



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:55 PM UTC

PDB ID : 3DM2 / pdb_00003dm2
Title : Crystal structure of HIV-1 K103N mutant reverse transcriptase in complex with GW564511.
Authors : Ren, J.; Chamberlain, P.P.; Stammers, D.K.
Deposited on : 2008-06-30
Resolution : 3.10 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

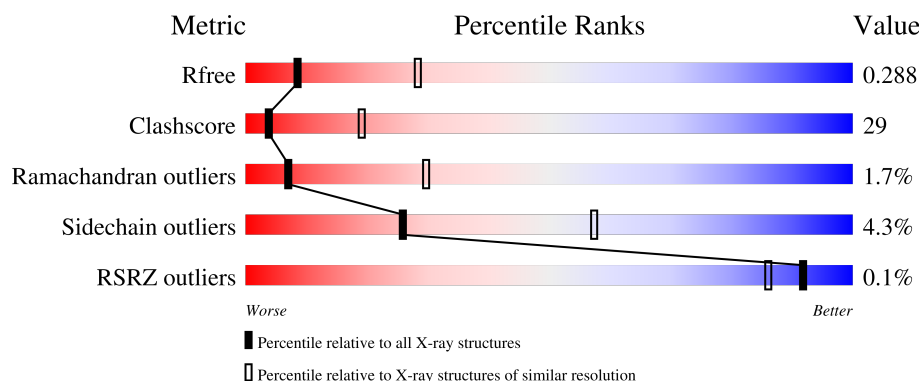
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	B	1300	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7702 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	532	Total	C	N	O	S	0	0	0
			4354	2820	723	803	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	engineered mutation	UNP P04585

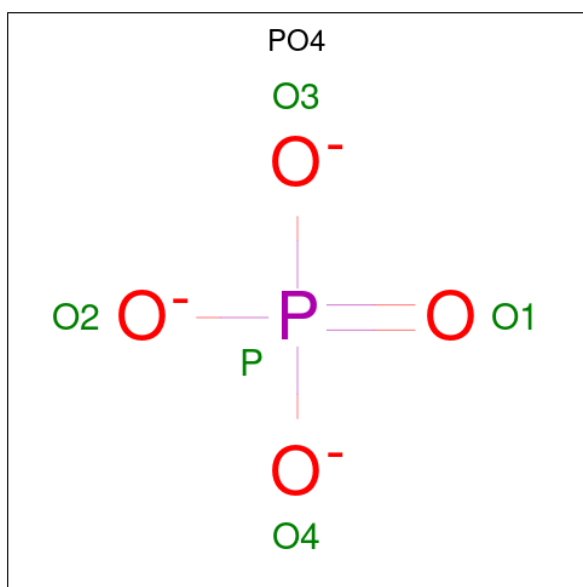
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	400	Total	C	N	O	S	0	0	0
			3302	2146	550	599	7			

There is a discrepancy between the modelled and reference sequences:

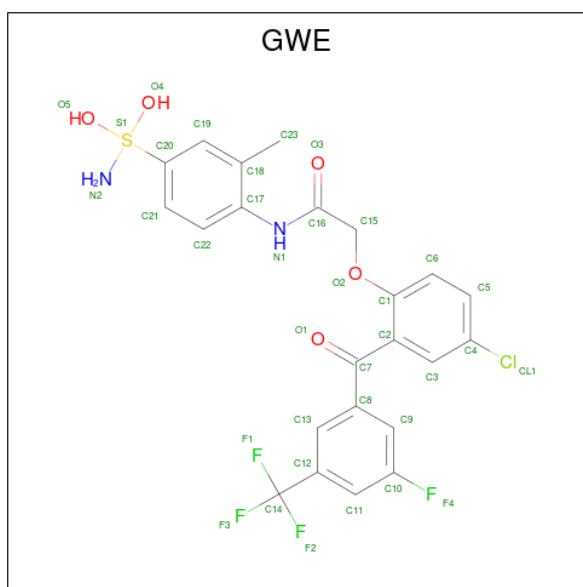
Chain	Residue	Modelled	Actual	Comment	Reference
B	103	ASN	LYS	engineered mutation	UNP P04585

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



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

- Molecule 4 is N-{4-[amino(dihydroxy)-lambda 4 -sulfanyl]-2-methylphenyl}-2-(4-chloro-2-{[3-fluoro-5-(trifluoromethyl)phenyl]carbonyl}phenoxy)acetamide (CCD ID: GWE) (formula: C₂₃H₁₉ClF₄N₂O₅S).

