.33	0.44
2:B:380:ILE:O	2:B:384:GLY:CA	2.64	0.44
2:B:395:LYS:HG3	2:B:416:PHE:CE1	2.53	0.44
1:A:13:LYS:O	1:A:14:PRO:C	2.61	0.43
1:A:410:TRP:CZ2	1:A:412:PRO:HA	2.53	0.43
1:A:547:GLN:HG3	2:B:286:THR:HG22	1.99	0.43
2:B:98:ALA:O	2:B:101:LYS:CG	2.62	0.43
1:A:16:MET:HE1	1:A:82:LYS:CE	2.48	0.43
1:A:108:ILE:HD12	1:A:188:TYR:CE2	2.53	0.43
1:A:126:LYS:HE3	1:A:127:TYR:CE2	2.53	0.43
1:A:238:LYS:HG2	1:A:239:TRP:N	2.33	0.43
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.47	0.43
2:B:422:LEU:C	2:B:424:LYS:N	2.76	0.43
2:B:426:TRP:CE3	2:B:426:TRP:CA	3.02	0.43
1:A:102:LYS:HE2	1:A:102:LYS:HB3	1.79	0.43
1:A:524:GLN:O	1:A:527:LYS:HB2	2.17	0.43
2:B:210:LEU:C	2:B:212:TRP:H	2.26	0.43
2:B:402:TRP:HZ3	2:B:406:TRP:CD2	2.36	0.43
1:A:442:VAL:HG12	1:A:457:TYR:HB3	2.00	0.43
2:B:41:MET:HB3	2:B:46:LYS:HB2	2.00	0.43
2:B:178:ILE:HG21	2:B:189:VAL:HG12	1.99	0.43
2:B:274:ILE:HD11	2:B:310:LEU:HD21	2.00	0.43
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.18	0.43
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.64	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LYS:HA	1:A:366:LYS:HD2	1.80	0.43
2:B:61:PHE:CD2	2:B:61:PHE:N	2.86	0.43
2:B:120:LEU:O	2:B:121:ASP:C	2.61	0.43
2:B:418:ASN:ND2	4:B:1021:HOH:O	2.51	0.43
1:A:107:THR:HG22	1:A:108:ILE:N	2.33	0.43
2:B:88:TRP:CE3	2:B:88:TRP:HA	2.53	0.43
2:B:372:VAL:HG13	2:B:389:PHE:CD2	2.54	0.43
1:A:58:THR:CG2	1:A:76:ASP:O	2.63	0.43
1:A:344:GLU:O	1:A:345:PRO:C	2.62	0.43
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.54	0.43
2:B:11:LYS:O	2:B:85:GLN:HB3	2.19	0.43
2:B:325:LEU:HD22	2:B:385:LYS:HG3	2.00	0.43
1:A:18:GLY:HA2	1:A:83:ARG:CD	2.48	0.43
1:A:488:ASP:OD2	1:A:488:ASP:N	2.49	0.43
1:A:492:GLU:OE2	1:A:530:LYS:HD2	2.19	0.43
2:B:236:PRO:O	2:B:238:LYS:N	2.51	0.43
2:B:61:PHE:CE1	2:B:74:LEU:HD23	2.54	0.43
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.17	0.43
1:A:241:VAL:CG2	1:A:314:VAL:HB	2.49	0.43
2:B:282:LEU:CD2	2:B:296:THR:HG23	2.45	0.43
1:A:77:PHE:O	1:A:79:GLU:N	2.51	0.42
1:A:299:ALA:C	1:A:301:LEU:N	2.76	0.42
2:B:119:PRO:HA	2:B:148:VAL:HA	2.00	0.42
2:B:205:LEU:CD1	2:B:209:LEU:HD22	2.49	0.42
2:B:369:THR:O	2:B:373:GLN:HG3	2.19	0.42
1:A:89:GLU:O	1:A:89:GLU:OE1	2.36	0.42
1:A:516:GLU:O	1:A:520:GLN:HG3	2.19	0.42
2:B:101:LYS:HB3	2:B:382:ILE:HA	2.01	0.42
2:B:319:TYR:OH	2:B:321:PRO:HA	2.19	0.42
1:A:255:ASN:HD22	1:A:255:ASN:HA	1.58	0.42
1:A:282:LEU:N	1:A:282:LEU:CD1	2.82	0.42
1:A:519:ASN:HA	1:A:522:ILE:HD12	2.02	0.42
2:B:108:ILE:HG12	2:B:188:TYR:CD2	2.54	0.42
1:A:218:ASP:OD1	1:A:221:HIS:HD2	2.03	0.42
2:B:310:LEU:C	2:B:312:GLU:H	2.27	0.42
2:B:368:LEU:O	2:B:372:VAL:HG23	2.20	0.42
1:A:493:VAL:CG1	1:A:494:ASN:N	2.83	0.42
