



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:38 AM UTC

PDB ID : 2OPQ / pdb_00002opq
Title : Crystal Structure of L100I Mutant HIV-1 Reverse Transcriptase in Complex with GW420867X.
Authors : Ren, J.; Nichols, C.E.; Chamberlain, P.P.; Weaver, K.L.; Short, S.A.; Chan, J.H.; Kleim, J.; Stammers, D.K.
Deposited on : 2007-01-30
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

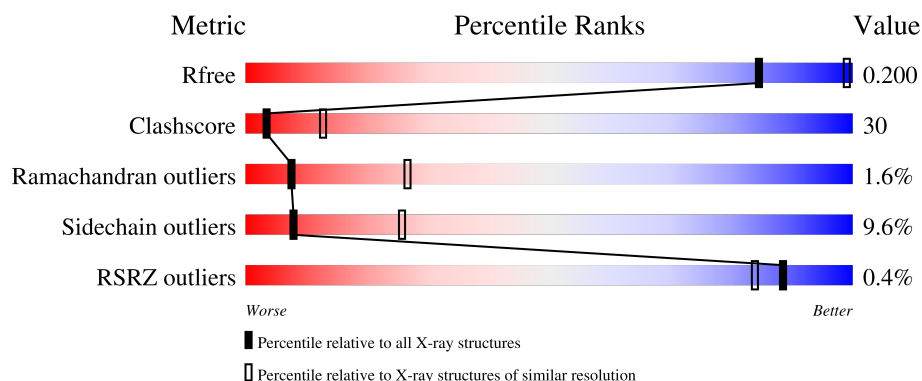
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

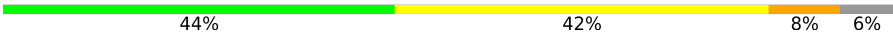
The reported resolution of this entry is 2.80 Å.

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))
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	534	
2	B	424	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7605 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/ribonuclease H.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ILE	LEU	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

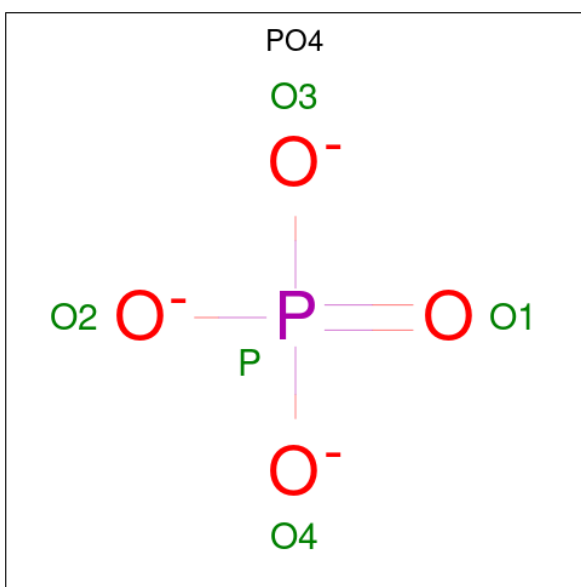
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	400	Total	C	N	O	S	0	0	0
			3317	2162	547	601	7			

There is a discrepancy between the modelled and reference sequences:

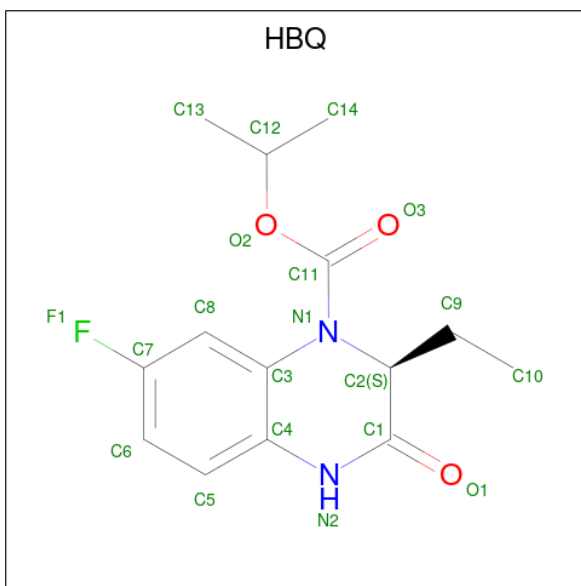
Chain	Residue	Modelled	Actual	Comment	Reference
B	100	ILE	LEU	engineered mutation	UNP P04585

- 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			

- Molecule 4 is ISOPROPYL (2S)-2-ETHYL-7-FLUORO-3-OXO-3,4-DIHYDROQUINOXALINE-1(2H)-CARBOXYLATE (CCD ID: HBQ) (formula: C₁₄H₁₇FN₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	
			20	14	1	2	3	

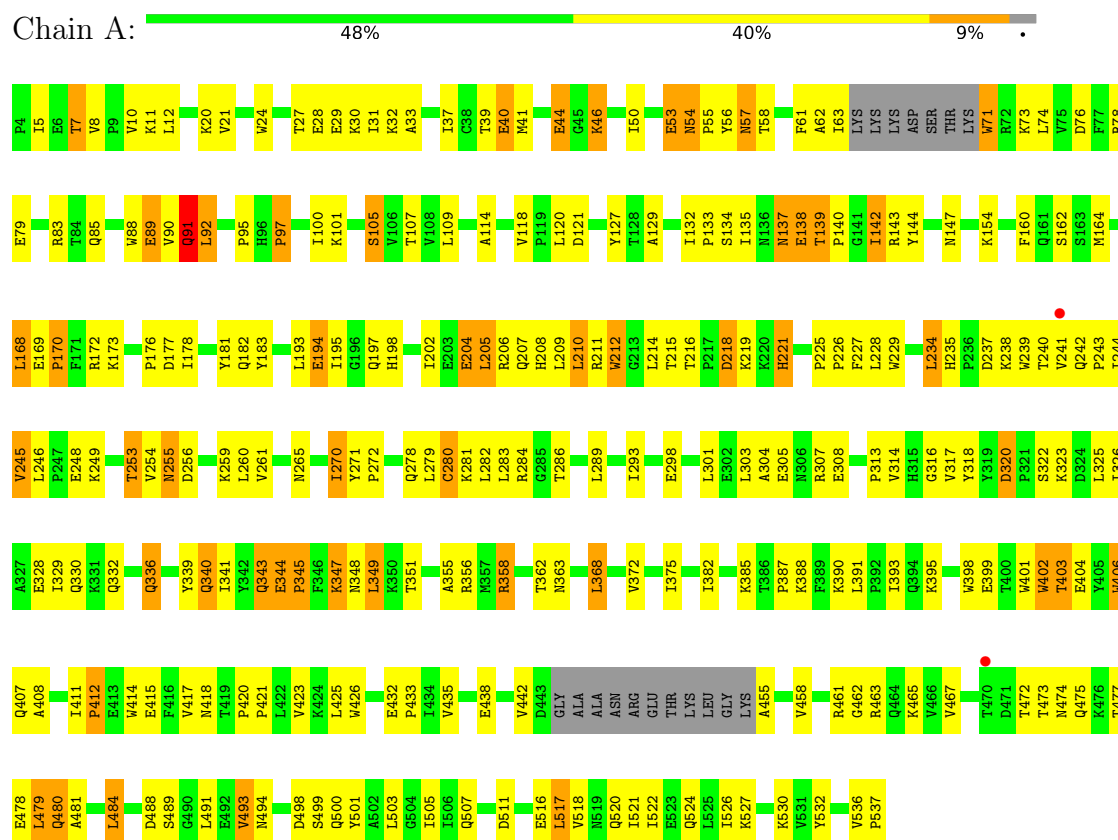
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total 12	O 12	0	0
5	B	13	Total 13	O 13	0	0

