



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:35 PM UTC

PDB ID : 3OTQ / pdb_00003otq
Title : Soluble Epoxide Hydrolase in complex with pyrazole antagonist
Authors : Farrow, N.A.
Deposited on : 2010-09-13
Resolution : 3.00 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

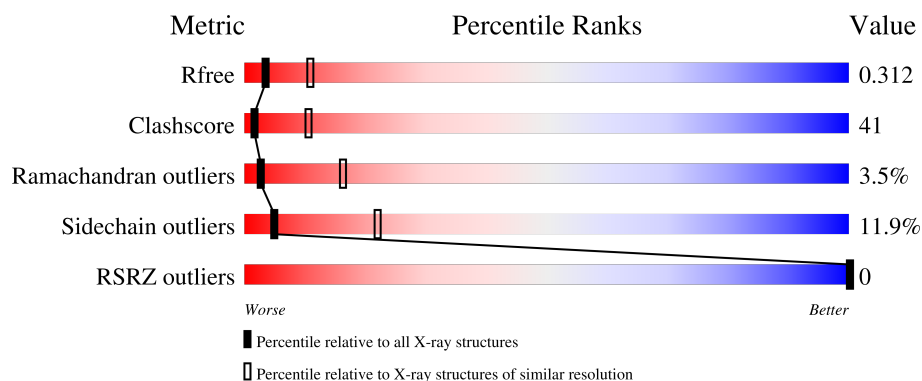
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	555	

2 Entry composition [i](#)

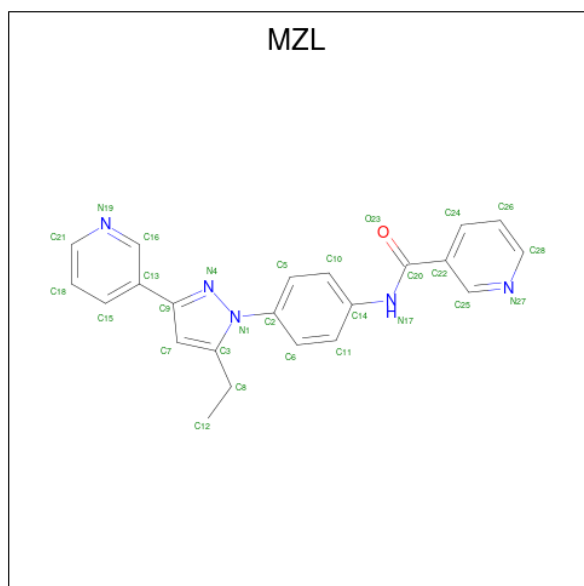
There are 3 unique types of molecules in this entry. The entry contains 4385 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Epoxide hydrolase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	545	4316	2765	728	787	36	0	0	0

- Molecule 2 is N-[4-(5-ethyl-3-pyridin-3-yl-1H-pyrazol-1-yl)phenyl]pyridine-3-carboxamide (CCD ID: MZL) (formula: C₂₂H₁₉N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	28	22	5	1	0	0

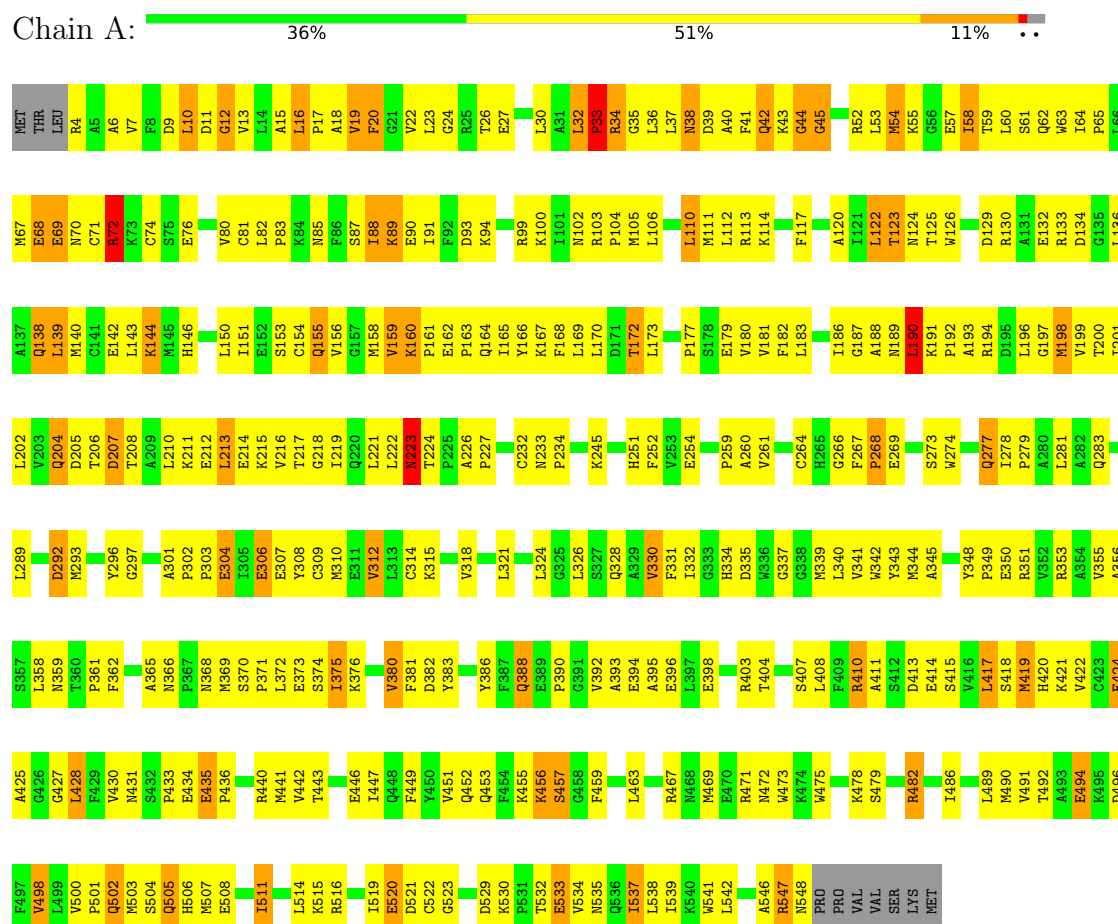
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	41	Total 41 O 41	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: Epoxide hydrolase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.99Å 92.99Å 243.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 97.3 (50.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 3.01Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.230 , 0.318 0.225 , 0.312	Depositor DCC
R_{free} test set	676 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4385	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: MZL