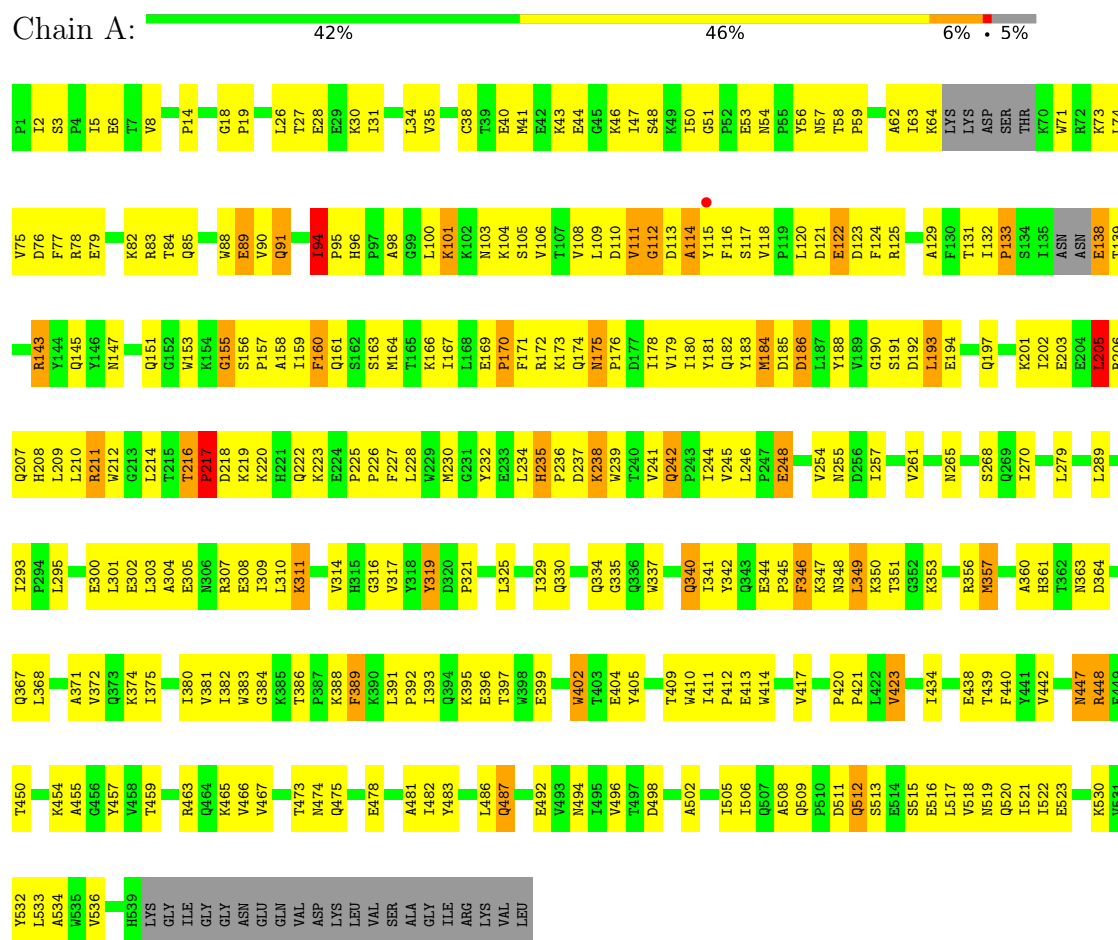


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	S	0	0
			36	23	1	4	2	5	1		

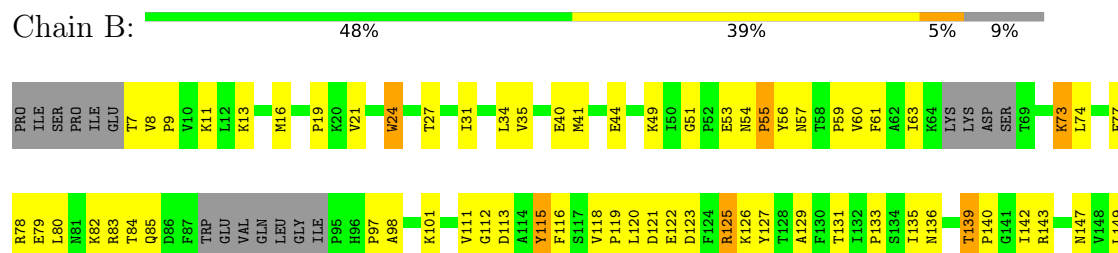
3 Residue-property plots

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

• Molecule 1: Reverse transcriptase/ribonuclease H



• Molecule 2: p51 RT



K388	F389	K390	L391	P392	I393	Q394	K398		T403	E404	Y405	V417		P421	L422	V423	K424	L425	W426	Y427	Q428	L429	E430	K431	E432	P433	I434	V435	G436	A437	GLU	THR	PHE																			
K388	F389	K390	L391	P392	I393	Q394	K398		T403	E404	Y405	V417		P421	L422	V423	K424	L425	W426	Y427	Q428	L429	E430	K431	E432	P433	I434	V435	G436	A437	GLU	THR	PHE																			
E312	D320	P321	S322	L325	I326	A327	E328	I329	Q330	K331	Q332	T338	Y339	Q340	I341	Y342	Q343	E344	F345	F346	K347	N348	L349	K353	Y354	A355	R356	G359	T362	N363	D364	V365	K366	Q367	L368	T369	E370	A371	V372	Q373	T376	T377	E378	S379	I380	V381	I382	W383	G384	A385	T386	P387
K150	Q151	K154	G155	S156	F160	Q161	S162	S163	M164	T165	K166	I167	L168	E169	P170	F171	N175	I178	V179	I180	M184	D185	D186	V189	G190	S191	E194	I195	G196	R199	T200	K201	I202	L205	R206	L209	L210	R211	W212	GLY	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN			
LYS	GLU	PRO	PRO	PHE	LEU	TRP	MET	GLY	TYR	E233	L234	H235	K238	W239	Q242	P243	I244	V245	D250	S251	W252	L260	K263	L264	N265	W266	A267	S268	Q269	I270	I274	L282	L283	L289	I293	T296	E297	E298	A299	E300	L303	N306	R307	E308	I309	L310	K311					

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.91Å 109.21Å 71.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.54 – 3.10 29.54 – 3.10	Depositor EDS
% Data completeness (in resolution range)	88.9 (29.54-3.10) 88.7 (29.54-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.307 0.212 , 0.288	Depositor DCC
R_{free} test set	938 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.690	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7702	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: GWE, PO4, 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	0.46	0/4461	1.02	29/6064 (0.5%)
2	B	0.44	0/3393	0.98	20/4608 (0.4%)
All	All	0.45	0/7854	1.00	49/10672 (0.5%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	VAL	N-CA-C	8.23	117.76	108.05
1	A	114	ALA	N-CA-C	-8.16	103.31	113.18
1	A	216	THR	CA-C-N	7.57	129.31	119.84
1	A	216	THR	C-N-CA	7.57	129.31	119.84
2	B	428	GLN	N-CA-C	-7.35	103.57	112.54
2	B	349	LEU	N-CA-C	-7.33	103.29	112.90
1	A	349	LEU	N-CA-C	-7.31	104.33	113.55
2	B	115	TYR	N-CA-C	7.08	118.64	111.07
2	B	242	GLN	CA-C-N	7.05	128.46	120.85
2	B	242	GLN	C-N-CA	7.05	128.46	120.85
1	A	319	TYR	N-CA-C	6.47	119.14	109.25
2	B	147	ASN	N-CA-C	-6.42	105.98	113.88
1	A	447	ASN	N-CA-C	-6.32	100.05	109.15
1	A	51	GLY	CA-C-N	6.21	125.91	119.64
1	A	51	GLY	C-N-CA	6.21	125.91	119.64
1	A	175	ASN	CA-C-N	6.14	125.54	118.85
1	A	175	ASN	C-N-CA	6.14	125.54	118.85
1	A	388	LYS	N-CA-C	-6.12	99.26	109.24
2	B	312	GLU	CA-C-N	6.02	125.78	119.76
2	B	312	GLU	C-N-CA	6.02	125.78	119.76
2	B	139	THR	CA-C-N	-5.98	113.62	119.78
2	B	139	THR	C-N-CA	-5.98	113.62	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	LYS	N-CA-C	-5.91	105.93	113.02
1	A	184	MET	CB-CA-C	-5.78	109.89	116.54
1	A	186	ASP	N-CA-C	5.73	118.57	110.14
1	A	245	VAL	N-CA-C	5.72	116.34	107.99
2	B	389	PHE	N-CA-C	5.68	119.08	109.76
1	A	94	ILE	CA-C-N	5.67	125.96	119.83
1	A	94	ILE	C-N-CA	5.67	125.96	119.83
2	B	186	ASP	N-CA-C	5.65	119.31	110.32
1	A	131	THR	N-CA-C	5.63	118.27	108.76
1	A	155	GLY	N-CA-C	5.59	120.82	114.67
2	B	125	ARG	N-CA-C	5.59	118.09	111.33
1	A	389	PHE	N-CA-C	5.42	119.06	109.96
2	B	250	ASP	N-CA-C	-5.41	104.42	111.02
1	A	364	ASP	N-CA-C	5.35	117.11	111.28
2	B	343	GLN	N-CA-C	-5.34	107.42	114.04
2	B	417	VAL	N-CA-C	5.30	116.33	108.65
2	B	391	LEU	N-CA-C	5.28	117.28	109.62
1	A	101	LYS	N-CA-C	-5.27	103.07	110.50
2	B	195	ILE	N-CA-C	5.16	116.51	110.62
1	A	235	HIS	CA-C-N	5.16	126.28	119.84
1	A	235	HIS	C-N-CA	5.16	126.28	119.84
2	B	332	GLN	N-CA-C	-5.15	106.85	113.23
1	A	242	GLN	N-CA-C	-5.08	103.19	109.64
1	A	205	LEU	N-CA-C	-5.06	105.45	110.97
1	A	96	HIS	CA-C-N	5.06	126.17	119.84
1	A	96	HIS	C-N-CA	5.06	126.17	119.84
2	B	382	ILE	N-CA-C	5.03	116.49	111.00

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	4354	0	4391	276	0
2	B	3302	0	3331	177	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	B	5	0	0	2	0
4	A	36	0	17	4	0
All	All	7702	0	7739	442	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 29.

