



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:12 AM EDT

PDB ID : 1TKT / pdb_00001tkt
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN
COMPLEX WITH GW426318
Authors : Hopkins, A.L.; Ren, J.; Stuart, D.I.; Stammers, D.K.
Deposited on : 2004-06-09
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

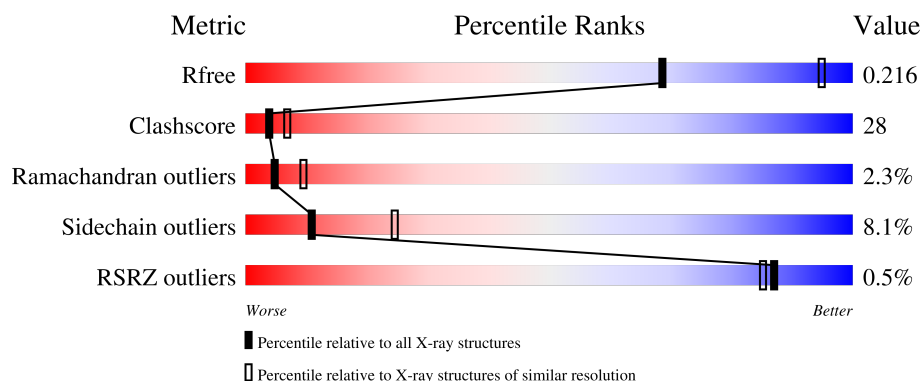
1 Overall quality at a glance

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))
R_{free}	180053	4008 (2.60-2.60)
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 [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7624 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 Pol polyproteins [Reverse transcriptase], Chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4238	2748	699	783	8			

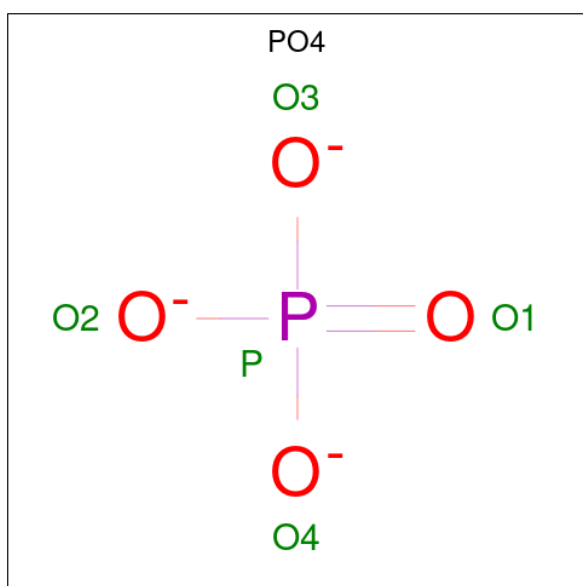
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	modified residue	UNP P04585

- Molecule 2 is a protein called Pol polyproteins [Reverse transcriptase], Chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	399	Total	C	N	O	S	0	0	0
			3311	2162	546	596	7			

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

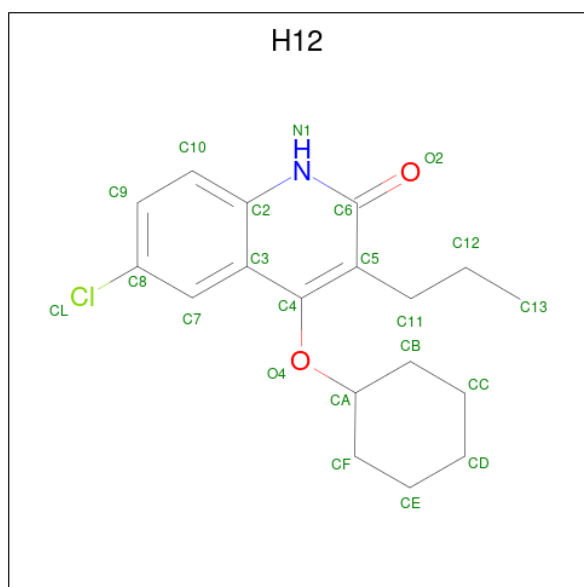


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	A	1	Total 5	O 4	P 1	0	0
3	A	1	Total 5	O 4	P 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is 6-CHLORO-4-(CYCLOHEXYLOXY)-3-PROPYLQUINOLIN-2(1H)-ONE (CCD ID: H12) (formula: $C_{18}H_{22}ClNO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			22	18	1	1	2		

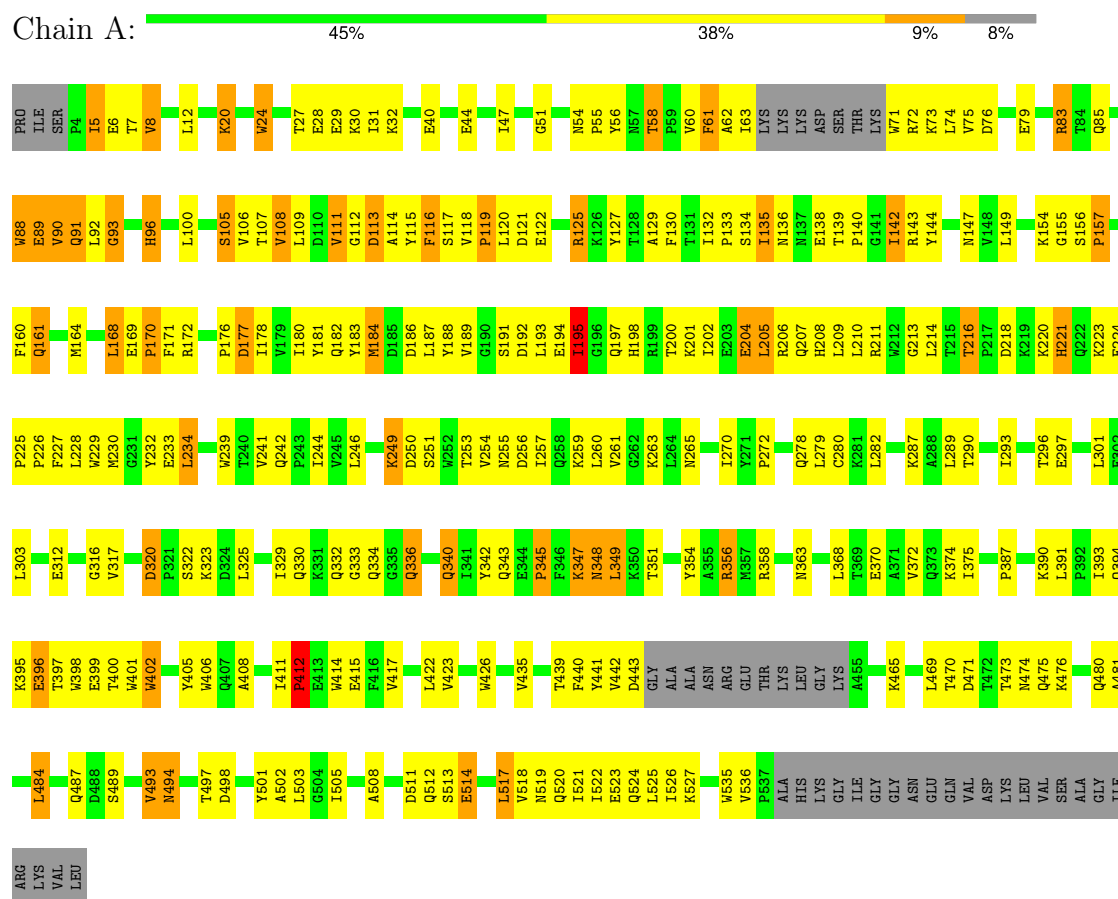
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	23	Total O 23 23	0	0
6	B	14	Total O 14 14	0	0