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	0.57	0/4421	1.10	28/5990 (0.5%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	LYS	N-CA-C	-8.89	102.42	113.18
1	A	72	ARG	N-CA-C	-7.94	102.57	114.64
1	A	88	ILE	N-CA-C	-7.02	102.74	112.50
1	A	388	GLN	N-CA-C	6.98	118.97	111.36
1	A	302	PRO	CA-C-N	6.87	126.11	118.97
1	A	302	PRO	C-N-CA	6.87	126.11	118.97
1	A	198	MET	N-CA-C	6.25	119.43	110.24
1	A	511	ILE	CA-C-N	6.16	127.54	119.84
1	A	511	ILE	C-N-CA	6.16	127.54	119.84
1	A	292	ASP	N-CA-C	-6.13	95.53	107.62
1	A	68	GLU	N-CA-C	-6.01	104.42	110.97
1	A	537	ILE	N-CA-C	5.89	116.67	110.72
1	A	57	GLU	N-CA-C	-5.87	106.46	113.97
1	A	318	VAL	N-CA-C	-5.84	105.04	110.53
1	A	467	ARG	N-CA-C	5.78	119.10	112.57
1	A	204	GLN	N-CA-C	-5.76	102.11	111.04
1	A	123	THR	N-CA-C	5.74	118.81	108.48
1	A	494	GLU	N-CA-C	5.58	117.81	111.11
1	A	113	ARG	N-CA-C	-5.46	105.22	111.07
1	A	227	PRO	N-CA-C	5.38	118.75	111.22
1	A	32	LEU	CA-C-N	5.32	126.50	119.84
1	A	32	LEU	C-N-CA	5.32	126.50	119.84
1	A	226	ALA	CA-C-N	5.17	125.17	120.21
1	A	226	ALA	C-N-CA	5.17	125.17	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	ASP	N-CA-C	-5.13	104.31	111.39
1	A	233	ASN	CA-C-N	5.12	126.25	119.84
1	A	233	ASN	C-N-CA	5.12	126.25	119.84
1	A	505	GLN	N-CA-C	5.08	117.71	111.82

