



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:06 PM UTC

PDB ID : 1X81 / pdb_00001x81
Title : Farnesyl transferase structure of Jansen compound
Authors : Li, Q.; Claiborne, A.; Li, T.; Hasvold, L.; Stoll, V.S.; Muchmore, S.; Jakob, C.G.; Gu, W.; Cohen, J.; Hutchins, C.; Frost, D.; Rosenberg, S.H.; Sham, H.L.
Deposited on : 2004-08-16
Resolution : 3.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

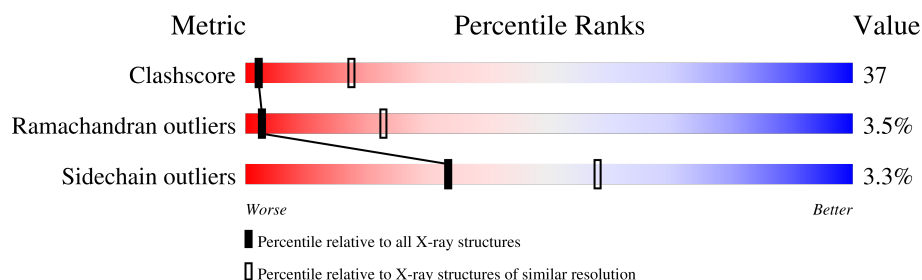
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	315	
2	B	397	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5849 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 Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2689	1712	473	499	5			

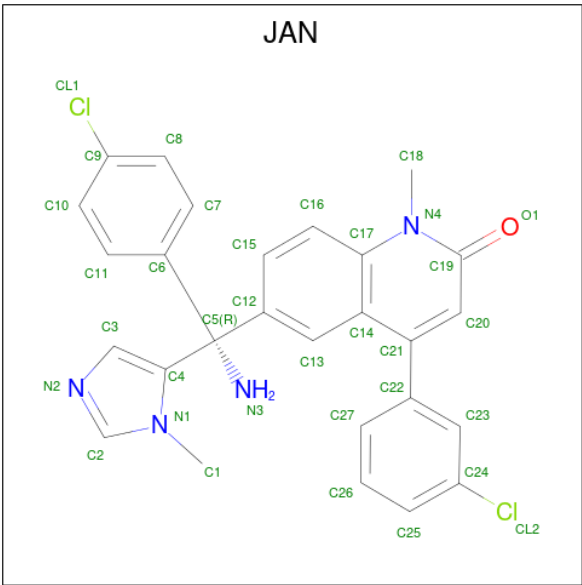
- Molecule 2 is a protein called Protein farnesyltransferase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	397	Total	C	N	O	S	0	0	0
			3125	1995	539	568	23			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 6-[(S)-AMINO(4-CHLOROPHENYL)(1-METHYL-1H-IMIDAZOL-5-YL)METHYL]-4-(3-CHLOROPHENYL)-1-METHYLQUINOLIN-2(1H)-ONE (CCD ID: JAN) (formula: C₂₇H₂₂Cl₂N₄O).



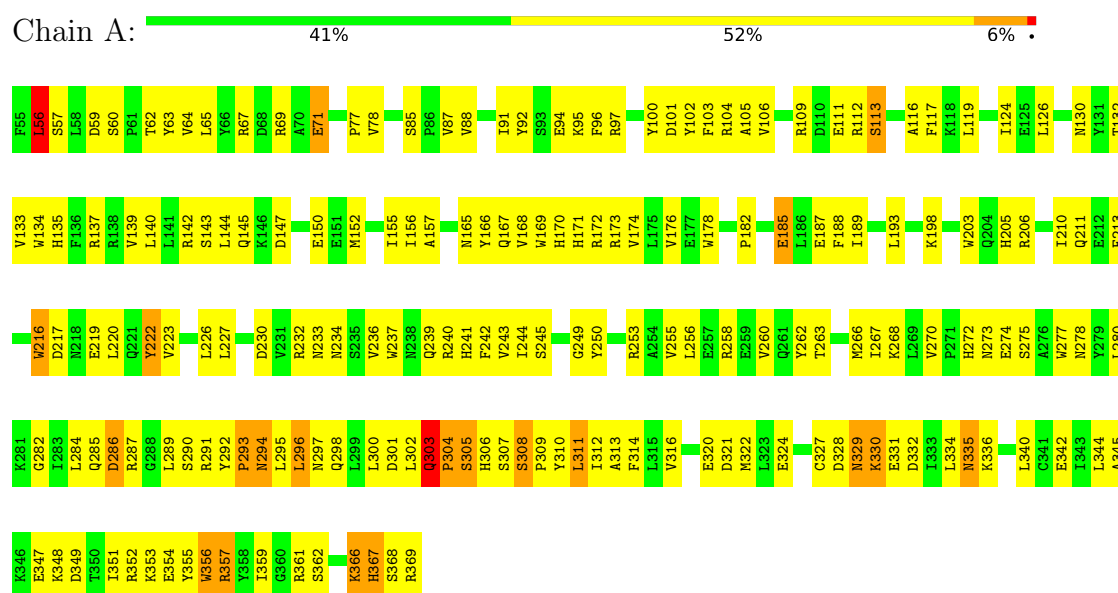
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
4	B	1	34	27	2	4	1	0	0

3 Residue-property plots

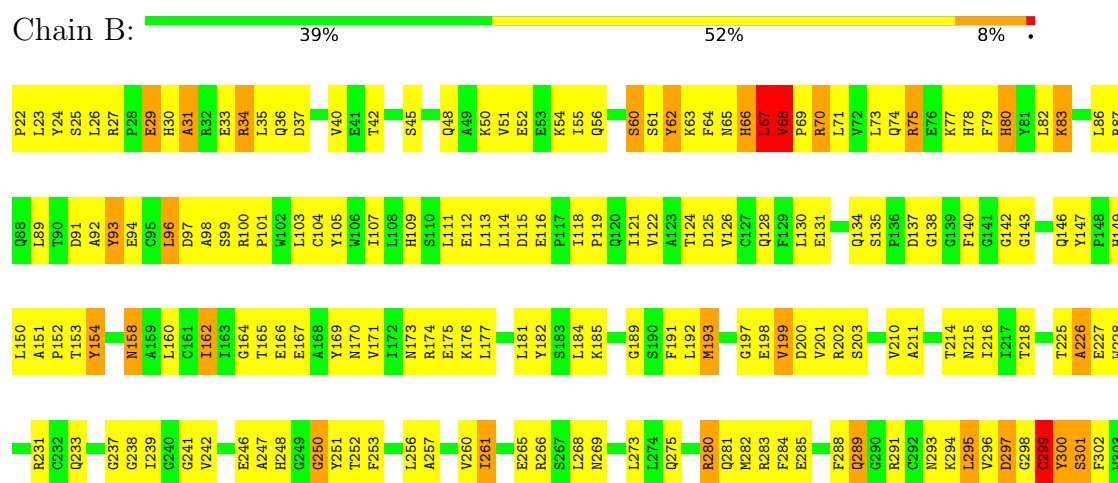
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit