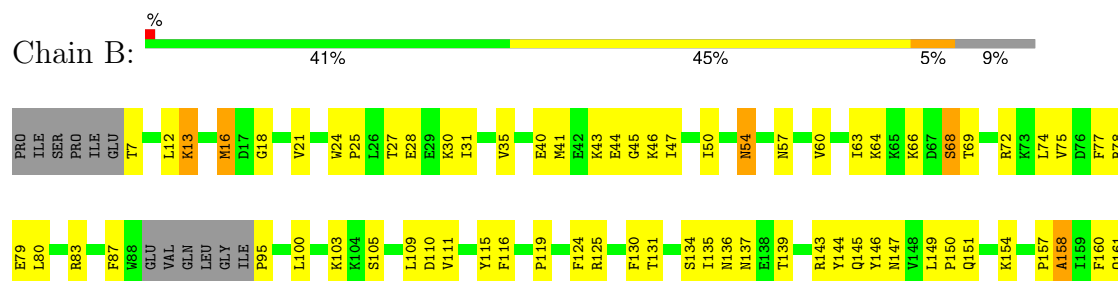
3 Residue-property plots

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: Pol polyproteins [Reverse transcriptase], Chain A



• Molecule 2: Pol polyproteins [Reverse transcriptase], Chain B



T376	T377	E378	S379	I380	V381	L382	W383	G384	P387	K388	F389	K390	K395	E396	T397	W398	E399	T400	W401	W402	Y405	W406	Q407	W410	I411	E412	E413	V417	N418	T419	P420	P421	L422	V423	K424	L425	W426	Y427	GLN	LEU	GLU	LYS	GLU	PRO	ILE	VAL	GLY	ALA	GLU	THR	PHE				
S162	S163	M164	T165	K166	I167	L168	E169	P170	F171	R172	K173	Q174	N175	P176	D177	I178	V179	Q182	Y183	M184	D185	D186	L187	G190	S191	D192	L193	E194	I195	R199	T200	K201	T202	E203	E204	L205	R206	Q207	H208	L209	W212	G213	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU	P225	P226
F227	L228	W229	M230	Q231	V232	E233	L234	H235	P236	D237	K238	W239	T240	V241	Q242	I244	D250	S251	W252	T253	V254	I257	Q258	L260	K263	W266	Q269	I274	K275	V276	R277	L282	L283	R284	G285	T286	K287	A288	L289	T290	E291	V292	T293	P294	L295	T296	E297	E298	L301						
E302	L303	A304	E305	N306	R307	E308	I309	L310	K311	V317	K323	D324	L325	I326	P243	E328	I329	Q330	K331	Q334	G335	Q336	W337	T338	Y339	Y342	Q343	E344	P345	F346	K347	N348	L349	K350	T351	G352	K353	R356	MET	ARG	GLY	ALA	HIS	T362	R363	D364	V365	V366	Q367	L368	T369	E370	A371	V372	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	138.20Å 115.10Å 65.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.60 29.83 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.7 (29.83-2.60) 86.7 (29.83-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.208 , 0.282 0.198 , 0.216	Depositor DCC
R_{free} test set	1380 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7624	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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, H12, MG, 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	0.68	0/4343	1.14	29/5907 (0.5%)
2	B	0.63	0/3408	1.10	23/4629 (0.5%)
All	All	0.66	0/7751	1.13	52/10536 (0.5%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	LEU	N-CA-C	-11.47	99.82	114.04
1	A	250	ASP	N-CA-C	-9.01	102.20	113.55
2	B	420	PRO	CA-C-N	8.72	130.75	119.84
2	B	420	PRO	C-N-CA	8.72	130.75	119.84
1	A	88	TRP	N-CA-C	-8.38	97.08	109.15
1	A	192	ASP	N-CA-C	-7.99	99.51	111.81
1	A	93	GLY	N-CA-C	-7.96	94.32	113.18
1	A	348	ASN	N-CA-C	7.83	120.03	110.41
2	B	417	VAL	N-CA-C	7.83	118.08	108.53
1	A	293	ILE	CA-C-N	-7.60	112.09	120.14
1	A	293	ILE	C-N-CA	-7.60	112.09	120.14
1	A	343	GLN	N-CA-C	-7.44	103.03	112.93
1	A	234	LEU	N-CA-C	7.35	120.50	108.52
1	A	58	THR	CA-C-N	6.98	127.02	119.90
1	A	58	THR	C-N-CA	6.98	127.02	119.90
2	B	231	GLY	N-CA-C	-6.75	105.92	115.30
1	A	51	GLY	CA-C-N	6.63	126.32	119.82
1	A	51	GLY	C-N-CA	6.63	126.32	119.82
2	B	234	LEU	N-CA-C	-6.62	99.80	110.32
1	A	493	VAL	N-CA-C	6.47	116.89	108.35
2	B	233	GLU	N-CA-C	6.46	120.57	110.17
1	A	147	ASN	N-CA-C	-6.40	105.22	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	382	ILE	N-CA-C	6.30	116.34	110.42
2	B	87	PHE	N-CA-C	6.13	118.84	107.99
2	B	343	GLN	N-CA-C	-6.11	105.73	113.43
1	A	96	HIS	N-CA-C	-6.01	99.79	109.40
2	B	395	LYS	N-CA-C	6.00	118.31	111.11
2	B	235	HIS	CA-C-N	5.98	126.14	119.32
2	B	235	HIS	C-N-CA	5.98	126.14	119.32
1	A	204	GLU	N-CA-C	-5.96	104.86	111.36
1	A	494	ASN	N-CA-C	-5.80	100.25	109.59
1	A	221	HIS	N-CA-C	5.70	120.94	113.30
1	A	142	ILE	N-CA-C	5.47	116.14	109.30
1	A	89	GLU	N-CA-C	5.45	117.56	110.53
2	B	147	ASN	N-CA-C	-5.44	106.78	113.41
1	A	184	MET	CB-CA-C	-5.39	109.90	117.23
1	A	111	VAL	N-CA-C	5.33	115.27	108.12
2	B	13	LYS	CA-C-N	5.29	125.59	119.93
2	B	13	LYS	C-N-CA	5.29	125.59	119.93
1	A	391	LEU	N-CA-C	5.26	117.92	110.40
2	B	349	LEU	N-CA-C	-5.22	106.06	112.90
2	B	401	TRP	N-CA-C	5.19	119.74	113.41
1	A	8	VAL	CB-CA-C	-5.16	104.84	110.78
1	A	514	GLU	N-CA-C	-5.16	106.50	112.89
2	B	18	GLY	CA-C-N	5.15	125.08	119.78
2	B	18	GLY	C-N-CA	5.15	125.08	119.78
2	B	290	THR	N-CA-C	5.14	118.65	112.38
1	A	320	ASP	CA-C-N	5.11	126.22	119.84
1	A	320	ASP	C-N-CA	5.11	126.22	119.84
2	B	21	VAL	CB-CA-C	-5.03	104.20	111.34
2	B	54	ASN	CA-C-N	5.01	124.70	119.64
2	B	54	ASN	C-N-CA	5.01	124.70	119.64

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	4238	0	4262	241	1
2	B	3311	0	3336	202	0
3	A	15	0	0	0	0
4	A	1	0	0	0	0
5	A	22	0	22	2	0
6	A	23	0	0	0	0
6	B	14	0	0	1	1
All	All	7624	0	7620	431	1

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 28.