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	4316	0	4317	360	1
2	A	28	0	19	3	0
3	A	41	0	0	2	0
All	All	4385	0	4336	360	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (360) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:HD12	1:A:100:LYS:HB2	1.32	1.11
1:A:80:VAL:HG12	1:A:81:CYS:H	1.01	1.08
1:A:17:PRO:HD2	1:A:99:ARG:HA	1.43	1.00
1:A:67:MET:HG3	1:A:88:ILE:HD13	1.45	0.99
1:A:170:LEU:HD13	1:A:198:MET:HE1	1.46	0.95
1:A:13:VAL:HG13	1:A:105:MET:HE3	1.48	0.94
1:A:217:THR:HB	1:A:219:ILE:HD12	1.47	0.93
1:A:80:VAL:CG1	1:A:81:CYS:H	1.84	0.90
1:A:208:THR:HA	1:A:211:LYS:HE3	1.52	0.89
1:A:69:GLU:HA	1:A:72:ARG:NH1	1.88	0.88
1:A:80:VAL:HG12	1:A:81:CYS:N	1.84	0.88
1:A:19:VAL:O	1:A:22:VAL:HG12	1.75	0.86
1:A:15:ALA:HB1	1:A:99:ARG:HD2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HG	1:A:169:LEU:HD22	1.60	0.83
1:A:27:GLU:HG3	1:A:37:LEU:HG	1.60	0.82
1:A:193:ALA:HB1	1:A:198:MET:HG3	1.62	0.81
1:A:498:VAL:HG11	2:A:556:MZL:H6	1.61	0.81
1:A:64:ILE:HB	1:A:65:PRO:HD3	1.63	0.80
1:A:447:ILE:O	1:A:451:VAL:HG23	1.81	0.80
1:A:37:LEU:C	1:A:39:ASP:H	1.90	0.79
1:A:16:LEU:HA	3:A:569:HOH:O	1.82	0.79
1:A:162:GLU:HB3	1:A:164:GLN:HG2	1.65	0.79
1:A:165:ILE:O	1:A:168:PHE:HB3	1.83	0.79
1:A:183:LEU:HD22	1:A:201:ILE:HB	1.65	0.78
1:A:16:LEU:CD1	1:A:100:LYS:HB2	2.15	0.77
1:A:199:VAL:HG11	1:A:216:VAL:HG21	1.66	0.75
1:A:519:ILE:HG22	1:A:522:CYS:HB2	1.68	0.75
1:A:159:VAL:HG22	1:A:161:PRO:HD2	1.68	0.75
1:A:502:GLN:HG3	1:A:503:MET:N	2.01	0.74
1:A:89:LYS:HG3	1:A:90:GLU:N	2.02	0.74
1:A:16:LEU:HB2	1:A:17:PRO:HD3	1.70	0.73
1:A:245:LYS:NZ	1:A:245:LYS:HB3	2.03	0.73
1:A:245:LYS:HB3	1:A:245:LYS:HZ3	1.53	0.73
1:A:530:LYS:HB3	1:A:533:GLU:CG	2.19	0.72
1:A:16:LEU:CB	1:A:17:PRO:HD3	2.19	0.72
1:A:479:SER:HB2	1:A:482:ARG:HG3	1.72	0.72
1:A:191:LYS:HB2	1:A:192:PRO:HD3	1.72	0.72
1:A:530:LYS:HB3	1:A:533:GLU:HG2	1.72	0.71
1:A:161:PRO:HG3	1:A:189:ASN:OD1	1.91	0.71
1:A:208:THR:HA	1:A:211:LYS:HB2	1.72	0.71
1:A:111:MET:HE3	1:A:114:LYS:HB3	1.71	0.71
1:A:533:GLU:O	1:A:537:ILE:HG13	1.90	0.70
1:A:269:GLU:HB3	1:A:273:SER:OG	1.92	0.70
1:A:26:THR:HG21	1:A:91:ILE:HD13	1.73	0.70
1:A:278:ILE:HB	1:A:279:PRO:HD3	1.73	0.70
1:A:380:VAL:HG11	1:A:498:VAL:HA	1.71	0.70
1:A:177:PRO:HA	1:A:198:MET:HE2	1.72	0.70
1:A:110:LEU:HD21	1:A:146:HIS:HB3	1.72	0.70
1:A:170:LEU:HD21	1:A:177:PRO:HG3	1.75	0.69
1:A:504:SER:HB2	1:A:507:MET:SD	2.33	0.69
1:A:194:ARG:HB2	1:A:194:ARG:NH1	2.06	0.69
1:A:124:ASN:ND2	1:A:160:LYS:HB2	2.08	0.69
1:A:261:VAL:HA	1:A:330:VAL:HG13	1.74	0.69
1:A:274:TRP:HE3	1:A:277:GLN:HG3	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:CD2	1:A:146:HIS:HB3	2.23	0.68
1:A:124:ASN:CG	1:A:160:LYS:HB2	2.18	0.68
1:A:321:LEU:HD11	1:A:331:PHE:HZ	1.58	0.68
1:A:43:LYS:CD	1:A:44:GLY:H	2.07	0.67
1:A:59:THR:OG1	1:A:62:GLN:HG3	1.94	0.67
1:A:266:GLY:HA3	1:A:335:ASP:HB3	1.76	0.67
1:A:252:PHE:CE2	1:A:289:LEU:HD22	2.29	0.67
1:A:382:ASP:OD2	1:A:422:VAL:N	2.27	0.67
1:A:410:ARG:NH2	1:A:414:GLU:HB3	2.09	0.67
1:A:68:GLU:HA	1:A:88:ILE:HD12	1.76	0.67
1:A:304:GLU:H	1:A:304:GLU:CD	2.01	0.66
1:A:23:LEU:HD22	1:A:38:ASN:HA	1.77	0.66
1:A:187:GLY:O	1:A:190:LEU:HB2	1.95	0.66
1:A:27:GLU:OE1	1:A:35:GLY:N	2.27	0.66
1:A:340:LEU:O	1:A:344:MET:HG2	1.95	0.66
1:A:372:LEU:H	1:A:372:LEU:HD22	1.61	0.66
1:A:23:LEU:HB2	1:A:38:ASN:OD1	1.95	0.66
1:A:23:LEU:HB2	1:A:38:ASN:CG	2.21	0.66
1:A:494:GLU:HB2	1:A:520:GLU:HA	1.77	0.66
1:A:190:LEU:H	1:A:192:PRO:HD2	1.61	0.65
1:A:43:LYS:CG	1:A:44:GLY:H	2.09	0.65
1:A:139:LEU:HD23	1:A:139:LEU:O	1.96	0.65
1:A:212:GLU:O	1:A:215:LYS:HB3	1.97	0.65
1:A:213:LEU:HD22	1:A:221:LEU:HD11	1.77	0.65
1:A:33:PRO:HG2	1:A:80:VAL:HG21	1.79	0.65
1:A:410:ARG:HH22	1:A:414:GLU:HB3	1.62	0.65
1:A:261:VAL:HG22	1:A:330:VAL:CG1	2.27	0.64
1:A:69:GLU:HG3	1:A:72:ARG:HH12	1.61	0.64
1:A:124:ASN:OD1	1:A:160:LYS:HB2	1.96	0.64
1:A:151:ILE:HD11	1:A:172:THR:HG21	1.79	0.64
1:A:371:PRO:HG2	1:A:473:TRP:HB2	1.79	0.64
1:A:60:LEU:HD23	1:A:130:ARG:HG3	1.79	0.63