All (442) 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:195:ILE:HB	2:B:199:ARG:HH12	1.22	1.03
1:A:106:VAL:H	4:A:999:GWE:HNS	1.05	0.98
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.29	0.96
2:B:242:GLN:HE21	2:B:243:PRO:HD2	1.29	0.96
2:B:353:LYS:HE3	2:B:430:GLU:HB3	1.48	0.94
2:B:359:GLY:N	3:B:1300:PO4:O1	2.08	0.87
1:A:183:TYR:HE1	1:A:184:MET:HE2	1.41	0.85
2:B:235:HIS:HB3	2:B:238:LYS:HE3	1.57	0.84
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.58	0.83
1:A:448:ARG:NH2	1:A:475:GLN:H	1.76	0.83
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.58	0.82
2:B:154:LYS:HA	2:B:184:MET:HE1	1.61	0.82
1:A:216:THR:OG1	1:A:217:PRO:HD2	1.80	0.82
2:B:73:LYS:NZ	2:B:73:LYS:HB3	1.95	0.81
2:B:195:ILE:HB	2:B:199:ARG:NH1	1.97	0.79
1:A:448:ARG:HE	1:A:473:THR:HB	1.47	0.78
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.65	0.78
1:A:211:ARG:HG2	1:A:211:ARG:NH1	1.92	0.77
1:A:502:ALA:HA	1:A:505:ILE:HD12	1.66	0.77
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.67	0.77
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.66	0.77
1:A:217:PRO:HB2	1:A:222:GLN:NE2	1.99	0.76
2:B:161:GLN:HE21	2:B:161:GLN:HA	1.49	0.76
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.66	0.76
1:A:41:MET:HE1	1:A:73:LYS:HE2	1.68	0.76
2:B:242:GLN:NE2	2:B:243:PRO:HD2	2.01	0.76
1:A:111:VAL:HG23	1:A:160:PHE:HZ	1.49	0.76
2:B:79:GLU:O	2:B:83:ARG:HG3	1.85	0.76
1:A:448:ARG:NE	1:A:474:ASN:H	1.84	0.75
1:A:114:ALA:HA	1:A:117:SER:OG	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:HG22	1:A:314:VAL:HG11	1.67	0.75
1:A:163:SER:O	1:A:167:ILE:HG13	1.86	0.74
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.27	0.74
2:B:235:HIS:HB2	2:B:238:LYS:HD2	1.67	0.74
2:B:379:SER:OG	2:B:387:PRO:HD3	1.87	0.73
1:A:183:TYR:CE1	1:A:184:MET:HE2	2.23	0.73
1:A:448:ARG:HH21	1:A:475:GLN:H	1.35	0.73
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.71	0.73
2:B:235:HIS:HB3	2:B:238:LYS:CE	2.18	0.73
1:A:257:ILE:O	1:A:261:VAL:HG23	1.87	0.73
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.23	0.72
1:A:181:TYR:HB2	1:A:188:TYR:HB2	1.71	0.72
1:A:237:ASP:OD1	1:A:238:LYS:HD2	1.88	0.72
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.04	0.71
2:B:235:HIS:CB	2:B:238:LYS:HD2	2.19	0.71
1:A:106:VAL:N	4:A:999:GWE:HNS	1.85	0.70
1:A:160:PHE:HD2	1:A:160:PHE:C	1.99	0.70
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.74	0.70
1:A:50:ILE:HG21	1:A:145:GLN:HG2	1.74	0.69
1:A:448:ARG:NE	1:A:473:THR:HB	2.07	0.69
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.73	0.68
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.75	0.67
1:A:94:ILE:HD11	1:A:230:MET:HG3	1.77	0.67
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.77	0.67
1:A:447:ASN:HB3	1:A:450:THR:OG1	1.95	0.66
2:B:376:THR:HG23	2:B:386:THR:HG22	1.76	0.66
1:A:483:TYR:CE2	1:A:487:GLN:NE2	2.63	0.66
2:B:265:ASN:O	2:B:268:SER:HB3	1.96	0.66
1:A:409:THR:O	2:B:364:ASP:HB2	1.94	0.66
1:A:357:MET:HE2	1:A:374:LYS:NZ	2.12	0.66
1:A:448:ARG:HE	1:A:473:THR:CB	2.08	0.66
2:B:31:ILE:O	2:B:35:VAL:HG23	1.96	0.66
2:B:376:THR:CG2	2:B:386:THR:HG22	2.25	0.66
2:B:164:MET:HA	2:B:167:ILE:HD11	1.78	0.65
2:B:116:PHE:HZ	2:B:151:GLN:NE2	1.92	0.65
1:A:160:PHE:C	1:A:160:PHE:CD2	2.72	0.65
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.32	0.65
2:B:194:GLU:CD	2:B:196:GLY:H	2.05	0.65
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.79	0.65
2:B:434:ILE:HG22	2:B:435:VAL:HG13	1.78	0.65
2:B:235:HIS:CB	2:B:238:LYS:CD	2.75	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:CZ	1:A:474:ASN:H	2.11	0.64
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.32	0.64
2:B:426:TRP:O	2:B:429:LEU:HB2	1.97	0.64
1:A:74:LEU:HD23	1:A:75:VAL:N	2.12	0.64
1:A:317:VAL:HG23	1:A:349:LEU:HD23	1.78	0.64
1:A:448:ARG:HG3	1:A:448:ARG:HH11	1.63	0.64
1:A:357:MET:HE2	1:A:374:LYS:HZ1	1.63	0.63
1:A:211:ARG:HH11	1:A:211:ARG:CG	2.07	0.63
2:B:162:SER:O	2:B:166:LYS:HG3	1.99	0.63
1:A:442:VAL:HG22	1:A:496:VAL:O	1.99	0.62
2:B:376:THR:O	2:B:380:ILE:HG13	1.99	0.62
1:A:116:PHE:CE2	1:A:151:GLN:HG2	2.35	0.62
2:B:31:ILE:HD13	2:B:133:PRO:O	1.99	0.62
1:A:246:LEU:O	1:A:307:ARG:NH1	2.26	0.62
2:B:433:PRO:HB3	2:B:436:GLY:O	2.00	0.61
1:A:335:GLY:O	1:A:356:ARG:HA	2.00	0.61
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.81	0.61
1:A:346:PHE:N	1:A:346:PHE:CD2	2.67	0.61
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.35	0.60
2:B:235:HIS:O	2:B:238:LYS:HG2	2.00	0.60
1:A:120:LEU:HD23	1:A:125:ARG:HG2	1.83	0.60
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.37	0.60
2:B:369:THR:O	2:B:373:GLN:HG3	2.00	0.60
1:A:40:GLU:O	1:A:43:LYS:HG2	2.01	0.60
1:A:448:ARG:HE	1:A:473:THR:CA	2.14	0.60
1:A:164:MET:HE1	1:A:209:LEU:HD22	1.84	0.60
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.82	0.59
1:A:214:LEU:C	1:A:214:LEU:HD23	2.27	0.59
1:A:203:GLU:HG3	1:A:207:GLN:HE21	1.66	0.59
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.00	0.59
2:B:425:LEU:O	2:B:429:LEU:HD13	2.02	0.59
1:A:40:GLU:O	1:A:44:GLU:HG3	2.03	0.59
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.84	0.59
1:A:114:ALA:HB3	1:A:160:PHE:CE1	2.37	0.59
2:B:366:LYS:HE3	2:B:405:TYR:CE2	2.38	0.59
1:A:420:PRO:HA	1:A:421:PRO:C	2.27	0.58
2:B:73:LYS:HB3	2:B:73:LYS:HZ3	1.65	0.58
2:B:175:ASN:HD21	2:B:201:LYS:HE3	1.67	0.58
1:A:114:ALA:HB3	1:A:160:PHE:CZ	2.37	0.58
2:B:73:LYS:HB3	2:B:73:LYS:HZ2	1.67	0.58
2:B:163:SER:O	2:B:167:ILE:HG12	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:HIS:HB2	2:B:238:LYS:CD	2.33	0.58
2:B:332:GLN:NE2	2:B:424:LYS:HE2	2.18	0.58
1:A:405:TYR:O	2:B:331:LYS:HD3	2.04	0.58
1:A:122:GLU:H	1:A:122:GLU:CD	2.11	0.58
2:B:344:GLU:HB2	2:B:347:LYS:HD2	1.85	0.58
1:A:194:GLU:HB2	1:A:197:GLN:HG3	1.83	0.58
1:A:46:LYS:CE	1:A:116:PHE:HB3	2.34	0.58
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.21	0.58
1:A:206:ARG:O	1:A:210:LEU:HD13	2.03	0.58
1:A:208:HIS:O	1:A:211:ARG:HB3	2.03	0.58
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.84	0.58
1:A:164:MET:HG2	1:A:182:GLN:HE21	1.69	0.57
1:A:171:PHE:HE2	1:A:175:ASN:HB2	1.69	0.57
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.39	0.57
2:B:308:GLU:OE1	2:B:311:LYS:HE3	2.05	0.57
2:B:365:VAL:O	2:B:369:THR:HG23	2.04	0.57
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.69	0.57
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.22	0.57
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.87	0.57
1:A:112:GLY:C	1:A:114:ALA:H	2.10	0.57
2:B:78:ARG:O	2:B:82:LYS:HG3	2.05	0.57
1:A:138:GLU:OE1	1:A:139:THR:HG23	2.04	0.57
2:B:34:LEU:CD2	2:B:73:LYS:HG3	2.34	0.57
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.40	0.57
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.38	0.57
1:A:518:VAL:O	1:A:522:ILE:HG13	2.04	0.57
1:A:380:ILE:O	1:A:384:GLY:HA2	2.04	0.57
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.87	0.56
1:A:50:ILE:CG2	1:A:145:GLN:HG2	2.35	0.56