All (431) 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:O	1:A:168:LEU:HD23	1.52	1.10
2:B:66:LYS:HE3	2:B:230:MET:HG3	1.35	1.06
1:A:195:ILE:HD12	1:A:195:ILE:H	1.22	1.04
1:A:206:ARG:HH12	1:A:218:ASP:HA	1.28	0.98
1:A:28:GLU:HG3	1:A:135:ILE:CG2	1.98	0.92
2:B:13:LYS:HB2	2:B:16:MET:HE3	1.48	0.92
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.35	0.91
2:B:66:LYS:CE	2:B:230:MET:HG3	2.01	0.91
1:A:28:GLU:HG3	1:A:135:ILE:HG21	1.55	0.88
2:B:227:PHE:HB3	2:B:231:GLY:HA2	1.53	0.88
2:B:40:GLU:HG3	2:B:44:GLU:OE2	1.76	0.86
1:A:5:ILE:HD12	1:A:5:ILE:H	1.39	0.84
2:B:169:GLU:HG2	2:B:170:PRO:HD3	1.60	0.84
1:A:469:LEU:HD21	1:A:480:GLN:HG3	1.60	0.84
2:B:323:LYS:HE3	2:B:323:LYS:HA	1.58	0.83
1:A:161:GLN:HA	1:A:182:GLN:HE22	1.46	0.80
1:A:206:ARG:NH1	1:A:218:ASP:HA	1.97	0.79
2:B:175:ASN:ND2	2:B:201:LYS:HD3	1.98	0.79
1:A:191:SER:HB2	1:A:193:LEU:HG	1.64	0.78
2:B:295:LEU:H	2:B:295:LEU:HD12	1.49	0.78
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.65	0.78
2:B:13:LYS:HD2	2:B:16:MET:CE	2.16	0.75
1:A:358:ARG:HD3	1:A:370:GLU:CD	2.11	0.75
2:B:234:LEU:HD21	2:B:377:THR:CG2	2.15	0.75
2:B:295:LEU:HD12	2:B:295:LEU:N	2.02	0.75
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.22	0.75
1:A:5:ILE:HD13	1:A:119:PRO:HD2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PHE:CE2	1:A:74:LEU:HG	2.24	0.73
1:A:253:THR:HG22	1:A:289:LEU:O	1.90	0.72
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.72	0.72
1:A:195:ILE:HD12	1:A:195:ILE:N	2.03	0.71
2:B:362:THR:HG22	2:B:366:LYS:HD3	1.71	0.71
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.25	0.71
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.73	0.71
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.06	0.71
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.56	0.70
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.27	0.70
2:B:13:LYS:CB	2:B:16:MET:HE3	2.22	0.70
1:A:116:PHE:H	1:A:116:PHE:HD2	1.37	0.70
2:B:151:GLN:HB3	2:B:185:ASP:OD1	1.93	0.69
1:A:354:TYR:CZ	1:A:356:ARG:HB3	2.28	0.69
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.28	0.69
2:B:163:SER:O	2:B:167:ILE:HG13	1.93	0.69
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.90	0.69
2:B:297:GLU:O	2:B:301:LEU:HG	1.93	0.68
2:B:234:LEU:HD21	2:B:377:THR:HG21	1.74	0.68
1:A:108:VAL:C	1:A:109:LEU:HD23	2.19	0.68
1:A:228:LEU:HD21	1:A:233:GLU:HG3	1.76	0.68
1:A:5:ILE:HD12	1:A:5:ILE:N	2.08	0.68
1:A:194:GLU:OE1	1:A:194:GLU:HA	1.92	0.67
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.76	0.67
1:A:62:ALA:C	1:A:63:ILE:HD12	2.19	0.67
1:A:89:GLU:C	1:A:91:GLN:H	2.03	0.66
2:B:227:PHE:CB	2:B:231:GLY:HA2	2.26	0.66
2:B:331:LYS:O	2:B:424:LYS:HE2	1.95	0.66
2:B:345:PRO:O	2:B:347:LYS:HG3	1.96	0.66
1:A:27:THR:HG22	1:A:29:GLU:H	1.60	0.65
2:B:242:GLN:HG2	2:B:353:LYS:NZ	2.11	0.65
1:A:105:SER:HB2	1:A:198:HIS:CD2	2.32	0.65
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.31	0.65
2:B:79:GLU:O	2:B:83:ARG:HG3	1.96	0.65
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.78	0.65
2:B:131:THR:OG1	2:B:143:ARG:HD2	1.95	0.65
1:A:30:LYS:HE3	1:A:71:TRP:CH2	2.32	0.64
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.79	0.64
2:B:66:LYS:HB2	2:B:407:GLN:HE22	1.62	0.64
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.33	0.63
1:A:296:THR:HG22	1:A:297:GLU:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ARG:O	2:B:287:LYS:NZ	2.31	0.63
1:A:253:THR:CG2	1:A:289:LEU:O	2.46	0.63
2:B:103:LYS:HE3	2:B:191:SER:HA	1.79	0.63
1:A:96:HIS:H	2:B:136:ASN:HD21	1.47	0.63
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.80	0.62
1:A:469:LEU:CD2	1:A:480:GLN:HG3	2.29	0.62
1:A:411:ILE:O	1:A:412:PRO:O	2.17	0.62
2:B:227:PHE:HB3	2:B:231:GLY:CA	2.25	0.62
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.34	0.62
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.34	0.62
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.82	0.62
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.80	0.62
1:A:116:PHE:CD2	1:A:116:PHE:N	2.63	0.62
2:B:366:LYS:O	2:B:370:GLU:HG3	1.99	0.62
1:A:72:ARG:HG2	1:A:73:LYS:N	2.14	0.62
2:B:167:ILE:O	2:B:208:HIS:HE1	1.81	0.62
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.35	0.61
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.30	0.61
2:B:208:HIS:CE1	2:B:212:TRP:HZ3	2.18	0.61
2:B:308:GLU:OE1	2:B:311:LYS:HD2	2.01	0.61
1:A:164:MET:SD	1:A:168:LEU:HD21	2.40	0.61
2:B:66:LYS:HE3	2:B:230:MET:CG	2.22	0.61
2:B:66:LYS:HB2	2:B:407:GLN:NE2	2.16	0.61
2:B:200:THR:O	2:B:204:GLU:HG3	1.99	0.61
2:B:372:VAL:HG13	2:B:389:PHE:CZ	2.36	0.61
1:A:195:ILE:H	1:A:195:ILE:CD1	1.99	0.61
2:B:175:ASN:N	2:B:176:PRO:HD3	2.16	0.61
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.31	0.61
1:A:24:TRP:HZ3	1:A:61:PHE:HB3	1.65	0.60
1:A:164:MET:HE3	1:A:168:LEU:HD21	1.83	0.60
1:A:171:PHE:CE2	1:A:205:LEU:HG	2.37	0.60
1:A:60:VAL:HG22	1:A:75:VAL:HG13	1.82	0.60
1:A:498:ASP:HA	1:A:536:VAL:O	2.00	0.60
1:A:61:PHE:HE2	1:A:74:LEU:HG	1.66	0.60
1:A:72:ARG:HG2	1:A:73:LYS:H	1.67	0.60
1:A:56:TYR:O	1:A:143:ARG:NH2	2.28	0.60
1:A:85:GLN:C	1:A:154:LYS:HZ3	2.09	0.60
2:B:282:LEU:HB3	2:B:293:ILE:HG21	1.83	0.60
1:A:111:VAL:CG1	1:A:114:ALA:HB2	2.31	0.60
1:A:129:ALA:HA	1:A:144:TYR:O	2.02	0.59
1:A:40:GLU:HG3	1:A:44:GLU:OE1	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.37	0.59
2:B:239:TRP:CZ2	2:B:378:GLU:HG2	2.37	0.59
2:B:274:ILE:HG23	2:B:306:ASN:OD1	2.03	0.59
2:B:169:GLU:N	2:B:170:PRO:HD2	2.17	0.59
1:A:136:ASN:OD1	1:A:139:THR:HG23	2.03	0.59
1:A:194:GLU:O	1:A:198:HIS:N	2.34	0.59
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.38	0.58
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.37	0.58
1:A:73:LYS:HE2	1:A:75:VAL:CG2	2.33	0.58
2:B:169:GLU:HG2	2:B:170:PRO:CD	2.33	0.58
2:B:13:LYS:HB2	2:B:16:MET:CE	2.27	0.58
2:B:172:ARG:O	2:B:176:PRO:HG3	2.03	0.58
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.39	0.58
1:A:393:ILE:HD12	1:A:423:VAL:CG2	2.34	0.58
1:A:115:TYR:O	1:A:149:LEU:HB2	2.03	0.58
1:A:142:ILE:HD12	1:A:144:TYR:OH	2.04	0.57
1:A:176:PRO:C	1:A:178:ILE:H	2.12	0.57
2:B:45:GLY:HA2	6:B:1020:HOH:O	2.02	0.57
1:A:61:PHE:N	1:A:61:PHE:HD2	2.01	0.57
1:A:347:LYS:O	1:A:347:LYS:HG2	2.05	0.57
1:A:24:TRP:HZ3	1:A:61:PHE:CG	2.22	0.57
2:B:105:SER:O	2:B:190:GLY:HA2	2.04	0.57
1:A:279:LEU:HD23	1:A:282:LEU:HD11	1.85	0.57
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.86	0.57
1:A:89:GLU:OE1	1:A:90:VAL:HG23	2.05	0.57
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.87	0.56
1:A:113:ASP:HB2	1:A:116:PHE:CD2	2.41	0.56
2:B:167:ILE:HG23	2:B:212:TRP:CE3	2.40	0.56
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.21	0.56
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.41	0.56
2:B:266:TRP:O	2:B:269:GLN:HG2	2.06	0.56
