



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:37 AM UTC

PDB ID : 2WON / pdb\_00002won  
Title : Crystal Structure of UK-453061 bound to HIV-1 Reverse Transcriptase (wild-type).  
Authors : Phillips, C.; Irving, S.L.; Knoechel, T.; Ringrose, H.  
Deposited on : 2009-07-27  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

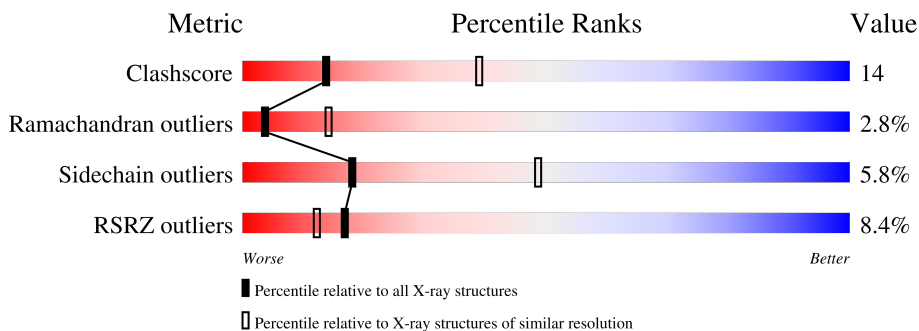
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	560	 8% 67% 28% . .
2	B	440	 9% 64% 26% . 6%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7944 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.

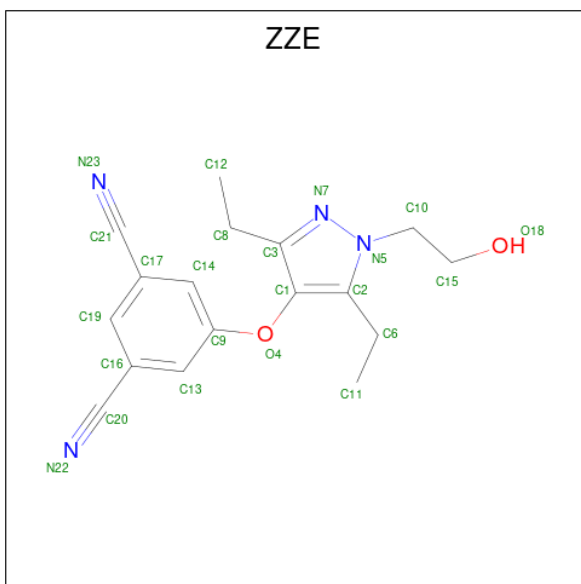
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	558	4537	2931	760	838	8	0	0	1

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	413	3384	2197	565	615	7	0	0	1

- Molecule 3 is 5-{{[3,5-diethyl-1-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy}benzene-1,3-dicarbonit rile (CCD ID: ZZE) (formula: C<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	23	17	4	2	0	0

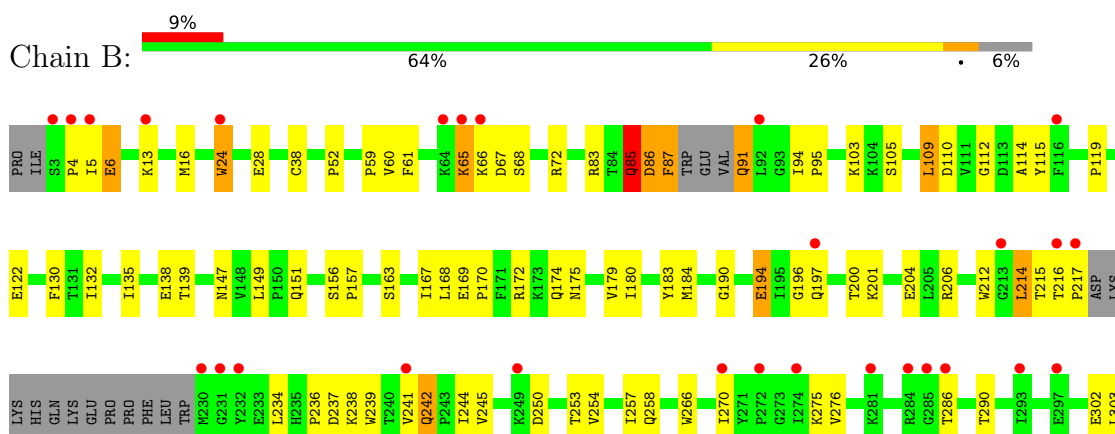
### 3 Residue-property plots [i](#)

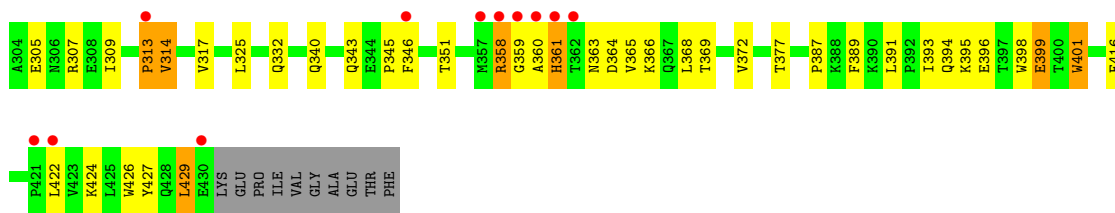
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HIV-1 REVERSE TRANSCRIPTASE