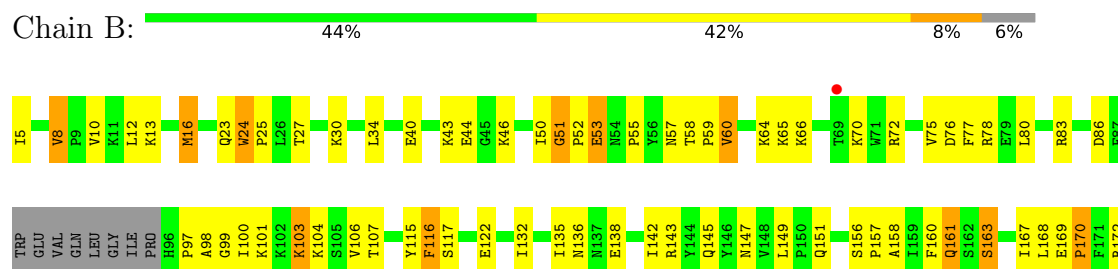
3 Residue-property plots

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: Reverse transcriptase/ribonuclease H



• Molecule 2: p51 RT



K173	D237	E308	S379
Q174	K238	I309	I380
M175	W239	P313	V381
P176	T240	V317	I382
D177	V241	Y318	V383
I178	Q242	Y319	G384
W179	P243	D320	P387
I180	I244	S321	K388
		S322	F389
Y183	K249	L325	K390
M184	D250	E328	I393
D185	S251	I329	Q394
D186	W252	Q330	K395
	T253	K331	
V189	V254	Q332	W401
G190	I257	Q336	
S191	Q258	Y339	E413
D192	K259	Q340	W414
	L260		E415
I195	V261		
G196	Q262		N418
	L264		T419
R199	W265		P420
T200	W266		P421
K201			L422
I202			V423
E203			K424
E204			L425
L205	I270		W426
R206	Y271		Y427
Q207	P272		Q428
H208	G273		
L209	I274		
R211	K275		
L210	V276		
	R277		
W212	Q278		
G213	L279		
LEU	C280	R356	
THR	K281	MEI	
THR	L282	ARG	
PRO	L283	GLY	
ASP	R284	ALA	
LYS		HIS	
LYS	K287	T362	
HIS	A288	R363	
GLN	L289	D364	
LYS	T290	V365	
GLU		K366	
P225		Q367	
P226	I293	L368	
F227		T369	
L228	E298	E370	
W229	A299	A371	
M230	E300	V372	
G231	L301	K373	
Y232	E302	K374	
E233	L303	I375	
L234	A304	T376	
H235	E305	T377	
P236	N306	E378	
	R307		

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 114.90Å 64.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 2.80 29.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.78-2.80) 98.8 (29.78-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.273 0.197 , 0.200	Depositor DCC
R_{free} test set	1250 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 78.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7605	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: PO4, HBQ, CSD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	0/4343	1.07	22/5907 (0.4%)
2	B	0.61	0/3411	1.13	27/4630 (0.6%)
All	All	0.62	0/7754	1.10	49/10537 (0.5%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	225	PRO	CA-C-N	10.86	133.42	119.84
2	B	225	PRO	C-N-CA	10.86	133.42	119.84
2	B	235	HIS	CA-C-N	9.86	130.12	119.28
2	B	235	HIS	C-N-CA	9.86	130.12	119.28
1	A	349	LEU	N-CA-C	-8.94	102.28	113.55
2	B	231	GLY	N-CA-C	-7.87	94.53	113.18
2	B	51	GLY	CA-C-N	7.57	127.20	119.56
2	B	51	GLY	C-N-CA	7.57	127.20	119.56
1	A	248	GLU	N-CA-C	-7.35	97.26	109.24
1	A	234	LEU	N-CA-C	7.09	120.80	109.24
2	B	395	LYS	N-CA-C	7.08	119.61	111.11
2	B	132	ILE	N-CA-C	-6.84	99.93	107.73
1	A	139	THR	N-CA-C	6.69	118.07	109.65
2	B	210	LEU	N-CA-C	-6.65	104.06	111.71
1	A	344	GLU	N-CA-C	-6.64	101.42	109.72
2	B	229	TRP	N-CA-C	-6.58	96.78	110.80
1	A	204	GLU	N-CA-C	-6.49	104.13	111.14
1	A	320	ASP	CA-C-N	6.32	127.74	119.84
1	A	320	ASP	C-N-CA	6.32	127.74	119.84
2	B	388	LYS	N-CA-C	-6.12	99.22	109.07
2	B	209	LEU	N-CA-C	-6.03	104.91	112.93
1	A	343	GLN	N-CA-C	-6.00	104.94	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	229	TRP	CA-CB-CG	-5.95	102.29	113.60
1	A	138	GLU	N-CA-C	-5.93	104.89	111.71
2	B	344	GLU	N-CA-C	-5.82	101.36	110.14
2	B	12	LEU	N-CA-C	-5.78	102.37	110.35
2	B	422	LEU	N-CA-C	5.77	117.57	111.28
2	B	208	HIS	N-CA-C	-5.65	106.37	113.20
2	B	98	ALA	N-CA-C	-5.62	106.50	113.19
1	A	147	ASN	N-CA-C	-5.53	106.43	114.12
1	A	221	HIS	N-CA-C	5.46	120.96	113.97
2	B	293	ILE	N-CA-C	5.46	114.49	108.05
1	A	245	VAL	N-CA-C	5.42	115.76	108.17
1	A	388	LYS	N-CA-C	-5.42	101.15	109.76
1	A	406	TRP	N-CA-C	5.41	117.93	111.71
1	A	462	GLY	N-CA-C	5.38	122.51	115.36
2	B	401	TRP	N-CA-C	5.37	120.85	113.97
1	A	382	ILE	N-CA-C	5.35	117.25	111.58
2	B	147	ASN	N-CA-C	-5.30	106.87	113.55
2	B	343	GLN	N-CA-C	-5.28	106.16	113.18
1	A	356	ARG	N-CA-C	5.27	117.34	109.59
1	A	118	VAL	CA-C-N	5.26	126.41	119.84
1	A	118	VAL	C-N-CA	5.26	126.41	119.84
1	A	212	TRP	N-CA-C	-5.22	105.63	112.41
2	B	382	ILE	N-CA-C	5.16	115.38	110.53
1	A	57	ASN	N-CA-C	5.10	116.16	108.46
2	B	8	VAL	CB-CA-C	-5.08	105.01	110.85
2	B	232	TYR	N-CA-C	5.05	118.31	110.17
2	B	24	TRP	N-CA-C	-5.05	103.23	109.64

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	4261	254	0
2	B	3317	0	3343	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
4	A	20	0	17	1	0
5	A	12	0	0	3	0
5	B	13	0	0	1	0
All	All	7605	0	7621	455	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 30.