2:B:154:LYS:O	2:B:157:PRO:HD2	2.06	0.55
1:A:27:THR:HG22	1:A:29:GLU:N	2.20	0.55
1:A:164:MET:CE	1:A:168:LEU:HD21	2.36	0.55
1:A:332:GLN:O	1:A:332:GLN:HG2	2.06	0.55
1:A:108:VAL:HG13	1:A:223:LYS:HB2	1.88	0.55
1:A:24:TRP:CZ3	1:A:61:PHE:HB3	2.40	0.55
1:A:27:THR:O	1:A:30:LYS:N	2.39	0.55
2:B:254:VAL:O	2:B:258:GLN:HG3	2.07	0.55
1:A:111:VAL:HG13	1:A:214:LEU:HD22	1.88	0.55
1:A:61:PHE:N	1:A:61:PHE:CD2	2.73	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLU:C	1:A:91:GLN:N	2.63	0.55
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.06	0.55
1:A:28:GLU:HG3	1:A:135:ILE:HG22	1.89	0.55
2:B:368:LEU:O	2:B:372:VAL:HG23	2.07	0.54
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.89	0.54
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.43	0.54
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.42	0.54
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.88	0.54
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.42	0.54
1:A:228:LEU:CD2	1:A:233:GLU:HG3	2.38	0.54
1:A:201:LYS:O	1:A:204:GLU:HB3	2.07	0.54
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.87	0.54
2:B:201:LYS:HE3	2:B:201:LYS:HA	1.88	0.54
1:A:169:GLU:HB2	1:A:170:PRO:CD	2.38	0.54
1:A:177:ASP:O	1:A:178:ILE:HD13	2.08	0.54
2:B:13:LYS:HD2	2:B:16:MET:HE1	1.90	0.54
2:B:178:ILE:CD1	2:B:201:LYS:HG2	2.35	0.54
1:A:74:LEU:HD12	1:A:75:VAL:N	2.24	0.53
2:B:295:LEU:H	2:B:295:LEU:CD1	2.20	0.53
2:B:13:LYS:HD2	2:B:16:MET:HE3	1.88	0.53
2:B:171:PHE:CE1	2:B:205:LEU:HA	2.44	0.53
2:B:174:GLN:C	2:B:176:PRO:HD3	2.34	0.53
1:A:106:VAL:HA	1:A:189:VAL:O	2.08	0.53
2:B:195:ILE:HD11	2:B:233:GLU:HG3	1.91	0.53
2:B:380:ILE:O	2:B:384:GLY:N	2.38	0.53
1:A:325:LEU:HB3	1:A:387:PRO:HB3	1.90	0.53
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.57	0.53
1:A:518:VAL:O	1:A:522:ILE:HG13	2.09	0.52
2:B:63:ILE:HG21	2:B:74:LEU:HD22	1.92	0.52
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.45	0.52
2:B:379:SER:CB	2:B:387:PRO:HD3	2.40	0.52
2:B:242:GLN:HG2	2:B:353:LYS:HZ3	1.72	0.52
1:A:417:VAL:O	1:A:417:VAL:HG13	2.09	0.52
2:B:193:LEU:HD12	2:B:193:LEU:H	1.74	0.52
1:A:399:GLU:OE1	1:A:402:TRP:HZ3	1.93	0.52
2:B:423:VAL:HA	2:B:426:TRP:CE3	2.45	0.52
1:A:111:VAL:HG11	1:A:114:ALA:HB2	1.92	0.51
2:B:168:LEU:O	2:B:172:ARG:HG3	2.10	0.51
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.92	0.51
1:A:168:LEU:O	1:A:172:ARG:HB2	2.09	0.51
1:A:31:ILE:HG12	1:A:133:PRO:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:HG12	1:A:114:ALA:HB2	1.93	0.51
2:B:258:GLN:HG2	2:B:283:LEU:HD21	1.91	0.51
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.39	0.51
2:B:64:LYS:HE2	2:B:68:SER:O	2.10	0.51
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.45	0.51
2:B:12:LEU:O	2:B:13:LYS:C	2.53	0.51
1:A:90:VAL:O	1:A:91:GLN:C	2.54	0.51
1:A:278:GLN:NE2	1:A:278:GLN:HA	2.25	0.50
2:B:193:LEU:HD12	2:B:193:LEU:N	2.26	0.50
1:A:329:ILE:HG22	1:A:330:GLN:N	2.26	0.50
1:A:523:GLU:O	1:A:527:LYS:HG2	2.11	0.50
1:A:28:GLU:O	1:A:32:LYS:HG3	2.11	0.50
1:A:188:TYR:CD2	5:A:999:H12:HF1	2.45	0.50
1:A:522:ILE:HA	1:A:525:LEU:HD12	1.93	0.50
1:A:368:LEU:O	1:A:372:VAL:HG23	2.12	0.50
2:B:202:ILE:HG21	2:B:227:PHE:HE1	1.77	0.50
2:B:276:VAL:O	2:B:277:ARG:C	2.53	0.50
1:A:88:TRP:HB2	2:B:54:ASN:O	2.11	0.50
2:B:161:GLN:O	2:B:164:MET:HB3	2.12	0.50
1:A:73:LYS:HE2	1:A:75:VAL:HG22	1.94	0.49
1:A:396:GLU:HG3	1:A:397:THR:N	2.26	0.49
2:B:27:THR:OG1	2:B:30:LYS:HG2	2.12	0.49
2:B:254:VAL:HG23	2:B:291:GLU:O	2.12	0.49
2:B:326:ILE:HG22	2:B:327:ALA:N	2.26	0.49
1:A:29:GLU:OE1	1:A:71:TRP:CZ2	2.65	0.49
2:B:160:PHE:CD1	2:B:164:MET:HB2	2.47	0.49
1:A:5:ILE:H	1:A:5:ILE:CD1	2.16	0.49
1:A:93:GLY:O	2:B:137:ASN:HB3	2.12	0.49
2:B:234:LEU:HD21	2:B:377:THR:HG22	1.92	0.49
2:B:398:TRP:O	2:B:402:TRP:HD1	1.95	0.49
1:A:226:PRO:HA	1:A:234:LEU:O	2.13	0.49
2:B:229:TRP:HA	2:B:229:TRP:CE3	2.48	0.49
2:B:44:GLU:O	2:B:46:LYS:HE3	2.13	0.49
1:A:333:GLY:O	1:A:334:GLN:C	2.55	0.49
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.69	0.49
1:A:210:LEU:O	1:A:213:GLY:N	2.41	0.49
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.41	0.49
2:B:323:LYS:HB2	2:B:343:GLN:NE2	2.28	0.49
1:A:398:TRP:NE1	1:A:411:ILE:HD12	2.27	0.48
2:B:41:MET:HE2	2:B:46:LYS:HB2	1.95	0.48
2:B:193:LEU:H	2:B:193:LEU:CD1	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:THR:HA	2:B:292:VAL:HA	1.93	0.48
1:A:340:GLN:HA	1:A:351:THR:HA	1.95	0.48
2:B:183:TYR:CD1	2:B:184:MET:HG2	2.49	0.48
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.95	0.48
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.47	0.48
1:A:253:THR:HG22	1:A:254:VAL:N	2.29	0.48
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.78	0.48
1:A:194:GLU:O	1:A:195:ILE:C	2.57	0.48
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.96	0.48
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.96	0.48
2:B:257:ILE:HG21	2:B:283:LEU:HD13	1.95	0.48
1:A:393:ILE:CB	1:A:423:VAL:HG22	2.42	0.48
2:B:40:GLU:OE2	2:B:43:LYS:HD2	2.14	0.48
2:B:136:ASN:O	2:B:137:ASN:HB2	2.14	0.48
2:B:396:GLU:CD	2:B:396:GLU:H	2.22	0.48
1:A:120:LEU:HD12	1:A:121:ASP:N	2.29	0.47
1:A:473:THR:O	1:A:474:ASN:C	2.56	0.47
2:B:110:ASP:HB3	2:B:226:PRO:HG2	1.96	0.47
1:A:90:VAL:O	1:A:90:VAL:HG12	2.14	0.47
1:A:390:LYS:HD2	1:A:415:GLU:OE2	2.13	0.47
2:B:57:ASN:ND2	2:B:143:ARG:NH1	2.60	0.47
2:B:63:ILE:HD11	2:B:72:ARG:HD3	1.95	0.47
1:A:24:TRP:HZ3	1:A:61:PHE:CB	2.27	0.47
2:B:285:GLY:O	2:B:287:LYS:HG3	2.14	0.47
1:A:218:ASP:O	1:A:221:HIS:N	2.45	0.47
1:A:393:ILE:HD12	1:A:423:VAL:HG21	1.96	0.47
2:B:205:LEU:HD22	2:B:209:LEU:HG	1.95	0.47
1:A:108:VAL:O	1:A:109:LEU:HD23	2.14	0.47
1:A:206:ARG:HG2	1:A:216:THR:OG1	2.14	0.47
1:A:253:THR:CG2	1:A:290:THR:HA	2.45	0.47
1:A:169:GLU:N	1:A:170:PRO:HD2	2.30	0.47
1:A:255:ASN:O	1:A:259:LYS:HG3	2.15	0.47
1:A:342:TYR:HA	1:A:349:LEU:CD1	2.44	0.47
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.96	0.47
2:B:168:LEU:C	2:B:170:PRO:HD2	2.40	0.47
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.97	0.47
1:A:29:GLU:OE1	1:A:71:TRP:HZ2	1.97	0.47
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.80	0.47
2:B:28:GLU:CA	2:B:135:ILE:HD11	2.45	0.47
1:A:198:HIS:C	1:A:200:THR:N	2.72	0.47
1:A:253:THR:HG22	1:A:255:ASN:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:THR:CG2	1:A:297:GLU:N	2.78	0.47
1:A:469:LEU:HD11	1:A:480:GLN:HE21	1.80	0.47
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.50	0.47
1:A:107:THR:HG23	1:A:198:HIS:NE2	2.30	0.46
1:A:270:ILE:O	1:A:272:PRO:HD3	2.15	0.46
1:A:401:TRP:CH2	1:A:508:ALA:O	2.68	0.46
1:A:522:ILE:O	1:A:526:ILE:HG13	2.15	0.46
2:B:371:ALA:O	2:B:372:VAL:C	2.57	0.46
2:B:103:LYS:CE	2:B:191:SER:HA	2.45	0.46
1:A:426:TRP:CD1	1:A:426:TRP:N	2.83	0.46
1:A:465:LYS:HD2	1:A:484:LEU:HD21	1.97	0.46
2:B:388:LYS:HE2	2:B:413:GLU:OE1	2.15	0.46