1:A:255:ASN:O	1:A:259:LYS:HG2	2.19	0.42
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.55	0.42
1:A:511:ASP:OD1	1:A:511:ASP:C	2.62	0.42
2:B:33:ALA:O	2:B:37:ILE:HG13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:GLU:OE1	2:B:53:GLU:N	2.35	0.42
2:B:379:SER:OG	2:B:387:PRO:HD3	2.20	0.42
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.52	0.42
1:A:41:MET:CB	1:A:47:ILE:HG12	2.50	0.42
1:A:103:LYS:HD3	1:A:103:LYS:HA	1.80	0.42
1:A:278:GLN:NE2	1:A:281:LYS:HD2	2.35	0.42
1:A:521:ILE:O	1:A:522:ILE:C	2.62	0.42
2:B:65:LYS:HE2	2:B:72:ARG:HD3	1.96	0.42
1:A:169:GLU:O	1:A:173:LYS:HD3	2.19	0.41
1:A:206:ARG:HH11	1:A:216:THR:CG2	2.22	0.41
1:A:271:TYR:CZ	1:A:314:VAL:HG23	2.55	0.41
1:A:120:LEU:O	1:A:122:GLU:N	2.53	0.41
2:B:166:LYS:O	2:B:168:LEU:N	2.53	0.41
2:B:178:ILE:HG12	2:B:191:SER:CB	2.47	0.41
2:B:208:HIS:O	2:B:211:ARG:HG3	2.20	0.41
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.81	0.41
2:B:423:VAL:O	2:B:427:TYR:HD2	2.03	0.41
1:A:276:VAL:O	1:A:280:CSD:HB3	2.20	0.41
2:B:373:GLN:O	2:B:377:THR:HG23	2.21	0.41
1:A:24:TRP:O	1:A:25:PRO:C	2.64	0.41
1:A:90:VAL:O	1:A:91:GLN:C	2.63	0.41
1:A:288:ALA:O	1:A:291:GLU:HB3	2.21	0.41
1:A:362:THR:HB	1:A:363:ASN:H	1.37	0.41
2:B:165:THR:O	2:B:166:LYS:C	2.64	0.41
1:A:402:TRP:CH2	2:B:362:THR:HA	2.55	0.41
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.49	0.41
1:A:239:TRP:HD1	1:A:318:TYR:CE1	2.39	0.41
1:A:344:GLU:HB2	1:A:347:LYS:HD2	2.02	0.41
2:B:114:ALA:N	2:B:214:LEU:HD21	2.34	0.41
2:B:166:LYS:C	2:B:168:LEU:N	2.77	0.41
2:B:244:ILE:HD13	2:B:266:TRP:HZ3	1.85	0.41
2:B:260:LEU:HD21	2:B:303:LEU:HD21	2.03	0.41
1:A:160:PHE:O	1:A:161:GLN:C	2.64	0.41
1:A:317:VAL:HG12	1:A:318:TYR:N	2.36	0.41
1:A:522:ILE:HG22	1:A:526:ILE:HD11	2.02	0.41
1:A:118:VAL:O	1:A:148:VAL:HB	2.20	0.41
1:A:170:PRO:O	1:A:171:PHE:C	2.63	0.41
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.56	0.41
1:A:363:ASN:HA	1:A:511:ASP:CG	2.46	0.41
2:B:137:ASN:C	2:B:139:THR:N	2.78	0.41
2:B:171:PHE:CG	2:B:205:LEU:HD23	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:HIS:O	2:B:211:ARG:CG	2.69	0.40
1:A:131:THR:CG2	1:A:132:ILE:N	2.84	0.40
1:A:241:VAL:CG2	1:A:270:ILE:HD13	2.52	0.40
1:A:427:TYR:CD2	1:A:427:TYR:C	2.99	0.40
1:A:37:ILE:CG2	1:A:41:MET:HE3	2.51	0.40
1:A:184:MET:HB3	1:A:185:ASP:H	1.40	0.40
2:B:249:LYS:HZ3	2:B:249:LYS:CB	2.22	0.40
1:A:38:CYS:O	1:A:39:THR:C	2.63	0.40
2:B:195:ILE:CG2	2:B:196:GLY:H	2.29	0.40
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.57	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	539/560 (96%)	446 (83%)	74 (14%)	19 (4%)	3	10
2	B	389/440 (88%)	335 (86%)	45 (12%)	9 (2%)	5	18
All	All	928/1000 (93%)	781 (84%)	119 (13%)	28 (3%)	3	12