All (455) 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:230:MET:HG3	2:B:231:GLY:H	1.12	1.10
2:B:362:THR:HG22	2:B:367:GLN:HE21	1.20	1.03
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.38	1.02
2:B:16:MET:HE3	2:B:83:ARG:HA	1.41	0.99
2:B:330:GLN:HE22	2:B:340:GLN:HE22	0.96	0.95
1:A:286:THR:HG22	1:A:293:ILE:HD11	1.48	0.95
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.35	0.91
1:A:142:ILE:HD13	1:A:142:ILE:H	1.35	0.91
1:A:33:ALA:O	1:A:37:ILE:HG12	1.71	0.90
1:A:208:HIS:O	1:A:211:ARG:HG2	1.71	0.90
2:B:195:ILE:HG12	2:B:199:ARG:HE	1.38	0.89
2:B:206:ARG:HA	2:B:209:LEU:HD12	1.55	0.88
1:A:344:GLU:HB3	1:A:347:LYS:HB2	1.56	0.86
2:B:330:GLN:NE2	2:B:340:GLN:HE22	1.76	0.83
2:B:366:LYS:O	2:B:370:GLU:HG3	1.79	0.82
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.62	0.81
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.77	0.81
1:A:54:ASN:HD22	1:A:143:ARG:NH2	1.79	0.81
2:B:330:GLN:HE22	2:B:340:GLN:NE2	1.78	0.81
1:A:332:GLN:O	1:A:332:GLN:HG2	1.79	0.80
1:A:474:ASN:O	1:A:477:THR:HG22	1.83	0.78
2:B:230:MET:HG3	2:B:231:GLY:N	1.95	0.78
1:A:253:THR:HG22	1:A:256:ASP:H	1.48	0.78
1:A:27:THR:HG22	1:A:29:GLU:H	1.49	0.77
1:A:101:LYS:HD2	1:A:101:LYS:N	1.99	0.77
1:A:210:LEU:HD22	1:A:214:LEU:O	1.84	0.77
1:A:8:VAL:HG13	2:B:53:GLU:HG3	1.68	0.76
2:B:97:PRO:HG2	2:B:100:ILE:HD11	1.67	0.76
2:B:66:LYS:HG2	2:B:230:MET:HA	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:PRO:CG	2:B:100:ILE:HD11	2.14	0.76
2:B:422:LEU:HA	2:B:425:LEU:HD13	1.67	0.75
1:A:503:LEU:O	1:A:507:GLN:HB2	1.87	0.74
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.69	0.74
2:B:362:THR:CG2	2:B:367:GLN:HG3	2.18	0.74
1:A:344:GLU:HB3	1:A:347:LYS:CB	2.18	0.73
1:A:347:LYS:HE2	1:A:347:LYS:HA	1.69	0.73
1:A:41:MET:HE2	1:A:46:LYS:HZ1	1.53	0.73
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.69	0.73
2:B:229:TRP:HA	2:B:229:TRP:CE3	2.22	0.73
2:B:151:GLN:HB3	2:B:185:ASP:OD1	1.89	0.72
2:B:362:THR:CG2	2:B:367:GLN:HE21	1.99	0.72
2:B:16:MET:CE	2:B:83:ARG:HA	2.18	0.72
1:A:71:TRP:CD1	1:A:71:TRP:N	2.58	0.71
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.05	0.71
2:B:270:ILE:O	2:B:272:PRO:HD3	1.89	0.71
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.04	0.71
2:B:174:GLN:C	2:B:176:PRO:HD3	2.16	0.70
1:A:225:PRO:HA	1:A:226:PRO:C	2.15	0.70
2:B:97:PRO:O	2:B:100:ILE:HG12	1.91	0.70
1:A:24:TRP:HZ2	1:A:61:PHE:HD2	1.36	0.70
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.27	0.70
2:B:103:LYS:NZ	2:B:191:SER:HA	2.07	0.70
1:A:142:ILE:HD13	1:A:142:ILE:N	2.06	0.69
1:A:41:MET:HE2	1:A:46:LYS:NZ	2.07	0.69
2:B:72:ARG:HH21	2:B:409:THR:HB	1.57	0.69
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.28	0.68
1:A:61:PHE:HE1	1:A:63:ILE:HD11	1.59	0.68
2:B:40:GLU:OE2	2:B:43:LYS:HD2	1.94	0.68
2:B:230:MET:C	2:B:232:TYR:H	2.01	0.68
1:A:522:ILE:O	1:A:526:ILE:HG13	1.94	0.67
2:B:353:LYS:NZ	2:B:428:GLN:HG3	2.09	0.67
2:B:374:LYS:O	2:B:377:THR:HG22	1.94	0.67
1:A:28:GLU:OE1	1:A:135:ILE:HG23	1.94	0.67
1:A:90:VAL:HG23	5:A:1001:HOH:O	1.94	0.67
2:B:208:HIS:CE1	2:B:212:TRP:HZ3	2.13	0.67
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.09	0.66
1:A:194:GLU:CD	1:A:194:GLU:H	2.03	0.66
1:A:61:PHE:CE1	1:A:74:LEU:HD23	2.30	0.66
1:A:28:GLU:O	1:A:32:LYS:HG3	1.96	0.66
1:A:347:LYS:HA	1:A:347:LYS:CE	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HD12	1:A:307:ARG:HB3	1.75	0.66
2:B:237:ASP:OD1	2:B:238:LYS:HG2	1.94	0.66
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.31	0.66
2:B:97:PRO:C	2:B:99:GLY:H	2.04	0.66
1:A:105:SER:HB2	1:A:198:HIS:CE1	2.30	0.65
1:A:301:LEU:O	1:A:305:GLU:HG3	1.95	0.65
1:A:473:THR:HG22	1:A:475:GLN:H	1.61	0.65
2:B:13:LYS:HD2	2:B:16:MET:HE2	1.76	0.65
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.77	0.65
1:A:202:ILE:O	1:A:206:ARG:HG3	1.97	0.65
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.77	0.64
2:B:254:VAL:O	2:B:258:GLN:HG3	1.98	0.64
2:B:379:SER:OG	2:B:387:PRO:HG3	1.98	0.64
1:A:28:GLU:CD	1:A:135:ILE:HG23	2.23	0.64
2:B:104:LYS:HD2	2:B:192:ASP:O	1.97	0.64
2:B:332:GLN:HA	2:B:424:LYS:HE2	1.79	0.64
2:B:344:GLU:HB2	2:B:347:LYS:HG3	1.80	0.64
2:B:13:LYS:HB2	2:B:16:MET:HE2	1.80	0.63
1:A:226:PRO:HG3	1:A:235:HIS:CE1	2.33	0.63
2:B:101:LYS:O	2:B:236:PRO:HB2	1.98	0.63
1:A:197:GLN:HA	1:A:197:GLN:NE2	2.14	0.63
1:A:344:GLU:HG2	1:A:347:LYS:HG3	1.81	0.62
2:B:234:LEU:N	2:B:234:LEU:HD12	2.14	0.62
2:B:298:GLU:CD	2:B:298:GLU:H	2.07	0.62
1:A:255:ASN:HD22	1:A:259:LYS:HE3	1.64	0.62
1:A:244:ILE:O	1:A:244:ILE:HG23	2.00	0.62
2:B:27:THR:OG1	2:B:30:LYS:HG2	1.98	0.62
2:B:106:VAL:HA	2:B:189:VAL:O	2.00	0.62
2:B:175:ASN:HD21	2:B:201:LYS:CE	2.12	0.62
2:B:353:LYS:HZ1	2:B:428:GLN:HG3	1.65	0.62
1:A:24:TRP:CZ2	1:A:61:PHE:HD2	2.17	0.62
1:A:61:PHE:CE1	1:A:63:ILE:HD11	2.35	0.62
1:A:218:ASP:HB3	1:A:221:HIS:ND1	2.15	0.62
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.35	0.61
1:A:197:GLN:HA	1:A:197:GLN:HE21	1.65	0.61
1:A:28:GLU:OE1	1:A:135:ILE:HA	2.00	0.61
2:B:30:LYS:HG3	5:B:1017:HOH:O	1.99	0.61
2:B:239:TRP:CZ3	2:B:378:GLU:HG3	2.35	0.61
1:A:455:ALA:HB3	1:A:467:VAL:O	2.00	0.61
1:A:54:ASN:HD22	1:A:143:ARG:HH21	1.49	0.61
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ALA:C	1:A:63:ILE:HD12	2.26	0.60