1:A:401:TRP:HH2	1:A:508:ALA:O	1.97	0.46
1:A:517:LEU:CA	1:A:520:GLN:HE21	2.18	0.46
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.50	0.46
2:B:103:LYS:HE3	2:B:191:SER:CA	2.45	0.46
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.46	0.46
2:B:160:PHE:O	2:B:161:GLN:C	2.58	0.46
2:B:203:GLU:O	2:B:206:ARG:HB2	2.16	0.46
1:A:134:SER:OG	1:A:139:THR:O	2.28	0.45
1:A:363:ASN:ND2	1:A:401:TRP:CH2	2.84	0.45
2:B:60:VAL:HG11	2:B:130:PHE:CD1	2.51	0.45
1:A:114:ALA:HA	1:A:117:SER:OG	2.16	0.45
1:A:180:ILE:HA	1:A:188:TYR:O	2.16	0.45
2:B:208:HIS:CE1	2:B:212:TRP:CZ3	3.02	0.45
1:A:107:THR:OG1	1:A:202:ILE:HD12	2.16	0.45
1:A:195:ILE:N	1:A:195:ILE:CD1	2.73	0.45
1:A:405:TYR:O	2:B:331:LYS:HD3	2.16	0.45
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.51	0.45
2:B:227:PHE:CG	2:B:231:GLY:HA2	2.52	0.45
1:A:320:ASP:CG	1:A:322:SER:OG	2.59	0.45
1:A:349:LEU:HD12	1:A:349:LEU:N	2.32	0.45
1:A:502:ALA:O	1:A:505:ILE:HB	2.17	0.45
1:A:71:TRP:HA	1:A:71:TRP:CE3	2.52	0.45
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.51	0.45
1:A:183:TYR:O	1:A:184:MET:HB2	2.17	0.45
1:A:120:LEU:O	1:A:121:ASP:C	2.60	0.45
1:A:279:LEU:HA	1:A:282:LEU:CD1	2.46	0.45
2:B:31:ILE:O	2:B:35:VAL:HG23	2.16	0.45
2:B:100:LEU:O	2:B:103:LYS:HG2	2.16	0.45
2:B:328:GLU:O	2:B:339:TYR:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG12	1:A:227:PHE:HE2	1.82	0.45
1:A:228:LEU:HA	1:A:232:TYR:O	2.17	0.45
1:A:320:ASP:C	1:A:322:SER:N	2.74	0.45
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.16	0.45
2:B:425:LEU:C	2:B:425:LEU:HD23	2.42	0.45
1:A:108:VAL:HA	1:A:187:LEU:O	2.16	0.45
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.99	0.45
1:A:249:LYS:HZ3	1:A:256:ASP:CG	2.25	0.45
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.52	0.44
1:A:261:VAL:O	1:A:265:ASN:OD1	2.35	0.44
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.47	0.44
2:B:285:GLY:O	2:B:287:LYS:N	2.50	0.44
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.51	0.44
1:A:332:GLN:HB3	1:A:336:GLN:HB3	1.98	0.44
2:B:208:HIS:NE2	2:B:212:TRP:HZ3	2.14	0.44
1:A:194:GLU:HB2	1:A:197:GLN:HB3	1.99	0.44
2:B:206:ARG:NH2	2:B:227:PHE:CG	2.86	0.44
1:A:20:LYS:HD2	1:A:55:PRO:HB2	1.99	0.44
1:A:63:ILE:HD12	1:A:63:ILE:N	2.33	0.44
2:B:330:GLN:HB2	2:B:338:THR:HG1	1.82	0.44
1:A:208:HIS:O	1:A:211:ARG:HB2	2.18	0.44
2:B:376:THR:O	2:B:377:THR:C	2.60	0.44
1:A:253:THR:HG23	1:A:290:THR:C	2.43	0.44
2:B:229:TRP:HA	2:B:229:TRP:HE3	1.82	0.44
1:A:497:THR:O	1:A:535:TRP:HA	2.18	0.44
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.53	0.44
1:A:320:ASP:OD2	1:A:322:SER:OG	2.32	0.43
2:B:325:LEU:O	2:B:387:PRO:HA	2.18	0.43
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.31	0.43
1:A:111:VAL:CG1	1:A:214:LEU:HD22	2.49	0.43
1:A:132:ILE:HB	1:A:142:ILE:HG13	2.01	0.43
2:B:170:PRO:HG2	2:B:208:HIS:NE2	2.33	0.43
2:B:242:GLN:HG2	2:B:353:LYS:HZ2	1.80	0.43
2:B:406:TRP:HZ2	2:B:410:TRP:O	2.00	0.43
2:B:24:TRP:CD1	2:B:25:PRO:HD2	2.53	0.43
2:B:160:PHE:HD1	2:B:164:MET:HB2	1.82	0.43
2:B:173:LYS:C	2:B:176:PRO:HD3	2.43	0.43
1:A:155:GLY:O	1:A:156:SER:C	2.60	0.43
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.48	0.43
2:B:169:GLU:N	2:B:170:PRO:CD	2.82	0.43
2:B:205:LEU:O	2:B:209:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.99	0.43
1:A:89:GLU:O	1:A:91:GLN:N	2.51	0.43
1:A:100:LEU:HB3	5:A:999:H12:C6	2.48	0.43
2:B:66:LYS:HG2	2:B:230:MET:SD	2.59	0.43
1:A:118:VAL:HA	1:A:119:PRO:HD2	1.86	0.43
2:B:124:PHE:O	2:B:125:ARG:C	2.60	0.43
2:B:134:SER:HB2	2:B:139:THR:OG1	2.19	0.43
2:B:173:LYS:HA	2:B:176:PRO:HG3	2.00	0.43
2:B:239:TRP:CZ3	2:B:378:GLU:HG2	2.53	0.43
2:B:227:PHE:CB	2:B:231:GLY:CA	2.93	0.43
2:B:241:VAL:O	2:B:243:PRO:HD3	2.18	0.43
1:A:139:THR:HA	1:A:140:PRO:HD3	1.82	0.42
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.54	0.42
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.54	0.42
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.54	0.42
2:B:157:PRO:O	2:B:161:GLN:N	2.51	0.42
2:B:242:GLN:CG	2:B:353:LYS:NZ	2.80	0.42
1:A:198:HIS:C	1:A:200:THR:H	2.26	0.42
2:B:115:TYR:HB3	2:B:149:LEU:HB2	2.01	0.42
1:A:513:SER:HB3	1:A:519:ASN:ND2	2.33	0.42
1:A:521:ILE:HG22	1:A:525:LEU:HD11	2.01	0.42
1:A:90:VAL:O	1:A:92:LEU:N	2.53	0.42
1:A:227:PHE:HB2	1:A:234:LEU:HB2	2.02	0.42
1:A:411:ILE:C	1:A:412:PRO:O	2.62	0.42
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.17	0.42
2:B:158:ALA:O	2:B:161:GLN:N	2.50	0.42
1:A:194:GLU:O	1:A:197:GLN:N	2.53	0.42
1:A:395:LYS:H	1:A:395:LYS:HG2	1.65	0.42
2:B:24:TRP:CE2	2:B:399:GLU:HB3	2.54	0.42
2:B:423:VAL:O	2:B:427:TYR:HD2	2.03	0.42
1:A:239:TRP:CD1	1:A:316:GLY:C	2.98	0.42
2:B:13:LYS:CG	2:B:16:MET:HE3	2.50	0.42
2:B:305:GLU:O	2:B:309:ILE:HG13	2.19	0.42
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.02	0.42
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.85	0.42
1:A:197:GLN:HA	1:A:197:GLN:OE1	2.19	0.42
2:B:233:GLU:H	2:B:233:GLU:HG2	1.65	0.42
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.55	0.42
1:A:239:TRP:HZ2	1:A:349:LEU:O	2.03	0.42
1:A:241:VAL:O	1:A:242:GLN:C	2.63	0.42
2:B:175:ASN:HB3	2:B:178:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:TRP:O	2:B:402:TRP:C	2.62	0.42
2:B:422:LEU:HB3	2:B:426:TRP:CZ2	2.55	0.42
1:A:253:THR:HG21	1:A:290:THR:HA	2.01	0.41
1:A:417:VAL:O	1:A:417:VAL:CG1	2.68	0.41
1:A:225:PRO:HA	1:A:226:PRO:C	2.44	0.41
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.83	0.41
2:B:365:VAL:O	2:B:366:LYS:C	2.64	0.41
1:A:253:THR:O	1:A:257:ILE:HG13	2.20	0.41
1:A:399:GLU:HA	1:A:402:TRP:HB3	2.03	0.41
2:B:44:GLU:O	2:B:46:LYS:CE	2.68	0.41
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.54	0.41
1:A:120:LEU:O	1:A:125:ARG:NE	2.54	0.41
1:A:107:THR:HG22	1:A:224:GLU:OE1	2.20	0.41
1:A:342:TYR:HA	1:A:349:LEU:HD13	2.02	0.41
1:A:514:GLU:H	1:A:514:GLU:HG3	1.66	0.41
2:B:239:TRP:HB3	2:B:350:LYS:NZ	2.36	0.41
1:A:58:THR:CG2	1:A:76:ASP:O	2.69	0.41
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.55	0.41
1:A:263:LYS:HA	1:A:263:LYS:HD3	1.83	0.41
1:A:354:TYR:HD2	1:A:374:LYS:HD3	1.86	0.41
2:B:28:GLU:HB2	2:B:135:ILE:HD11	2.03	0.41
2:B:263:LYS:HE3	2:B:426:TRP:HA	2.03	0.41
2:B:336:GLN:HE21	2:B:336:GLN:HB2	1.64	0.41
1:A:521:ILE:O	1:A:524:GLN:HB2	2.20	0.40
2:B:199:ARG:CZ	2:B:233:GLU:OE1	2.69	0.40
1:A:8:VAL:O	1:A:121:ASP:HB2	2.21	0.40
1:A:60:VAL:HG12	1:A:61:PHE:N	2.36	0.40
1:A:112:GLY:O	1:A:113:ASP:C	2.65	0.40
1:A:205:LEU:HD22	1:A:209:LEU:HG	2.03	0.40
1:A:279:LEU:HA	1:A:282:LEU:HD11	2.03	0.40
2:B:78:ARG:HD3	2:B:411:ILE:O	2.21	0.40
2:B:379:SER:OG	2:B:387:PRO:HD3	2.21	0.40
1:A:54:ASN:HA	1:A:55:PRO:HD2	1.99	0.40
2:B:296:THR:O	2:B:297:GLU:C	2.64	0.40
2:B:350:LYS:CG	2:B:351:THR:N	2.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ASP:OD1	6:B:1035:HOH:O[2_555]	1.97	0.23

