



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:08 PM UTC

PDB ID : 2RKI / pdb_00002rki
Title : Crystal Structure of HIV-1 Reverse Transcriptase (RT) in Complex with a triazole derived NNRTI
Authors : Lansdon, E.B.; Kirschberg, T.A.
Deposited on : 2007-10-16
Resolution : 2.30 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

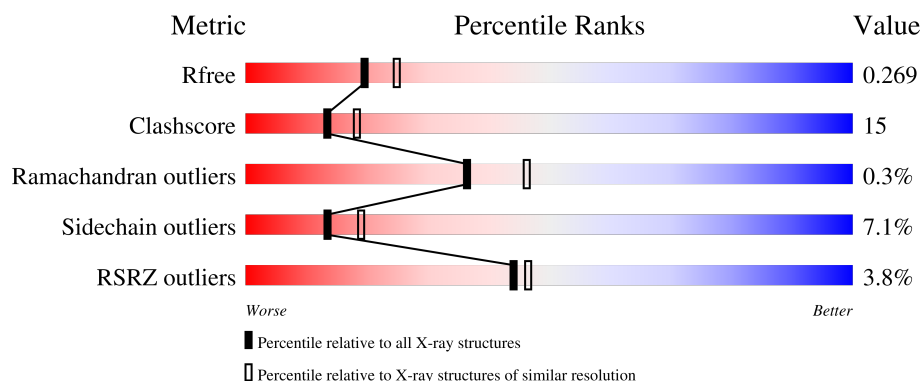
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	560	2% 67% 28% • •
2	B	440	6% 65% 23% • 9%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8224 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.

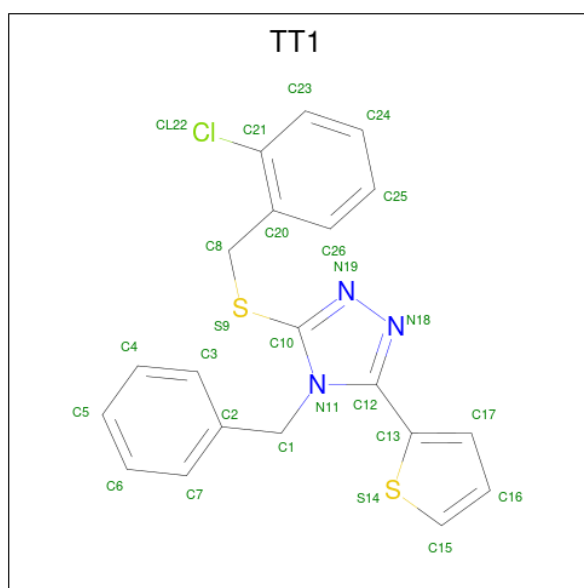
- Molecule 1 is a protein called HIV-1 reverse transcriptase (RT) p66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4536	2931	759	838	8			

- Molecule 2 is a protein called HIV-1 reverse transcriptase (RT) p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3328	2168	549	605	6			

- Molecule 3 is 4-benzyl-3-[(2-chlorobenzyl)sulfanyl]-5-thiophen-2-yl-4H-1,2,4-triazole (CCD ID: TT1) (formula: C₂₀H₁₆ClN₃S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	S	0	0
			26	20	1	3	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	4	Total	Cl	0	0
			4	4		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