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.33	0.56
2:B:209:LEU:C	2:B:211:ARG:H	2.13	0.56
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.06	0.56
2:B:344:GLU:CB	2:B:347:LYS:HD2	2.35	0.56
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.05	0.56
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.86	0.56
1:A:111:VAL:HG22	1:A:185:ASP:O	2.05	0.56
1:A:340:GLN:CB	1:A:351:THR:HG22	2.36	0.56
1:A:58:THR:HG23	1:A:76:ASP:O	2.05	0.56
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.41	0.56
1:A:46:LYS:NZ	1:A:116:PHE:HB3	2.20	0.55
1:A:307:ARG:HH11	1:A:307:ARG:HG2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:OE1	1:A:248:GLU:HA	2.07	0.55
2:B:160:PHE:O	2:B:160:PHE:CD1	2.60	0.55
1:A:101:LYS:HA	1:A:319:TYR:O	2.06	0.55
1:A:454:LYS:HA	1:A:467:VAL:O	2.07	0.55
1:A:334:GLN:O	1:A:356:ARG:HD3	2.06	0.55
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.37	0.55
1:A:5:ILE:HD11	1:A:166:LYS:HD2	1.88	0.54
1:A:57:ASN:HA	1:A:129:ALA:O	2.07	0.54
1:A:90:VAL:O	1:A:91:GLN:C	2.51	0.54
1:A:88:TRP:CH2	2:B:57:ASN:CB	2.90	0.54
1:A:301:LEU:O	1:A:304:ALA:HB3	2.07	0.54
2:B:54:ASN:O	2:B:143:ARG:NH2	2.40	0.54
1:A:74:LEU:HD23	1:A:74:LEU:C	2.32	0.54
1:A:63:ILE:HD12	1:A:64:LYS:N	2.23	0.54
1:A:206:ARG:HH11	1:A:216:THR:HG21	1.73	0.54
1:A:175:ASN:CB	1:A:178:ILE:HD12	2.33	0.54
1:A:28:GLU:O	1:A:28:GLU:HG2	2.08	0.54
2:B:40:GLU:O	2:B:44:GLU:HG3	2.07	0.54
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.89	0.54
2:B:328:GLU:O	2:B:339:TYR:HA	2.08	0.53
1:A:346:PHE:N	1:A:346:PHE:HD2	2.07	0.53
2:B:27:THR:O	2:B:31:ILE:HG13	2.09	0.53
1:A:79:GLU:CD	1:A:83:ARG:HH21	2.16	0.53
2:B:326:ILE:O	2:B:341:ILE:HA	2.09	0.53
2:B:118:VAL:HB	2:B:149:LEU:HG	1.91	0.53
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.08	0.53
2:B:235:HIS:HB3	2:B:238:LYS:CD	2.39	0.52
1:A:108:VAL:C	1:A:109:LEU:HD12	2.34	0.52
2:B:111:VAL:HG22	2:B:185:ASP:O	2.09	0.52
1:A:217:PRO:HB2	1:A:222:GLN:HE21	1.73	0.52
1:A:110:ASP:HB3	1:A:217:PRO:HG3	1.90	0.52
1:A:241:VAL:HG22	1:A:242:GLN:O	2.09	0.52
2:B:206:ARG:O	2:B:210:LEU:HB2	2.09	0.52
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.40	0.52
1:A:492:GLU:OE2	1:A:530:LYS:HD2	2.08	0.52
1:A:90:VAL:O	1:A:90:VAL:HG23	2.10	0.52
1:A:244:ILE:HB	1:A:310:LEU:HD13	1.91	0.52
1:A:57:ASN:HD22	1:A:143:ARG:HH12	1.57	0.52
1:A:31:ILE:O	1:A:35:VAL:HG23	2.10	0.51
1:A:63:ILE:HD12	1:A:63:ILE:C	2.34	0.51
1:A:227:PHE:O	1:A:234:LEU:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:HG23	1:A:349:LEU:CD2	2.39	0.51
1:A:516:GLU:O	1:A:519:ASN:HB2	2.09	0.51
1:A:171:PHE:CE2	1:A:175:ASN:HB2	2.44	0.51
2:B:51:GLY:HA3	2:B:53:GLU:OE1	2.10	0.51
2:B:245:VAL:HG23	2:B:431:LYS:HB2	1.93	0.51
1:A:78:ARG:O	1:A:82:LYS:HG3	2.11	0.51
1:A:110:ASP:C	1:A:112:GLY:H	2.18	0.51
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.92	0.51
1:A:205:LEU:O	1:A:206:ARG:C	2.53	0.51
1:A:382:ILE:O	2:B:136:ASN:HB2	2.09	0.51
1:A:508:ALA:O	1:A:509:GLN:C	2.54	0.51
1:A:38:CYS:O	1:A:47:ILE:HD11	2.11	0.51
1:A:216:THR:O	1:A:217:PRO:O	2.29	0.50
1:A:225:PRO:HA	1:A:226:PRO:C	2.36	0.50
1:A:235:HIS:HB2	1:A:238:LYS:O	2.11	0.50
1:A:307:ARG:NH1	1:A:307:ARG:HG2	2.26	0.50
1:A:417:VAL:O	1:A:417:VAL:HG13	2.11	0.50
2:B:263:LYS:HE2	2:B:425:LEU:HB3	1.93	0.50
2:B:209:LEU:C	2:B:211:ARG:N	2.70	0.50
1:A:112:GLY:O	1:A:114:ALA:N	2.33	0.50
2:B:139:THR:HG22	2:B:140:PRO:O	2.11	0.50
2:B:167:ILE:HG22	2:B:212:TRP:CZ2	2.47	0.50
1:A:111:VAL:CG2	1:A:160:PHE:HZ	2.22	0.49
1:A:440:PHE:CD2	1:A:459:THR:HG22	2.47	0.49
2:B:379:SER:CB	2:B:387:PRO:HD3	2.42	0.49
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.46	0.49
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.93	0.49
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.11	0.49
2:B:142:ILE:N	2:B:142:ILE:HD12	2.27	0.49
2:B:366:LYS:HE3	2:B:405:TYR:CD2	2.46	0.49
1:A:76:ASP:OD2	1:A:78:ARG:HG3	2.12	0.49
1:A:164:MET:HG2	1:A:182:GLN:NE2	2.27	0.49
2:B:122:GLU:HG3	2:B:123:ASP:N	2.26	0.49
1:A:161:GLN:NE2	2:B:140:PRO:HB3	2.26	0.49
1:A:98:ALA:HB2	1:A:350:LYS:HB2	1.94	0.49
1:A:176:PRO:C	1:A:178:ILE:H	2.19	0.49
1:A:396:GLU:HG3	1:A:397:THR:N	2.28	0.49
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.95	0.49
1:A:206:ARG:HH11	1:A:216:THR:CG2	2.26	0.49
1:A:171:PHE:O	1:A:172:ARG:C	2.55	0.49
1:A:46:LYS:NZ	1:A:116:PHE:CB	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:C	1:A:74:LEU:CD2	2.86	0.48
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.48	0.48
2:B:169:GLU:O	2:B:170:PRO:C	2.55	0.48
1:A:101:LYS:HG2	1:A:321:PRO:HD3	1.94	0.48
1:A:335:GLY:HA3	1:A:356:ARG:CD	2.44	0.48
1:A:334:GLN:NE2	1:A:512:GLN:HB3	2.29	0.48
2:B:11:LYS:O	2:B:85:GLN:HB3	2.13	0.48
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.48	0.48
1:A:455:ALA:O	1:A:466:VAL:HA	2.14	0.48
1:A:103:ASN:ND2	4:A:999:GWE:H5	2.28	0.48
1:A:235:HIS:O	1:A:238:LYS:O	2.32	0.48
1:A:448:ARG:HE	1:A:474:ASN:H	1.62	0.48
1:A:112:GLY:C	1:A:114:ALA:N	2.71	0.47
2:B:303:LEU:O	2:B:307:ARG:HG3	2.13	0.47
1:A:392:PRO:O	1:A:423:VAL:HG12	2.14	0.47
1:A:19:PRO:O	1:A:56:TYR:HA	2.15	0.47
1:A:27:THR:O	1:A:31:ILE:HG13	2.15	0.47
1:A:79:GLU:O	1:A:83:ARG:HG3	2.15	0.47
1:A:169:GLU:CG	1:A:173:LYS:HE3	2.43	0.47
1:A:171:PHE:HD2	1:A:171:PHE:C	2.22	0.47
1:A:48:SER:O	1:A:50:ILE:HG23	2.15	0.47
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.97	0.47
2:B:84:THR:HB	2:B:154:LYS:HE2	1.95	0.47
2:B:120:LEU:O	2:B:121:ASP:C	2.58	0.47
2:B:298:GLU:CD	2:B:298:GLU:H	2.22	0.47
1:A:111:VAL:HG23	1:A:111:VAL:O	2.14	0.47
1:A:344:GLU:HG3	1:A:347:LYS:HD2	1.96	0.47
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.50	0.47
1:A:329:ILE:O	1:A:392:PRO:HD3	2.14	0.47
2:B:126:LYS:HE3	2:B:127:TYR:CE1	2.50	0.47
2:B:421:PRO:O	2:B:425:LEU:HG	2.14	0.47
2:B:112:GLY:HA2	2:B:115:TYR:CE2	2.49	0.47
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.29	0.47
2:B:211:ARG:HG3	2:B:212:TRP:CD1	2.50	0.47
1:A:183:TYR:CE1	1:A:184:MET:HG3	2.50	0.46
1:A:381:VAL:O	2:B:136:ASN:N	2.46	0.46
2:B:8:VAL:HG23	2:B:9:PRO:HD2	1.96	0.46
1:A:171:PHE:C	1:A:171:PHE:CD2	2.91	0.46
1:A:279:LEU:HG	1:A:302:GLU:OE1	2.16	0.46
2:B:320:ASP:OD1	2:B:322:SER:N	2.48	0.46
1:A:295:LEU:HD12	1:A:300:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.46	0.46
1:A:57:ASN:HB2	1:A:143:ARG:HH22	1.80	0.46
2:B:7:THR:CG2	2:B:119:PRO:HG2	2.39	0.46
1:A:26:LEU:HD12	1:A:133:PRO:HG3	1.97	0.46
1:A:110:ASP:C	1:A:112:GLY:N	2.73	0.46
2:B:178:ILE:HG12	2:B:191:SER:CB	2.44	0.46
1:A:478:GLU:O	1:A:482:ILE:HG13	2.16	0.46
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.48	0.46
2:B:31:ILE:HD12	2:B:135:ILE:HG13	1.98	0.46
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.97	0.46
2:B:49:LYS:HA	2:B:143:ARG:O	2.16	0.46
2:B:167:ILE:HG12	2:B:167:ILE:H	1.55	0.46
2:B:206:ARG:O	2:B:210:LEU:N	2.40	0.46
1:A:254:VAL:HB	1:A:289:LEU:HA	1.98	0.46
1:A:255:ASN:HD22	1:A:289:LEU:HB3	1.80	0.46
1:A:94:ILE:CD1	1:A:230:MET:HE2	2.45	0.45
1:A:208:HIS:CE1	1:A:212:TRP:NE1	2.84	0.45