#### • Molecule 2: HIV-1 REVERSE TRANSCRIPTASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.49Å 154.25Å 154.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.88 – 2.80 24.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (24.88-2.80) 88.4 (24.88-2.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.98 (at 2.80Å)	Xtrriage
Refinement program	BUSTER-TNT 2.9.2	Depositor
R, $R_{free}$	0.253 , 0.271 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtrriage
Anisotropy	0.349	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.59	1/4654 (0.0%)	1.02	11/6323 (0.2%)
2	B	0.55	1/3477 (0.0%)	1.00	9/4724 (0.2%)
All	All	0.57	2/8131 (0.0%)	1.01	20/11047 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	557	ARG	C-N	-5.85	1.25	1.33
2	B	429	LEU	C-N	-5.39	1.25	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	TRP	N-CA-C	7.03	122.97	113.97
1	A	349	LEU	N-CA-C	-6.94	103.49	112.23
2	B	85	GLN	CA-C-N	6.38	133.18	121.70
2	B	85	GLN	C-N-CA	6.38	133.18	121.70
2	B	391	LEU	N-CA-C	6.19	117.85	109.24
2	B	87	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	89	GLU	N-CA-C	-5.89	98.26	110.80
1	A	356	ARG	CA-C-N	5.79	132.59	121.54
1	A	356	ARG	C-N-CA	5.79	132.59	121.54
1	A	218	ASP	CA-CB-CG	-5.78	106.82	112.60
1	A	111	VAL	N-CA-C	5.73	121.26	109.34
1	A	147	ASN	N-CA-C	-5.72	106.93	114.31
2	B	4	PRO	N-CA-C	5.67	120.12	111.11
1	A	37	ILE	CB-CG1-CD1	5.55	125.47	113.80
1	A	529	GLU	N-CA-C	-5.48	107.14	113.88
2	B	363	ASN	N-CA-C	5.47	117.76	108.02
2	B	343	GLN	N-CA-C	-5.44	107.19	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ASP	CA-CB-CG	5.38	117.98	112.60
2	B	147	ASN	N-CA-C	-5.29	107.20	113.97
1	A	491	LEU	N-CA-C	5.14	121.74	110.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	4537	0	4590	139	0
2	B	3384	0	3417	102	0
3	A	23	0	18	2	0
All	All	7944	0	8025	231	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 14.