1:A:177:ASP:O	1:A:178:ILE:HD13	2.01	0.60
2:B:276:VAL:O	2:B:277:ARG:C	2.43	0.60
2:B:348:ASN:HD22	2:B:351:THR:HG22	1.67	0.59
2:B:46:LYS:HE2	2:B:116:PHE:HB3	1.84	0.59
2:B:362:THR:HG22	2:B:367:GLN:NE2	2.04	0.59
1:A:85:GLN:C	1:A:154:LYS:HZ3	2.10	0.59
1:A:253:THR:HG23	1:A:289:LEU:O	2.03	0.59
2:B:178:ILE:HG22	2:B:179:VAL:N	2.16	0.59
2:B:253:THR:O	2:B:257:ILE:HG12	2.03	0.59
2:B:277:ARG:O	2:B:281:LYS:HG3	2.01	0.59
2:B:362:THR:HG21	2:B:367:GLN:HG3	1.84	0.59
1:A:208:HIS:O	1:A:212:TRP:HD1	1.85	0.59
1:A:278:GLN:NE2	1:A:278:GLN:HA	2.17	0.59
1:A:498:ASP:HA	1:A:536:VAL:O	2.03	0.59
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.38	0.58
1:A:308:GLU:HA	1:A:308:GLU:OE1	2.03	0.58
1:A:368:LEU:O	1:A:372:VAL:HG23	2.03	0.58
1:A:465:LYS:HG2	1:A:484:LEU:HD11	1.86	0.58
1:A:418:ASN:C	1:A:418:ASN:HD22	2.09	0.58
1:A:54:ASN:ND2	1:A:143:ARG:NH2	2.49	0.58
1:A:261:VAL:O	1:A:265:ASN:OD1	2.22	0.58
1:A:54:ASN:ND2	1:A:56:TYR:H	2.02	0.58
2:B:195:ILE:HG12	2:B:199:ARG:NE	2.15	0.58
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.39	0.57
2:B:97:PRO:HG2	2:B:100:ILE:CD1	2.34	0.57
2:B:298:GLU:OE1	2:B:298:GLU:N	2.37	0.57
1:A:137:ASN:N	1:A:137:ASN:ND2	2.51	0.56
1:A:50:ILE:HD12	1:A:54:ASN:CB	2.35	0.56
1:A:137:ASN:N	1:A:137:ASN:HD22	2.03	0.56
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.39	0.56
1:A:474:ASN:O	1:A:478:GLU:HG3	2.04	0.56
1:A:516:GLU:O	1:A:520:GLN:HG3	2.05	0.56
2:B:158:ALA:O	2:B:161:GLN:HB2	2.05	0.56
2:B:202:ILE:O	2:B:205:LEU:HB3	2.05	0.56
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.87	0.56
2:B:135:ILE:N	2:B:135:ILE:HD12	2.20	0.56
1:A:8:VAL:CG1	2:B:53:GLU:HG3	2.33	0.56
2:B:142:ILE:H	2:B:142:ILE:HD12	1.71	0.56
1:A:53:GLU:O	1:A:55:PRO:HD3	2.06	0.56
1:A:219:LYS:HD3	1:A:219:LYS:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.88	0.56
1:A:255:ASN:ND2	1:A:259:LYS:HE3	2.21	0.55
1:A:339:TYR:CD1	1:A:339:TYR:C	2.84	0.55
2:B:332:GLN:HB3	2:B:428:GLN:NE2	2.21	0.55
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.86	0.55
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.89	0.55
1:A:363:ASN:HA	1:A:511:ASP:CG	2.31	0.55
1:A:401:TRP:HB2	1:A:425:LEU:HD11	1.88	0.55
2:B:195:ILE:O	2:B:199:ARG:HD2	2.06	0.55
2:B:103:LYS:HZ3	2:B:191:SER:HA	1.71	0.55
1:A:7:THR:CG2	1:A:121:ASP:HA	2.36	0.55
2:B:97:PRO:C	2:B:99:GLY:N	2.63	0.55
2:B:100:ILE:HD13	2:B:179:VAL:HG11	1.87	0.55
2:B:282:LEU:HB3	2:B:293:ILE:HG21	1.89	0.55
1:A:142:ILE:H	1:A:142:ILE:CD1	2.08	0.55
1:A:225:PRO:HD3	1:A:227:PHE:CZ	2.42	0.55
2:B:175:ASN:HD21	2:B:201:LYS:HZ2	1.54	0.55
1:A:132:ILE:HB	1:A:142:ILE:HG12	1.90	0.54
1:A:253:THR:HB	1:A:256:ASP:OD2	2.07	0.54
2:B:103:LYS:HE3	2:B:179:VAL:CG2	2.37	0.54
2:B:422:LEU:HD23	2:B:425:LEU:HD22	1.88	0.54
1:A:40:GLU:OE2	1:A:44:GLU:OE1	2.23	0.54
1:A:279:LEU:HD23	1:A:282:LEU:HD11	1.88	0.54
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.90	0.54
2:B:228:LEU:O	2:B:229:TRP:HB2	2.07	0.54
1:A:76:ASP:OD2	1:A:78:ARG:HG2	2.07	0.54
2:B:97:PRO:HG2	2:B:100:ILE:CG1	2.36	0.54
2:B:230:MET:C	2:B:232:TYR:N	2.65	0.54
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.41	0.54
1:A:28:GLU:OE1	1:A:135:ILE:HG12	2.07	0.54
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.43	0.54
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.43	0.54
2:B:175:ASN:N	2:B:176:PRO:HD3	2.23	0.53
2:B:390:LYS:HE2	2:B:415:GLU:OE1	2.08	0.53
1:A:8:VAL:HG13	2:B:53:GLU:CG	2.38	0.53
1:A:358:ARG:NH2	2:B:394:GLN:HG3	2.24	0.53
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.90	0.53
2:B:420:PRO:O	2:B:423:VAL:HG12	2.09	0.53
2:B:167:ILE:HG23	2:B:212:TRP:CE3	2.44	0.53
1:A:28:GLU:OE1	1:A:28:GLU:HA	2.09	0.53
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASN:HA	1:A:129:ALA:O	2.08	0.53
1:A:20:LYS:HG2	1:A:55:PRO:O	2.10	0.52
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.90	0.52
2:B:345:PRO:C	2:B:347:LYS:H	2.17	0.52
1:A:336:GLN:OE1	1:A:355:ALA:HB2	2.09	0.52
2:B:257:ILE:HB	2:B:283:LEU:HD11	1.92	0.52
1:A:532:TYR:OH	2:B:259:LYS:HE2	2.10	0.52
2:B:60:VAL:CG1	2:B:75:VAL:HG22	2.36	0.52
2:B:5:ILE:HG23	2:B:5:ILE:O	2.09	0.52
2:B:234:LEU:HD12	2:B:234:LEU:H	1.74	0.52
2:B:230:MET:HB3	2:B:232:TYR:HB2	1.91	0.52
2:B:64:LYS:HG2	2:B:65:LYS:N	2.25	0.52
2:B:332:GLN:HB3	2:B:428:GLN:HE22	1.75	0.52
2:B:8:VAL:O	2:B:10:VAL:HG23	2.10	0.52
2:B:163:SER:O	2:B:167:ILE:HG13	2.10	0.52
2:B:228:LEU:HD11	2:B:409:THR:HG23	1.92	0.51
1:A:253:THR:HG23	1:A:255:ASN:H	1.76	0.51
1:A:458:VAL:HG23	1:A:458:VAL:O	2.11	0.51
2:B:160:PHE:O	2:B:160:PHE:CD1	2.64	0.51
1:A:7:THR:HG21	1:A:121:ASP:HA	1.92	0.51
1:A:417:VAL:O	1:A:417:VAL:HG13	2.09	0.51
2:B:64:LYS:HG2	2:B:65:LYS:H	1.76	0.51
1:A:328:GLU:O	1:A:339:TYR:HA	2.09	0.51
1:A:517:LEU:CA	1:A:520:GLN:HE21	2.17	0.51
2:B:186:ASP:OD1	2:B:228:LEU:HD12	2.11	0.51
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.45	0.50
1:A:420:PRO:HA	1:A:421:PRO:C	2.35	0.50
1:A:61:PHE:CZ	1:A:74:LEU:HD23	2.46	0.50
1:A:239:TRP:CD1	1:A:316:GLY:C	2.90	0.50
1:A:289:LEU:HD12	1:A:289:LEU:N	2.27	0.50
2:B:276:VAL:O	2:B:279:LEU:N	2.45	0.50
2:B:365:VAL:O	2:B:369:THR:HG23	2.12	0.50
1:A:120:LEU:O	1:A:121:ASP:C	2.54	0.49
1:A:240:THR:OG1	1:A:241:VAL:N	2.40	0.49