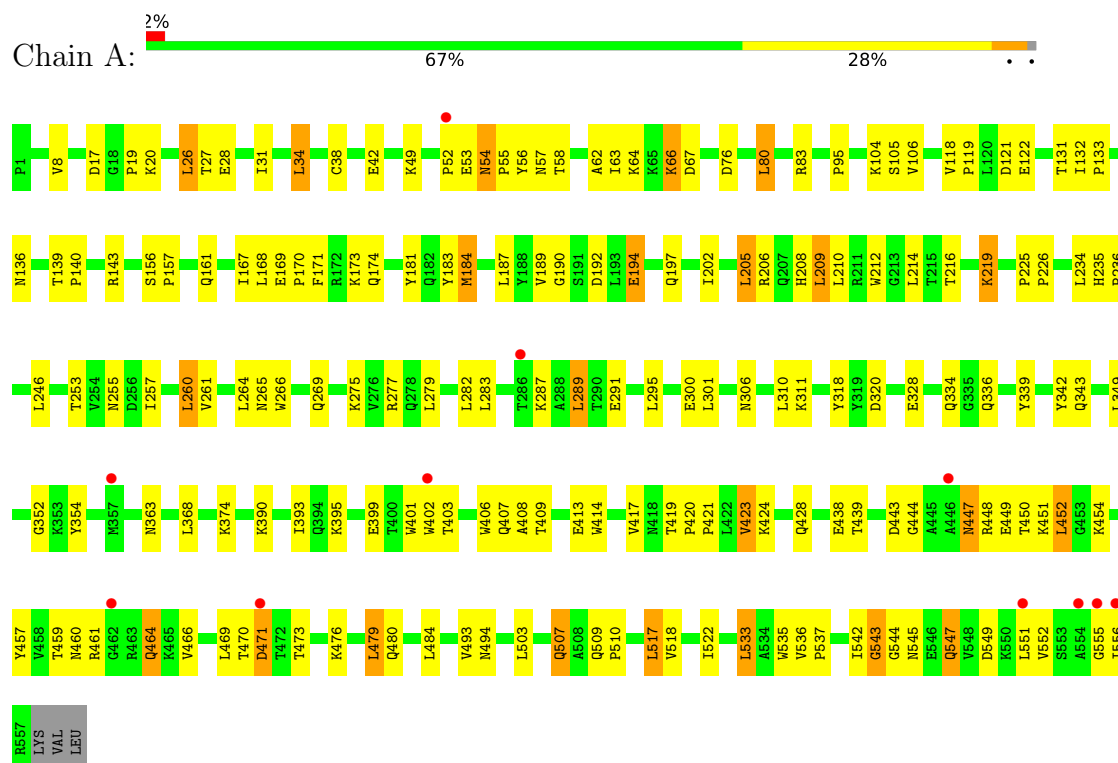
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	186	Total	O	0	0
			186	186		
8	B	111	Total	O	0	0
			111	111		

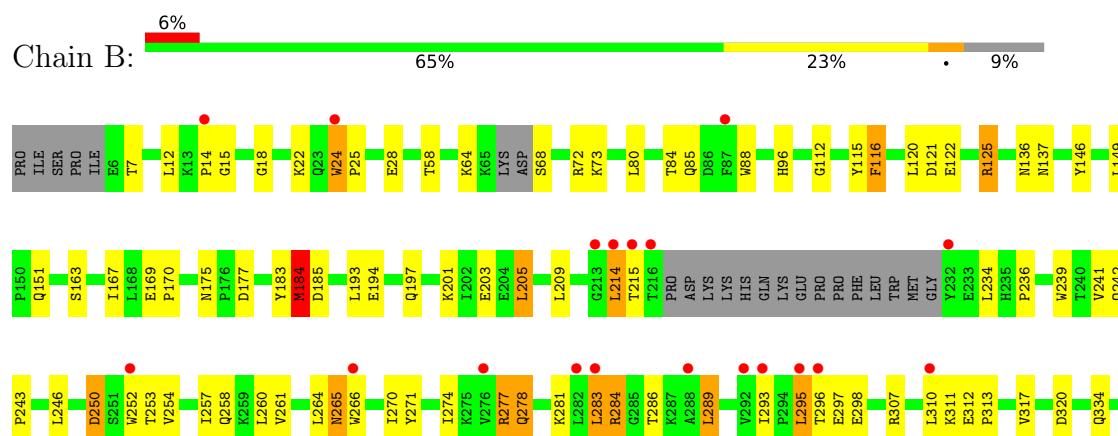
3 Residue-property plots

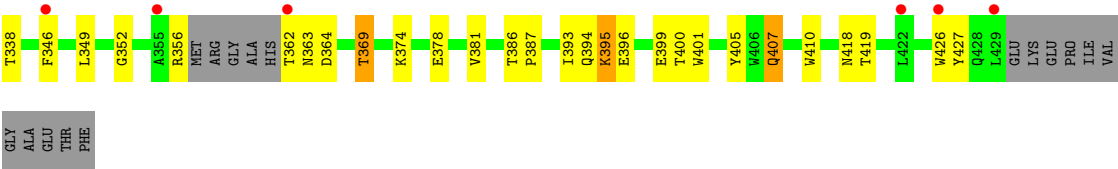
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HIV-1 reverse transcriptase (RT) p66