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	509/560 (91%)	457 (90%)	39 (8%)	13 (3%)	4	7
2	B	391/440 (89%)	342 (88%)	41 (10%)	8 (2%)	6	12
All	All	900/1000 (90%)	799 (89%)	80 (9%)	21 (2%)	5	9

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	ARG
1	A	412	PRO
2	B	250	ASP
2	B	334	GLN
1	A	91	GLN
1	A	195	ILE
2	B	277	ARG
2	B	286	THR
2	B	116	PHE
2	B	162	SER
1	A	113	ASP
1	A	177	ASP
2	B	193	LEU
1	A	90	VAL
1	A	125	ARG
1	A	170	PRO
1	A	345	PRO
1	A	402	TRP
2	B	158	ALA
1	A	119	PRO
1	A	157	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	465/499 (93%)	417 (90%)	48 (10%)	7	15
2	B	364/400 (91%)	345 (95%)	19 (5%)	21	44
All	All	829/899 (92%)	762 (92%)	67 (8%)	11	24

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	20	LYS
1	A	24	TRP
1	A	61	PHE
1	A	83	ARG
1	A	105	SER
1	A	108	VAL
1	A	116	PHE
1	A	135	ILE
1	A	138	GLU
1	A	161	GLN
1	A	168	LEU
1	A	195	ILE
1	A	205	LEU
1	A	207	GLN
1	A	216	THR
1	A	220	LYS
1	A	229	TRP
1	A	230	MET
1	A	244	ILE
1	A	249	LYS
1	A	251	SER
1	A	287	LYS
1	A	301	LEU
1	A	303	LEU