All (231) 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:139:THR:HB	1:A:140:PRO:HD2	1.38	1.05
1:A:23:GLN:HE22	1:A:60:VAL:H	1.02	0.95
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.57	0.86
1:A:23:GLN:NE2	1:A:60:VAL:H	1.74	0.86
1:A:296:THR:HG23	1:A:299:ALA:H	1.42	0.84
1:A:278:GLN:HG2	1:A:298:GLU:HB3	1.61	0.82
2:B:85:GLN:HA	2:B:87:PHE:N	1.99	0.78
1:A:111:VAL:O	1:A:111:VAL:HG12	1.82	0.78
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.66	0.77
1:A:500:GLN:NE2	2:B:422:LEU:HG	2.01	0.75
2:B:5:ILE:HG22	2:B:6:GLU:H	1.52	0.74
2:B:360:ALA:HB2	2:B:366:LYS:HD2	1.69	0.74
1:A:175:ASN:OD1	1:A:201:LYS:HE3	1.87	0.74
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:HG2	1:A:139:THR:N	2.04	0.71
2:B:85:GLN:HA	2:B:87:PHE:H	1.55	0.71
1:A:111:VAL:O	1:A:111:VAL:CG1	2.39	0.71
1:A:311:LYS:HE2	1:A:311:LYS:HA	1.72	0.70
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.57	0.69
2:B:24:TRP:H	2:B:24:TRP:CD1	2.09	0.68
2:B:86:ASP:HA	2:B:91:GLN:HB2	1.77	0.67
1:A:362:THR:HG22	1:A:363:ASN:N	2.10	0.67
1:A:458:VAL:HG12	1:A:548:VAL:HG22	1.76	0.67
1:A:500:GLN:HE22	2:B:422:LEU:HG	1.59	0.67
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.78	0.66
1:A:263:LYS:HE2	1:A:263:LYS:HA	1.78	0.66
1:A:27:THR:CG2	1:A:29:GLU:HG2	2.26	0.65
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.61	0.65
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.78	0.64
1:A:139:THR:HB	1:A:140:PRO:CD	2.21	0.64
2:B:24:TRP:HE1	2:B:59:PRO:HB3	1.62	0.64
1:A:277:ARG:HB3	1:A:336:GLN:OE1	1.98	0.64
1:A:551:LEU:HD23	1:A:551:LEU:H	1.63	0.64
1:A:451:LYS:HE2	1:A:471:ASP:HA	1.80	0.64
1:A:444:GLY:HA2	1:A:552:VAL:HG11	1.81	0.63
1:A:500:GLN:HE21	1:A:500:GLN:HA	1.64	0.63
2:B:215:THR:O	2:B:217:PRO:HD3	1.98	0.62
1:A:122:GLU:H	1:A:122:GLU:CD	2.07	0.62
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.82	0.62
1:A:194:GLU:CD	1:A:194:GLU:H	2.07	0.61
2:B:242:GLN:HE22	2:B:429:LEU:CD1	2.12	0.61
2:B:66:LYS:HG3	2:B:67:ASP:OD1	2.01	0.61
2:B:24:TRP:NE1	2:B:59:PRO:HB3	2.16	0.61
2:B:206:ARG:HD2	2:B:216:THR:O	2.01	0.61
1:A:106:VAL:HG21	3:A:1558:ZZE:H152	1.83	0.60
2:B:365:VAL:O	2:B:369:THR:HG23	2.00	0.60
1:A:23:GLN:HE22	1:A:60:VAL:N	1.86	0.60
2:B:16:MET:HE3	2:B:83:ARG:HA	1.81	0.60
1:A:27:THR:O	1:A:31:ILE:HG13	2.02	0.60
1:A:286:THR:O	1:A:287:LYS:HG2	2.01	0.60
1:A:27:THR:HG21	1:A:29:GLU:HG2	1.82	0.60
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.35	0.60
1:A:548:VAL:HA	1:A:551:LEU:HD21	1.84	0.60
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.37	0.59
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.84	0.59
1:A:23:GLN:NE2	1:A:60:VAL:N	2.49	0.59
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.85	0.59
2:B:360:ALA:CB	2:B:366:LYS:HD2	2.34	0.58
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.40	0.57
1:A:64:LYS:NZ	1:A:69:THR:HG23	2.20	0.57
2:B:13:LYS:HD2	2:B:16:MET:HE2	1.84	0.57
2:B:172:ARG:HH21	2:B:180:ILE:HB	1.68	0.57
1:A:111:VAL:HG21	1:A:164:MET:CE	2.34	0.57
2:B:13:LYS:HD2	2:B:16:MET:CE	2.34	0.57
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.86	0.57
1:A:206:ARG:HG3	1:A:216:THR:OG1	2.06	0.56
2:B:110:ASP:O	2:B:216:THR:HG23	2.05	0.56
1:A:268:SER:O	1:A:351:THR:HG22	2.05	0.55
2:B:303:LEU:HD22	2:B:307:ARG:HH21	1.71	0.55
2:B:5:ILE:HG22	2:B:6:GLU:N	2.19	0.55
1:A:556:ILE:HG22	1:A:556:ILE:O	2.07	0.55
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.04	0.55
1:A:454:LYS:HG3	1:A:556:ILE:CD1	2.36	0.55
1:A:195:ILE:HB	1:A:199:ARG:NH2	2.21	0.54
1:A:454:LYS:HG3	1:A:556:ILE:HD11	1.89	0.54
1:A:454:LYS:O	1:A:552:VAL:HG13	2.08	0.54
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.43	0.53