• Molecule 2: HIV-1 reverse transcriptase (RT) p51





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.39Å 154.17Å 154.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.30 29.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.0 (29.88-2.30) 90.0 (29.88-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.32Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.216 , 0.270 0.212 , 0.269	Depositor DCC
R_{free} test set	2860 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8224	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: SO4, TT1, CL, MG, GOL

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	0.41	1/4653 (0.0%)	0.75	1/6321 (0.0%)
2	B	0.41	0/3420	0.78	7/4647 (0.2%)
All	All	0.41	1/8073 (0.0%)	0.76	8/10968 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	MET	SD-CE	-6.31	1.63	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	18	GLY	CA-C-N	6.12	125.88	119.76
2	B	18	GLY	C-N-CA	6.12	125.88	119.76
2	B	184	MET	CB-CA-C	-5.71	109.46	117.23
2	B	320	ASP	CA-C-N	5.70	125.41	119.82
2	B	320	ASP	C-N-CA	5.70	125.41	119.82
1	A	493	VAL	N-CA-C	5.33	114.89	108.06
2	B	293	ILE	CA-C-N	5.25	125.41	119.90
2	B	293	ILE	C-N-CA	5.25	125.41	119.90

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	4536	0	4590	149	0
2	B	3328	0	3359	93	0
3	A	26	0	16	2	0
4	A	6	0	8	2	0
5	A	25	0	0	0	0
6	A	1	0	0	0	0
6	B	4	0	0	0	0
7	A	1	0	0	0	0
8	A	186	0	0	7	0
8	B	111	0	0	7	0
All	All	8224	0	7973	233	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 15.