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Mol	Chain	Res	Type
1	A	312	GLU
1	A	317	VAL
1	A	323	LYS
1	A	336	GLN
1	A	340	GLN
1	A	345	PRO
1	A	347	LYS
1	A	348	ASN
1	A	394	GLN
1	A	396	GLU
1	A	400	THR
1	A	412	PRO
1	A	422	LEU
1	A	443	ASP
1	A	470	THR
1	A	476	LYS
1	A	484	LEU
1	A	487	GLN
1	A	493	VAL
1	A	512	GLN
1	A	517	LEU
2	B	16	MET
2	B	68	SER
2	B	69	THR
2	B	95	PRO
2	B	109	LEU
2	B	165	THR
2	B	200	THR
2	B	201	LYS
2	B	205	LEU
2	B	233	GLU
2	B	242	GLN
2	B	251	SER
2	B	289	LEU
2	B	295	LEU
2	B	297	GLU
2	B	298	GLU
2	B	303	LEU
2	B	323	LYS
2	B	423	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	161	GLN
1	A	182	GLN
1	A	207	GLN
1	A	208	HIS
1	A	222	GLN
1	A	242	GLN
1	A	265	ASN
1	A	278	GLN
1	A	334	GLN
1	A	336	GLN
1	A	394	GLN
1	A	407	GLN
1	A	428	GLN
1	A	480	GLN
1	A	507	GLN
1	A	509	GLN
1	A	512	GLN
1	A	519	ASN
1	A	520	GLN
2	B	57	ASN
2	B	147	ASN
2	B	175	ASN
2	B	207	GLN
2	B	269	GLN
2	B	278	GLN
2	B	334	GLN
2	B	336	GLN
2	B	348	ASN
2	B	394	GLN
2	B	407	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	2.31	1 (25%)	1,8,10	5.28	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	4.36	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	5.28	115.33	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	1300	-	4,4,4	1.72	1 (25%)	6,6,6	0.46	0
3	PO4	A	1302	-	4,4,4	1.71	1 (25%)	6,6,6	0.47	0
5	H12	A	999	-	24,24,24	1.92	5 (20%)	31,33,33	1.54	7 (22%)
3	PO4	A	1301	-	4,4,4	1.64	0	6,6,6	0.48	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
5	H12	A	999	-	-	2/7/15/15	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	H12	CF-CA	4.40	1.62	1.51
5	A	999	H12	CB-CA	3.64	1.60	1.51
5	A	999	H12	C6-N1	3.31	1.40	1.35
5	A	999	H12	C3-C4	-3.07	1.39	1.45
5	A	999	H12	C10-C9	2.87	1.43	1.38
3	A	1300	PO4	P-O2	-2.06	1.48	1.54
3	A	1302	PO4	P-O2	-2.06	1.48	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	999	H12	O4-CA-CB	3.95	117.71	108.37
5	A	999	H12	O2-C6-C5	-3.07	120.78	124.56
5	A	999	H12	C2-N1-C6	-2.87	120.81	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	999	H12	C5-C6-N1	2.63	118.28	115.92
5	A	999	H12	O4-C4-C3	2.28	121.18	114.94
5	A	999	H12	CE-CF-CA	2.22	116.24	110.76
5	A	999	H12	O4-CA-CF	2.07	113.26	108.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

