



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:31 PM GMT

PDB ID : 3OTQ
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

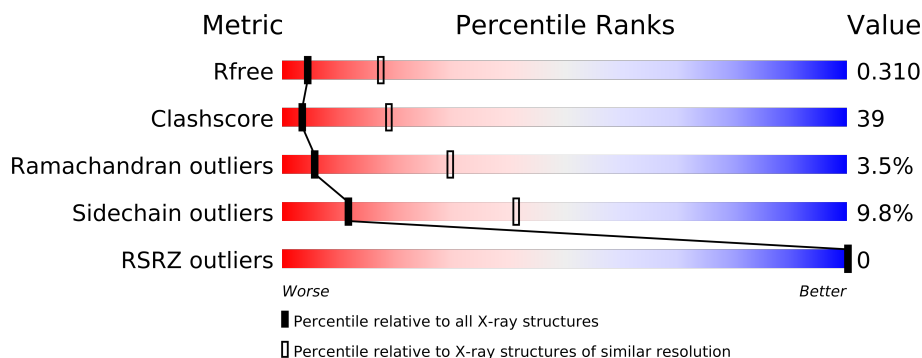
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	555	

2 Entry composition i

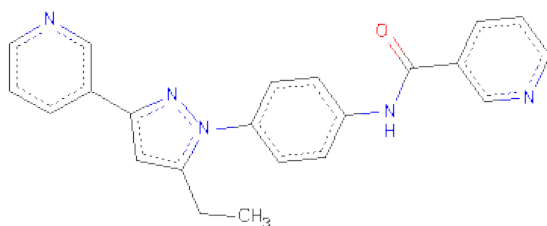
There are 3 unique types of molecules in this entry. The entry contains 4385 atoms, of which 0 are hydrogen and 0 are deuterium.

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]PYRIDIN E-3-CARBOXAMIDE (three-letter code: 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

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 40.35 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 97.1 (40.35-2.99)	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 0.226 , 0.310	Depositor DCC
R_{free} test set	661 reflections (5.38%)	DCC
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 , 32.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 13270 reflections	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.

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	0.48	0/4421	0.71	1/5990 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	ASP	N-CA-C	-5.73	95.53	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4316	0	4317	339	1
2	A	28	0	19	3	0
3	A	41	0	0	2	0
All	All	4385	0	4336	339	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 39.