All (233) 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:459:THR:HG22	1:A:461:ARG:H	1.07	1.11
1:A:131:THR:HG22	1:A:143:ARG:HD2	1.30	1.06
1:A:459:THR:HG22	1:A:461:ARG:N	1.82	0.94
1:A:320:ASP:H	1:A:343:GLN:HE22	1.18	0.92
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.52	0.91
1:A:547:GLN:H	1:A:547:GLN:HE21	1.21	0.88
1:A:275:LYS:H	1:A:306:ASN:HD21	1.20	0.87
1:A:503:LEU:HD12	1:A:533:LEU:HD13	1.59	0.85
1:A:547:GLN:HE21	1:A:547:GLN:N	1.77	0.83
1:A:194:GLU:CD	1:A:194:GLU:H	1.86	0.82
2:B:184:MET:HE3	2:B:410:TRP:HB3	1.63	0.81
1:A:131:THR:CG2	1:A:143:ARG:HD2	2.09	0.80
1:A:131:THR:CG2	1:A:143:ARG:HH11	1.97	0.78
1:A:555:GLY:N	1:A:556:ILE:HA	1.99	0.77
1:A:459:THR:CG2	1:A:461:ARG:H	1.91	0.77
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.66	0.75
2:B:278:GLN:HG2	2:B:298:GLU:HB2	1.69	0.74
2:B:58:THR:HG23	8:B:480:HOH:O	1.86	0.74
1:A:450:THR:HG22	1:A:452:LEU:HB3	1.68	0.74
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.86	0.73
2:B:24:TRP:CE3	2:B:25:PRO:HD2	2.24	0.73
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HG2	1:A:277:ARG:HH11	1.54	0.73
1:A:406:TRP:HD1	1:A:407:GLN:HE21	1.38	0.71
2:B:12:LEU:O	2:B:14:PRO:HD3	1.92	0.70
1:A:555:GLY:H	1:A:556:ILE:HA	1.54	0.70
1:A:277:ARG:NH1	1:A:334:GLN:HB3	2.06	0.69
2:B:394:GLN:HG2	2:B:396:GLU:OE1	1.93	0.69
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.74	0.68
2:B:395:LYS:O	2:B:399:GLU:HG2	1.92	0.68
1:A:54:ASN:ND2	1:A:56:TYR:H	1.91	0.68
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.74	0.68
2:B:116:PHE:C	2:B:116:PHE:HD1	2.01	0.68
1:A:401:TRP:HD1	1:A:402:TRP:CD1	2.11	0.68
1:A:57:ASN:OD1	1:A:131:THR:HG23	1.95	0.67
2:B:116:PHE:C	2:B:116:PHE:CD1	2.73	0.67
2:B:120:LEU:O	2:B:125:ARG:HD3	1.94	0.66
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.11	0.66
1:A:66:LYS:O	1:A:67:ASP:HB3	1.96	0.65
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.77	0.65
1:A:447:ASN:ND2	1:A:450:THR:H	1.95	0.65
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.77	0.65
1:A:205:LEU:HD13	1:A:209:LEU:HD22	1.80	0.64
1:A:265:ASN:HD21	4:A:569:GOL:H32	1.62	0.64
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.80	0.64
1:A:202:ILE:O	1:A:206:ARG:HG3	1.98	0.63
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.80	0.63
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.81	0.63
2:B:184:MET:HE3	2:B:410:TRP:CB	2.29	0.62
2:B:296:THR:CG2	2:B:298:GLU:HG2	2.29	0.62
2:B:24:TRP:CD2	2:B:25:PRO:HD2	2.35	0.61
1:A:54:ASN:HB3	1:A:143:ARG:HH21	1.66	0.61
2:B:84:THR:O	2:B:84:THR:HG22	2.00	0.61
1:A:54:ASN:C	1:A:54:ASN:HD22	2.10	0.59
2:B:72:ARG:NH2	8:B:552:HOH:O	2.36	0.59
1:A:450:THR:CG2	1:A:452:LEU:HB3	2.33	0.59
1:A:184:MET:HE1	8:A:753:HOH:O	2.02	0.59
1:A:536:VAL:HG13	1:A:537:PRO:HD2	1.85	0.59
2:B:374:LYS:HE2	2:B:378:GLU:OE1	2.03	0.59
1:A:473:THR:OG1	1:A:476:LYS:HD3	2.02	0.58
2:B:253:THR:O	2:B:257:ILE:HG12	2.04	0.58
1:A:53:GLU:H	1:A:53:GLU:CD	2.12	0.58
1:A:122:GLU:HG3	8:A:608:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HG2	1:A:277:ARG:NH1	2.18	0.58
2:B:177:ASP:HB2	8:B:462:HOH:O	2.03	0.57
2:B:400:THR:HG1	2:B:401:TRP:CD1	2.22	0.57
2:B:295:LEU:N	2:B:295:LEU:HD23	2.19	0.57
2:B:241:VAL:O	2:B:243:PRO:HD3	2.04	0.57
1:A:406:TRP:HZ3	1:A:507:GLN:HG2	1.69	0.56
1:A:287:LYS:HB2	8:A:702:HOH:O	2.06	0.56
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.87	0.56
2:B:296:THR:HG21	2:B:298:GLU:HG2	1.87	0.56
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.88	0.56
1:A:473:THR:HG23	1:A:476:LYS:NZ	2.20	0.56
1:A:209:LEU:HD23	1:A:216:THR:HG21	1.88	0.56
2:B:307:ARG:O	2:B:311:LYS:HG3	2.06	0.56
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.86	0.56