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.62	0.45
2:B:24:TRP:HH2	2:B:61:PHE:CD2	2.34	0.45
2:B:282:LEU:HB3	2:B:293:ILE:HG21	1.97	0.45
2:B:202:ILE:O	2:B:205:LEU:HB3	2.17	0.45
2:B:206:ARG:NH1	2:B:206:ARG:HG2	2.31	0.45
1:A:412:PRO:O	1:A:413:GLU:C	2.60	0.45
2:B:342:TYR:CD1	2:B:342:TYR:C	2.94	0.45
1:A:2:ILE:HG22	1:A:3:SER:N	2.31	0.45
1:A:371:ALA:O	1:A:375:ILE:HG13	2.16	0.45
2:B:206:ARG:HG2	2:B:206:ARG:HH11	1.82	0.45
1:A:218:ASP:C	1:A:220:LYS:N	2.72	0.45
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.99	0.45
1:A:201:LYS:O	1:A:202:ILE:C	2.57	0.45
2:B:393:ILE:HG12	2:B:394:GLN:N	2.31	0.45
1:A:155:GLY:O	1:A:159:ILE:HG13	2.17	0.45
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.98	0.45
2:B:425:LEU:HA	2:B:428:GLN:HE21	1.81	0.45
1:A:308:GLU:OE1	1:A:311:LYS:NZ	2.46	0.45
1:A:438:GLU:HG2	1:A:459:THR:HB	1.99	0.45
2:B:242:GLN:HE21	2:B:243:PRO:CD	2.14	0.45
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.99	0.44
1:A:169:GLU:HG2	1:A:173:LYS:HE3	1.98	0.44
1:A:498:ASP:HA	1:A:536:VAL:O	2.17	0.44
2:B:63:ILE:HD13	2:B:74:LEU:CD2	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.46	0.44
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.52	0.44
1:A:8:VAL:O	1:A:121:ASP:HB2	2.17	0.44
1:A:511:ASP:O	1:A:512:GLN:HB3	2.16	0.44
2:B:139:THR:HG23	2:B:140:PRO:HD2	2.00	0.44
2:B:265:ASN:O	2:B:268:SER:CB	2.65	0.44
2:B:359:GLY:CA	3:B:1300:PO4:O1	2.65	0.44
1:A:225:PRO:HG2	4:A:999:GWE:O4	2.17	0.44
1:A:303:LEU:O	1:A:307:ARG:HG3	2.17	0.44
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.51	0.44
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.99	0.44
1:A:516:GLU:O	1:A:520:GLN:HG3	2.18	0.44
1:A:115:TYR:HE1	1:A:185:ASP:OD2	2.01	0.44
1:A:143:ARG:HG2	1:A:143:ARG:NH1	2.31	0.44
1:A:335:GLY:HA3	1:A:356:ARG:HD2	1.99	0.44
1:A:342:TYR:HB3	1:A:348:ASN:HA	2.00	0.44
1:A:389:PHE:HB3	1:A:391:LEU:HD21	2.00	0.44
1:A:114:ALA:O	1:A:117:SER:HB2	2.18	0.44
1:A:205:LEU:HD22	1:A:209:LEU:HD11	1.99	0.44
1:A:228:LEU:HA	1:A:232:TYR:O	2.18	0.44
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.52	0.44
2:B:169:GLU:OE2	2:B:169:GLU:HA	2.17	0.44
2:B:170:PRO:O	2:B:171:PHE:C	2.59	0.44
1:A:88:TRP:CH2	2:B:57:ASN:HB2	2.52	0.44
1:A:90:VAL:HG12	1:A:158:ALA:HA	2.00	0.44
1:A:180:ILE:C	1:A:181:TYR:HD2	2.26	0.44
1:A:439:THR:O	1:A:459:THR:HA	2.17	0.44
1:A:492:GLU:HA	1:A:530:LYS:O	2.18	0.44
2:B:274:ILE:HD11	2:B:310:LEU:HD21	2.00	0.44
1:A:482:ILE:O	1:A:486:LEU:HG	2.19	0.43
2:B:168:LEU:HD23	2:B:168:LEU:HA	1.88	0.43
1:A:440:PHE:CG	1:A:459:THR:HG22	2.53	0.43
1:A:478:GLU:O	1:A:481:ALA:HB3	2.18	0.43
2:B:57:ASN:HD21	2:B:131:THR:N	2.16	0.43
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.18	0.43
2:B:343:GLN:HG3	2:B:349:LEU:HD11	2.00	0.43
1:A:170:PRO:O	1:A:173:LYS:HB2	2.18	0.43
1:A:138:GLU:CD	1:A:139:THR:HG23	2.44	0.43
1:A:337:TRP:O	1:A:353:LYS:HA	2.18	0.43
1:A:305:GLU:O	1:A:309:ILE:HG13	2.19	0.43
2:B:160:PHE:O	2:B:160:PHE:HD1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:HA	2:B:332:GLN:HE21	1.82	0.43
1:A:46:LYS:HE2	1:A:116:PHE:HB3	1.99	0.43
1:A:94:ILE:HD13	1:A:230:MET:HE2	2.00	0.43
2:B:325:LEU:HD12	2:B:325:LEU:HA	1.88	0.43
1:A:410:TRP:CD1	2:B:362:THR:O	2.72	0.43
1:A:515:SER:CB	1:A:518:VAL:HG23	2.47	0.43
2:B:24:TRP:CH2	2:B:61:PHE:CD2	3.07	0.43
1:A:34:LEU:O	1:A:35:VAL:C	2.62	0.43
1:A:164:MET:HE3	1:A:164:MET:HA	2.01	0.43
1:A:100:LEU:CD2	1:A:181:TYR:HE1	2.31	0.43
1:A:111:VAL:HG23	1:A:160:PHE:CZ	2.41	0.43
1:A:457:TYR:CE1	1:A:463:ARG:HD2	2.54	0.43
1:A:448:ARG:NH2	1:A:474:ASN:N	2.66	0.42
1:A:186:ASP:OD2	1:A:223:LYS:NZ	2.51	0.42
1:A:212:TRP:C	1:A:214:LEU:H	2.27	0.42
1:A:88:TRP:CH2	2:B:57:ASN:HB3	2.53	0.42
1:A:125:ARG:HD3	1:A:147:ASN:HA	2.02	0.42
1:A:399:GLU:OE2	1:A:402:TRP:HZ3	2.03	0.42
1:A:402:TRP:CD1	1:A:402:TRP:C	2.97	0.42
2:B:57:ASN:HA	2:B:129:ALA:O	2.19	0.42
2:B:84:THR:O	2:B:85:GLN:C	2.63	0.42
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.49	0.42
1:A:84:THR:HG21	1:A:153:TRP:CZ2	2.54	0.42
1:A:171:PHE:HE2	1:A:175:ASN:CB	2.32	0.42
1:A:171:PHE:O	1:A:174:GLN:N	2.53	0.42
1:A:30:LYS:HE2	1:A:71:TRP:CH2	2.53	0.42
1:A:54:ASN:OD1	1:A:56:TYR:N	2.51	0.42
1:A:94:ILE:HA	1:A:95:PRO:HD3	1.82	0.42
1:A:448:ARG:HE	1:A:473:THR:HA	1.84	0.42
1:A:519:ASN:O	1:A:523:GLU:HG2	2.19	0.42
2:B:235:HIS:CD2	2:B:238:LYS:NZ	2.88	0.42
1:A:95:PRO:HA	2:B:136:ASN:OD1	2.19	0.42
1:A:448:ARG:HH11	1:A:448:ARG:CG	2.30	0.42
2:B:175:ASN:ND2	2:B:201:LYS:HE3	2.32	0.42
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.55	0.42
2:B:209:LEU:O	2:B:211:ARG:N	2.53	0.42
1:A:465:LYS:CG	1:A:466:VAL:N	2.83	0.41
1:A:465:LYS:HG2	1:A:466:VAL:N	2.34	0.41
2:B:41:MET:HE3	2:B:116:PHE:HE2	1.85	0.41
1:A:218:ASP:O	1:A:219:LYS:C	2.62	0.41
1:A:77:PHE:O	1:A:78:ARG:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:HIS:HA	1:A:236:PRO:HD3	1.91	0.41
2:B:41:MET:HE3	2:B:116:PHE:CE2	2.55	0.41
2:B:380:ILE:O	2:B:384:GLY:N	2.46	0.41
1:A:63:ILE:O	1:A:71:TRP:HE3	2.03	0.41
1:A:265:ASN:O	1:A:268:SER:OG	2.33	0.41
1:A:293:ILE:N	1:A:293:ILE:HD12	2.35	0.41
2:B:53:GLU:O	2:B:55:PRO:HD3	2.20	0.41
2:B:332:GLN:NE2	2:B:332:GLN:HA	2.35	0.41
2:B:354:TYR:CD2	2:B:371:ALA:HB2	2.55	0.41
2:B:404:GLU:HB2	2:B:405:TYR:CE1	2.55	0.41
1:A:169:GLU:O	1:A:173:LYS:HG3	2.21	0.41
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.51	0.41
2:B:19:PRO:O	2:B:56:TYR:HB3	2.21	0.41
2:B:115:TYR:CD1	2:B:156:SER:HB3	2.56	0.41
1:A:170:PRO:O	1:A:174:GLN:HG3	2.20	0.41
1:A:457:TYR:HE1	1:A:463:ARG:HD2	1.85	0.41
2:B:378:GLU:O	2:B:382:ILE:HG13	2.21	0.41
2:B:60:VAL:HG22	2:B:61:PHE:N	2.35	0.41
2:B:98:ALA:O	2:B:101:LYS:HG2	2.20	0.41
2:B:422:LEU:O	2:B:423:VAL:C	2.64	0.41
1:A:360:ALA:O	1:A:513:SER:HB2	2.21	0.41
1:A:502:ALA:O	1:A:506:ILE:HG13	2.20	0.41
2:B:245:VAL:CG2	2:B:431:LYS:HB2	2.50	0.41
1:A:88:TRP:O	1:A:89:GLU:C	2.64	0.41
1:A:121:ASP:O	1:A:124:PHE:N	2.49	0.41
1:A:192:ASP:O	1:A:193:LEU:O	2.39	0.41
1:A:325:LEU:HA	1:A:325:LEU:HD12	1.89	0.41
2:B:63:ILE:CD1	2:B:74:LEU:HD22	2.46	0.41
2:B:111:VAL:HG23	2:B:111:VAL:O	2.20	0.41
2:B:121:ASP:O	2:B:125:ARG:HG3	2.21	0.41
2:B:168:LEU:O	2:B:169:GLU:C	2.62	0.41
2:B:235:HIS:O	2:B:238:LYS:CG	2.68	0.41
2:B:116:PHE:CZ	2:B:151:GLN:NE2	2.81	0.40
2:B:169:GLU:CB	2:B:170:PRO:HD3	2.51	0.40
2:B:266:TRP:C	2:B:268:SER:N	2.77	0.40
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.57	0.40
1:A:101:LYS:HE2	1:A:321:PRO:CG	2.48	0.40
1:A:116:PHE:CZ	1:A:151:GLN:HG2	2.56	0.40
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.87	0.40
1:A:105:SER:O	1:A:190:GLY:HA2	2.22	0.40
1:A:179:VAL:O	1:A:179:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:HIS:CB	2:B:238:LYS:CE	2.95	0.40
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.04	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	525/560 (94%)	463 (88%)	49 (9%)	13 (2%)	4	21
2	B	392/440 (89%)	361 (92%)	28 (7%)	3 (1%)	16	47
All	All	917/1000 (92%)	824 (90%)	77 (8%)	16 (2%)	7	30