All (339) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:217:THR:HB	1:A:219:ILE:HD12	1.47	0.93
1:A:80:VAL:HG12	1:A:81:CYS:N	1.84	0.92
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: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
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: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:170:LEU:HD13	1:A:198:MET:HE1	1.69	0.75
1:A:37:LEU:C	1:A:39:ASP:H	1.90	0.74
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: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: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:111:MET:HE3	1:A:114:LYS:HB3	1.74	0.70
1:A:380:VAL:HG11	1:A:498:VAL:HA	1.71	0.70
1:A:26:THR:HG21	1:A:91:ILE:HD13	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:278:ILE:HB	1:A:279:PRO:HD3	1.73	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:NH1	1:A:194:ARG:HB2	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
1:A:110:LEU:CD2	1:A:146:HIS:HB3	2.23	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:382:ASP:OD2	1:A:422:VAL:N	2.27	0.67
1:A:252:PHE:CE2	1:A:289:LEU:HD22	2.29	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: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:HD22	1:A:372:LEU:H	1.61	0.66
1:A:23:LEU:HB2	1:A:38:ASN:OD1	1.95	0.66
1:A:494:GLU:HB2	1:A:520:GLU:HA	1.77	0.66
1:A:170:LEU:HD13	1:A:198:MET:CE	2.26	0.65
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:212:GLU:O	1:A:215:LYS:HB3	1.97	0.65
1:A:139:LEU:HD23	1:A:139:LEU:O	1.96	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:124:ASN:CG	1:A:160:LYS:HB2	2.18	0.64
1:A:60:LEU:HD23	1:A:130:ARG:HG3	1.79	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:HD3	1:A:315:LYS:O	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:304:GLU:H	1:A:304:GLU:CD	2.01	0.61
1:A:394:GLU:O	1:A:398:GLU:HG3	2.01	0.61
1:A:23:LEU:HB2	1:A:38:ASN:CG	2.21	0.61
1:A:261:VAL:HG22	1:A:330:VAL:HG11	1.83	0.60
1:A:358:LEU:O	1:A:359:ASN:HB2	2.02	0.60
1:A:160:LYS:HB3	1:A:161:PRO:HD3	1.82	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:23:LEU:HB3	1:A:37:LEU:HB2	1.84	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: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: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: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:267:PHE:HD2	1:A:296:TYR:HH	1.54	0.56
1:A:36:LEU:C	1:A:36:LEU:HD13	2.26	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:44:GLY:O	1:A:45:GLY:C	2.45	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:388:GLN:O	1:A:390:PRO:HD3	2.06	0.55
1:A:64:ILE:O	1:A:68:GLU:HG2	2.06	0.54
1:A:414:GLU:CD	1:A:440:ARG:HG2	2.28	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:245:LYS:HB3	1:A:245:LYS:HZ3	1.73	0.54
1:A:69:GLU:O	1:A:72:ARG:N	2.42	0.53
1:A:177:PRO:HB3	1:A:198:MET:H	1.72	0.53
1:A:43:LYS:HG3	1:A:44:GLY:N	2.24	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: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:37:LEU:C	1:A:39:ASP:N	2.61	0.51
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:530:LYS:HB3	1:A:533:GLU:HG3	1.90	0.51
1:A:494:GLU:CB	1:A:520:GLU:HA	2.39	0.51
1:A:383:TYR:HD2	1:A:419:MET:HB3	1.75	0.51
1:A:471:ARG:HG3	1:A:471:ARG:HH11	1.76	0.51
1:A:112:LEU:C	1:A:117:PHE:HB2	2.31	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:511:ILE:HB	1:A:514:LEU:HB2	1.94	0.50
1:A:321:LEU:HD11	1:A:331:PHE:CZ	2.43	0.50
1:A:43:LYS:HD2	1:A:44:GLY:H	1.76	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: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:112:LEU:O	1:A:117:PHE:HB2	2.12	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:177:PRO:HA	1:A:198:MET:CE	2.42	0.49
1:A:479:SER:CB	1:A:482:ARG:HG3	2.41	0.49
1:A:496:ASP:O	1:A:500:VAL:HG12	2.12	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:479:SER:HA	1:A:482:ARG:HG2	1.95	0.49
1:A:61:SER:HB2	1:A:129:ASP:OD2	2.13	0.49
1:A:281:LEU:HD23	1:A:539:ILE:HG12	1.94	0.49
1:A:251:HIS:O	1:A:292:ASP:HB2	2.12	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: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:222:LEU:O	1:A:223:ASN:C	2.50	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
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:375:ILE:HD12	1:A:381:PHE:CD2	2.49	0.48
1:A:222:LEU:O	1:A:223:ASN:ND2	2.46	0.48