2:B:122:GLU:CD	2:B:122:GLU:H	2.17	0.53
1:A:288:ALA:HB3	1:A:291:GLU:HG2	1.89	0.53
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.91	0.53
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.43	0.53
2:B:242:GLN:HE22	2:B:429:LEU:HD13	1.73	0.53
1:A:285:GLY:O	1:A:287:LYS:N	2.42	0.52
1:A:17:ASP:O	1:A:83:ARG:HD3	2.10	0.52
1:A:198:HIS:O	1:A:202:ILE:HG12	2.09	0.52
1:A:228:LEU:HD22	1:A:242:GLN:OE1	2.09	0.52
2:B:314:VAL:HG13	2:B:317:VAL:HG22	1.92	0.52
2:B:157:PRO:HG2	2:B:184:MET:HA	1.90	0.52
2:B:266:TRP:HH2	2:B:427:TYR:CE1	2.27	0.52
1:A:23:GLN:NE2	1:A:59:PRO:HA	2.24	0.52
1:A:173:LYS:NZ	1:A:173:LYS:HB3	2.24	0.52
2:B:163:SER:O	2:B:167:ILE:HG13	2.10	0.52
1:A:362:THR:HG22	1:A:363:ASN:H	1.75	0.52
1:A:362:THR:CG2	1:A:363:ASN:N	2.73	0.52
2:B:266:TRP:HH2	2:B:427:TYR:CZ	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:ARG:H	2:B:358:ARG:HD3	1.75	0.52
1:A:466:VAL:HB	1:A:551:LEU:HD12	1.92	0.51
2:B:13:LYS:HZ1	2:B:85:GLN:HG2	1.75	0.51
2:B:60:VAL:HG21	2:B:130:PHE:CD2	2.46	0.51
2:B:65:LYS:O	2:B:68:SER:HB3	2.11	0.51
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.24	0.51
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.45	0.51
2:B:266:TRP:CH2	2:B:427:TYR:CZ	2.98	0.51
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.93	0.51
1:A:183:TYR:CE1	1:A:184:MET:HG3	2.45	0.51
1:A:162:SER:OG	2:B:52:PRO:HD3	2.10	0.50
1:A:417:VAL:HG13	1:A:419:THR:HG22	1.93	0.50
1:A:438:GLU:CG	1:A:461:ARG:HD2	2.41	0.50
2:B:24:TRP:NE1	2:B:61:PHE:CZ	2.80	0.50
1:A:106:VAL:HG11	3:A:1558:ZZE:C1	2.41	0.50
2:B:194:GLU:HG3	2:B:196:GLY:H	1.75	0.50
1:A:27:THR:HG22	1:A:29:GLU:HG2	1.94	0.50
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.94	0.50
2:B:242:GLN:O	2:B:242:GLN:HG3	2.10	0.50
1:A:332:GLN:HG3	1:A:338:THR:HG23	1.94	0.49
1:A:359:GLY:C	1:A:361:HIS:H	2.19	0.49
1:A:357:MET:O	1:A:359:GLY:N	2.32	0.49
1:A:458:VAL:CG1	1:A:548:VAL:HG22	2.42	0.49
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.95	0.49
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.13	0.49
1:A:467:VAL:HG23	1:A:484:LEU:HD11	1.94	0.49
1:A:511:ASP:OD1	1:A:512:GLN:HG3	2.12	0.49
2:B:112:GLY:HA3	2:B:151:GLN:HE21	1.77	0.49
1:A:402:TRP:CZ2	1:A:403:THR:HG22	2.48	0.49
1:A:60:VAL:HG22	1:A:130:PHE:HB2	1.95	0.48
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.95	0.48
1:A:194:GLU:O	1:A:195:ILE:C	2.55	0.48
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.47	0.48
2:B:109:LEU:HG	2:B:216:THR:HG22	1.94	0.48
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.48	0.48
1:A:96:HIS:HD1	1:A:98:ALA:H	1.61	0.48
1:A:27:THR:HG22	1:A:29:GLU:H	1.77	0.48
2:B:200:THR:O	2:B:204:GLU:HG3	2.14	0.48
1:A:139:THR:CB	1:A:140:PRO:HD2	2.27	0.47
1:A:457:TYR:HA	1:A:548:VAL:HG11	1.95	0.47
2:B:253:THR:O	2:B:257:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:GLU:H	1:A:396:GLU:CD	2.22	0.47
1:A:78:ARG:O	1:A:82:LYS:HG3	2.14	0.47
1:A:361:HIS:HD2	1:A:513:SER:OG	1.97	0.47
2:B:13:LYS:NZ	2:B:85:GLN:HG2	2.29	0.47
2:B:275:LYS:HB2	2:B:302:GLU:HG3	1.97	0.47
2:B:254:VAL:O	2:B:258:GLN:HG3	2.15	0.47
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.97	0.46
2:B:276:VAL:HA	2:B:302:GLU:OE2	2.16	0.46
1:A:64:LYS:HZ1	1:A:69:THR:HG23	1.81	0.46
2:B:234:LEU:HD21	2:B:377:THR:CG2	2.45	0.46
1:A:438:GLU:HG3	1:A:461:ARG:HD2	1.96	0.46
2:B:266:TRP:HE1	2:B:346:PHE:HE1	1.63	0.46
1:A:30:LYS:HE2	1:A:62:ALA:O	2.16	0.46
1:A:438:GLU:OE1	1:A:463:ARG:NH2	2.46	0.45
2:B:266:TRP:CE3	2:B:426:TRP:HB3	2.51	0.45
2:B:393:ILE:HG12	2:B:394:GLN:N	2.32	0.45
1:A:66:LYS:NZ	1:A:67:ASP:H	2.15	0.45
1:A:195:ILE:HB	1:A:199:ARG:HH22	1.81	0.45
1:A:362:THR:CG2	1:A:363:ASN:H	2.29	0.45