1:A:407:GLN:HE22	2:B:419:THR:H	1.54	0.55
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.05	0.55
1:A:54:ASN:HD22	1:A:56:TYR:H	1.54	0.54
2:B:296:THR:HG22	2:B:297:GLU:N	2.22	0.54
1:A:536:VAL:HG11	1:A:542:ILE:HG21	1.89	0.54
1:A:277:ARG:HH12	1:A:334:GLN:HB3	1.73	0.54
1:A:318:TYR:OH	3:A:568:TT1:H8	2.07	0.53
1:A:420:PRO:HA	1:A:421:PRO:C	2.33	0.53
1:A:447:ASN:HB3	1:A:450:THR:HB	1.90	0.53
2:B:64:LYS:HD3	2:B:68:SER:O	2.09	0.53
1:A:544:GLY:CA	2:B:286:THR:HG22	2.38	0.53
1:A:295:LEU:HD12	1:A:300:GLU:OE2	2.08	0.53
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.39	0.53
2:B:257:ILE:HB	2:B:283:LEU:HD11	1.91	0.52
1:A:518:VAL:O	1:A:522:ILE:HG13	2.09	0.52
1:A:470:THR:O	1:A:471:ASP:OD1	2.27	0.52
2:B:214:LEU:HG	2:B:215:THR:N	2.24	0.52
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.44	0.52
1:A:503:LEU:CD1	1:A:533:LEU:HD13	2.34	0.52
1:A:63:ILE:HG12	1:A:64:LYS:N	2.25	0.52
2:B:252:TRP:HD1	2:B:295:LEU:HD22	1.73	0.52
1:A:27:THR:HG22	1:A:28:GLU:N	2.26	0.51
1:A:459:THR:CG2	1:A:460:ASN:N	2.73	0.51
1:A:167:ILE:O	1:A:208:HIS:HE1	1.92	0.51
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.92	0.51
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.46	0.51
1:A:406:TRP:CZ3	1:A:507:GLN:HG2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LYS:HE2	1:A:55:PRO:HB2	1.92	0.51
1:A:447:ASN:ND2	1:A:449:GLU:H	2.09	0.51
1:A:34:LEU:HD13	1:A:62:ALA:HB2	1.93	0.51
1:A:260:LEU:HD13	1:A:279:LEU:HD13	1.94	0.50
2:B:266:TRP:HH2	2:B:427:TYR:OH	1.95	0.50
1:A:542:ILE:O	1:A:543:GLY:C	2.55	0.50
2:B:266:TRP:CD1	2:B:426:TRP:CZ3	3.00	0.50
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.94	0.50
2:B:125:ARG:HB3	2:B:146:TYR:O	2.12	0.49
2:B:297:GLU:HG2	2:B:298:GLU:N	2.26	0.49
1:A:277:ARG:NH1	1:A:334:GLN:CB	2.75	0.49
2:B:356:ARG:N	2:B:356:ARG:HD2	2.28	0.49
1:A:266:TRP:O	1:A:269:GLN:HG2	2.13	0.49
1:A:67:ASP:CG	1:A:67:ASP:O	2.56	0.49
2:B:296:THR:HG22	2:B:298:GLU:H	1.78	0.49
1:A:255:ASN:HB2	1:A:289:LEU:HG	1.95	0.48
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.13	0.48
2:B:254:VAL:O	2:B:258:GLN:HG3	2.12	0.48
1:A:27:THR:O	1:A:31:ILE:HG13	2.12	0.48
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.76	0.48
1:A:54:ASN:HD21	1:A:56:TYR:HB2	1.78	0.48
2:B:312:GLU:HB3	2:B:313:PRO:HD2	1.94	0.48
2:B:246:LEU:HD22	2:B:260:LEU:HD11	1.95	0.48
1:A:64:LYS:HD2	1:A:64:LYS:HA	1.69	0.48
1:A:17:ASP:O	1:A:83:ARG:NE	2.37	0.48
1:A:76:ASP:HA	8:A:692:HOH:O	2.14	0.48
1:A:139:THR:HB	1:A:140:PRO:HD2	1.96	0.47
1:A:118:VAL:HG13	1:A:119:PRO:HD2	1.96	0.47
1:A:363:ASN:ND2	1:A:401:TRP:CH2	2.79	0.47
2:B:205:LEU:HD22	2:B:209:LEU:CD2	2.44	0.47
2:B:250:ASP:OD2	2:B:250:ASP:N	2.43	0.47
1:A:443:ASP:OD2	1:A:444:GLY:N	2.45	0.47
2:B:112:GLY:HA3	2:B:151:GLN:HE21	1.80	0.47
2:B:356:ARG:HH11	2:B:356:ARG:HG2	1.80	0.47
1:A:464:GLN:NE2	8:A:648:HOH:O	2.47	0.47
1:A:26:LEU:HD22	1:A:133:PRO:HG3	1.97	0.47
1:A:354:TYR:CD1	1:A:374:LYS:HD2	2.49	0.47
2:B:14:PRO:HA	2:B:15:GLY:HA2	1.55	0.47
1:A:447:ASN:C	1:A:447:ASN:HD22	2.22	0.46
1:A:542:ILE:O	1:A:543:GLY:O	2.33	0.46
2:B:356:ARG:HG3	8:B:514:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:THR:CG2	2:B:297:GLU:OE1	2.63	0.46
2:B:214:LEU:HG	2:B:215:THR:H	1.80	0.46
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.56	0.46
1:A:95:PRO:HA	2:B:136:ASN:O	2.16	0.46
1:A:413:GLU:HA	8:A:737:HOH:O	2.14	0.46
1:A:336:GLN:NE2	8:A:644:HOH:O	2.43	0.46
2:B:64:LYS:O	2:B:407:GLN:NE2	2.49	0.45
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.50	0.45
1:A:194:GLU:OE1	1:A:197:GLN:HG3	2.16	0.45
1:A:395:LYS:HA	1:A:414:TRP:CH2	2.51	0.45
1:A:459:THR:HG22	1:A:460:ASN:N	2.30	0.45