- Molecule 2: Protein farnesyltransferase beta subunit



A373	A374	A375	F376	M381	L382	H383	V386	V389	P390	E391	N392	V393	L394	Q395	P396	T397	V400	Y401	N402	L403	A411	H414	F415	L416	Q417	K418	A373	A374	A375	F376	M381	L382	H383	V386	V389	P390	E391	N392	V393	L394	Q395	P396	T397	V400	Y401	N402	L403	A411	H414	F415	L416	Q417	K418	Q304	A305	G306	L307	L308	P309	L310	L311	L315	H316	A317	Q318	G319	D320	L323	S324	M325	M328	K329	F330	H331	G332	Q333	A334	L335	G336	M341	C342	G343	Q344	C345	G349	L350	L351	K352	K353	P354	G355	K356	S357	R358	D359	F360	T361	H362	T363	C364	Y365	C366	L367	S368	G369	L370	S371	L372
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	170.09Å 170.09Å 69.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.0	Depositor
R, R_{free}	0.223 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5849	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, JAN

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	0.67	1/2755 (0.0%)	1.13	17/3738 (0.5%)
2	B	0.64	0/3208	1.21	29/4353 (0.7%)
All	All	0.65	1/5963 (0.0%)	1.17	46/8091 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	HIS	C-O	-6.36	1.17	1.24

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	SER	N-CA-C	-11.55	99.17	113.38
1	A	270	VAL	CA-C-N	8.66	129.52	119.47
1	A	270	VAL	C-N-CA	8.66	129.52	119.47
1	A	85	SER	CA-C-N	8.57	128.59	119.76
1	A	85	SER	C-N-CA	8.57	128.59	119.76
2	B	351	LEU	N-CA-C	8.50	123.00	110.17
2	B	295	LEU	N-CA-C	8.26	120.98	110.24
1	A	150	GLU	N-CA-C	-8.03	102.11	112.23
2	B	62	TYR	N-CA-C	-7.98	102.34	113.20
2	B	96	LEU	N-CA-C	-7.65	103.51	112.92
2	B	199	VAL	N-CA-C	7.01	117.92	108.11
1	A	311	LEU	N-CA-C	-6.76	103.69	112.68
2	B	242	VAL	N-CA-C	-6.68	103.71	109.19
2	B	328	TRP	N-CA-C	-6.47	101.42	110.35
2	B	70	ARG	N-CA-C	6.44	121.30	113.38
2	B	269	ASN	N-CA-C	-6.38	99.24	109.39
2	B	366	CYS	N-CA-C	-6.36	104.56	112.90
2	B	162	ILE	N-CA-C	-6.30	104.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	ARG	N-CA-C	-6.25	105.31	113.12
2	B	80	HIS	N-CA-C	-6.15	104.49	111.07
1	A	113	SER	N-CA-C	6.11	119.79	109.76
1	A	187	GLU	N-CA-C	-6.09	104.56	111.14
1	A	329	ASN	N-CA-C	-6.02	105.52	112.86
1	A	59	ASP	N-CA-C	5.99	121.51	113.72
2	B	395	GLN	CA-C-N	5.91	125.87	119.78
2	B	395	GLN	C-N-CA	5.91	125.87	119.78
2	B	60	SER	N-CA-C	5.90	120.21	112.89
2	B	226	ALA	N-CA-C	-5.78	104.17	111.11
2	B	300	TYR	N-CA-C	-5.78	106.62	113.38
2	B	67	LEU	N-CA-C	5.75	118.66	111.24
2	B	237	GLY	N-CA-C	-5.63	107.27	114.37
2	B	165	THR	N-CA-C	-5.56	101.52	110.14
2	B	261	ILE	N-CA-C	-5.49	105.37	110.53
2	B	297	ASP	N-CA-C	5.45	117.55	108.99
2	B	31	ALA	N-CA-C	-5.39	105.80	112.38
1	A	157	ALA	N-CA-C	5.32	117.08	111.28
1	A	222	TYR	N-CA-C	-5.26	105.63	111.36
1	A	335	ASN	N-CA-C	-5.25	106.94	113.55
2	B	250	GLY	N-CA-C	-5.21	106.46	112.50
2	B	289	GLN	N-CA-C	-5.18	102.39	110.42
2	B	154	TYR	N-CA-C	-5.15	105.84	111.82
1	A	244	ILE	N-CA-C	5.14	115.42	110.74
2	B	352	ASP	N-CA-C	-5.12	99.89	110.80
1	A	237	TRP	N-CA-C	-5.11	106.56	112.89
1	A	303	GLN	N-CA-C	5.07	121.00	109.81
2	B	150	LEU	N-CA-C	5.02	119.11	112.89

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	2689	0	2614	185	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3125	0	3059	263	0
3	B	1	0	0	0	0
4	B	34	0	22	0	0
All	All	5849	0	5695	428	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 37.