2:B:305:GLU:O	2:B:309:ILE:HG13	2.16	0.45
1:A:218:ASP:O	1:A:220:LYS:N	2.50	0.45
1:A:454:LYS:C	1:A:552:VAL:HG13	2.41	0.45
1:A:175:ASN:CG	1:A:201:LYS:HE3	2.41	0.45
2:B:13:LYS:HB2	2:B:16:MET:CG	2.39	0.45
1:A:334:GLN:CD	1:A:334:GLN:H	2.24	0.45
1:A:461:ARG:HH11	1:A:461:ARG:CG	2.28	0.45
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.99	0.44
1:A:194:GLU:CD	1:A:194:GLU:N	2.74	0.44
1:A:278:GLN:NE2	1:A:281:LYS:HD2	2.32	0.44
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.98	0.44
2:B:358:ARG:HD3	2:B:358:ARG:N	2.32	0.44
1:A:283:LEU:O	1:A:286:THR:HG23	2.17	0.44
1:A:491:LEU:H	1:A:491:LEU:HD23	1.82	0.44
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.99	0.44
1:A:206:ARG:HD3	1:A:218:ASP:OD1	2.18	0.44
1:A:548:VAL:HA	1:A:551:LEU:CD2	2.47	0.44
2:B:359:GLY:C	2:B:361:HIS:H	2.26	0.44
1:A:460:ASN:HA	2:B:286:THR:O	2.17	0.44
2:B:332:GLN:HA	2:B:424:LYS:HE3	2.00	0.44
1:A:23:GLN:NE2	1:A:60:VAL:HG23	2.33	0.43
1:A:406:TRP:HE3	1:A:407:GLN:NE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:GLU:HB3	2:B:197:GLN:NE2	2.33	0.43
2:B:65:LYS:HE2	2:B:72:ARG:HD2	1.99	0.43
2:B:270:ILE:HG12	2:B:346:PHE:HB3	2.00	0.43
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.54	0.43
1:A:255:ASN:HB2	1:A:289:LEU:HG	2.01	0.43
1:A:540:LYS:C	1:A:542:ILE:H	2.26	0.43
2:B:24:TRP:HE1	2:B:59:PRO:CB	2.29	0.43
2:B:105:SER:O	2:B:190:GLY:HA2	2.19	0.43
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.59	0.43
1:A:286:THR:C	1:A:288:ALA:H	2.27	0.42
1:A:454:LYS:HB2	1:A:552:VAL:O	2.19	0.42
2:B:276:VAL:HG22	2:B:276:VAL:O	2.19	0.42
2:B:395:LYS:HG2	2:B:399:GLU:CG	2.50	0.42
1:A:181:TYR:CE1	2:B:138:GLU:HB3	2.54	0.42
2:B:241:VAL:HG13	2:B:351:THR:OG1	2.20	0.42
1:A:216:THR:HB	1:A:217:PRO:HD2	2.01	0.42
2:B:103:LYS:O	2:B:236:PRO:HG2	2.20	0.42
2:B:5:ILE:H	2:B:119:PRO:HG3	1.83	0.42
1:A:31:ILE:O	1:A:35:VAL:HG23	2.20	0.42
2:B:358:ARG:H	2:B:358:ARG:CD	2.32	0.42
2:B:340:GLN:HG2	2:B:427:TYR:CZ	2.55	0.41
1:A:195:ILE:O	1:A:196:GLY:C	2.63	0.41
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.49	0.41
1:A:311:LYS:HA	1:A:311:LYS:CE	2.45	0.41
1:A:379:SER:CB	1:A:387:PRO:HD3	2.50	0.41
1:A:459:THR:O	2:B:286:THR:HG21	2.21	0.41
2:B:314:VAL:HG13	2:B:317:VAL:CG2	2.50	0.41
2:B:94:ILE:HA	2:B:95:PRO:HD3	1.93	0.41
2:B:115:TYR:HB3	2:B:149:LEU:HB2	2.02	0.41
2:B:183:TYR:CE2	2:B:184:MET:HE3	2.54	0.41
2:B:303:LEU:HD22	2:B:307:ARG:NH2	2.36	0.41
2:B:313:PRO:HB2	2:B:314:VAL:H	1.64	0.41
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.56	0.41
2:B:396:GLU:CD	2:B:396:GLU:H	2.29	0.41
1:A:175:ASN:N	1:A:176:PRO:HD3	2.35	0.41
1:A:362:THR:HG22	1:A:363:ASN:O	2.20	0.41
1:A:429:LEU:HD11	1:A:506:ILE:HG22	2.01	0.41
1:A:242:GLN:NE2	1:A:243:PRO:HD2	2.35	0.41
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.02	0.41
2:B:167:ILE:HG12	2:B:212:TRP:CD2	2.55	0.41
1:A:351:THR:CG2	1:A:352:GLY:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.56	0.41
1:A:253:THR:HA	1:A:292:VAL:HA	2.02	0.41
1:A:457:TYR:CD1	1:A:457:TYR:C	2.99	0.41
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.50	0.41
2:B:201:LYS:HD3	2:B:201:LYS:HA	1.96	0.41
2:B:395:LYS:O	2:B:399:GLU:HG2	2.21	0.41
1:A:28:GLU:HG2	1:A:32:LYS:HE3	2.03	0.40
1:A:242:GLN:O	1:A:243:PRO:C	2.65	0.40
1:A:540:LYS:HB2	1:A:542:ILE:HG13	2.03	0.40
2:B:368:LEU:O	2:B:372:VAL:HG23	2.20	0.40
1:A:396:GLU:HA	1:A:399:GLU:HG2	2.03	0.40
2:B:345:PRO:O	2:B:346:PHE:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	556/560 (99%)	505 (91%)	31 (6%)	20 (4%)	<b>2</b>   <b>10</b>
2	B	407/440 (92%)	381 (94%)	19 (5%)	7 (2%)	<b>7</b>   <b>25</b>
All	All	963/1000 (96%)	886 (92%)	50 (5%)	27 (3%)	<b>4</b>   <b>14</b>