1:A:466:VAL:HG21	1:A:551:LEU:HG	1.98	0.45
1:A:54:ASN:ND2	1:A:54:ASN:C	2.73	0.45
2:B:175:ASN:HD21	2:B:201:LYS:HZ2	1.65	0.45
2:B:7:THR:HG23	2:B:7:THR:O	2.16	0.45
2:B:270:ILE:HG12	2:B:346:PHE:O	2.17	0.45
1:A:58:THR:HG23	1:A:76:ASP:O	2.16	0.45
1:A:106:VAL:HA	1:A:189:VAL:O	2.16	0.45
1:A:393:ILE:CB	1:A:423:VAL:HG13	2.46	0.45
1:A:194:GLU:CD	1:A:194:GLU:N	2.62	0.45
1:A:448:ARG:O	1:A:451:LYS:HD2	2.16	0.44
2:B:393:ILE:HG12	2:B:394:GLN:N	2.32	0.44
1:A:8:VAL:O	1:A:121:ASP:HB2	2.17	0.44
1:A:407:GLN:NE2	2:B:419:THR:H	2.15	0.44
1:A:395:LYS:HA	1:A:414:TRP:HH2	1.82	0.44
2:B:7:THR:HG21	8:B:506:HOH:O	2.17	0.44
1:A:52:PRO:HD2	1:A:53:GLU:OE1	2.18	0.44
1:A:173:LYS:NZ	1:A:174:GLN:HG3	2.33	0.44
1:A:457:TYR:CD1	1:A:457:TYR:C	2.95	0.44
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.99	0.44
1:A:257:ILE:O	1:A:261:VAL:HG23	2.18	0.44
1:A:105:SER:O	1:A:190:GLY:HA2	2.18	0.44
1:A:26:LEU:CD2	1:A:133:PRO:HG3	2.48	0.44
2:B:266:TRP:HH2	2:B:427:TYR:HH	1.59	0.44
2:B:277:ARG:O	2:B:281:LYS:HG3	2.18	0.44
1:A:545:ASN:O	1:A:549:ASP:HB2	2.18	0.43
2:B:24:TRP:CH2	2:B:400:THR:HG22	2.53	0.43
2:B:163:SER:O	2:B:167:ILE:HG13	2.18	0.43
2:B:242:GLN:HB2	2:B:352:GLY:HA2	2.00	0.43
2:B:96:HIS:HE1	2:B:381:VAL:O	2.01	0.43
2:B:296:THR:HG22	2:B:297:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:THR:O	2:B:364:ASP:HB2	2.18	0.43
2:B:283:LEU:O	2:B:284:ARG:C	2.62	0.43
1:A:210:LEU:C	1:A:212:TRP:H	2.25	0.43
1:A:169:GLU:N	1:A:170:PRO:HD2	2.33	0.43
2:B:295:LEU:HD23	2:B:295:LEU:H	1.81	0.43
1:A:454:LYS:CB	1:A:552:VAL:HG13	2.49	0.43
1:A:42:GLU:OE2	1:A:49:LYS:HE3	2.19	0.42
1:A:471:ASP:O	1:A:471:ASP:CG	2.62	0.42
1:A:473:THR:HG23	1:A:476:LYS:HZ3	1.83	0.42
1:A:509:GLN:N	1:A:510:PRO:CD	2.82	0.42
2:B:205:LEU:HD22	2:B:209:LEU:HD23	2.01	0.42
1:A:104:LYS:HB2	1:A:192:ASP:HA	2.01	0.42
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.55	0.42
2:B:194:GLU:HG3	2:B:197:GLN:HG3	2.01	0.42
1:A:27:THR:CG2	1:A:28:GLU:N	2.83	0.42
2:B:24:TRP:CZ3	2:B:400:THR:HG22	2.55	0.42
1:A:210:LEU:C	1:A:212:TRP:N	2.76	0.42
1:A:402:TRP:CD2	1:A:409:THR:HG21	2.55	0.42
2:B:122:GLU:HA	2:B:125:ARG:CG	2.50	0.42
2:B:137:ASN:ND2	8:B:540:HOH:O	2.53	0.42
2:B:271:TYR:O	2:B:274:ILE:HG12	2.20	0.42
1:A:171:PHE:CG	1:A:205:LEU:HD23	2.55	0.41
2:B:362:THR:OG1	2:B:363:ASN:N	2.53	0.41
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.35	0.41
2:B:338:THR:HG21	2:B:427:TYR:O	2.20	0.41
1:A:399:GLU:O	1:A:403:THR:HG23	2.19	0.41
2:B:116:PHE:HB3	8:B:520:HOH:O	2.20	0.41
1:A:253:THR:HA	1:A:291:GLU:O	2.21	0.41
2:B:125:ARG:H	2:B:125:ARG:HG2	1.59	0.41
1:A:34:LEU:HD12	1:A:34:LEU:HA	1.79	0.41
1:A:246:LEU:HD11	1:A:310:LEU:HD12	2.02	0.41
1:A:265:ASN:ND2	4:A:569:GOL:H32	2.31	0.41
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.78	0.41
1:A:225:PRO:CG	3:A:568:TT1:H25	2.50	0.41
2:B:7:THR:OG1	2:B:121:ASP:HA	2.21	0.41
2:B:120:LEU:O	2:B:121:ASP:C	2.63	0.41
2:B:261:VAL:O	2:B:265:ASN:HB3	2.21	0.41
1:A:225:PRO:HA	1:A:226:PRO:C	2.45	0.41
1:A:447:ASN:HD22	1:A:449:GLU:N	2.18	0.41
2:B:257:ILE:HG22	2:B:283:LEU:HD21	2.03	0.41
1:A:156:SER:HB2	1:A:157:PRO:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PRO:HD3	1:A:80:LEU:HD23	2.04	0.40
1:A:173:LYS:HZ2	1:A:174:GLN:HG3	1.86	0.40
1:A:219:LYS:HB3	1:A:219:LYS:HE3	1.89	0.40
1:A:447:ASN:ND2	1:A:447:ASN:C	2.78	0.40
2:B:386:THR:HA	2:B:387:PRO:HD3	1.88	0.40
1:A:479:LEU:HB3	1:A:517:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	555/560 (99%)	531 (96%)	22 (4%)	2 (0%)	30	38
2	B	394/440 (90%)	380 (96%)	13 (3%)	1 (0%)	36	46
All	All	949/1000 (95%)	911 (96%)	35 (4%)	3 (0%)	36	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	543	GLY
2	B	284	ARG