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	133	PRO
1	A	193	LEU
1	A	217	PRO
1	A	112	GLY
1	A	113	ASP
1	A	170	PRO
1	A	345	PRO
2	B	170	PRO
2	B	210	LEU
1	A	85	GLN
1	A	361	HIS
1	A	14	PRO
1	A	512	GLN
1	A	111	VAL
2	B	97	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	476/499 (95%)	450 (94%)	26 (6%)	19	50
2	B	363/400 (91%)	353 (97%)	10 (3%)	38	66
All	All	839/899 (93%)	803 (96%)	36 (4%)	26	57

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	53	GLU
1	A	89	GLU
1	A	94	ILE
1	A	122	GLU
1	A	123	ASP
1	A	138	GLU
1	A	143	ARG
1	A	160	PHE
1	A	191	SER
1	A	205	LEU
1	A	211	ARG
1	A	217	PRO
1	A	238	LYS
1	A	248	GLU
1	A	340	GLN
1	A	346	PHE
1	A	357	MET
1	A	368	LEU
1	A	402	TRP
1	A	404	GLU
1	A	423	VAL
1	A	448	ARG
1	A	487	GLN
1	A	517	LEU
1	A	533	LEU
2	B	24	TRP

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Mol	Chain	Res	Type
2	B	55	PRO
2	B	73	LYS
2	B	113	ASP
2	B	167	ILE
2	B	189	VAL
2	B	243	PRO
2	B	283	LEU
2	B	300	GLU
2	B	325	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	145	GLN
1	A	161	GLN
1	A	174	GLN
1	A	182	GLN
1	A	207	GLN
1	A	208	HIS
1	A	242	GLN
1	A	255	ASN
1	A	278	GLN
1	A	334	GLN
1	A	336	GLN
1	A	363	ASN
1	A	428	GLN
1	A	474	ASN
1	A	487	GLN
1	A	500	GLN
1	A	512	GLN
1	A	519	ASN
2	B	57	ASN
2	B	151	GLN
2	B	161	GLN
2	B	175	ASN
2	B	182	GLN
2	B	197	GLN
2	B	235	HIS
2	B	242	GLN
2	B	330	GLN
2	B	332	GLN