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	135	ILE
1	A	195	ILE
1	A	219	LYS
1	A	286	THR
1	A	358	ARG

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Mol	Chain	Res	Type
1	A	491	LEU
2	B	85	GLN
2	B	313	PRO
2	B	314	VAL
1	A	111	VAL
1	A	114	ALA
1	A	196	GLY
1	A	357	MET
2	B	86	ASP
2	B	361	HIS
1	A	14	PRO
1	A	88	TRP
1	A	345	PRO
1	A	360	ALA
1	A	361	HIS
1	A	138	GLU
1	A	287	LYS
1	A	356	ARG
2	B	245	VAL
2	B	358	ARG
1	A	139	THR

### 5.3.2 Protein sidechains [i](#)

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	497/500 (99%)	463 (93%)	34 (7%)	14	42
2	B	372/400 (93%)	356 (96%)	16 (4%)	26	60
All	All	869/900 (97%)	819 (94%)	50 (6%)	18	49

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	23	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	37	ILE
1	A	60	VAL
1	A	66	LYS
1	A	89	GLU
1	A	91	GLN
1	A	102	LYS
1	A	104	LYS
1	A	107	THR
1	A	122	GLU
1	A	136	ASN
1	A	145	GLN
1	A	195	ILE
1	A	215	THR
1	A	219	LYS
1	A	230	MET
1	A	241	VAL
1	A	308	GLU
1	A	311	LYS
1	A	334	GLN
1	A	340	GLN
1	A	356	ARG
1	A	357	MET
1	A	402	TRP
1	A	406	TRP
1	A	448	ARG
1	A	474	ASN
1	A	480	GLN
1	A	493	VAL
1	A	496	VAL
1	A	500	GLN
1	A	517	LEU
1	A	548	VAL
2	B	6	GLU
2	B	24	TRP
2	B	65	LYS
2	B	91	GLN
2	B	109	LEU
2	B	139	THR
2	B	174	GLN
2	B	194	GLU
2	B	214	LEU
2	B	237	ASP

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Mol	Chain	Res	Type
2	B	238	LYS
2	B	242	GLN
2	B	244	ILE
2	B	250	ASP
2	B	325	LEU
2	B	399	GLU

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	23	GLN
1	A	137	ASN
1	A	145	GLN
1	A	174	GLN
1	A	207	GLN
1	A	269	GLN
1	A	278	GLN
1	A	334	GLN
1	A	361	HIS
1	A	373	GLN
1	A	428	GLN
1	A	480	GLN
1	A	487	GLN
1	A	500	GLN
1	A	512	GLN
1	A	520	GLN
1	A	545	ASN
2	B	85	GLN
2	B	91	GLN
2	B	147	ASN
2	B	151	GLN
2	B	175	ASN
2	B	182	GLN
2	B	208	HIS
2	B	242	GLN
2	B	269	GLN
2	B	278	GLN
2	B	332	GLN
2	B	334	GLN
2	B	336	GLN
2	B	361	HIS
2	B	394	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](#)

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
3	ZZE	A	1558	-	23,24,24	2.49	11 (47%)	24,32,32	3.82	10 (41%)

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
3	ZZE	A	1558	-	-	4/15/15/15	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1558	ZZE	C13-C9	6.54	1.49	1.39
3	A	1558	ZZE	C19-C17	4.84	1.48	1.39
3	A	1558	ZZE	C13-C16	3.50	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1558	ZZE	C10-N5	-3.45	1.41	1.46
3	A	1558	ZZE	C19-C16	2.83	1.44	1.39
3	A	1558	ZZE	C21-N23	2.50	1.20	1.14
3	A	1558	ZZE	O4-C9	-2.33	1.36	1.41
3	A	1558	ZZE	O4-C1	2.27	1.43	1.38
3	A	1558	ZZE	C11-C6	-2.25	1.42	1.51
3	A	1558	ZZE	C16-C20	-2.04	1.40	1.44
3	A	1558	ZZE	C10-C15	2.02	1.58	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1558	ZZE	C14-C17-C21	-11.19	104.46	119.55
3	A	1558	ZZE	C19-C17-C21	8.78	131.40	119.55
3	A	1558	ZZE	C9-O4-C1	7.64	133.61	118.51
3	A	1558	ZZE	C8-C3-N7	4.17	126.80	119.65
3	A	1558	ZZE	C10-N5-C2	-3.76	125.54	129.15
3	A	1558	ZZE	C15-C10-N5	-3.59	105.95	112.37
3	A	1558	ZZE	C19-C17-C14	2.87	124.14	119.70
3	A	1558	ZZE	C16-C13-C9	-2.65	116.12	119.30
3	A	1558	ZZE	C10-N5-N7	2.31	122.43	118.89
3	A	1558	ZZE	O4-C1-C2	-2.29	120.89	124.07

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1558	ZZE	C1-C2-C6-C11
3	A	1558	ZZE	N5-C2-C6-C11
3	A	1558	ZZE	C15-C10-N5-C2
3	A	1558	ZZE	N5-C10-C15-O18