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLU
1	A	135	ILE
1	A	538	ALA
2	B	65	LYS
2	B	423	VAL
1	A	113	ASP
1	A	121	ASP
1	A	543	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	85	GLN
2	B	213	GLY
1	A	4	PRO
1	A	89	GLU
1	A	461	ARG
1	A	503	LEU
2	B	237	ASP
2	B	267	ALA
1	A	16	MET
1	A	27	THR
1	A	345	PRO
1	A	40	GLU
1	A	78	ARG
1	A	170	PRO
2	B	311	LYS
1	A	151	GLN
2	B	166	LYS
1	A	169	GLU
2	B	14	PRO
1	A	19	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	487/499 (98%)	438 (90%)	49 (10%)	7	23
2	B	362/400 (90%)	337 (93%)	25 (7%)	14	41
All	All	849/899 (94%)	775 (91%)	74 (9%)	9	30

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	4	PRO
1	A	19	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	21	VAL
1	A	46	LYS
1	A	52	PRO
1	A	53	GLU
1	A	86	ASP
1	A	89	GLU
1	A	91	GLN
1	A	92	LEU
1	A	94	ILE
1	A	111	VAL
1	A	113	ASP
1	A	120	LEU
1	A	137	ASN
1	A	138	GLU
1	A	143	ARG
1	A	145	GLN
1	A	151	GLN
1	A	184	MET
1	A	187	LEU
1	A	194	GLU
1	A	195	ILE
1	A	197	GLN
1	A	205	LEU
1	A	206	ARG
1	A	216	THR
1	A	218	ASP
1	A	224	GLU
1	A	238	LYS
1	A	240	THR
1	A	249	LYS
1	A	255	ASN
1	A	279	LEU
1	A	317	VAL
1	A	324	ASP
1	A	340	GLN
1	A	362	THR
1	A	368	LEU
1	A	402	TRP
1	A	403	THR
1	A	413	GLU
1	A	423	VAL
1	A	459	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	474	ASN
1	A	488	ASP
1	A	496	VAL
1	A	517	LEU
2	B	8	VAL
2	B	11	LYS
2	B	40	GLU
2	B	61	PHE
2	B	65	LYS
2	B	70	LYS
2	B	88	TRP
2	B	139	THR
2	B	165	THR
2	B	167	ILE
2	B	189	VAL
2	B	202	ILE
2	B	209	LEU
2	B	233	GLU
2	B	234	LEU
2	B	277	ARG
2	B	287	LYS
2	B	291	GLU
2	B	301	LEU
2	B	325	LEU
2	B	350	LYS
2	B	358	ARG
2	B	365	VAL
2	B	368	LEU
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	147	ASN
1	A	151	GLN
1	A	174	GLN
1	A	221	HIS
1	A	222	GLN
1	A	255	ASN
1	A	265	ASN
1	A	278	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	332	GLN
1	A	336	GLN
1	A	428	GLN
1	A	474	ASN
1	A	500	GLN
1	A	509	GLN
1	A	547	GLN
2	B	57	ASN
2	B	147	ASN
2	B	175	ASN
2	B	197	GLN
2	B	208	HIS
2	B	255	ASN
2	B	269	GLN
2	B	278	GLN
2	B	332	GLN
2	B	336	GLN
2	B	348	ASN
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	2.19	1 (25%)	1,8,10	7.27	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	4.01	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	7.27	118.99	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1.51	3 (13%)	34,34,34	2.08	8 (23%)

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	-	-	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)
3	A	999	NVP	C10-C9	4.59	1.55	1.49
3	A	999	NVP	C15-N1	2.82	1.45	1.42
3	A	999	NVP	C5-C4	2.14	1.42	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	NVP	C7-C2-N1	-7.07	117.43	120.14
3	A	999	NVP	C7-N8-C9	4.94	132.36	128.29
3	A	999	NVP	N3-C2-N1	4.42	120.01	116.67
3	A	999	NVP	N14-C15-N1	3.92	119.63	116.67
3	A	999	NVP	C15-C10-C9	-2.79	121.28	124.01
3	A	999	NVP	C10-C15-N1	-2.31	118.07	120.95
3	A	999	NVP	C11-C10-C9	2.10	120.27	116.76
3	A	999	NVP	C2-N1-CA	-2.08	114.69	116.34

There are no chirality outliers.