1:A:36:LEU:HD12	1:A:37:LEU:HD23	1.95	0.48
1:A:245:LYS:HB3	1:A:245:LYS:HZ2	1.78	0.48
1:A:505:GLN:HA	1:A:516:ARG:HH22	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:13:VAL:HG13	1:A:105:MET:CE	2.43	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: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: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:CB	1:A:245:LYS:NZ	2.76	0.47
1:A:125:THR:O	1:A:154:CYS:HB3	2.14	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:HG2	1:A:547:ARG:NH1	2.30	0.46
1:A:223:ASN:HD22	1:A:223:ASN:C	2.18	0.46
1:A:168:PHE:O	1:A:172:THR:HG22	2.15	0.46
1:A:498:VAL:HG21	2:A:556:MZL:H11	1.98	0.46
1:A:451:VAL:HG12	1:A:455:LYS:HZ2	1.80	0.46
1:A:7:VAL:HA	1:A:120:ALA:O	2.17	0.45
1:A:13:VAL:HG13	1:A:105:MET:HE3	1.98	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
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:547:ARG:HH11	1:A:547:ARG:CG	2.30	0.45
1:A:218:GLY:C	1:A:219:ILE:HG13	2.37	0.45
1:A:55:LYS:HE2	1:A:162:GLU:OE1	2.16	0.45
1:A:413:ASP:CG	1:A:440:ARG:HH21	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:187:GLY:O	1:A:188:ALA:C	2.55	0.45
1:A:331:PHE:HB3	1:A:341:VAL:HG22	1.99	0.45
1:A:268:PRO:HA	1:A:296:TYR:HE2	1.82	0.45
1:A:471:ARG:HG3	1:A:471:ARG:NH1	2.32	0.44
1:A:205:ASP:HB2	1:A:207:ASP:OD2	2.16	0.44
1:A:140:MET:CE	1:A:140:MET:HA	2.47	0.44
1:A:206:THR:HG22	1:A:210:LEU:HD11	1.99	0.44
1:A:190:LEU:O	1:A:191:LYS:C	2.53	0.44
1:A:9:ASP:O	1:A:13:VAL:HB	2.17	0.44
1:A:142:GLU:HG3	1:A:283:GLN:CD	2.37	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:519:ILE:O	1:A:522:CYS:HB3	2.18	0.44
1:A:134:ASP:O	1:A:138:GLN:HB2	2.17	0.44
1:A:546:ALA:O	1:A:547:ARG:C	2.56	0.44
1:A:214:GLU:HB2	1:A:219:ILE:O	2.18	0.44
1:A:112:LEU:HD22	1:A:117:PHE:CE2	2.52	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:70:ASN:C	2.55	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:23:LEU:HB3	1:A:37:LEU:CB	2.48	0.43
1:A:22:VAL:HG13	1:A:23:LEU:N	2.33	0.43
1:A:303:PRO:HG2	1:A:304:GLU:OE2	2.18	0.43
1:A:216:VAL:HG13	1:A:217:THR:HG23	1.99	0.43
1:A:393:ALA:O	1:A:394:GLU:C	2.57	0.43
1:A:417:LEU:HD21	1:A:428:LEU:CD1	2.48	0.43
1:A:103:ARG:HB2	1:A:104:PRO:HD3	2.01	0.43
1:A:122:LEU:HD12	1:A:182:PHE:CE2	2.51	0.43
1:A:155:GLN:HA	1:A:155:GLN:OE1	2.19	0.43
1:A:500:VAL:CG2	1:A:502:GLN:HG2	2.49	0.43
1:A:375:ILE:HD13	1:A:375:ILE:HA	1.89	0.43
1:A:19:VAL:O	1:A:20:PHE:C	2.57	0.43
1:A:309:CYS:SG	1:A:312:VAL:CG1	3.07	0.43
1:A:430:VAL:HG12	1:A:431:ASN:ND2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:217:THR:O	1:A:219:ILE:HG13	2.18	0.42
1:A:89:LYS:HE2	1:A:93:ASP:OD2	2.19	0.42
1:A:159:VAL:HG22	1:A:161:PRO:CD	2.45	0.42
1:A:168:PHE:C	1:A:168:PHE:CD2	2.93	0.42
1:A:508:GLU:OE2	1:A:516:ARG:NH2	2.42	0.42
1:A:111:MET:HE1	1:A:115:LYS:HE3	2.02	0.42
1:A:43:LYS:O	1:A:44:GLY:C	2.57	0.42
1:A:443:THR:OG1	1:A:446:GLU:HG3	2.19	0.42
1:A:72:ARG:O	1:A:76:GLU:HB2	2.19	0.42
1:A:254:GLU:OE2	1:A:289:LEU:HD21	2.20	0.42
1:A:261:VAL:HG22	1:A:330:VAL:HG13	1.97	0.42
1:A:136:LEU:C	1:A:136:LEU:HD23	2.40	0.42
1:A:42:GLN:HB2	1:A:42:GLN:HE21	1.72	0.42
1:A:519:ILE:HD11	1:A:537:ILE:HD12	2.02	0.41
1:A:281:LEU:CD2	1:A:539:ILE:HG12	2.50	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:451:VAL:HG12	1:A:455:LYS:HZ1	1.85	0.41
1:A:422:VAL:O	1:A:425:ALA:HB3	2.20	0.41
1:A:418:SER:O	1:A:420:HIS:N	2.53	0.41
1:A:7:VAL:CG1	1:A:122:LEU:HB2	2.51	0.41
1:A:324:LEU:HA	1:A:324:LEU:HD23	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:388:GLN:NE2	1:A:469:MET:HE1	2.35	0.41
1:A:71:CYS:SG	1:A:88:ILE:HD11	2.61	0.41
1:A:177:PRO:O	1:A:198:MET:HA	2.21	0.41
1:A:133:ARG:HG3	1:A:134:ASP:N	2.35	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:177:PRO:HA	1:A:198:MET:HE3	2.02	0.41
1:A:345:ALA:CB	1:A:486:ILE:HD11	2.50	0.41
1:A:264:CYS:O	1:A:337:GLY:HA3	2.21	0.41
1:A:475:TRP:HA	1:A:478:LYS:HE2	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:6:ALA:HA	1:A:181:VAL:HG23	2.03	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: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:143:LEU:O	1:A:144:LYS:C	2.59	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:32:LEU:CD2	1:A:33:PRO:HD2	2.52	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	Distance(Å)	Clash(Å)
1:A:254:GLU:OE1	1:A:254:GLU:OE1[11_655]	1.95	0.25