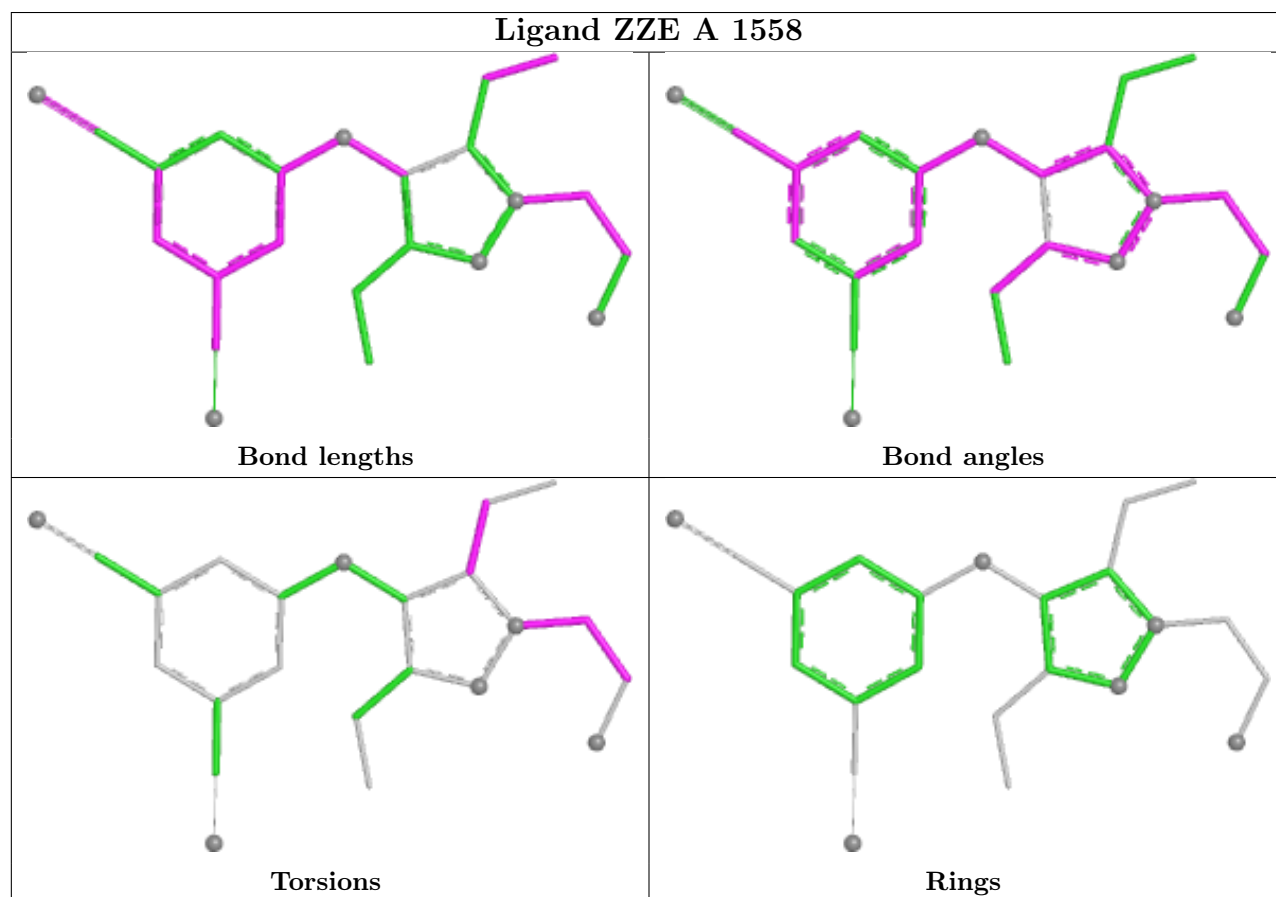
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1558	ZZE	2	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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	558/560 (99%)	0.55	43 (7%)	19   14	31, 58, 105, 194	0
2	B	413/440 (93%)	0.58	39 (9%)	14   10	29, 57, 108, 128	0
All	All	971/1000 (97%)	0.56	82 (8%)	17   12	29, 57, 107, 194	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	548	VAL	6.9
1	A	551	LEU	6.8
2	B	216	THR	6.7
2	B	4	PRO	6.4
2	B	217	PRO	6.3
1	A	545	ASN	6.0
2	B	360	ALA	5.7
2	B	357	MET	5.4
1	A	549	ASP	5.3
1	A	554	ALA	5.1
1	A	359	GLY	5.1
1	A	544	GLY	4.9
2	B	232	TYR	4.7
2	B	13	LYS	4.7
2	B	3	SER	4.1
1	A	552	VAL	4.0
1	A	360	ALA	3.9
1	A	24	TRP	3.8
1	A	161	GLN	3.7
2	B	430	GLU	3.7
2	B	92	LEU	3.7
2	B	66	LYS	3.6
2	B	231	GLY	3.6
2	B	286	THR	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	65	LYS	3.4
1	A	66	LYS	3.4
2	B	116	PHE	3.3
2	B	241	VAL	3.3
2	B	346	PHE	3.3
2	B	5	ILE	3.2
1	A	289	LEU	3.2
1	A	91	GLN	3.2
1	A	268	SER	3.1
1	A	556	ILE	3.1
2	B	422	LEU	3.1
1	A	539	HIS	3.0
2	B	272	PRO	2.9
1	A	206	ARG	2.9
1	A	555	GLY	2.9
2	B	313	PRO	2.9
1	A	547	GLN	2.9
1	A	288	ALA	2.8
1	A	550	LYS	2.8
2	B	359	GLY	2.8
1	A	290	THR	2.7
1	A	542	ILE	2.7
2	B	361	HIS	2.7
2	B	362	THR	2.7
2	B	230	MET	2.7
1	A	65	LYS	2.6
1	A	358	ARG	2.6
1	A	406	TRP	2.6
1	A	553	SER	2.5
1	A	448	ARG	2.5
2	B	293	ILE	2.5
2	B	24	TRP	2.4
1	A	287	LYS	2.4
1	A	557	ARG	2.4
2	B	197	GLN	2.4
1	A	543	GLY	2.3
1	A	90	VAL	2.3
2	B	213	GLY	2.3
2	B	281	LYS	2.3
1	A	144	TYR	2.3
2	B	297	GLU	2.3
1	A	541	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	270	ILE	2.2
2	B	284	ARG	2.2
2	B	358	ARG	2.2
1	A	401	TRP	2.2
1	A	419	THR	2.2
2	B	421	PRO	2.1
2	B	285	GLY	2.1
1	A	92	LEU	2.1
1	A	286	THR	2.1
1	A	445	ALA	2.1
1	A	373	GLN	2.1
2	B	64	LYS	2.1
1	A	105	SER	2.0
1	A	185	ASP	2.0
2	B	274	ILE	2.0
2	B	249	LYS	2.0