1:A:140:MET:HE3	1:A:140:MET:HA	1.80	0.63
1:A:310:MET:HG2	1:A:472:ASN:ND2	2.13	0.63
1:A:310:MET:HG3	1:A:343:TYR:CE1	2.33	0.63
1:A:315:LYS:O	1:A:315:LYS:HD3	1.99	0.63
1:A:62:GLN:O	1:A:65:PRO:HD2	1.98	0.62
1:A:217:THR:CB	1:A:219:ILE:HD12	2.24	0.62
1:A:69:GLU:HA	1:A:72:ARG:HH11	1.65	0.62
1:A:169:LEU:O	1:A:173:LEU:HB2	1.99	0.62
1:A:498:VAL:HG11	2:A:556:MZL:C6	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:PRO:CD	1:A:99:ARG:HA	2.24	0.62
1:A:37:LEU:O	1:A:39:ASP:N	2.32	0.62
1:A:111:MET:O	1:A:114:LYS:HB3	2.00	0.62
1:A:394:GLU:O	1:A:398:GLU:HG3	2.01	0.61
1:A:490:MET:HE3	1:A:491:VAL:N	2.15	0.60
1:A:261:VAL:HG22	1:A:330:VAL:HG11	1.83	0.60
1:A:36:LEU:C	1:A:36:LEU:HD13	2.26	0.60
1:A:44:GLY:O	1:A:45:GLY:C	2.45	0.59
1:A:160:LYS:HB3	1:A:161:PRO:HD3	1.82	0.59
1:A:170:LEU:HD13	1:A:198:MET:CE	2.26	0.59
1:A:420:HIS:O	1:A:421:LYS:HB3	2.01	0.59
1:A:345:ALA:HB1	1:A:486:ILE:HD11	1.84	0.59
1:A:37:LEU:C	1:A:39:ASP:N	2.61	0.59
1:A:23:LEU:HB3	1:A:37:LEU:HB2	1.84	0.59
1:A:414:GLU:CD	1:A:440:ARG:HG2	2.28	0.59
1:A:54:MET:HA	1:A:54:MET:HE3	1.85	0.59
1:A:158:MET:HG2	1:A:164:GLN:OE1	2.03	0.59
1:A:170:LEU:CD2	1:A:177:PRO:HG3	2.32	0.58
1:A:232:CYS:O	1:A:234:PRO:HD3	2.04	0.58
1:A:411:ALA:N	1:A:441:MET:HE2	2.19	0.58
1:A:368:ASN:HB3	1:A:369:MET:HE2	1.84	0.58
1:A:451:VAL:HG12	1:A:455:LYS:NZ	2.19	0.58
1:A:328:GLN:OE1	1:A:353:ARG:HB2	2.03	0.58
1:A:358:LEU:O	1:A:359:ASN:HB2	2.02	0.58
1:A:361:PRO:HB3	1:A:504:SER:HB3	1.86	0.57
1:A:403:ARG:NH1	1:A:434:GLU:HG2	2.19	0.57
1:A:30:LEU:HD13	1:A:83:PRO:HG2	1.86	0.57
1:A:309:CYS:SG	1:A:312:VAL:HG13	2.45	0.57
1:A:10:LEU:HD22	1:A:140:MET:HE1	1.85	0.57
1:A:372:LEU:HD22	1:A:372:LEU:N	2.19	0.57
1:A:163:PRO:HA	1:A:166:TYR:HD1	1.69	0.56
1:A:372:LEU:H	1:A:372:LEU:CD2	2.18	0.56
1:A:19:VAL:HG23	1:A:99:ARG:HD3	1.87	0.56
1:A:43:LYS:CG	1:A:44:GLY:N	2.68	0.56
1:A:112:LEU:C	1:A:117:PHE:HB2	2.31	0.56
1:A:260:ALA:O	1:A:330:VAL:HG12	2.06	0.56
1:A:124:ASN:HD21	1:A:160:LYS:HB2	1.71	0.55
1:A:163:PRO:HA	1:A:166:TYR:CD1	2.41	0.55
1:A:190:LEU:CD2	1:A:200:THR:HB	2.36	0.55
1:A:43:LYS:HG3	1:A:44:GLY:H	1.71	0.55
1:A:183:LEU:CD2	1:A:201:ILE:HD12	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:PRO:HB2	1:A:197:GLY:HA3	1.87	0.55
1:A:23:LEU:HD12	1:A:23:LEU:H	1.71	0.55
1:A:60:LEU:HD22	1:A:126:TRP:CD1	2.41	0.55
1:A:69:GLU:HG3	1:A:72:ARG:NH1	2.21	0.55
1:A:535:ASN:O	1:A:539:ILE:HG13	2.06	0.55
1:A:490:MET:HB3	1:A:514:LEU:HD11	1.87	0.55
1:A:388:GLN:O	1:A:390:PRO:HD3	2.06	0.55
1:A:404:THR:O	1:A:408:LEU:HG	2.07	0.55
1:A:459:PHE:O	1:A:463:LEU:HD12	2.07	0.55
1:A:64:ILE:O	1:A:68:GLU:HG2	2.06	0.54
1:A:373:GLU:O	1:A:375:ILE:N	2.40	0.54
1:A:4:ARG:HA	1:A:179:GLU:O	2.07	0.54
1:A:170:LEU:HD21	1:A:177:PRO:CG	2.37	0.54
1:A:356:ALA:HB2	1:A:541:TRP:CH2	2.43	0.54
1:A:27:GLU:OE2	1:A:37:LEU:N	2.34	0.54
1:A:538:LEU:O	1:A:542:LEU:HG	2.08	0.54
1:A:216:VAL:HG22	1:A:216:VAL:O	2.06	0.54
1:A:403:ARG:CZ	1:A:434:GLU:HG2	2.37	0.54
1:A:362:PHE:HB3	1:A:507:MET:HE3	1.90	0.54
1:A:69:GLU:O	1:A:72:ARG:N	2.42	0.53
1:A:222:LEU:O	1:A:223:ASN:C	2.50	0.53
1:A:43:LYS:HG3	1:A:44:GLY:N	2.24	0.53
1:A:177:PRO:HB3	1:A:198:MET:H	1.72	0.53
1:A:356:ALA:HB2	1:A:541:TRP:CZ3	2.43	0.53
1:A:16:LEU:HB2	1:A:100:LYS:H	1.74	0.53
1:A:122:LEU:HD12	1:A:182:PHE:HE2	1.73	0.53
1:A:502:GLN:HG3	1:A:503:MET:H	1.73	0.53
1:A:213:LEU:HD22	1:A:221:LEU:CD1	2.39	0.53
1:A:523:GLY:HA3	3:A:565:HOH:O	2.08	0.52
1:A:58:ILE:HA	1:A:62:GLN:OE1	2.08	0.52
1:A:421:LYS:HE2	1:A:424:GLU:OE1	2.10	0.52
1:A:433:PRO:HB2	1:A:435:GLU:OE2	2.09	0.52
1:A:451:VAL:HG12	1:A:455:LYS:HZ2	1.73	0.52
1:A:547:ARG:O	1:A:548:ASN:HB3	2.08	0.52
1:A:181:VAL:HG12	1:A:199:VAL:HB	1.91	0.52
1:A:40:ALA:HB1	1:A:70:ASN:HB2	1.91	0.52
1:A:65:PRO:HA	1:A:68:GLU:CG	2.40	0.52
1:A:170:LEU:HD21	1:A:177:PRO:CD	2.40	0.51
1:A:332:ILE:HG12	1:A:356:ALA:HB3	1.93	0.51
1:A:383:TYR:HD2	1:A:419:MET:HB3	1.75	0.51
1:A:471:ARG:HH11	1:A:471:ARG:HG3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:GLU:CB	1:A:520:GLU:HA	2.39	0.51