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	543/555 (98%)	436 (80%)	88 (16%)	19 (4%)	6	30

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	425 (90%)	46 (10%)	12	41

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PHE
1	A	34	ARG
1	A	42	GLN
1	A	54	MET
1	A	72	ARG
1	A	74	CYS
1	A	82	LEU
1	A	85	ASN
1	A	94	LYS
1	A	106	LEU
1	A	110	LEU
1	A	122	LEU
1	A	123	THR
1	A	128	ASP
1	A	132	GLU
1	A	140	MET
1	A	159	VAL
1	A	172	THR
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	233	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	277	GLN
1	A	330	VAL
1	A	339	MET
1	A	370	SER
1	A	380	VAL
1	A	417	LEU
1	A	424	GLU
1	A	435	GLU
1	A	457	SER
1	A	469	MET
1	A	471	ARG
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	536	GLN
1	A	545	ASP
1	A	547	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	204	GLN
1	A	220	GLN
1	A	223	ASN
1	A	233	ASN
1	A	388	GLN
1	A	431	ASN
1	A	448	GLN
1	A	506	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	3.59	18 (58%)	42,42,42	2.29	12 (28%)

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	-	-	0/18/18/18	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	C3-N1	8.67	1.49	1.36
2	A	556	MZL	C6-C2	7.22	1.50	1.38
2	A	556	MZL	C10-C5	6.67	1.51	1.38
2	A	556	MZL	C25-C22	6.14	1.49	1.39
2	A	556	MZL	C18-C15	4.52	1.49	1.39
2	A	556	MZL	C11-C14	4.31	1.46	1.39
2	A	556	MZL	C16-C13	4.31	1.47	1.39
2	A	556	MZL	C21-N19	4.21	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	556	MZL	C26-C24	4.02	1.48	1.39
2	A	556	MZL	C7-C9	3.95	1.47	1.40
2	A	556	MZL	C7-C3	-3.88	1.33	1.39
2	A	556	MZL	C2-N1	3.71	1.51	1.43
2	A	556	MZL	C9-N4	-3.40	1.28	1.34
2	A	556	MZL	C20-N17	2.78	1.42	1.35
2	A	556	MZL	C8-C3	2.77	1.55	1.50
2	A	556	MZL	C28-N27	2.66	1.42	1.33
2	A	556	MZL	C11-C6	-2.43	1.34	1.38
2	A	556	MZL	C24-C22	-2.19	1.35	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	556	MZL	C2-N1-N4	8.03	125.06	118.85
2	A	556	MZL	C7-C9-C13	-5.40	122.02	129.37
2	A	556	MZL	C3-N1-N4	-5.08	106.72	111.82
2	A	556	MZL	C13-C9-N4	4.01	125.90	120.76
2	A	556	MZL	C21-N19-C16	3.63	123.37	116.85
2	A	556	MZL	C8-C3-C7	-3.27	125.73	128.75
2	A	556	MZL	C11-C6-C2	3.14	122.56	119.29
2	A	556	MZL	C28-N27-C25	3.03	122.29	116.85
2	A	556	MZL	C8-C3-N1	2.86	126.85	121.80
2	A	556	MZL	C7-C3-N1	2.38	107.42	105.84
2	A	556	MZL	C22-C25-N27	-2.31	120.14	123.51
2	A	556	MZL	C6-C2-C5	-2.09	118.09	121.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.34	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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MZL	A	556	28/28	0.23	1.99	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.