All (428) 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:280:ARG:HH11	2:B:280:ARG:HA	1.19	1.03
2:B:193:MET:HA	2:B:193:MET:HE3	1.37	1.02
2:B:119:PRO:HB2	2:B:122:VAL:HG23	1.47	0.96
2:B:308:LEU:HD12	2:B:330:PHE:HD1	1.31	0.94
2:B:192:LEU:HA	2:B:199:VAL:HG12	1.51	0.93
1:A:69:ARG:HB3	1:A:71:GLU:OE2	1.70	0.92
2:B:73:LEU:HD12	2:B:344:GLN:NE2	1.88	0.89
1:A:287:ARG:H	1:A:287:ARG:HD2	1.38	0.87
2:B:34:ARG:HH11	2:B:34:ARG:HB3	1.41	0.86
2:B:285:GLU:HG2	2:B:296:VAL:HG11	1.59	0.84
2:B:73:LEU:HA	2:B:344:GLN:HE22	1.41	0.83
1:A:334:LEU:HD21	1:A:368:SER:HB3	1.60	0.83
2:B:66:HIS:HA	2:B:70:ARG:HD2	1.60	0.83
2:B:308:LEU:HD12	2:B:330:PHE:CD1	2.12	0.83
1:A:282:GLY:HA2	1:A:285:GLN:HE21	1.41	0.83
2:B:67:LEU:HD12	2:B:67:LEU:H	1.42	0.82
2:B:280:ARG:HA	2:B:280:ARG:NH1	1.94	0.82
1:A:287:ARG:HD2	1:A:287:ARG:N	1.95	0.82
2:B:361:TYR:CD2	2:B:362:HIS:HD2	1.98	0.81
2:B:71:LEU:HD21	2:B:341:MET:HE2	1.62	0.80
1:A:170:HIS:O	1:A:174:VAL:HG23	1.83	0.79
1:A:362:SER:O	1:A:366:LYS:HG2	1.82	0.78
1:A:260:VAL:HG13	1:A:280:LEU:HD11	1.63	0.78
1:A:334:LEU:HD22	1:A:367:HIS:O	1.84	0.77
1:A:189:ILE:HG21	1:A:206:ARG:HB2	1.65	0.77
2:B:349:GLY:HA2	2:B:363:THR:HG23	1.66	0.76
2:B:62:TYR:HA	2:B:70:ARG:NH1	2.01	0.75
1:A:173:ARG:HE	2:B:198:GLU:CD	1.95	0.74
1:A:71:GLU:CD	1:A:71:GLU:H	1.96	0.74
2:B:304:GLN:HA	2:B:304:GLN:HE21	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:LEU:HD12	2:B:36:GLN:N	2.04	0.73
2:B:101:PRO:HD3	2:B:142:GLY:O	1.89	0.73
2:B:361:TYR:CD2	2:B:362:HIS:CD2	2.78	0.72
1:A:347:GLU:OE1	1:A:348:LYS:HG2	1.88	0.71
2:B:124:THR:HG23	2:B:167:GLU:OE2	1.91	0.71
2:B:62:TYR:HA	2:B:70:ARG:HH12	1.55	0.71
2:B:202:ARG:HH11	2:B:202:ARG:HB3	1.55	0.71
1:A:334:LEU:CD2	1:A:368:SER:HB3	2.21	0.70
1:A:282:GLY:HA2	1:A:285:GLN:NE2	2.06	0.70
1:A:303:GLN:O	1:A:307:SER:HB2	1.92	0.69
2:B:119:PRO:HD2	2:B:122:VAL:HG21	1.75	0.68
2:B:370:LEU:HD23	2:B:394:LEU:HD11	1.76	0.68
2:B:69:PRO:HB2	2:B:389:VAL:HG12	1.75	0.67
1:A:112:ARG:HA	1:A:140:LEU:HD21	1.76	0.67
1:A:293:PRO:HG2	1:A:294:ASN:H	1.60	0.67
2:B:60:SER:O	2:B:63:LYS:HB2	1.95	0.67
2:B:34:ARG:HB3	2:B:34:ARG:NH1	2.09	0.67
1:A:223:VAL:HG11	1:A:240:ARG:HB2	1.77	0.66
2:B:361:TYR:HD2	2:B:362:HIS:CD2	2.12	0.66
2:B:266:ARG:HG2	2:B:318:GLN:HE21	1.61	0.66
1:A:357:ARG:HB3	1:A:361:ARG:HH12	1.59	0.66
2:B:266:ARG:HG2	2:B:318:GLN:NE2	2.10	0.66
2:B:185:LYS:NZ	2:B:189:GLY:HA2	2.11	0.66
1:A:132:THR:HG23	2:B:147:TYR:CD2	2.31	0.65
2:B:308:LEU:CD1	2:B:330:PHE:HB3	2.25	0.65
1:A:65:LEU:O	1:A:69:ARG:HG3	1.96	0.65
1:A:170:HIS:ND1	2:B:198:GLU:HG3	2.12	0.65
1:A:303:GLN:HE22	1:A:312:ILE:CD1	2.08	0.65
2:B:265:GLU:CD	2:B:265:GLU:H	2.05	0.65
2:B:61:SER:C	2:B:63:LYS:H	2.05	0.64
1:A:77:PRO:HB3	1:A:102:TYR:CE1	2.32	0.64
2:B:25:SER:HA	2:B:30:HIS:CE1	2.32	0.64
1:A:77:PRO:HB3	1:A:102:TYR:CD1	2.32	0.64
2:B:73:LEU:HD12	2:B:344:GLN:HE21	1.61	0.64
2:B:202:ARG:NH1	2:B:202:ARG:CB	2.61	0.64
2:B:282:MET:HG3	2:B:296:VAL:HB	1.79	0.64
1:A:152:MET:O	1:A:156:ILE:HG13	1.98	0.64
2:B:246:GLU:OE1	2:B:291:ARG:HD2	1.98	0.64
1:A:263:THR:HG21	1:A:280:LEU:HB2	1.78	0.64
2:B:283:ARG:HG2	2:B:283:ARG:HH11	1.63	0.64
2:B:68:VAL:HB	2:B:69:PRO:CD	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLN:HG3	1:A:242:PHE:HZ	1.63	0.63
1:A:165:ASN:ND2	1:A:167:GLN:H	1.97	0.63
2:B:297:ASP:HB3	2:B:300:TYR:HD2	1.63	0.63
2:B:345:CYS:SG	2:B:358:ARG:HD2	2.37	0.63
1:A:312:ILE:O	1:A:316:VAL:HG23	1.99	0.62
1:A:232:ARG:CZ	2:B:45:SER:HB2	2.29	0.62
1:A:165:ASN:HB3	1:A:168:VAL:HG12	1.80	0.62
2:B:185:LYS:HZ1	2:B:189:GLY:HA2	1.65	0.62
2:B:199:VAL:HG23	2:B:199:VAL:O	1.99	0.62
1:A:369:ARG:HG3	1:A:369:ARG:O	2.00	0.62
2:B:60:SER:HA	2:B:63:LYS:HD2	1.82	0.62
2:B:273:LEU:HD23	2:B:311:LEU:HD21	1.82	0.62
2:B:105:TYR:OH	2:B:402:ASN:ND2	2.33	0.61
1:A:263:THR:CG2	1:A:280:LEU:HB2	2.31	0.61
1:A:78:VAL:O	1:A:104:ARG:HD2	2.00	0.61
2:B:193:MET:HA	2:B:193:MET:CE	2.20	0.61
2:B:248:HIS:CE1	2:B:300:TYR:OH	2.54	0.61
1:A:260:VAL:HG13	1:A:280:LEU:CD1	2.32	0.60
2:B:50:LYS:O	2:B:54:LYS:HG3	2.01	0.60
2:B:82:LEU:HD12	2:B:111:LEU:HD23	1.84	0.60
1:A:198:LYS:NZ	2:B:293:ASN:O	2.33	0.60
2:B:281:GLN:HB2	2:B:288:PHE:CE2	2.36	0.60
2:B:316:HIS:HB2	2:B:323:LEU:HD12	1.84	0.60
2:B:227:GLU:O	2:B:231:ARG:HG3	2.02	0.59
2:B:299:CYS:C	2:B:301:SER:H	2.11	0.59
2:B:201:VAL:HA	2:B:228:TRP:HZ3	1.67	0.59
1:A:256:LEU:O	1:A:260:VAL:HG23	2.03	0.59
1:A:255:VAL:HG13	1:A:258:ARG:NH2	2.17	0.58
1:A:320:GLU:O	1:A:324:GLU:HG2	2.03	0.58
2:B:35:LEU:HD12	2:B:36:GLN:H	1.67	0.58
2:B:281:GLN:HB2	2:B:288:PHE:CZ	2.39	0.58
2:B:149:HIS:O	2:B:153:THR:OG1	2.19	0.58
2:B:256:LEU:O	2:B:260:VAL:HG23	2.03	0.58
1:A:100:TYR:O	1:A:104:ARG:HG3	2.03	0.58
2:B:112:GLU:OE2	2:B:162:ILE:HG23	2.04	0.58