1:A:530:LYS:HB3	1:A:533:GLU:HG3	1.90	0.51
1:A:16:LEU:CB	1:A:17:PRO:CD	2.89	0.51
1:A:326:LEU:O	1:A:351:ARG:NH1	2.44	0.51
1:A:65:PRO:HA	1:A:68:GLU:HG3	1.93	0.50
1:A:194:ARG:HB2	1:A:194:ARG:HH11	1.73	0.50
1:A:314:CYS:SG	1:A:340:LEU:HD22	2.51	0.50
1:A:125:THR:HG23	1:A:154:CYS:SG	2.51	0.50
1:A:223:ASN:C	1:A:223:ASN:HD22	2.18	0.50
1:A:43:LYS:HD2	1:A:44:GLY:H	1.76	0.50
1:A:321:LEU:HD11	1:A:331:PHE:CZ	2.43	0.50
1:A:511:ILE:HB	1:A:514:LEU:HB2	1.94	0.50
1:A:15:ALA:CB	1:A:99:ARG:HD2	2.36	0.50
1:A:23:LEU:HD21	1:A:41:PHE:HB2	1.93	0.50
1:A:112:LEU:O	1:A:117:PHE:HB2	2.12	0.50
1:A:122:LEU:O	1:A:160:LYS:HE2	2.12	0.50
1:A:170:LEU:HD21	1:A:177:PRO:HD3	1.93	0.50
1:A:417:LEU:HD21	1:A:428:LEU:HD11	1.94	0.50
1:A:191:LYS:HB2	1:A:192:PRO:CD	2.41	0.49
1:A:348:TYR:N	1:A:349:PRO:HD3	2.26	0.49
1:A:413:ASP:CG	1:A:440:ARG:HH21	2.21	0.49
1:A:479:SER:CB	1:A:482:ARG:HG3	2.41	0.49
1:A:187:GLY:O	1:A:188:ALA:C	2.55	0.49
1:A:496:ASP:O	1:A:500:VAL:HG12	2.12	0.49
1:A:218:GLY:C	1:A:219:ILE:HG13	2.37	0.49
1:A:12:GLY:CA	1:A:18:ALA:HB2	2.43	0.49
1:A:449:PHE:O	1:A:453:GLN:HG2	2.13	0.49
1:A:61:SER:HB2	1:A:129:ASP:OD2	2.13	0.49
1:A:190:LEU:O	1:A:191:LYS:C	2.53	0.49
1:A:264:CYS:HB3	1:A:293:MET:HE2	1.94	0.49
1:A:479:SER:HA	1:A:482:ARG:HG2	1.95	0.49
1:A:142:GLU:HG3	1:A:283:GLN:CD	2.37	0.49
1:A:251:HIS:O	1:A:292:ASP:HB2	2.12	0.49
1:A:281:LEU:HD23	1:A:539:ILE:HG12	1.94	0.49
1:A:392:VAL:O	1:A:395:ALA:HB3	2.13	0.49
1:A:87:SER:O	1:A:91:ILE:HG13	2.12	0.49
1:A:546:ALA:O	1:A:547:ARG:C	2.56	0.49
1:A:11:ASP:HA	1:A:15:ALA:HB3	1.94	0.49
1:A:53:LEU:HD13	1:A:63:TRP:HB2	1.95	0.49
1:A:160:LYS:O	1:A:166:TYR:CE1	2.66	0.48
1:A:530:LYS:O	1:A:534:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLU:O	1:A:70:ASN:C	2.55	0.48
1:A:186:ILE:O	1:A:190:LEU:HD12	2.13	0.48
1:A:328:GLN:HB2	1:A:351:ARG:O	2.13	0.48
1:A:334:HIS:O	1:A:337:GLY:N	2.46	0.48
1:A:68:GLU:O	1:A:71:CYS:HB2	2.14	0.48
1:A:222:LEU:O	1:A:223:ASN:ND2	2.46	0.48
1:A:375:ILE:HD12	1:A:381:PHE:CD2	2.49	0.48
1:A:36:LEU:HD12	1:A:37:LEU:HD23	1.95	0.48
1:A:393:ALA:O	1:A:394:GLU:C	2.57	0.48
1:A:505:GLN:HA	1:A:516:ARG:HH22	1.78	0.48
1:A:12:GLY:HA2	1:A:18:ALA:HB2	1.96	0.48
1:A:52:ARG:HB2	1:A:58:ILE:HD11	1.96	0.48
1:A:53:LEU:HD11	1:A:60:LEU:HA	1.96	0.47
1:A:422:VAL:HG13	1:A:427:GLY:O	2.14	0.47
1:A:19:VAL:O	1:A:20:PHE:C	2.57	0.47
1:A:156:VAL:HG11	1:A:168:PHE:CZ	2.49	0.47
1:A:190:LEU:HD22	1:A:200:THR:HB	1.97	0.47
1:A:23:LEU:CD2	1:A:41:PHE:HB2	2.44	0.47
1:A:183:LEU:HD21	1:A:201:ILE:HD12	1.96	0.47
1:A:306:GLU:HG2	1:A:471:ARG:HH22	1.80	0.47
1:A:441:MET:SD	1:A:529:ASP:HB2	2.54	0.47
1:A:168:PHE:C	1:A:168:PHE:CD2	2.93	0.47
1:A:43:LYS:O	1:A:44:GLY:C	2.57	0.47
1:A:142:GLU:HG3	1:A:283:GLN:NE2	2.29	0.47
1:A:514:LEU:HD13	1:A:515:LYS:O	2.15	0.47
1:A:245:LYS:NZ	1:A:245:LYS:CB	2.76	0.47
1:A:125:THR:O	1:A:154:CYS:HB3	2.14	0.46
1:A:136:LEU:HD23	1:A:136:LEU:C	2.40	0.46
1:A:22:VAL:HG13	1:A:23:LEU:HD12	1.97	0.46
1:A:530:LYS:O	1:A:533:GLU:HG2	2.16	0.46
1:A:208:THR:O	1:A:212:GLU:HG3	2.15	0.46
1:A:191:LYS:CB	1:A:192:PRO:HD3	2.44	0.46
1:A:301:ALA:HB3	1:A:457:SER:HB3	1.97	0.46
1:A:547:ARG:NH1	1:A:547:ARG:HG2	2.30	0.46
1:A:168:PHE:O	1:A:172:THR:HG22	2.15	0.46
1:A:177:PRO:HA	1:A:198:MET:CE	2.42	0.46
1:A:498:VAL:HG21	2:A:556:MZL:H11	1.98	0.46
1:A:7:VAL:HA	1:A:120:ALA:O	2.17	0.45
1:A:144:LYS:HG3	1:A:150:LEU:CD2	2.46	0.45
1:A:105:MET:SD	1:A:210:LEU:HD21	2.56	0.45
1:A:386:TYR:CE2	1:A:396:GLU:OE1	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:HG21	1:A:447:ILE:HD11	1.98	0.45
1:A:490:MET:HG2	1:A:507:MET:SD	2.56	0.45
1:A:124:ASN:HD21	1:A:160:LYS:CB	2.29	0.45
1:A:259:PRO:HG2	1:A:547:ARG:HD3	1.98	0.45
1:A:407:SER:OG	1:A:436:PRO:HG2	2.15	0.45
1:A:143:LEU:O	1:A:144:LYS:C	2.59	0.45
1:A:362:PHE:CB	1:A:507:MET:HE3	2.46	0.45
1:A:547:ARG:HH11	1:A:547:ARG:CG	2.30	0.45
1:A:55:LYS:HE2	1:A:162:GLU:OE1	2.16	0.45
1:A:492:THR:HB	1:A:501:PRO:HG3	1.98	0.45
1:A:68:GLU:OE1	1:A:88:ILE:HB	2.17	0.45