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Mol	Chain	Res	Type
2	B	340	GLN
2	B	394	GLN
2	B	418	ASN
2	B	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSD	A	280	1	4,7,8	0.81	0	1,8,10	0.16	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
1	CSD	A	280	1	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	PO4	B	1300	-	4,4,4	1.84	2 (50%)	6,6,6	0.50	0
4	GWE	A	999	-	34,38,38	2.94	11 (32%)	49,57,57	1.35	7 (14%)
3	PO4	A	1301	-	4,4,4	1.71	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
4	GWE	A	999	-	-	4/25/29/29	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	GWE	C6-C5	7.13	1.50	1.38
4	A	999	GWE	C22-C21	6.83	1.49	1.38
4	A	999	GWE	C2-C1	6.30	1.52	1.40
4	A	999	GWE	C17-C18	6.26	1.53	1.40
4	A	999	GWE	C3-C4	6.23	1.48	1.38
4	A	999	GWE	C19-C20	4.89	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	GWE	C9-C10	2.42	1.41	1.37
4	A	999	GWE	C11-C10	2.37	1.41	1.37
4	A	999	GWE	C9-C8	2.34	1.43	1.39
4	A	999	GWE	C8-C7	2.19	1.53	1.49
3	B	1300	PO4	P-O3	-2.07	1.48	1.54
3	B	1300	PO4	P-O4	-2.07	1.48	1.54
4	A	999	GWE	C16-N1	2.02	1.39	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	GWE	C2-C7-C8	2.77	123.99	119.56
4	A	999	GWE	C11-C10-C9	-2.69	120.23	123.50
4	A	999	GWE	C15-O2-C1	2.66	123.15	117.60
4	A	999	GWE	C22-C17-C18	-2.43	117.92	120.70
4	A	999	GWE	C1-C2-C7	-2.27	119.34	122.85
4	A	999	GWE	O2-C15-C16	-2.27	104.57	110.80
4	A	999	GWE	F2-C14-C12	-2.12	108.35	112.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	999	GWE	C15-C16-N1-C17
4	A	999	GWE	O3-C16-N1-C17
4	A	999	GWE	C1-C2-C7-C8
4	A	999	GWE	C1-C2-C7-O1