2:B:16:MET:HE3	2:B:83:ARG:CA	2.29	0.49
1:A:56:TYR:O	1:A:143:ARG:NH2	2.37	0.49
1:A:205:LEU:HD22	1:A:209:LEU:HG	1.94	0.49
1:A:282:LEU:O	1:A:293:ILE:HD13	2.12	0.49
1:A:347:LYS:HE2	1:A:347:LYS:CA	2.41	0.49
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.47	0.49
1:A:320:ASP:OD1	1:A:322:SER:OG	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:THR:HG22	1:A:293:ILE:CD1	2.33	0.49
1:A:391:LEU:C	1:A:417:VAL:HG12	2.38	0.49
2:B:13:LYS:HB2	2:B:16:MET:CE	2.41	0.49
2:B:263:LYS:HE3	2:B:426:TRP:O	2.13	0.49
1:A:31:ILE:HD11	1:A:133:PRO:HB2	1.95	0.49
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.43	0.49
2:B:328:GLU:O	2:B:339:TYR:HA	2.12	0.49
1:A:317:VAL:HG12	1:A:318:TYR:N	2.27	0.49
2:B:303:LEU:HD21	2:B:307:ARG:HH21	1.78	0.48
2:B:252:TRP:HB3	2:B:257:ILE:HD11	1.95	0.48
1:A:134:SER:HB2	1:A:139:THR:O	2.14	0.48
1:A:91:GLN:O	1:A:91:GLN:HG2	2.08	0.48
2:B:241:VAL:HG11	2:B:313:PRO:HG3	1.96	0.48
2:B:271:TYR:O	2:B:274:ILE:HG12	2.14	0.48
1:A:193:LEU:HD13	1:A:197:GLN:HG3	1.95	0.48
2:B:100:ILE:CD1	2:B:179:VAL:CG1	2.92	0.48
2:B:227:PHE:HB3	2:B:230:MET:O	2.13	0.48
1:A:79:GLU:HG3	1:A:83:ARG:HD2	1.95	0.48
1:A:169:GLU:O	1:A:172:ARG:HB2	2.14	0.48
2:B:24:TRP:CG	2:B:25:PRO:HD2	2.48	0.48
1:A:226:PRO:HA	1:A:234:LEU:O	2.14	0.48
1:A:282:LEU:HB3	1:A:293:ILE:HG21	1.95	0.47
2:B:260:LEU:O	2:B:264:LEU:HG	2.14	0.47
1:A:97:PRO:O	1:A:100:ILE:HG12	2.14	0.47
1:A:169:GLU:N	1:A:170:PRO:HD2	2.29	0.47
1:A:283:LEU:O	1:A:286:THR:HG23	2.13	0.47
1:A:340:GLN:HA	1:A:351:THR:HA	1.96	0.47
1:A:24:TRP:HE1	1:A:61:PHE:HB3	1.80	0.47
1:A:10:VAL:HG12	1:A:11:LYS:N	2.30	0.47
1:A:41:MET:SD	1:A:73:LYS:HE2	2.55	0.47
1:A:79:GLU:O	1:A:83:ARG:HG3	2.15	0.47
1:A:516:GLU:O	1:A:517:LEU:C	2.57	0.47
2:B:100:ILE:CD1	2:B:179:VAL:HG11	2.43	0.47
1:A:208:HIS:O	1:A:212:TRP:CD1	2.67	0.47
1:A:489:SER:OG	1:A:493:VAL:HG21	2.15	0.47
2:B:266:TRP:CE3	2:B:426:TRP:HB3	2.49	0.47
2:B:299:ALA:O	2:B:302:GLU:HB3	2.14	0.47
2:B:305:GLU:O	2:B:309:ILE:HG13	2.15	0.47
1:A:253:THR:O	1:A:254:VAL:C	2.58	0.47
1:A:402:TRP:HE1	2:B:364:ASP:CG	2.23	0.47
1:A:28:GLU:CG	1:A:135:ILE:HG23	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.14	0.47
1:A:168:LEU:O	1:A:169:GLU:C	2.58	0.46
1:A:206:ARG:HH12	1:A:218:ASP:HA	1.81	0.46
1:A:289:LEU:N	1:A:289:LEU:CD1	2.77	0.46
1:A:344:GLU:CB	1:A:347:LYS:HB2	2.38	0.46
2:B:228:LEU:HD23	2:B:228:LEU:HA	1.57	0.46
2:B:24:TRP:CD1	2:B:25:PRO:HD2	2.51	0.46
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.98	0.46
1:A:58:THR:CG2	1:A:76:ASP:O	2.64	0.46
2:B:180:ILE:HD12	2:B:189:VAL:HG22	1.98	0.46
2:B:421:PRO:O	2:B:425:LEU:HD13	2.16	0.46
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.15	0.46
2:B:362:THR:HG21	2:B:367:GLN:CG	2.46	0.46
1:A:320:ASP:CG	1:A:322:SER:HG	2.22	0.46
2:B:284:ARG:O	2:B:287:LYS:HE2	2.15	0.46
1:A:91:GLN:HE22	1:A:183:TYR:HE2	1.64	0.46
1:A:281:LYS:HE3	1:A:284:ARG:CZ	2.46	0.46
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.50	0.46
2:B:242:GLN:NE2	2:B:243:PRO:O	2.45	0.46
1:A:226:PRO:HG3	1:A:235:HIS:HE1	1.79	0.46
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.16	0.46
1:A:101:LYS:N	1:A:101:LYS:CD	2.74	0.46
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.44	0.46
2:B:103:LYS:HA	2:B:103:LYS:HD2	1.70	0.46
2:B:115:TYR:C	2:B:117:SER:H	2.24	0.46
2:B:340:GLN:HB3	2:B:348:ASN:ND2	2.31	0.46
1:A:27:THR:HG22	1:A:29:GLU:N	2.26	0.46
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.51	0.46
1:A:134:SER:OG	1:A:140:PRO:C	2.59	0.45
1:A:472:THR:OG1	1:A:473:THR:N	2.49	0.45
2:B:65:LYS:HG3	2:B:70:LYS:O	2.15	0.45
1:A:129:ALA:HA	1:A:144:TYR:O	2.17	0.45
1:A:279:LEU:HA	1:A:282:LEU:CD1	2.47	0.45
1:A:399:GLU:O	1:A:402:TRP:HB3	2.15	0.45
2:B:353:LYS:NZ	2:B:428:GLN:CG	2.79	0.45
1:A:27:THR:CG2	1:A:29:GLU:HB3	2.47	0.45
1:A:63:ILE:HD12	1:A:63:ILE:N	2.31	0.45
1:A:95:PRO:O	1:A:229:TRP:HH2	1.98	0.45
1:A:107:THR:HG21	1:A:202:ILE:HD12	1.97	0.45
2:B:175:ASN:ND2	2:B:201:LYS:HD2	2.32	0.45
1:A:255:ASN:O	1:A:259:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:TYR:CE1	2:B:184:MET:CG	2.99	0.45
2:B:278:GLN:CD	2:B:298:GLU:HB3	2.42	0.45
1:A:95:PRO:HB3	2:B:136:ASN:O	2.16	0.45
1:A:100:ILE:HD11	1:A:318:TYR:CE1	2.51	0.45
1:A:204:GLU:O	1:A:207:GLN:HB2	2.16	0.45
1:A:438:GLU:HB2	1:A:461:ARG:NH1	2.31	0.45
2:B:51:GLY:HA3	2:B:53:GLU:OE2	2.17	0.45
2:B:161:GLN:HE21	2:B:161:GLN:HB3	1.46	0.45
1:A:463:ARG:NH2	1:A:488:ASP:O	2.50	0.45
2:B:371:ALA:O	2:B:372:VAL:C	2.57	0.45
1:A:40:GLU:OE2	1:A:40:GLU:CA	2.64	0.44
1:A:433:PRO:HA	1:A:532:TYR:CG	2.53	0.44
2:B:350:LYS:HG2	2:B:351:THR:N	2.32	0.44
1:A:500:GLN:O	1:A:503:LEU:HB3	2.16	0.44
1:A:74:LEU:HD12	1:A:74:LEU:HA	1.74	0.44
1:A:465:LYS:NZ	1:A:484:LEU:HD21	2.33	0.44
1:A:518:VAL:O	1:A:522:ILE:HG13	2.16	0.44
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.14	0.44
2:B:78:ARG:HD2	2:B:413:GLU:OE1	2.17	0.44
2:B:319:TYR:CD1	2:B:319:TYR:C	2.94	0.44
1:A:173:LYS:O	1:A:176:PRO:HD3	2.17	0.44
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.33	0.44
1:A:344:GLU:O	1:A:347:LYS:HB2	2.16	0.44
2:B:50:ILE:CG2	2:B:145:GLN:HB3	2.48	0.44
2:B:203:GLU:OE1	2:B:206:ARG:HD3	2.18	0.44
1:A:100:ILE:C	1:A:101:LYS:HD2	2.43	0.44