1:A:102:ASN:OD1	1:A:104:PRO:HD2	2.16	0.45
1:A:268:PRO:HA	1:A:296:TYR:HE2	1.82	0.45
1:A:331:PHE:HB3	1:A:341:VAL:HG22	1.99	0.45
1:A:205:ASP:HB2	1:A:207:ASP:OD2	2.16	0.44
1:A:267:PHE:HD2	1:A:296:TYR:HH	1.65	0.44
1:A:471:ARG:HG3	1:A:471:ARG:NH1	2.32	0.44
1:A:206:THR:HG22	1:A:210:LEU:HD11	1.99	0.44
1:A:9:ASP:O	1:A:13:VAL:HB	2.17	0.44
1:A:144:LYS:HG3	1:A:150:LEU:HD23	1.98	0.44
1:A:60:LEU:HD23	1:A:130:ARG:CG	2.47	0.44
1:A:134:ASP:O	1:A:138:GLN:HB2	2.17	0.44
1:A:519:ILE:O	1:A:522:CYS:HB3	2.18	0.44
1:A:70:ASN:C	1:A:72:ARG:H	2.25	0.44
1:A:112:LEU:HD22	1:A:117:PHE:CE2	2.52	0.44
1:A:214:GLU:HB2	1:A:219:ILE:O	2.18	0.44
1:A:297:GLY:O	1:A:456:LYS:HD3	2.18	0.44
1:A:53:LEU:HA	1:A:58:ILE:HG13	2.00	0.44
1:A:36:LEU:CD1	1:A:37:LEU:HD23	2.48	0.44
1:A:40:ALA:HB1	1:A:70:ASN:CB	2.47	0.44
1:A:124:ASN:HA	1:A:153:SER:HB3	2.00	0.44
1:A:413:ASP:OD2	1:A:440:ARG:NH2	2.51	0.44
1:A:69:GLU:O	1:A:72:ARG:HB2	2.18	0.43
1:A:451:VAL:O	1:A:455:LYS:HG3	2.18	0.43
1:A:266:GLY:CA	1:A:335:ASP:HB3	2.46	0.43
1:A:365:ALA:HB1	1:A:473:TRP:CD1	2.54	0.43
1:A:373:GLU:C	1:A:375:ILE:H	2.25	0.43
1:A:22:VAL:HG13	1:A:23:LEU:N	2.33	0.43
1:A:23:LEU:HB3	1:A:37:LEU:CB	2.48	0.43
1:A:303:PRO:HG2	1:A:304:GLU:OE2	2.18	0.43
1:A:18:ALA:O	1:A:19:VAL:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:HB2	1:A:104:PRO:HD3	2.01	0.43
1:A:216:VAL:HG13	1:A:217:THR:HG23	1.99	0.43
1:A:417:LEU:HD21	1:A:428:LEU:CD1	2.48	0.43
1:A:122:LEU:HD12	1:A:182:PHE:CE2	2.51	0.43
1:A:375:ILE:HD13	1:A:375:ILE:HA	1.89	0.43
1:A:500:VAL:CG2	1:A:502:GLN:HG2	2.49	0.43
1:A:309:CYS:SG	1:A:312:VAL:CG1	3.07	0.43
1:A:340:LEU:HD13	1:A:340:LEU:C	2.44	0.43
1:A:366:ASN:OD1	1:A:366:ASN:C	2.62	0.43
1:A:430:VAL:HG12	1:A:431:ASN:ND2	2.34	0.43
1:A:10:LEU:HD12	1:A:10:LEU:C	2.44	0.42
1:A:89:LYS:HE2	1:A:93:ASP:OD2	2.19	0.42
1:A:155:GLN:OE1	1:A:155:GLN:HA	2.19	0.42
1:A:217:THR:O	1:A:219:ILE:HG13	2.18	0.42
1:A:159:VAL:HG22	1:A:161:PRO:CD	2.45	0.42
1:A:383:TYR:CD1	1:A:383:TYR:C	2.97	0.42
1:A:508:GLU:OE2	1:A:516:ARG:NH2	2.42	0.42
1:A:33:PRO:O	1:A:34:ARG:C	2.62	0.42
1:A:350:GLU:H	1:A:350:GLU:CD	2.26	0.42
1:A:443:THR:OG1	1:A:446:GLU:HG3	2.19	0.42
1:A:533:GLU:CD	1:A:533:GLU:H	2.25	0.42
1:A:72:ARG:O	1:A:76:GLU:HB2	2.19	0.42
1:A:161:PRO:O	1:A:162:GLU:C	2.62	0.42
1:A:254:GLU:OE2	1:A:289:LEU:HD21	2.20	0.42
1:A:20:PHE:C	1:A:20:PHE:CD1	2.96	0.42
1:A:22:VAL:C	1:A:24:GLY:N	2.77	0.42
1:A:42:GLN:HE21	1:A:42:GLN:HB2	1.72	0.42
1:A:261:VAL:HG22	1:A:330:VAL:HG13	1.97	0.42
1:A:342:TRP:CZ2	1:A:507:MET:HE1	2.55	0.42
1:A:281:LEU:CD2	1:A:539:ILE:HG12	2.50	0.41
1:A:519:ILE:HD11	1:A:537:ILE:HD12	2.02	0.41
1:A:505:GLN:HG3	1:A:506:HIS:CD2	2.54	0.41
1:A:422:VAL:HA	1:A:425:ALA:HB3	2.02	0.41
1:A:418:SER:O	1:A:420:HIS:N	2.53	0.41
1:A:422:VAL:O	1:A:425:ALA:HB3	2.20	0.41
1:A:7:VAL:CG1	1:A:122:LEU:HB2	2.51	0.41
1:A:139:LEU:HD23	1:A:139:LEU:C	2.45	0.41
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.89	0.41
1:A:36:LEU:O	1:A:39:ASP:HB3	2.21	0.41
1:A:213:LEU:O	1:A:217:THR:HG23	2.21	0.41
1:A:71:CYS:SG	1:A:88:ILE:HD11	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ARG:HG3	1:A:134:ASP:N	2.35	0.41
1:A:177:PRO:O	1:A:198:MET:HA	2.21	0.41
1:A:306:GLU:C	1:A:308:TYR:H	2.29	0.41
1:A:11:ASP:OD2	1:A:18:ALA:HA	2.21	0.41
1:A:213:LEU:HA	1:A:216:VAL:HG12	2.02	0.41
1:A:264:CYS:O	1:A:337:GLY:HA3	2.21	0.41
1:A:345:ALA:CB	1:A:486:ILE:HD11	2.50	0.41
1:A:475:TRP:HA	1:A:478:LYS:HE2	2.03	0.41
1:A:6:ALA:HA	1:A:181:VAL:HG23	2.03	0.41
1:A:16:LEU:HB3	1:A:17:PRO:HD3	1.99	0.41
1:A:32:LEU:HD22	1:A:33:PRO:HD2	2.02	0.41
1:A:306:GLU:HG2	1:A:471:ARG:NH2	2.36	0.41
1:A:425:ALA:O	1:A:430:VAL:HG21	2.21	0.40
1:A:194:ARG:C	1:A:196:LEU:H	2.30	0.40
1:A:162:GLU:O	1:A:165:ILE:HG22	2.22	0.40
1:A:383:TYR:CD2	1:A:419:MET:HB3	2.54	0.40
1:A:32:LEU:CD2	1:A:33:PRO:HD2	2.52	0.40
1:A:166:TYR:O	1:A:167:LYS:C	2.63	0.40
1:A:264:CYS:HB3	1:A:293:MET:CE	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLU:OE1	1:A:254:GLU:OE1[11_655]	1.95	0.25