## 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](#)

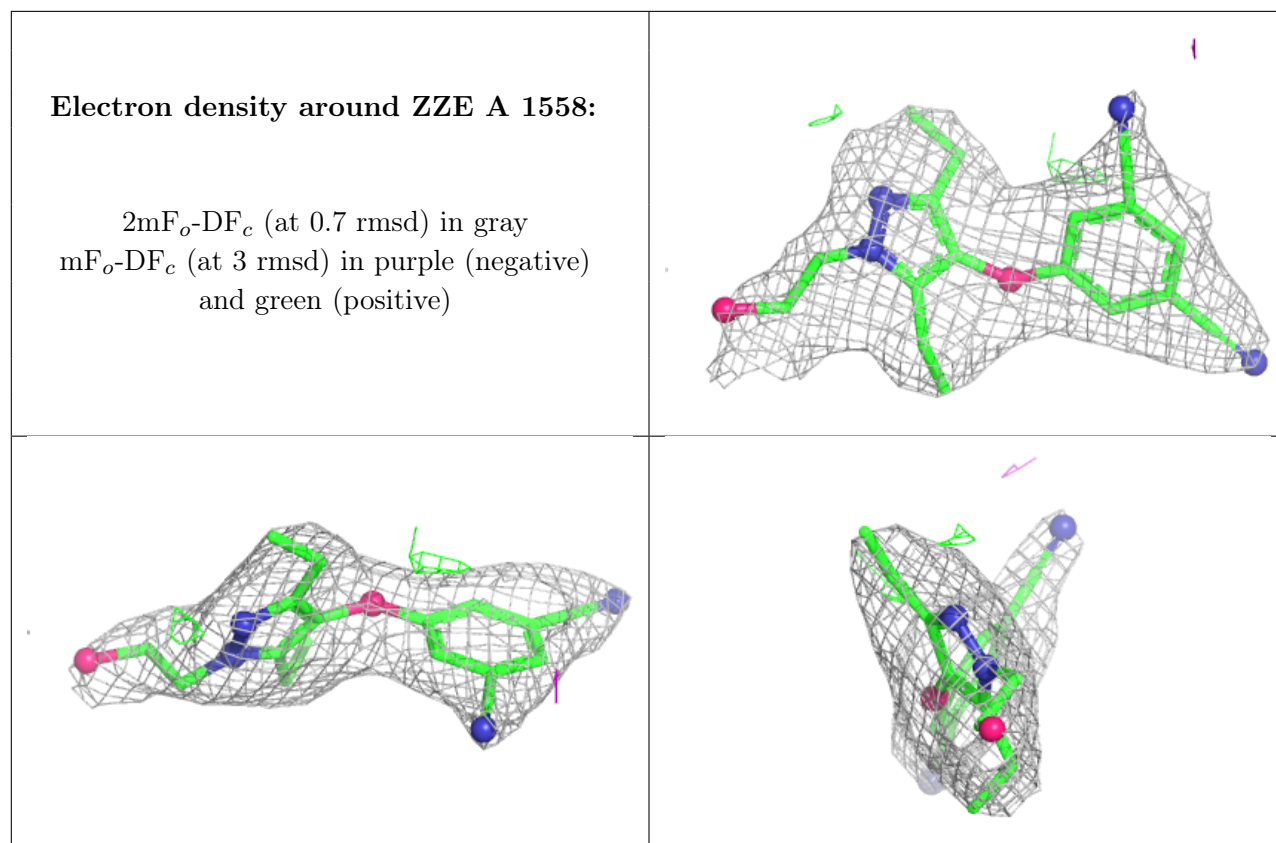
There are no oligosaccharides in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	ZZE	A	1558	23/23	0.89	0.14	46,50,55,59	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.