2:B:335:LEU:HD23	2:B:373:ALA:HB2	1.85	0.58
1:A:331:GLU:H	1:A:331:GLU:CD	2.11	0.58
2:B:79:PHE:CE2	2:B:83:LYS:HD2	2.39	0.58
2:B:247:ALA:O	2:B:291:ARG:HG2	2.05	0.57
2:B:87:ARG:HH22	2:B:125:ASP:CG	2.12	0.57
2:B:370:LEU:O	2:B:374:GLN:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ALA:O	2:B:261:ILE:HG13	2.04	0.57
2:B:202:ARG:NH2	2:B:251:TYR:CE1	2.73	0.57
2:B:202:ARG:HH11	2:B:202:ARG:CB	2.17	0.57
1:A:356:TRP:HA	1:A:356:TRP:CE3	2.40	0.57
2:B:138:GLY:HA3	2:B:176:LYS:O	2.05	0.56
1:A:298:GLN:O	1:A:301:ASP:HB2	2.05	0.56
2:B:69:PRO:CB	2:B:389:VAL:HG12	2.35	0.56
1:A:334:LEU:HD21	1:A:368:SER:CB	2.35	0.56
1:A:307:SER:HA	1:A:311:LEU:HD13	1.87	0.56
1:A:357:ARG:HB3	1:A:361:ARG:NH1	2.21	0.56
1:A:100:TYR:C	1:A:104:ARG:NH1	2.64	0.56
1:A:170:HIS:HD1	2:B:198:GLU:HG3	1.71	0.56
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.41	0.56
2:B:134:GLN:HE22	2:B:173:ASN:H	1.54	0.56
2:B:386:VAL:HG21	2:B:393:VAL:HG22	1.87	0.56
2:B:389:VAL:H	2:B:392:ASN:ND2	2.04	0.56
1:A:328:ASP:O	1:A:329:ASN:HB2	2.06	0.55
1:A:342:GLU:OE1	1:A:342:GLU:HA	2.06	0.55
1:A:262:TYR:O	1:A:266:MET:HB2	2.07	0.55
2:B:202:ARG:HB3	2:B:202:ARG:NH1	2.20	0.55
1:A:65:LEU:N	1:A:65:LEU:HD22	2.21	0.55
2:B:368:SER:O	2:B:372:ILE:HG12	2.05	0.55
1:A:232:ARG:NH1	2:B:42:THR:OG1	2.40	0.55
1:A:256:LEU:O	1:A:256:LEU:HD23	2.07	0.55
2:B:280:ARG:NH1	2:B:289:GLN:NE2	2.55	0.55
2:B:299:CYS:C	2:B:301:SER:N	2.63	0.55
2:B:118:ILE:HD12	2:B:118:ILE:N	2.21	0.55
2:B:29:GLU:CD	2:B:29:GLU:H	2.13	0.55
1:A:87:VAL:O	1:A:88:VAL:C	2.51	0.54
1:A:347:GLU:OE1	1:A:348:LYS:HE3	2.07	0.54
2:B:64:PHE:O	2:B:64:PHE:CD1	2.60	0.54
1:A:165:ASN:O	1:A:169:TRP:HD1	1.90	0.54
2:B:33:GLU:O	2:B:284:PHE:HB2	2.07	0.54
2:B:135:SER:C	2:B:137:ASP:H	2.13	0.54
2:B:350:LEU:HD12	2:B:350:LEU:N	2.21	0.54
1:A:97:ARG:HG2	1:A:101:ASP:OD2	2.06	0.54
2:B:252:THR:HG22	2:B:307:LEU:HD11	1.90	0.54
1:A:111:GLU:HG2	1:A:113:SER:OG	2.08	0.54
1:A:268:LYS:HE2	1:A:302:LEU:HD21	1.90	0.54
2:B:86:LEU:HB2	2:B:107:ILE:HG21	1.90	0.54
1:A:106:VAL:HG11	1:A:116:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:O	1:A:298:GLN:HG3	2.07	0.53
1:A:334:LEU:CD2	1:A:367:HIS:O	2.53	0.53
2:B:308:LEU:HD11	2:B:330:PHE:HB3	1.90	0.53
2:B:298:GLY:C	2:B:299:CYS:O	2.48	0.53
1:A:103:PHE:O	1:A:104:ARG:C	2.51	0.53
2:B:140:PHE:HD1	2:B:153:THR:HG23	1.73	0.53
2:B:352:ASP:HB3	2:B:356:LYS:HG2	1.91	0.53
1:A:168:VAL:HG22	1:A:168:VAL:O	2.08	0.53
2:B:48:GLN:HE21	2:B:52:GLU:HG3	1.73	0.53
2:B:166:GLU:HG2	2:B:170:ASN:OD1	2.09	0.53
2:B:302:PHE:O	2:B:306:GLY:HA3	2.08	0.53
1:A:284:LEU:C	1:A:286:ASP:H	2.17	0.53
2:B:308:LEU:HD12	2:B:330:PHE:HB3	1.89	0.52
1:A:263:THR:O	1:A:267:ILE:HG13	2.10	0.52
1:A:292:TYR:CD1	1:A:292:TYR:N	2.76	0.52
1:A:311:LEU:HD22	1:A:312:ILE:HD13	1.91	0.52
2:B:27:ARG:HG2	2:B:27:ARG:HH11	1.74	0.52
1:A:165:ASN:ND2	1:A:166:TYR:N	2.58	0.52
1:A:239:GLN:HE21	1:A:239:GLN:HA	1.75	0.52
2:B:67:LEU:HD12	2:B:67:LEU:N	2.19	0.52
2:B:192:LEU:HA	2:B:199:VAL:CG1	2.33	0.52
2:B:78:HIS:O	2:B:82:LEU:HG	2.10	0.52
2:B:79:PHE:CZ	2:B:83:LYS:HD2	2.45	0.52
2:B:192:LEU:HD22	2:B:197:GLY:O	2.10	0.52
1:A:65:LEU:HD22	1:A:65:LEU:H	1.75	0.52
1:A:290:SER:OG	1:A:322:MET:HA	2.10	0.51
2:B:192:LEU:CA	2:B:199:VAL:HG12	2.31	0.51
1:A:147:ASP:OD2	1:A:147:ASP:C	2.53	0.51
2:B:246:GLU:CD	2:B:291:ARG:HD2	2.34	0.51
2:B:285:GLU:HG2	2:B:296:VAL:CG1	2.38	0.51
2:B:151:ALA:HB3	2:B:152:PRO:CD	2.40	0.51
1:A:172:ARG:O	1:A:176:VAL:HG23	2.10	0.51
2:B:202:ARG:NH1	2:B:202:ARG:HB2	2.25	0.51
2:B:154:TYR:O	2:B:158:ASN:HB2	2.11	0.51
1:A:344:LEU:HB3	1:A:356:TRP:CD1	2.46	0.51
2:B:100:ARG:O	2:B:101:PRO:C	2.53	0.51
1:A:245:SER:HA	1:A:249:GLY:HA2	1.93	0.51
2:B:253:PHE:HA	2:B:307:LEU:HD21	1.92	0.51
1:A:155:ILE:HD13	1:A:171:HIS:HD2	1.76	0.50
1:A:170:HIS:CE1	2:B:198:GLU:HG3	2.45	0.50
1:A:303:GLN:HE22	1:A:312:ILE:HD11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:HIS:HB2	2:B:323:LEU:CD1	2.41	0.50
2:B:319:GLY:O	2:B:320:ASP:C	2.55	0.50
1:A:65:LEU:H	1:A:65:LEU:CD2	2.24	0.50
1:A:112:ARG:HA	1:A:140:LEU:CD2	2.41	0.50
1:A:165:ASN:HD22	1:A:166:TYR:N	2.10	0.50
1:A:273:ASN:O	1:A:277:TRP:HD1	1.94	0.50
2:B:291:ARG:NH2	2:B:294:LYS:HD2	2.26	0.50
1:A:293:PRO:O	1:A:295:LEU:N	2.45	0.50
2:B:119:PRO:HD2	2:B:122:VAL:CG2	2.41	0.50
2:B:113:LEU:HA	2:B:395:GLN:HB2	1.93	0.50
1:A:67:ARG:HA	1:A:102:TYR:OH	2.11	0.49
2:B:113:LEU:HD13	2:B:367:LEU:O	2.12	0.49
2:B:248:HIS:CE1	2:B:250:GLY:H	2.29	0.49
2:B:325:MET:HE3	2:B:381:MET:HE2	1.93	0.49
1:A:116:ALA:O	1:A:117:PHE:C	2.54	0.49
2:B:77:LYS:HE2	2:B:77:LYS:HA	1.94	0.49
2:B:389:VAL:H	2:B:392:ASN:HD21	1.58	0.49
1:A:289:LEU:HD11	1:A:314:PHE:HE1	1.78	0.49
2:B:124:THR:O	2:B:128:GLN:HG3	2.13	0.49
1:A:193:LEU:HD13	1:A:203:TRP:CZ2	2.48	0.49