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	543/555 (98%)	436 (80%)	88 (16%)	19 (4%)	3 16

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	38	ASN
1	A	44	GLY
1	A	190	LEU
1	A	374	SER
1	A	415	SER
1	A	419	MET
1	A	45	GLY
1	A	34	ARG
1	A	223	ASN
1	A	482	ARG
1	A	10	LEU
1	A	160	LYS
1	A	33	PRO
1	A	144	LYS
1	A	456	LYS
1	A	12	GLY
1	A	19	VAL
1	A	268	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	471/481 (98%)	415 (88%)	56 (12%)	5	22

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PHE
1	A	33	PRO
1	A	42	GLN
1	A	54	MET
1	A	58	ILE
1	A	69	GLU

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Mol	Chain	Res	Type
1	A	72	ARG
1	A	74	CYS
1	A	82	LEU
1	A	85	ASN
1	A	89	LYS
1	A	94	LYS
1	A	106	LEU
1	A	110	LEU
1	A	122	LEU
1	A	123	THR
1	A	132	GLU
1	A	138	GLN
1	A	139	LEU
1	A	155	GLN
1	A	159	VAL
1	A	172	THR
1	A	180	VAL
1	A	190	LEU
1	A	202	LEU
1	A	204	GLN
1	A	207	ASP
1	A	213	LEU
1	A	223	ASN
1	A	224	THR
1	A	277	GLN
1	A	304	GLU
1	A	306	GLU
1	A	307	GLU
1	A	312	VAL
1	A	330	VAL
1	A	339	MET
1	A	355	VAL
1	A	370	SER
1	A	375	ILE
1	A	380	VAL
1	A	410	ARG
1	A	417	LEU
1	A	424	GLU
1	A	428	LEU
1	A	435	GLU
1	A	452	GLN
1	A	457	SER

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Mol	Chain	Res	Type
1	A	469	MET
1	A	489	LEU
1	A	498	VAL
1	A	502	GLN
1	A	520	GLU
1	A	532	THR
1	A	533	GLU
1	A	547	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	220	GLN
1	A	223	ASN
1	A	233	ASN
1	A	277	GLN
1	A	448	GLN
1	A	468	ASN
1	A	506	HIS

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MZL	A	556	-	31,31,31	3.82	18 (58%)	38,42,42	2.02	10 (26%)

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
2	MZL	A	556	-	-	2/18/18/18	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	556	MZL	C10-C5	7.91	1.51	1.38
2	A	556	MZL	C3-N1	7.07	1.49	1.36
2	A	556	MZL	C25-C22	6.39	1.49	1.39
2	A	556	MZL	C18-C15	6.18	1.49	1.38
2	A	556	MZL	C6-C2	5.95	1.50	1.39
2	A	556	MZL	C26-C24	5.50	1.48	1.38
2	A	556	MZL	C16-C13	5.13	1.47	1.39
2	A	556	MZL	C21-N19	4.66	1.46	1.33
2	A	556	MZL	C2-N1	4.51	1.51	1.43
2	A	556	MZL	C9-N4	-4.34	1.28	1.34
2	A	556	MZL	C7-C9	4.27	1.47	1.40
2	A	556	MZL	C11-C14	4.27	1.46	1.39
2	A	556	MZL	C8-C3	4.21	1.55	1.50
2	A	556	MZL	C7-C3	-3.09	1.33	1.37
2	A	556	MZL	C11-C6	-2.94	1.34	1.38
2	A	556	MZL	C28-N27	2.93	1.42	1.33
2	A	556	MZL	C24-C22	-2.61	1.35	1.39
2	A	556	MZL	C20-N17	2.46	1.42	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	556	MZL	C9-N4-N1	5.61	108.05	104.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	556	MZL	C13-C9-C7	-4.76	122.02	128.69
2	A	556	MZL	C2-N1-N4	4.41	125.06	118.67
2	A	556	MZL	C13-C9-N4	4.11	125.90	120.49
2	A	556	MZL	C21-N19-C16	3.72	123.37	116.85
2	A	556	MZL	C28-N27-C25	3.10	122.29	116.85
2	A	556	MZL	C13-C16-N19	-2.72	119.45	123.50
2	A	556	MZL	C8-C3-C7	-2.54	125.73	130.15
2	A	556	MZL	C22-C25-N27	-2.26	120.14	123.50
2	A	556	MZL	C12-C8-C3	2.21	116.68	113.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