2:B:103:LYS:HE3	2:B:179:VAL:HG21	2.00	0.44
1:A:178:ILE:HD11	1:A:193:LEU:HD11	1.99	0.44
1:A:210:LEU:CD2	1:A:215:THR:HA	2.47	0.44
1:A:477:THR:CG2	1:A:478:GLU:N	2.80	0.44
1:A:517:LEU:HD22	1:A:521:ILE:HD11	2.00	0.44
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.53	0.44
2:B:135:ILE:N	2:B:135:ILE:CD1	2.81	0.44
2:B:207:GLN:C	2:B:209:LEU:H	2.26	0.44
1:A:255:ASN:OD1	1:A:289:LEU:HB3	2.18	0.44
2:B:206:ARG:O	2:B:209:LEU:HB2	2.17	0.44
1:A:139:THR:HA	1:A:140:PRO:HD3	1.83	0.43
1:A:218:ASP:CB	1:A:221:HIS:ND1	2.79	0.43
2:B:169:GLU:O	2:B:172:ARG:HB3	2.18	0.43
1:A:325:LEU:HB3	1:A:387:PRO:HB3	2.00	0.43
1:A:407:GLN:HG2	2:B:393:ILE:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:ILE:HG23	2:B:145:GLN:HB3	2.00	0.43
2:B:203:GLU:OE1	2:B:203:GLU:HA	2.18	0.43
1:A:89:GLU:OE1	1:A:92:LEU:N	2.52	0.43
1:A:40:GLU:OE2	1:A:40:GLU:HA	2.19	0.43
1:A:271:TYR:CE1	1:A:314:VAL:HG22	2.52	0.43
1:A:348:ASN:ND2	1:A:351:THR:CG2	2.82	0.43
1:A:478:GLU:HB3	1:A:499:SER:HB2	2.00	0.43
1:A:8:VAL:O	1:A:121:ASP:HB2	2.18	0.43
1:A:270:ILE:O	1:A:272:PRO:HD3	2.18	0.43
1:A:426:TRP:CD1	1:A:426:TRP:N	2.86	0.43
1:A:503:LEU:HD11	1:A:507:GLN:NE2	2.34	0.43
2:B:336:GLN:HE21	2:B:336:GLN:HB2	1.59	0.43
1:A:134:SER:HB3	1:A:139:THR:HB	2.00	0.43
1:A:242:GLN:HB2	1:A:243:PRO:HD2	2.00	0.43
1:A:271:TYR:OH	1:A:313:PRO:HA	2.19	0.43
2:B:234:LEU:HB3	2:B:239:TRP:HZ2	1.83	0.43
2:B:377:THR:HG23	2:B:378:GLU:N	2.33	0.43
2:B:418:ASN:O	2:B:420:PRO:HD3	2.19	0.43
1:A:20:LYS:HE2	1:A:55:PRO:HB2	2.01	0.43
1:A:164:MET:HG3	1:A:168:LEU:HD22	2.01	0.43
2:B:178:ILE:CG2	2:B:179:VAL:N	2.80	0.43
1:A:170:PRO:O	1:A:173:LYS:N	2.52	0.43
1:A:27:THR:O	1:A:30:LYS:N	2.52	0.43
2:B:72:ARG:HG3	2:B:72:ARG:HH11	1.82	0.43
1:A:31:ILE:HD13	1:A:133:PRO:O	2.19	0.43
1:A:235:HIS:O	4:A:999:HBQ:H6	2.18	0.42
1:A:465:LYS:HZ3	1:A:484:LEU:HD21	1.83	0.42
2:B:156:SER:O	2:B:157:PRO:C	2.61	0.42
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.99	0.42
1:A:105:SER:HB2	1:A:198:HIS:ND1	2.34	0.42
1:A:398:TRP:O	1:A:399:GLU:C	2.62	0.42
2:B:100:ILE:HD13	2:B:100:ILE:N	2.35	0.42
2:B:169:GLU:CB	2:B:170:PRO:HD3	2.49	0.42
2:B:169:GLU:CG	2:B:173:LYS:NZ	2.81	0.42
1:A:50:ILE:HD12	1:A:54:ASN:HB3	2.01	0.42
2:B:209:LEU:C	2:B:211:ARG:N	2.77	0.42
2:B:234:LEU:N	2:B:234:LEU:CD1	2.81	0.42
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.55	0.42
1:A:237:ASP:OD1	1:A:238:LYS:HG2	2.19	0.42
2:B:377:THR:CG2	2:B:378:GLU:N	2.82	0.42
1:A:411:ILE:O	1:A:412:PRO:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:THR:O	2:B:377:THR:C	2.62	0.42
1:A:253:THR:O	1:A:256:ASP:N	2.53	0.42
1:A:536:VAL:HA	1:A:537:PRO:HD3	1.85	0.42
2:B:58:THR:HG23	2:B:76:ASP:O	2.19	0.42
1:A:279:LEU:O	1:A:280:CSD:C	2.67	0.42
2:B:348:ASN:ND2	2:B:351:THR:HG22	2.33	0.42
1:A:432:GLU:OE2	1:A:433:PRO:HD2	2.20	0.42
2:B:423:VAL:HG13	2:B:424:LYS:N	2.35	0.42
1:A:246:LEU:HD13	1:A:303:LEU:CD1	2.50	0.41
1:A:325:LEU:O	1:A:326:ILE:HD13	2.20	0.41
2:B:261:VAL:HG22	2:B:276:VAL:HG13	2.02	0.41
1:A:142:ILE:N	1:A:142:ILE:CD1	2.76	0.41
1:A:326:ILE:O	1:A:341:ILE:HA	2.20	0.41
1:A:398:TRP:CZ2	1:A:411:ILE:HD12	2.56	0.41
2:B:173:LYS:O	2:B:176:PRO:HD3	2.21	0.41
2:B:195:ILE:CG2	2:B:196:GLY:N	2.84	0.41
2:B:234:LEU:H	2:B:234:LEU:CD1	2.32	0.41
1:A:298:GLU:H	1:A:298:GLU:CD	2.28	0.41
2:B:183:TYR:O	2:B:184:MET:C	2.62	0.41
2:B:270:ILE:O	2:B:272:PRO:CD	2.63	0.41
2:B:320:ASP:OD1	2:B:322:SER:OG	2.36	0.41
1:A:281:LYS:O	1:A:284:ARG:HG3	2.21	0.41
1:A:402:TRP:C	1:A:404:GLU:H	2.29	0.41
2:B:239:TRP:CE3	2:B:378:GLU:HG3	2.55	0.41
1:A:304:ALA:HA	1:A:307:ARG:HG2	2.01	0.41
2:B:169:GLU:CG	2:B:173:LYS:HZ1	2.33	0.41
2:B:249:LYS:HB3	2:B:249:LYS:HE2	1.74	0.41
2:B:300:GLU:OE1	2:B:300:GLU:HA	2.21	0.41
1:A:162:SER:HB2	2:B:52:PRO:HG3	2.02	0.41
1:A:210:LEU:HD21	1:A:215:THR:HA	2.02	0.41
2:B:136:ASN:HB3	2:B:138:GLU:OE2	2.21	0.41
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.55	0.41
1:A:239:TRP:O	1:A:316:GLY:N	2.41	0.41
1:A:246:LEU:HD22	1:A:260:LEU:HD11	2.03	0.41
1:A:278:GLN:NE2	1:A:278:GLN:CA	2.80	0.41
1:A:521:ILE:O	1:A:524:GLN:HB2	2.20	0.41
2:B:168:LEU:O	2:B:169:GLU:C	2.64	0.41
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.56	0.41
2:B:241:VAL:O	2:B:241:VAL:HG13	2.21	0.41
1:A:54:ASN:ND2	1:A:54:ASN:C	2.79	0.41
1:A:249:LYS:NZ	1:A:256:ASP:CG	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ARG:NH1	5:A:1013:HOH:O	2.54	0.41
2:B:421:PRO:O	2:B:425:LEU:CD1	2.69	0.41
1:A:320:ASP:C	1:A:322:SER:H	2.29	0.40
1:A:480:GLN:O	1:A:481:ALA:C	2.64	0.40
2:B:252:TRP:CH2	2:B:260:LEU:HD22	2.56	0.40
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.93	0.40
1:A:494:ASN:HB3	2:B:289:LEU:HD22	2.03	0.40
2:B:40:GLU:OE1	2:B:44:GLU:OE2	2.40	0.40
1:A:530:LYS:HA	5:A:1010:HOH:O	2.21	0.40
2:B:99:GLY:O	2:B:103:LYS:HG2	2.22	0.40
2:B:274:ILE:HG23	2:B:306:ASN:OD1	2.22	0.40
1:A:88:TRP:O	1:A:89:GLU:C	2.64	0.40
2:B:241:VAL:O	2:B:243:PRO:HD3	2.22	0.40
2:B:380:ILE:O	2:B:384:GLY:N	2.52	0.40
2:B:13:LYS:CD	2:B:16:MET:HE2	2.49	0.40
2:B:261:VAL:HG22	2:B:276:VAL:CG1	2.51	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	509/534 (95%)	462 (91%)	38 (8%)	9 (2%)	6	23
2	B	392/424 (92%)	347 (88%)	40 (10%)	5 (1%)	9	31
All	All	901/958 (94%)	809 (90%)	78 (9%)	14 (2%)	7	27