2:B:75:ARG:NH1	2:B:114:LEU:O	2.46	0.49
1:A:165:ASN:HD22	1:A:166:TYR:H	1.60	0.49
1:A:206:ARG:O	1:A:210:ILE:HG13	2.13	0.49
1:A:274:GLU:O	1:A:278:ASN:OD1	2.30	0.49
2:B:78:HIS:HD1	2:B:349:GLY:N	2.10	0.49
2:B:93:TYR:HD2	2:B:96:LEU:HD12	1.78	0.49
2:B:193:MET:HE1	2:B:203:SER:HA	1.94	0.49
2:B:376:PHE:CD1	2:B:376:PHE:C	2.91	0.49
1:A:91:ILE:HG22	1:A:91:ILE:O	2.13	0.48
1:A:219:GLU:O	1:A:223:VAL:HG23	2.13	0.48
2:B:192:LEU:HD23	2:B:199:VAL:HG13	1.93	0.48
1:A:165:ASN:HB3	1:A:168:VAL:CG1	2.43	0.48
2:B:34:ARG:HH11	2:B:34:ARG:CB	2.21	0.48
2:B:143:GLY:N	2:B:146:GLN:NE2	2.61	0.48
2:B:296:VAL:HG22	2:B:297:ASP:N	2.28	0.48
1:A:275:SER:C	1:A:277:TRP:H	2.20	0.48
1:A:241:HIS:HA	1:A:250:TYR:OH	2.13	0.48
1:A:56:LEU:HB3	1:A:57:SER:H	1.43	0.48
1:A:309:PRO:O	1:A:313:ALA:HB2	2.14	0.48
2:B:55:ILE:O	2:B:55:ILE:HG22	2.14	0.48
2:B:130:LEU:HD13	2:B:160:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.94	0.48
2:B:61:SER:C	2:B:63:LYS:N	2.70	0.48
2:B:304:GLN:HA	2:B:304:GLN:NE2	2.23	0.48
1:A:216:TRP:H	1:A:216:TRP:CD1	2.30	0.48
1:A:239:GLN:O	1:A:243:VAL:HG23	2.14	0.48
1:A:322:MET:HB3	1:A:327:CYS:SG	2.54	0.47
2:B:35:LEU:H	2:B:52:GLU:CD	2.22	0.47
2:B:189:GLY:O	2:B:225:THR:HA	2.14	0.47
2:B:214:THR:O	2:B:215:ASN:HB3	2.14	0.47
2:B:89:LEU:CD1	2:B:103:LEU:HD13	2.44	0.47
2:B:233:GLN:HG3	2:B:238:GLY:O	2.13	0.47
2:B:280:ARG:NH1	2:B:289:GLN:HE21	2.11	0.47
2:B:92:ALA:O	2:B:94:GLU:N	2.45	0.47
2:B:336:GLN:HG2	2:B:370:LEU:HD12	1.96	0.47
2:B:372:ILE:HD11	2:B:397:THR:HG23	1.96	0.47
1:A:222:TYR:CZ	1:A:226:LEU:HD11	2.50	0.47
2:B:82:LEU:O	2:B:83:LYS:C	2.58	0.47
2:B:302:PHE:CZ	2:B:402:ASN:HB2	2.50	0.47
1:A:291:ARG:NH1	1:A:291:ARG:HB3	2.29	0.47
1:A:336:LYS:O	1:A:340:LEU:HG	2.14	0.47
1:A:351:ILE:O	2:B:331:HIS:HB2	2.15	0.47
2:B:51:VAL:HG21	2:B:295:LEU:HD13	1.96	0.47
2:B:91:ASP:O	2:B:94:GLU:HB2	2.15	0.47
2:B:119:PRO:C	2:B:121:ILE:N	2.72	0.47
2:B:51:VAL:HG21	2:B:295:LEU:HD22	1.96	0.47
2:B:315:LEU:O	2:B:320:ASP:HB3	2.14	0.47
2:B:349:GLY:C	2:B:350:LEU:HD12	2.40	0.47
2:B:70:ARG:HE	2:B:70:ARG:HB2	1.55	0.47
2:B:280:ARG:O	2:B:289:GLN:HG2	2.15	0.47
2:B:282:MET:SD	2:B:289:GLN:HB3	2.55	0.47
1:A:112:ARG:O	1:A:144:LEU:HD21	2.14	0.46
1:A:64:VAL:HG23	1:A:69:ARG:HE	1.80	0.46
2:B:82:LEU:CD1	2:B:111:LEU:HD23	2.45	0.46
2:B:231:ARG:HE	2:B:231:ARG:HB3	1.47	0.46
2:B:24:TYR:HB2	2:B:333:GLN:NE2	2.31	0.46
2:B:280:ARG:HH11	2:B:289:GLN:HE21	1.63	0.46
2:B:78:HIS:HD1	2:B:349:GLY:H	1.64	0.46
2:B:122:VAL:O	2:B:126:VAL:HG23	2.16	0.46
2:B:239:ILE:HB	2:B:252:THR:HA	1.97	0.46
1:A:227:LEU:HG	1:A:236:VAL:CG1	2.46	0.46
1:A:277:TRP:CE3	1:A:314:PHE:HD2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASN:O	1:A:332:ASP:HB3	2.16	0.46
2:B:325:MET:O	2:B:376:PHE:CE1	2.69	0.46
2:B:415:PHE:C	2:B:417:GLN:H	2.22	0.46
1:A:268:LYS:HA	1:A:306:HIS:HD2	1.80	0.46
1:A:329:ASN:O	1:A:330:LYS:C	2.58	0.46
2:B:202:ARG:HB2	2:B:202:ARG:CZ	2.46	0.46
1:A:96:PHE:CD2	1:A:126:LEU:HB3	2.51	0.46
1:A:185:GLU:O	1:A:188:PHE:HB3	2.16	0.46
2:B:297:ASP:OD1	2:B:298:GLY:N	2.49	0.46
2:B:316:HIS:ND1	2:B:316:HIS:C	2.74	0.46
1:A:105:ALA:O	1:A:109:ARG:HG2	2.16	0.46
1:A:232:ARG:HH21	2:B:37:ASP:HA	1.80	0.46
2:B:68:VAL:HB	2:B:69:PRO:HD3	1.98	0.46
1:A:152:MET:O	1:A:155:ILE:HG22	2.16	0.45
1:A:185:GLU:OE1	1:A:205:HIS:HE1	1.99	0.45
2:B:174:ARG:HD2	2:B:415:PHE:CE1	2.51	0.45
2:B:266:ARG:C	2:B:268:LEU:N	2.72	0.45
1:A:268:LYS:HA	1:A:306:HIS:CD2	2.51	0.45
2:B:94:GLU:O	2:B:97:ASP:HB2	2.16	0.45
2:B:105:TYR:HE1	2:B:158:ASN:HD22	1.61	0.45
2:B:225:THR:O	2:B:226:ALA:C	2.59	0.45
1:A:60:SER:HB2	1:A:62:THR:HG22	1.97	0.45
1:A:290:SER:HB2	1:A:321:ASP:CG	2.41	0.45
1:A:308:SER:C	1:A:310:TYR:H	2.25	0.45
1:A:324:GLU:HA	1:A:324:GLU:OE2	2.17	0.45
2:B:35:LEU:HB3	2:B:52:GLU:OE1	2.16	0.45
2:B:248:HIS:HB3	2:B:251:TYR:HD2	1.80	0.45
2:B:288:PHE:HB2	2:B:300:TYR:O	2.15	0.45
2:B:114:LEU:HG	2:B:367:LEU:HD13	1.97	0.45
1:A:116:ALA:O	1:A:119:LEU:N	2.49	0.45
1:A:274:GLU:HG2	1:A:278:ASN:OD1	2.17	0.45
1:A:275:SER:C	1:A:277:TRP:N	2.75	0.45
2:B:184:LEU:HD13	2:B:192:LEU:O	2.17	0.45
1:A:253:ARG:HA	1:A:253:ARG:HD3	1.80	0.45
2:B:282:MET:HB2	2:B:285:GLU:HB2	1.98	0.45
2:B:105:TYR:CD1	2:B:158:ASN:HB3	2.52	0.45
2:B:167:GLU:O	2:B:171:VAL:HG23	2.17	0.45
2:B:248:HIS:HE1	2:B:300:TYR:OH	1.99	0.45
1:A:140:LEU:O	1:A:144:LEU:HB2	2.17	0.45
2:B:411:ALA:O	2:B:414:HIS:HB3	2.17	0.45
1:A:139:VAL:O	1:A:142:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:PHE:CD1	2:B:116:GLU:HG3	2.51	0.44
2:B:389:VAL:N	2:B:392:ASN:ND2	2.66	0.44
1:A:272:HIS:NE2	2:B:36:GLN:NE2	2.65	0.44
1:A:334:LEU:O	1:A:334:LEU:HD12	2.17	0.44
1:A:302:LEU:HB3	1:A:306:HIS:HB2	1.99	0.44
2:B:27:ARG:HB3	2:B:29:GLU:OE1	2.18	0.44
2:B:191:PHE:O	2:B:199:VAL:HG12	2.16	0.44