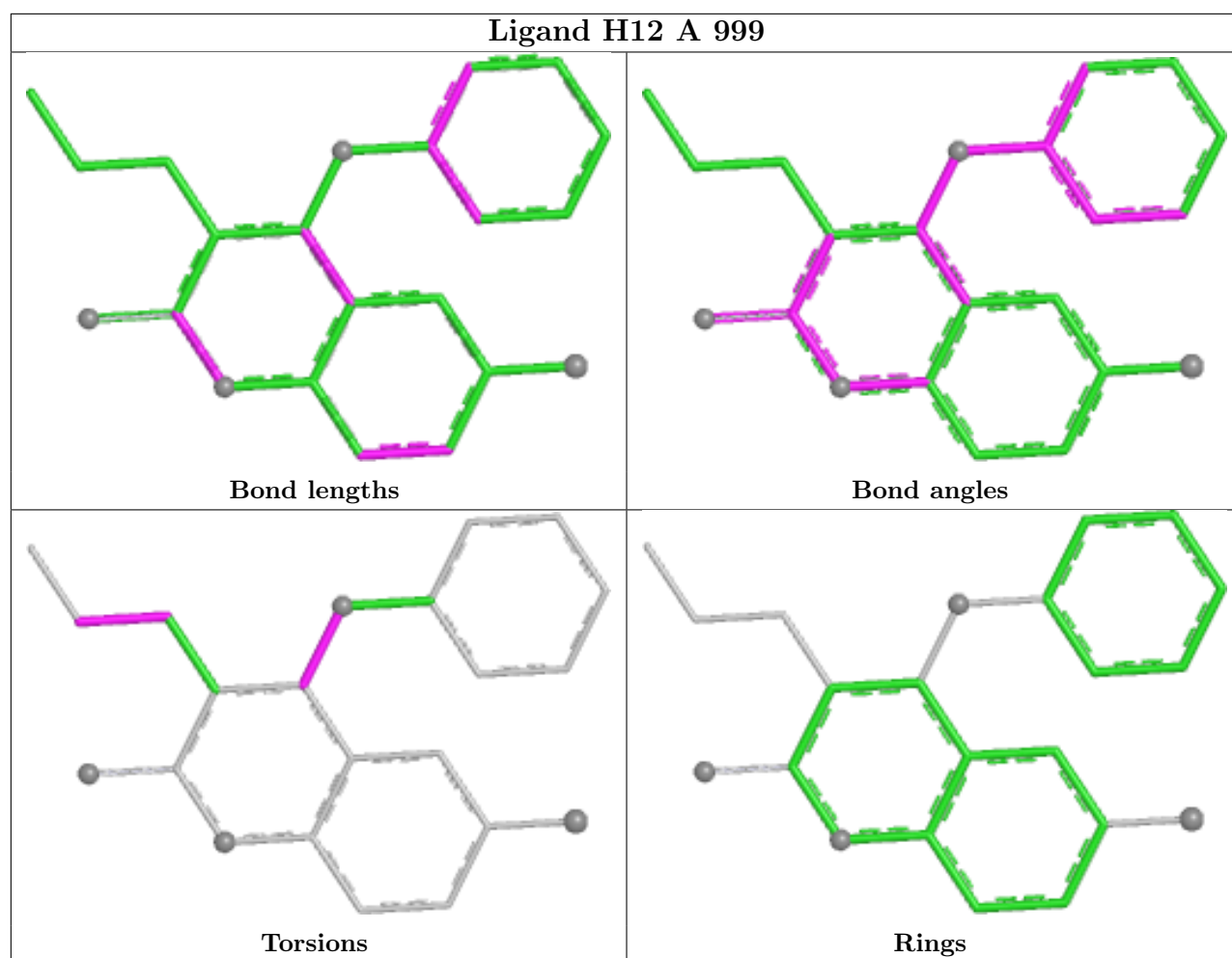
Mol	Chain	Res	Type	Atoms
5	A	999	H12	C5-C11-C12-C13
5	A	999	H12	C3-C4-O4-CA

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	999	H12	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	515/560 (91%)	-0.43	0 100 100	26, 62, 100, 143	0
2	B	399/440 (90%)	-0.41	5 (1%) 75 71	25, 60, 113, 139	0
All	All	914/1000 (91%)	-0.42	5 (0%) 87 85	25, 62, 104, 143	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	231	GLY	2.8
2	B	237	ASP	2.3
2	B	229	TRP	2.2
2	B	317	VAL	2.1
2	B	213	GLY	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	0.97	0.05	56,60,74,84	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

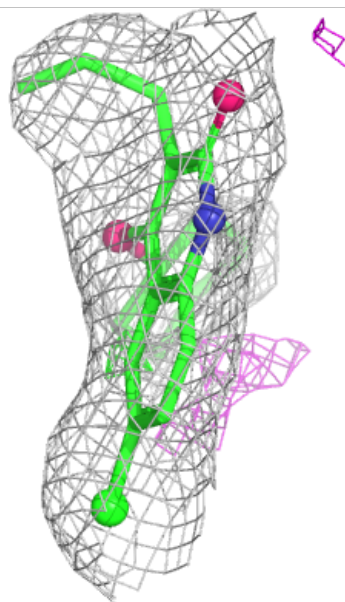
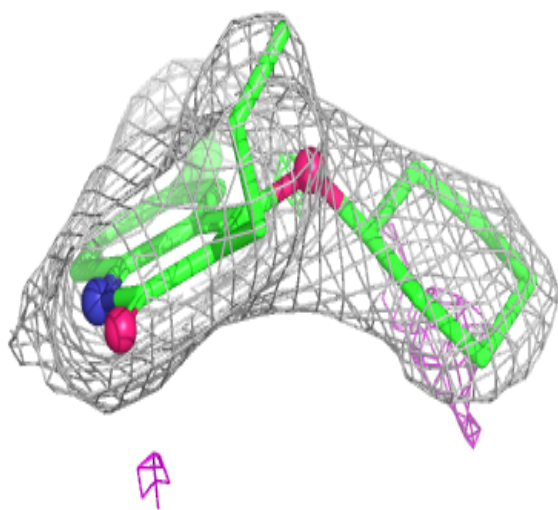
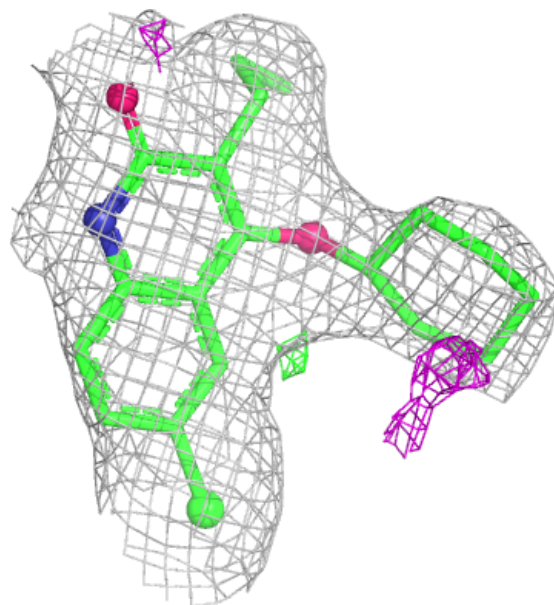
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	1300	5/5	0.75	0.08	127,128,130,131	0
3	PO4	A	1302	5/5	0.80	0.12	146,149,150,150	0
3	PO4	A	1301	5/5	0.89	0.14	120,123,129,129	0
4	MG	A	1303	1/1	0.91	0.14	62,62,62,62	0
5	H12	A	999	22/22	0.95	0.09	26,41,49,51	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.

Electron density around H12 A 999:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.