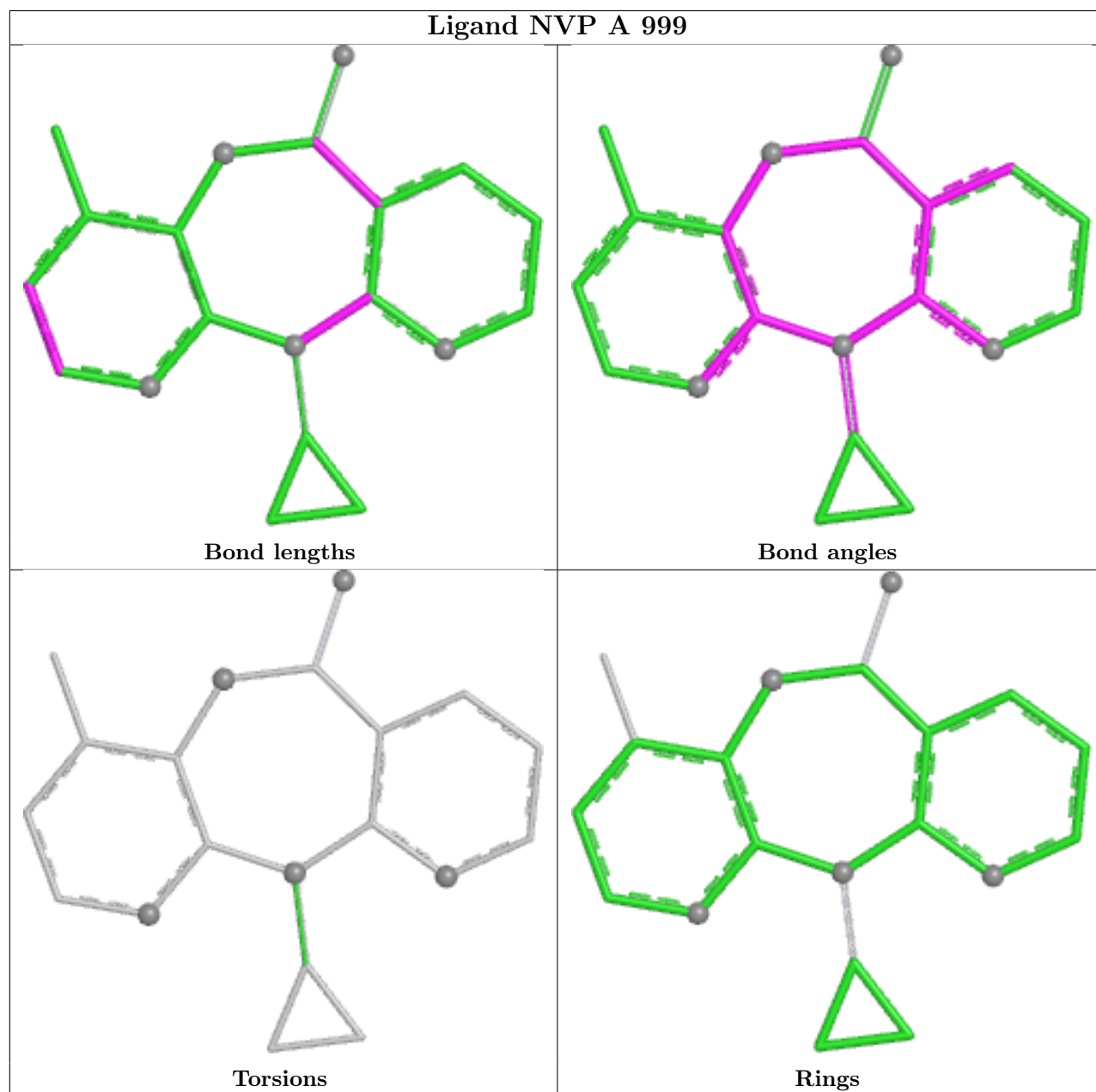
There are no torsion outliers.