1:A:156:ILE:HG23	1:A:188:PHE:CE1	2.53	0.44
1:A:344:LEU:HD13	1:A:356:TRP:CZ2	2.53	0.44
2:B:40:VAL:HG12	2:B:40:VAL:O	2.17	0.44
2:B:51:VAL:O	2:B:55:ILE:HG12	2.17	0.44
2:B:22:PRO:HG2	2:B:23:LEU:H	1.83	0.44
1:A:135:HIS:CD2	2:B:147:TYR:CE2	3.06	0.44
2:B:98:ALA:HA	2:B:146:GLN:HE22	1.82	0.44
2:B:389:VAL:HG22	2:B:392:ASN:ND2	2.33	0.44
2:B:64:PHE:O	2:B:65:ASN:OD1	2.35	0.44
2:B:119:PRO:O	2:B:121:ILE:N	2.51	0.44
2:B:304:GLN:O	2:B:307:LEU:HB2	2.18	0.44
2:B:329:MET:HE3	2:B:329:MET:HB2	1.77	0.44
2:B:298:GLY:O	2:B:299:CYS:O	2.35	0.43
2:B:305:ALA:O	2:B:309:PRO:HD3	2.18	0.43
1:A:96:PHE:CE2	1:A:126:LEU:HB3	2.54	0.43
1:A:234:ASN:ND2	2:B:246:GLU:OE2	2.44	0.43
1:A:239:GLN:HA	1:A:239:GLN:NE2	2.33	0.43
1:A:282:GLY:HA2	1:A:285:GLN:HG2	2.00	0.43
1:A:331:GLU:O	1:A:335:ASN:ND2	2.51	0.43
1:A:357:ARG:CB	1:A:361:ARG:HH12	2.29	0.43
2:B:304:GLN:HE21	2:B:304:GLN:CA	2.19	0.43
1:A:356:TRP:HA	1:A:356:TRP:HE3	1.79	0.43
2:B:26:LEU:HD12	2:B:26:LEU:N	2.32	0.43
2:B:113:LEU:HD13	2:B:367:LEU:C	2.43	0.43
2:B:362:HIS:CD2	2:B:362:HIS:N	2.85	0.43
1:A:124:ILE:HD11	1:A:137:ARG:HD2	2.00	0.43
1:A:189:ILE:HB	1:A:206:ARG:NH1	2.34	0.43
1:A:354:GLU:HG2	2:B:328:TRP:O	2.18	0.43
2:B:128:GLN:O	2:B:131:GLU:HB3	2.17	0.43
2:B:149:HIS:ND1	2:B:152:PRO:HD2	2.33	0.43
2:B:109:HIS:CE1	2:B:402:ASN:O	2.71	0.43
2:B:48:GLN:HE21	2:B:52:GLU:CG	2.32	0.43
2:B:301:SER:O	2:B:369:GLY:CA	2.67	0.43
1:A:155:ILE:HD13	1:A:171:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:PHE:O	2:B:65:ASN:CG	2.62	0.43
2:B:77:LYS:HE2	2:B:80:HIS:CD2	2.54	0.43
1:A:274:GLU:O	1:A:274:GLU:HG2	2.19	0.43
1:A:349:ASP:OD1	2:B:283:ARG:NH2	2.51	0.42
2:B:101:PRO:O	2:B:104:CYS:HB2	2.18	0.42
2:B:342:CYS:O	2:B:354:PRO:HG3	2.19	0.42
1:A:353:LYS:HE3	2:B:331:HIS:NE2	2.34	0.42
2:B:31:ALA:O	2:B:34:ARG:HG2	2.19	0.42
1:A:103:PHE:HA	1:A:119:LEU:HD21	2.00	0.42
1:A:284:LEU:C	1:A:286:ASP:N	2.77	0.42
1:A:291:ARG:NH1	1:A:291:ARG:CB	2.82	0.42
1:A:307:SER:O	1:A:308:SER:HB3	2.19	0.42
1:A:331:GLU:CD	1:A:331:GLU:N	2.77	0.42
2:B:182:TYR:OH	2:B:218:THR:OG1	2.22	0.42
2:B:266:ARG:C	2:B:268:LEU:H	2.27	0.42
2:B:295:LEU:HA	2:B:295:LEU:HD23	1.75	0.42
1:A:166:TYR:OH	2:B:198:GLU:HB2	2.20	0.42
1:A:345:ALA:HB2	1:A:356:TRP:HB3	2.01	0.42
2:B:158:ASN:ND2	2:B:403:ILE:HG23	2.35	0.42
1:A:176:VAL:HG21	1:A:185:GLU:OE1	2.20	0.42
1:A:303:GLN:NE2	1:A:312:ILE:HD11	2.34	0.42
1:A:356:TRP:CZ3	1:A:359:ILE:HG13	2.54	0.42
2:B:200:ASP:OD1	2:B:202:ARG:NH1	2.52	0.42
2:B:376:PHE:HB3	2:B:383:HIS:O	2.20	0.42
1:A:220:LEU:O	1:A:223:VAL:HB	2.19	0.42
2:B:328:TRP:CZ2	2:B:376:PHE:HA	2.55	0.42
1:A:291:ARG:CB	1:A:291:ARG:HH11	2.33	0.42
1:A:304:PRO:HB2	1:A:305:SER:H	1.73	0.42
2:B:158:ASN:ND2	2:B:403:ILE:CG2	2.83	0.42
2:B:177:LEU:HD21	2:B:210:VAL:CG1	2.50	0.42
2:B:177:LEU:HD21	2:B:210:VAL:HG12	2.02	0.42
2:B:301:SER:O	2:B:369:GLY:HA3	2.20	0.41
2:B:362:HIS:C	2:B:364:CYS:N	2.78	0.41
2:B:164:GLY:HA2	2:B:169:TYR:CZ	2.55	0.41
2:B:257:ALA:HB1	2:B:400:VAL:HG13	2.01	0.41
1:A:185:GLU:OE1	1:A:205:HIS:CE1	2.73	0.41
1:A:130:ASN:ND2	2:B:98:ALA:HB2	2.35	0.41
1:A:63:TYR:CE2	1:A:95:LYS:HE3	2.56	0.41
1:A:101:ASP:HA	1:A:104:ARG:HH11	1.86	0.41
1:A:296:LEU:HD22	1:A:322:MET:SD	2.60	0.41
2:B:216:ILE:O	2:B:216:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:389:VAL:HG23	2:B:391:GLU:H	1.85	0.41
1:A:103:PHE:CE2	1:A:133:VAL:HG22	2.56	0.41
1:A:134:TRP:HZ3	1:A:171:HIS:CD2	2.38	0.41
1:A:142:ARG:HD2	1:A:143:SER:N	2.35	0.41
1:A:106:VAL:HG13	1:A:111:GLU:HB3	2.03	0.41
1:A:112:ARG:HG2	1:A:112:ARG:HH11	1.86	0.41
1:A:297:ASN:O	1:A:300:LEU:N	2.53	0.41
2:B:25:SER:HA	2:B:30:HIS:ND1	2.36	0.41
2:B:54:LYS:C	2:B:56:GLN:N	2.78	0.41
2:B:64:PHE:O	2:B:64:PHE:HD1	2.03	0.41
2:B:93:TYR:CE2	2:B:360:PHE:HD2	2.39	0.41
2:B:181:LEU:CD1	2:B:211:ALA:HB2	2.51	0.41
2:B:266:ARG:CG	2:B:318:GLN:HE21	2.32	0.41
1:A:143:SER:C	1:A:145:GLN:N	2.78	0.41
1:A:198:LYS:HE2	1:A:233:ASN:HA	2.02	0.41
2:B:62:TYR:HE2	2:B:71:LEU:HD23	1.86	0.41
2:B:297:ASP:OD1	2:B:297:ASP:C	2.63	0.41
2:B:323:LEU:O	2:B:324:SER:C	2.62	0.41
2:B:175:GLU:H	2:B:175:GLU:CD	2.28	0.40
1:A:213:PHE:CD1	1:A:213:PHE:N	2.89	0.40
2:B:89:LEU:HD11	2:B:103:LEU:HD13	2.02	0.40
2:B:241:GLY:HA2	2:B:251:TYR:CD1	2.56	0.40
2:B:306:GLY:C	2:B:309:PRO:HD2	2.47	0.40
1:A:210:ILE:HD13	1:A:219:GLU:HG2	2.03	0.40
2:B:115:ASP:O	2:B:115:ASP:OD1	2.39	0.40
2:B:118:ILE:N	2:B:118:ILE:CD1	2.85	0.40
1:A:71:GLU:CD	1:A:71:GLU:N	2.73	0.40
1:A:170:HIS:HD1	2:B:198:GLU:CG	2.34	0.40
1:A:355:TYR:OH	2:B:275:GLN:HG2	2.21	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	313/315 (99%)	257 (82%)	42 (13%)	14 (4%)	2	17
2	B	395/397 (100%)	334 (85%)	50 (13%)	11 (3%)	4	26
All	All	708/712 (99%)	591 (84%)	92 (13%)	25 (4%)	3	23