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	403	THR
1	A	412	PRO

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Mol	Chain	Res	Type
2	B	250	ASP
2	B	277	ARG
1	A	402	TRP
2	B	116	PHE
1	A	91	GLN
1	A	170	PRO
1	A	270	ILE
2	B	170	PRO
1	A	92	LEU
1	A	345	PRO
2	B	229	TRP
1	A	195	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	465/479 (97%)	418 (90%)	47 (10%)	7	23
2	B	365/386 (95%)	332 (91%)	33 (9%)	9	28
All	All	830/865 (96%)	750 (90%)	80 (10%)	8	26

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	7	THR
1	A	21	VAL
1	A	39	THR
1	A	40	GLU
1	A	44	GLU
1	A	46	LYS
1	A	53	GLU
1	A	54	ASN
1	A	71	TRP
1	A	89	GLU

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Mol	Chain	Res	Type
1	A	91	GLN
1	A	97	PRO
1	A	105	SER
1	A	109	LEU
1	A	137	ASN
1	A	138	GLU
1	A	142	ILE
1	A	168	LEU
1	A	182	GLN
1	A	194	GLU
1	A	205	LEU
1	A	210	LEU
1	A	216	THR
1	A	218	ASP
1	A	245	VAL
1	A	253	THR
1	A	255	ASN
1	A	323	LYS
1	A	336	GLN
1	A	340	GLN
1	A	345	PRO
1	A	347	LYS
1	A	358	ARG
1	A	362	THR
1	A	368	LEU
1	A	385	LYS
1	A	390	LYS
1	A	403	THR
1	A	415	GLU
1	A	479	LEU
1	A	480	GLN
1	A	484	LEU
1	A	491	LEU
1	A	493	VAL
1	A	517	LEU
1	A	527	LYS
2	B	16	MET
2	B	34	LEU
2	B	53	GLU
2	B	55	PRO
2	B	60	VAL
2	B	86	ASP

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Mol	Chain	Res	Type
2	B	103	LYS
2	B	107	THR
2	B	122	GLU
2	B	161	GLN
2	B	163	SER
2	B	179	VAL
2	B	207	GLN
2	B	225	PRO
2	B	226	PRO
2	B	228	LEU
2	B	234	LEU
2	B	259	LYS
2	B	277	ARG
2	B	280	CYS
2	B	283	LEU
2	B	284	ARG
2	B	289	LEU
2	B	290	THR
2	B	298	GLU
2	B	317	VAL
2	B	319	TYR
2	B	322	SER
2	B	325	LEU
2	B	330	GLN
2	B	336	GLN
2	B	368	LEU
2	B	413	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	91	GLN
1	A	136	ASN
1	A	137	ASN
1	A	174	GLN
1	A	197	GLN
1	A	222	GLN
1	A	235	HIS
1	A	278	GLN
1	A	332	GLN
1	A	348	ASN

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Mol	Chain	Res	Type
1	A	418	ASN
1	A	475	GLN
1	A	480	GLN
1	A	500	GLN
1	A	509	GLN
1	A	520	GLN
2	B	57	ASN
2	B	137	ASN
2	B	161	GLN
2	B	175	ASN
2	B	258	GLN
2	B	278	GLN
2	B	330	GLN
2	B	332	GLN
2	B	336	GLN
2	B	348	ASN
2	B	367	GLN
2	B	394	GLN
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	2.34	1 (25%)	1,8,10	11.82	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	4.30	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	11.82	127.36	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](#)

2 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	1301	-	4,4,4	1.78	1 (25%)	6,6,6	0.49	0
4	HBQ	A	999	-	21,21,21	2.09	7 (33%)	28,30,30	1.07	1 (3%)

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	HBQ	A	999	-	-	0/10/26/26	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	HBQ	C11-N1	4.93	1.44	1.37
4	A	999	HBQ	O3-C11	4.06	1.27	1.21
4	A	999	HBQ	C3-N1	3.08	1.47	1.42
4	A	999	HBQ	C1-N2	3.04	1.38	1.34
4	A	999	HBQ	C6-C5	2.83	1.43	1.38
4	A	999	HBQ	C4-C3	2.24	1.43	1.40
4	A	999	HBQ	C2-N1	2.17	1.50	1.47
3	A	1301	PO4	P-O2	-2.02	1.48	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	HBQ	O2-C12-C13	-2.28	101.07	107.13

There are no chirality outliers.