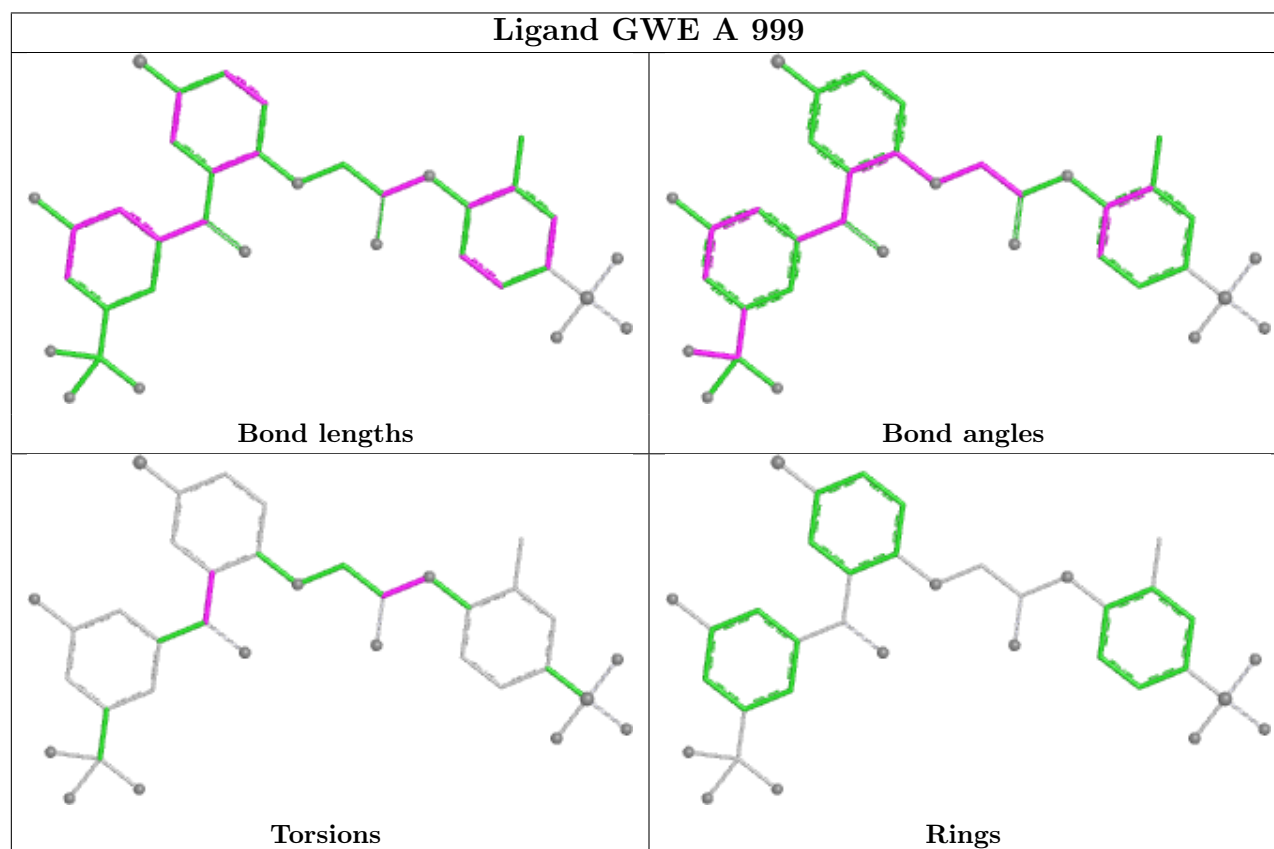
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1300	PO4	2	0
4	A	999	GWE	4	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	531/560 (94%)	-0.33	1 (0%) 91 83	18, 59, 103, 141	0
2	B	400/440 (90%)	-0.41	0 100 100	25, 58, 105, 133	0
All	All	931/1000 (93%)	-0.37	1 (0%) 92 86	18, 59, 103, 141	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	TYR	2.3

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	0.06	38,60,64,65	0

6.3 Carbohydrates [i](#)

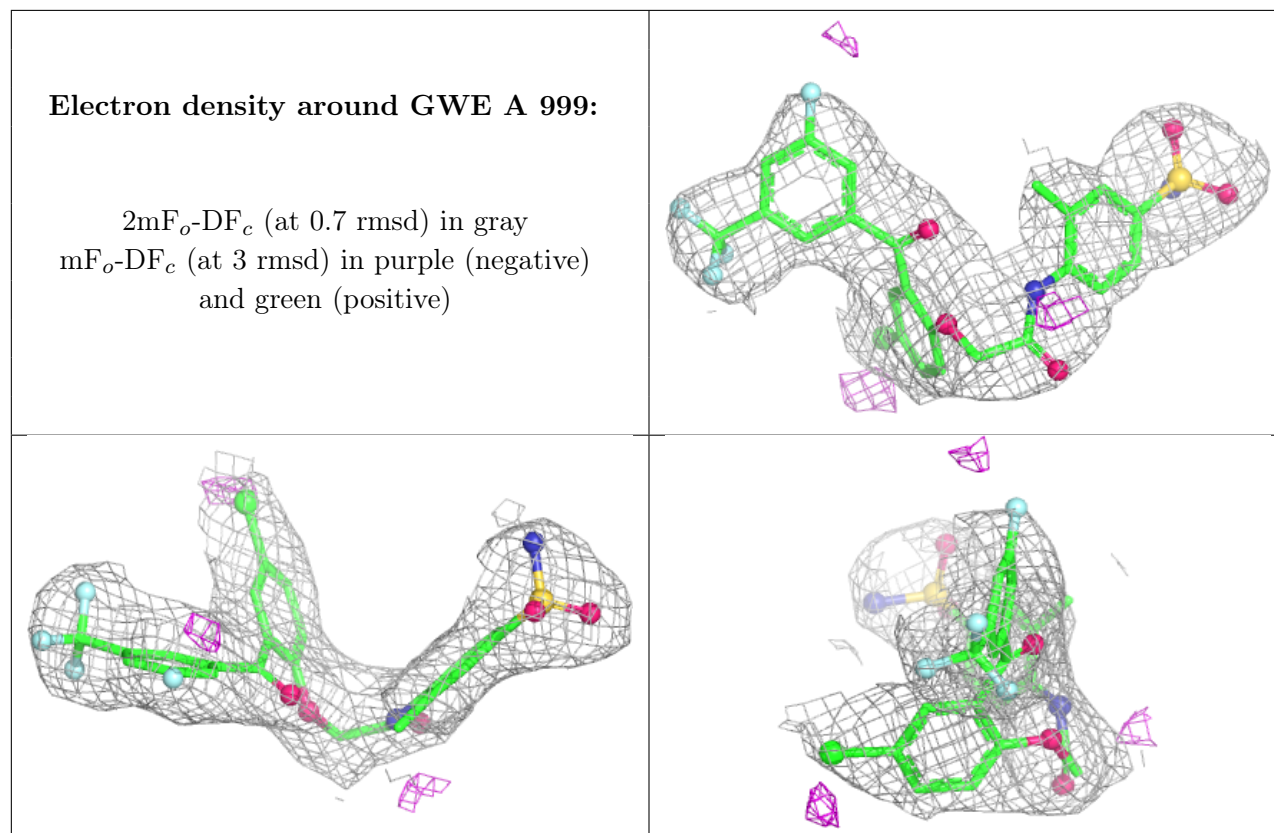
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	B	1300	5/5	0.62	0.12	124,130,137,145	0
3	PO4	A	1301	5/5	0.80	0.10	101,110,114,124	0
4	GWE	A	999	36/36	0.93	0.09	27,51,72,77	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.