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	185	GLU
1	A	294	ASN
1	A	304	PRO
2	B	66	HIS
1	A	217	ASP
2	B	299	CYS
2	B	360	PHE
1	A	216	TRP
1	A	296	LEU
2	B	93	TYR
1	A	92	TYR
1	A	230	ASP
1	A	293	PRO
1	A	305	SER
1	A	308	SER
1	A	330	LYS
2	B	320	ASP
2	B	68	VAL
2	B	74	GLN
2	B	75	ARG
2	B	83	LYS
2	B	352	ASP
2	B	357	SER
1	A	303	GLN

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	294/294 (100%)	285 (97%)	9 (3%)	35	59
2	B	335/335 (100%)	323 (96%)	12 (4%)	31	57
All	All	629/629 (100%)	608 (97%)	21 (3%)	33	58

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	71	GLU
1	A	94	GLU
1	A	178	TRP
1	A	182	PRO
1	A	286	ASP
1	A	352	ARG
1	A	356	TRP
1	A	366	LYS
2	B	29	GLU
2	B	34	ARG
2	B	67	LEU
2	B	68	VAL
2	B	99	SER
2	B	158	ASN
2	B	193	MET
2	B	280	ARG
2	B	299	CYS
2	B	304	GLN
2	B	316	HIS
2	B	354	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	127	ASN
1	A	130	ASN
1	A	135	HIS
1	A	165	ASN
1	A	167	GLN
1	A	195	GLN
1	A	218	ASN
1	A	221	GLN