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	20
2	B	367/400 (92%)	340 (93%)	27 (7%)	13	17
All	All	864/900 (96%)	803 (93%)	61 (7%)	13	19

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	34	LEU
1	A	54	ASN
1	A	66	LYS
1	A	80	LEU
1	A	161	GLN
1	A	168	LEU
1	A	187	LEU
1	A	194	GLU
1	A	205	LEU
1	A	209	LEU
1	A	214	LEU
1	A	219	LYS
1	A	234	LEU
1	A	260	LEU
1	A	264	LEU
1	A	282	LEU
1	A	283	LEU
1	A	289	LEU
1	A	301	LEU
1	A	311	LYS
1	A	368	LEU
1	A	423	VAL
1	A	424	LYS
1	A	428	GLN
1	A	447	ASN
1	A	452	LEU
1	A	464	GLN
1	A	471	ASP
1	A	479	LEU
1	A	507	GLN
1	A	517	LEU
1	A	533	LEU
1	A	547	GLN
2	B	22	LYS

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Mol	Chain	Res	Type
2	B	24	TRP
2	B	28	GLU
2	B	73	LYS
2	B	80	LEU
2	B	116	PHE
2	B	125	ARG
2	B	184	MET
2	B	193	LEU
2	B	203	GLU
2	B	205	LEU
2	B	214	LEU
2	B	234	LEU
2	B	250	ASP
2	B	264	LEU
2	B	265	ASN
2	B	277	ARG
2	B	278	GLN
2	B	283	LEU
2	B	289	LEU
2	B	295	LEU
2	B	310	LEU
2	B	334	GLN
2	B	369	THR
2	B	395	LYS
2	B	407	GLN
2	B	418	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	136	ASN
1	A	207	GLN
1	A	208	HIS
1	A	242	GLN
1	A	258	GLN
1	A	306	ASN
1	A	336	GLN
1	A	343	GLN
1	A	373	GLN
1	A	407	GLN
1	A	447	ASN