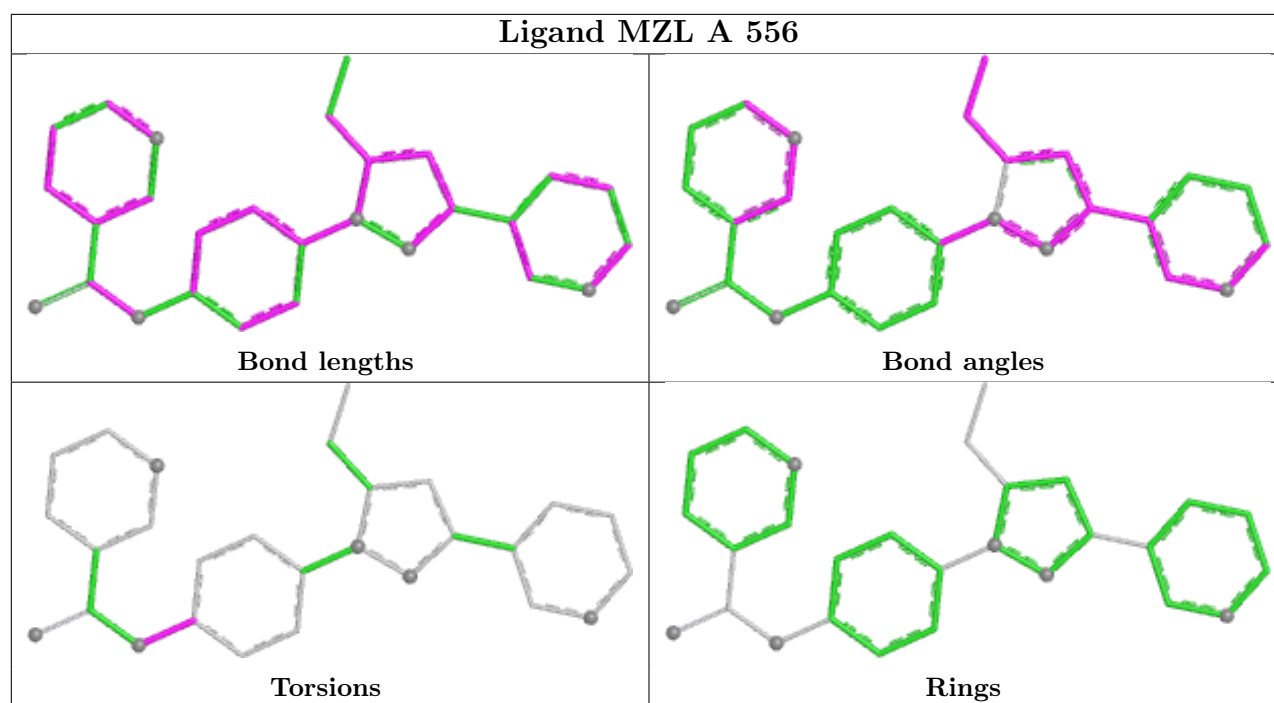
Mol	Chain	Res	Type	Atoms
2	A	556	MZL	C11-C14-N17-C20
2	A	556	MZL	C10-C14-N17-C20

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	556	MZL	3	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	545/555 (98%)	-0.42	0 100 100	15, 40, 79, 107	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

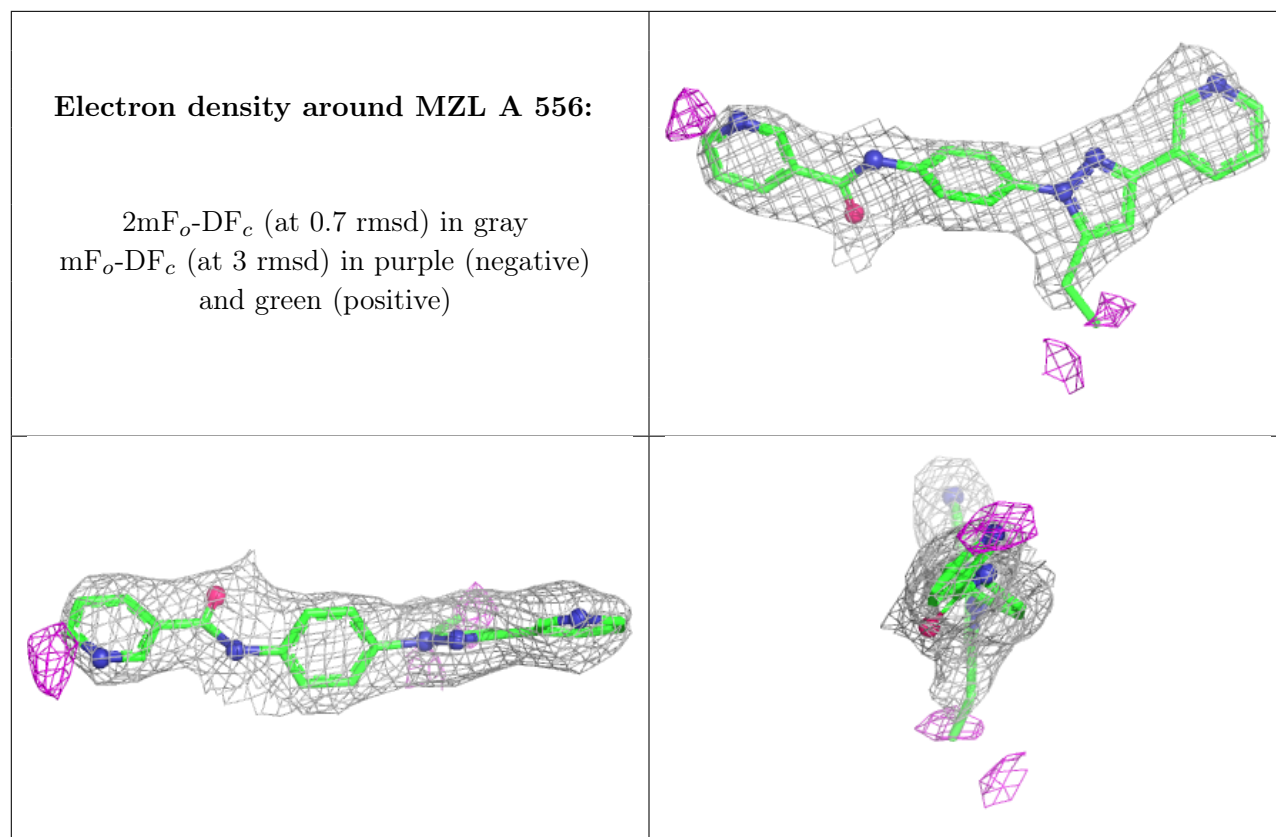
There are no oligosaccharides in this entry.

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
2	MZL	A	556	28/28	0.89	0.12	40,40,40,40	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.