There are no torsion outliers.

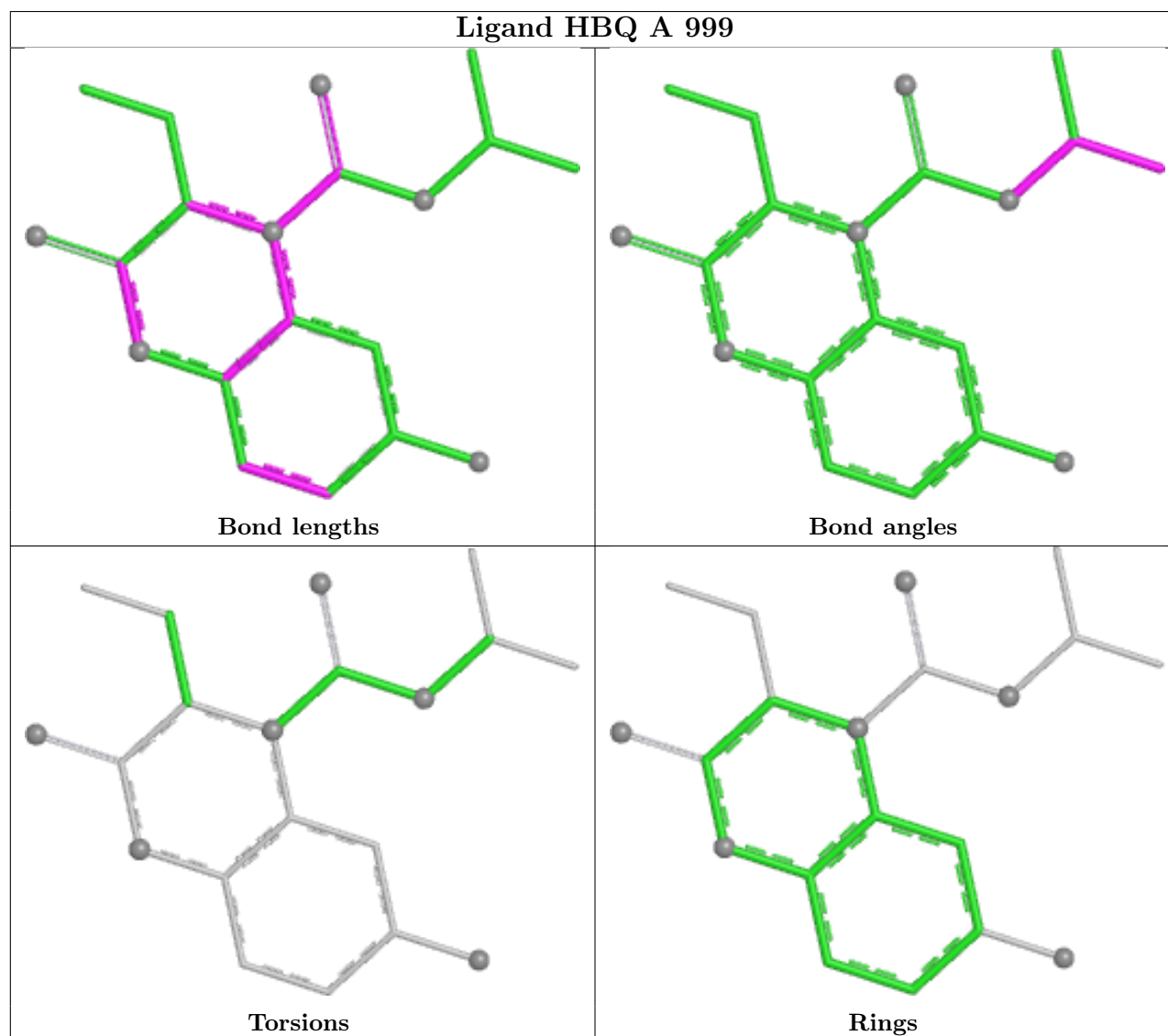
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	HBQ	1	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

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	515/534 (96%)	-0.43	2 (0%) 88 84	27, 56, 97, 122	0
2	B	400/424 (94%)	-0.42	2 (0%) 87 82	24, 56, 106, 132	0
All	All	915/958 (95%)	-0.42	4 (0%) 88 84	24, 56, 101, 132	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	69	THR	3.0
2	B	229	TRP	2.7
1	A	470	THR	2.1
1	A	241	VAL	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	0.95	0.07	45,52,74,74	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

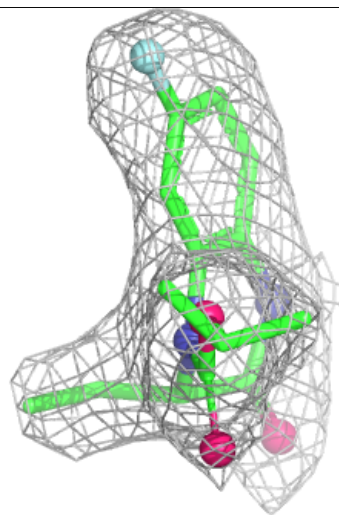
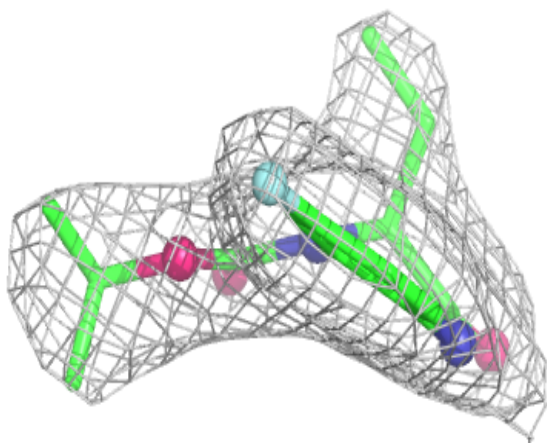
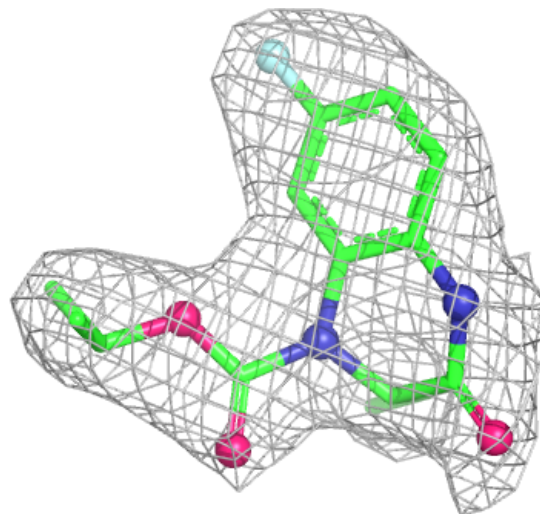
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	A	1301	5/5	0.85	0.13	123,127,131,133	0
4	HBQ	A	999	20/20	0.97	0.06	25,36,48,55	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 HBQ 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 [i](#)

There are no such residues in this entry.