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Mol	Chain	Res	Type
1	A	239	GLN
1	A	246	ASN
1	A	285	GLN
1	A	298	GLN
1	A	303	GLN
1	A	325	ASN
1	A	335	ASN
1	A	364	GLN
2	B	36	GLN
2	B	48	GLN
2	B	128	GLN
2	B	134	GLN
2	B	146	GLN
2	B	158	ASN
2	B	289	GLN
2	B	293	ASN
2	B	304	GLN
2	B	318	GLN
2	B	333	GLN
2	B	344	GLN
2	B	362	HIS
2	B	383	HIS
2	B	417	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
4	JAN	B	1	-	33,38,38	3.35	16 (48%)	47,57,57	1.32	7 (14%)

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	JAN	B	1	-	-	1/16/22/22	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	JAN	C14-C17	11.20	1.57	1.41
4	B	1	JAN	C20-C21	8.08	1.44	1.35
4	B	1	JAN	C7-C6	4.53	1.46	1.39
4	B	1	JAN	C23-C24	4.16	1.45	1.38
4	B	1	JAN	C25-C24	3.99	1.45	1.38
4	B	1	JAN	C11-C6	3.81	1.45	1.39
4	B	1	JAN	C26-C25	3.64	1.45	1.38
4	B	1	JAN	C26-C27	3.51	1.44	1.38
4	B	1	JAN	C8-C7	3.34	1.44	1.38
4	B	1	JAN	C15-C12	3.32	1.44	1.39
4	B	1	JAN	C10-C9	3.32	1.44	1.38
4	B	1	JAN	C16-C15	2.85	1.43	1.38
4	B	1	JAN	C14-C21	-2.70	1.41	1.47
4	B	1	JAN	C27-C22	2.67	1.43	1.39
4	B	1	JAN	C8-C9	2.47	1.42	1.38
4	B	1	JAN	C24-CL2	-2.10	1.69	1.74

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	JAN	N1-C2-N2	3.82	115.22	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	JAN	C20-C19-N4	2.97	118.35	115.44
4	B	1	JAN	O1-C19-C20	-2.30	119.93	125.61
4	B	1	JAN	C16-C17-N4	2.20	123.97	121.04
4	B	1	JAN	C17-C14-C21	-2.04	117.24	119.56
4	B	1	JAN	C14-C13-C12	2.03	125.13	121.98
4	B	1	JAN	C6-C5-N3	2.00	111.87	108.60

There are no chirality outliers.

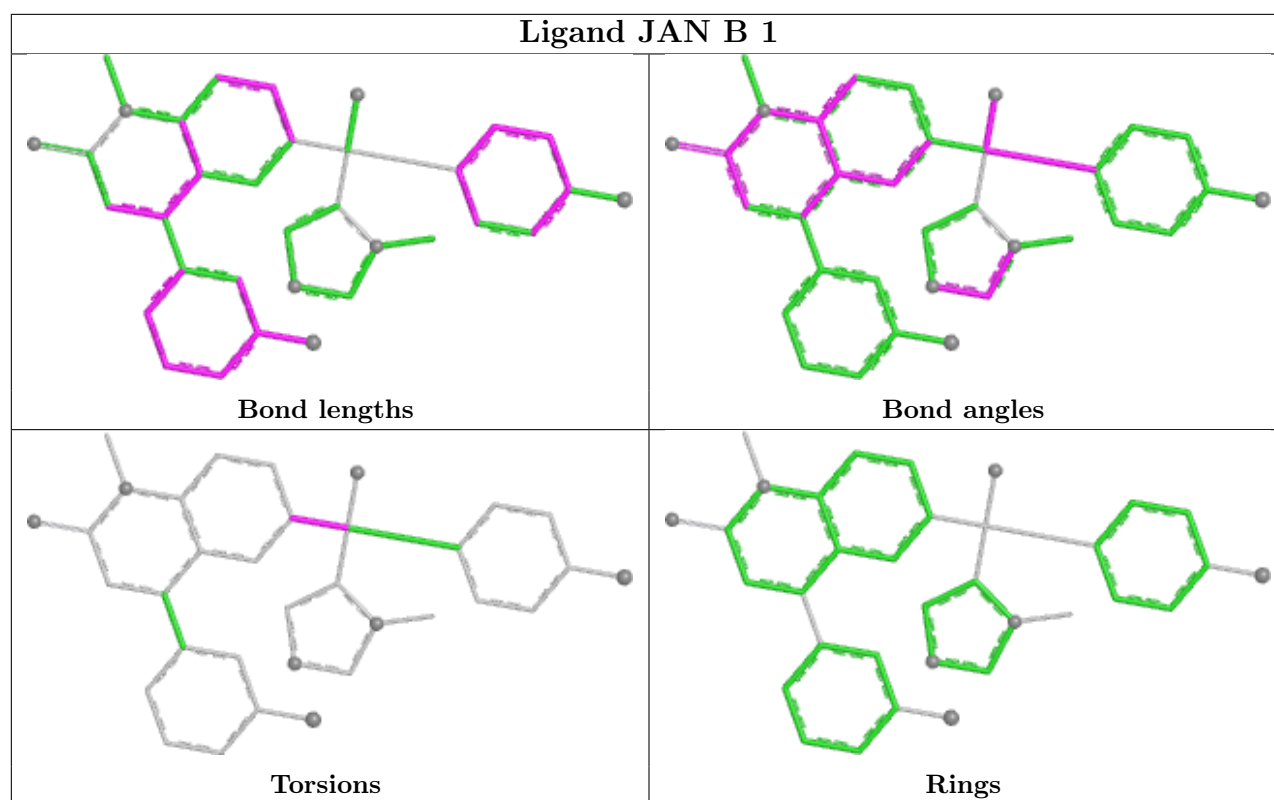
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	JAN	C13-C12-C5-C4

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.