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	545/560 (97%)	-0.17	4 (0%) 84 77	31, 79, 133, 150	0
2	B	397/440 (90%)	-0.20	0 100 100	39, 81, 130, 150	0
All	All	942/1000 (94%)	-0.19	4 (0%) 88 84	31, 80, 132, 150	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	PHE	2.7
1	A	2	ILE	2.4
1	A	468	THR	2.4
1	A	19	PRO	2.2

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	0.09	71,79,95,99	0

6.3 Carbohydrates [i](#)

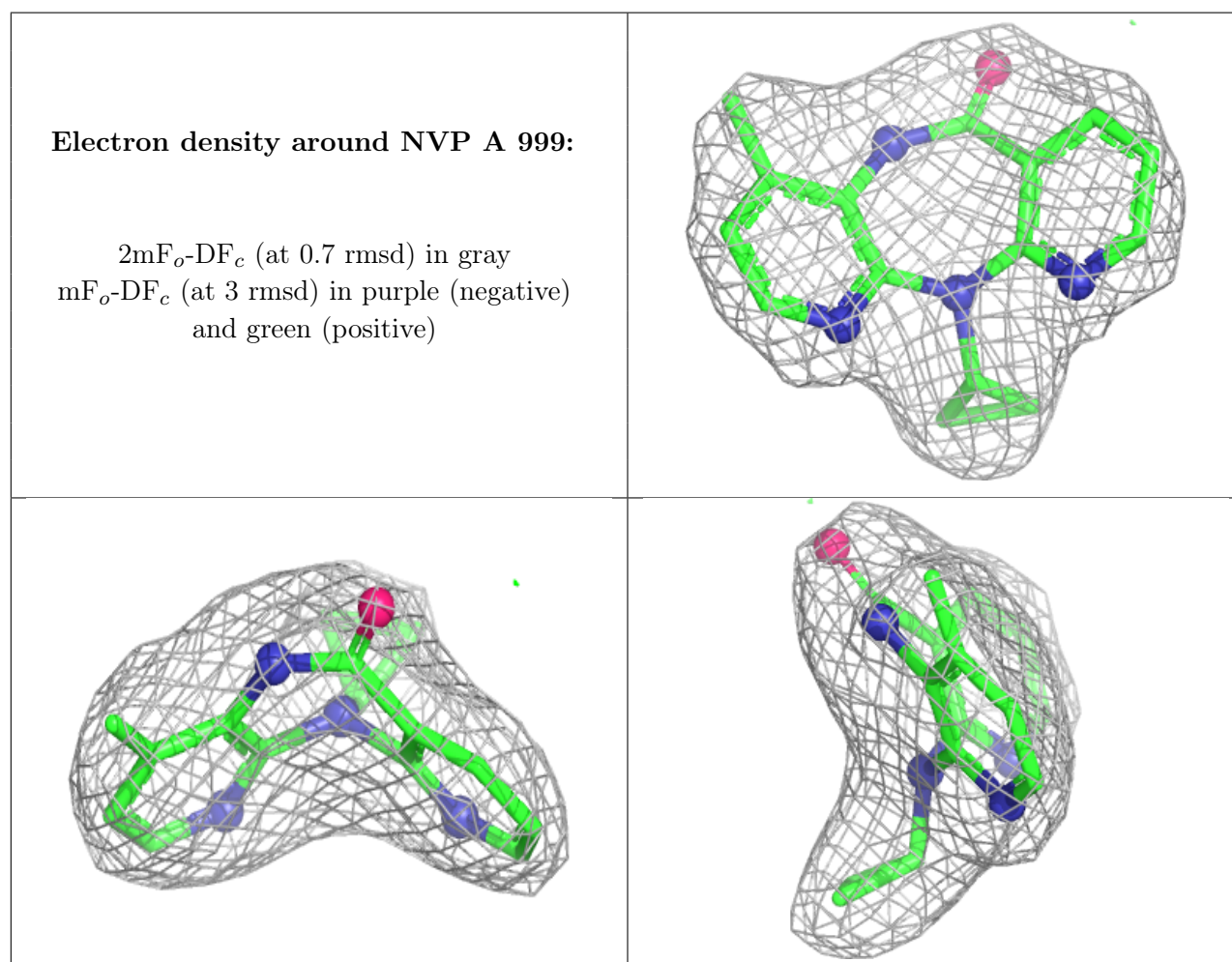
There are no oligosaccharides in this entry.

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	NVP	A	999	20/20	0.97	0.07	47,55,61,67	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.