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Mol	Chain	Res	Type
1	A	464	GLN
1	A	480	GLN
1	A	500	GLN
1	A	512	GLN
1	A	520	GLN
1	A	524	GLN
1	A	539	HIS
1	A	547	GLN
2	B	96	HIS
2	B	151	GLN
2	B	161	GLN
2	B	175	ASN
2	B	182	GLN
2	B	255	ASN
2	B	278	GLN
2	B	315	HIS
2	B	348	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	563	-	4,4,4	0.36	0	6,6,6	0.08	0
3	TT1	A	568	-	29,29,29	3.23	19 (65%)	37,39,39	1.50	4 (10%)
5	SO4	A	561	-	4,4,4	0.37	0	6,6,6	0.17	0
5	SO4	A	562	-	4,4,4	0.37	0	6,6,6	0.13	0
5	SO4	A	564	-	4,4,4	0.38	0	6,6,6	0.08	0
4	GOL	A	569	-	5,5,5	0.33	0	5,5,5	0.31	0
5	SO4	A	565	-	4,4,4	0.40	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TT1	A	568	-	-	4/13/13/13	0/4/4/4
4	GOL	A	569	-	-	0/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	568	TT1	C25-C26	9.37	1.54	1.38
3	A	568	TT1	C8-C20	5.47	1.58	1.51
3	A	568	TT1	C21-C20	4.68	1.46	1.39
3	A	568	TT1	C10-N11	-3.96	1.30	1.38
3	A	568	TT1	C3-C2	3.72	1.46	1.38
3	A	568	TT1	C12-N11	-3.69	1.31	1.38
3	A	568	TT1	C12-N18	-3.59	1.27	1.32
3	A	568	TT1	C6-C7	3.49	1.44	1.38
3	A	568	TT1	C5-C6	3.49	1.45	1.38
3	A	568	TT1	C10-S9	3.33	1.80	1.74
3	A	568	TT1	C4-C3	3.06	1.44	1.38
3	A	568	TT1	C4-C5	3.05	1.44	1.38
3	A	568	TT1	C7-C2	2.95	1.44	1.38
3	A	568	TT1	C23-C21	2.52	1.44	1.38
3	A	568	TT1	C13-S14	2.46	1.79	1.71
3	A	568	TT1	C10-N19	-2.29	1.28	1.31
3	A	568	TT1	C24-C23	2.18	1.42	1.38
3	A	568	TT1	C26-C20	2.12	1.43	1.39
3	A	568	TT1	C13-C12	2.06	1.48	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	568	TT1	N11-C12-N18	6.73	113.50	110.40
3	A	568	TT1	C13-C12-N18	-2.25	120.43	124.79
3	A	568	TT1	S9-C10-N19	-2.07	124.79	127.78
3	A	568	TT1	C15-S14-C13	-2.02	88.70	92.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

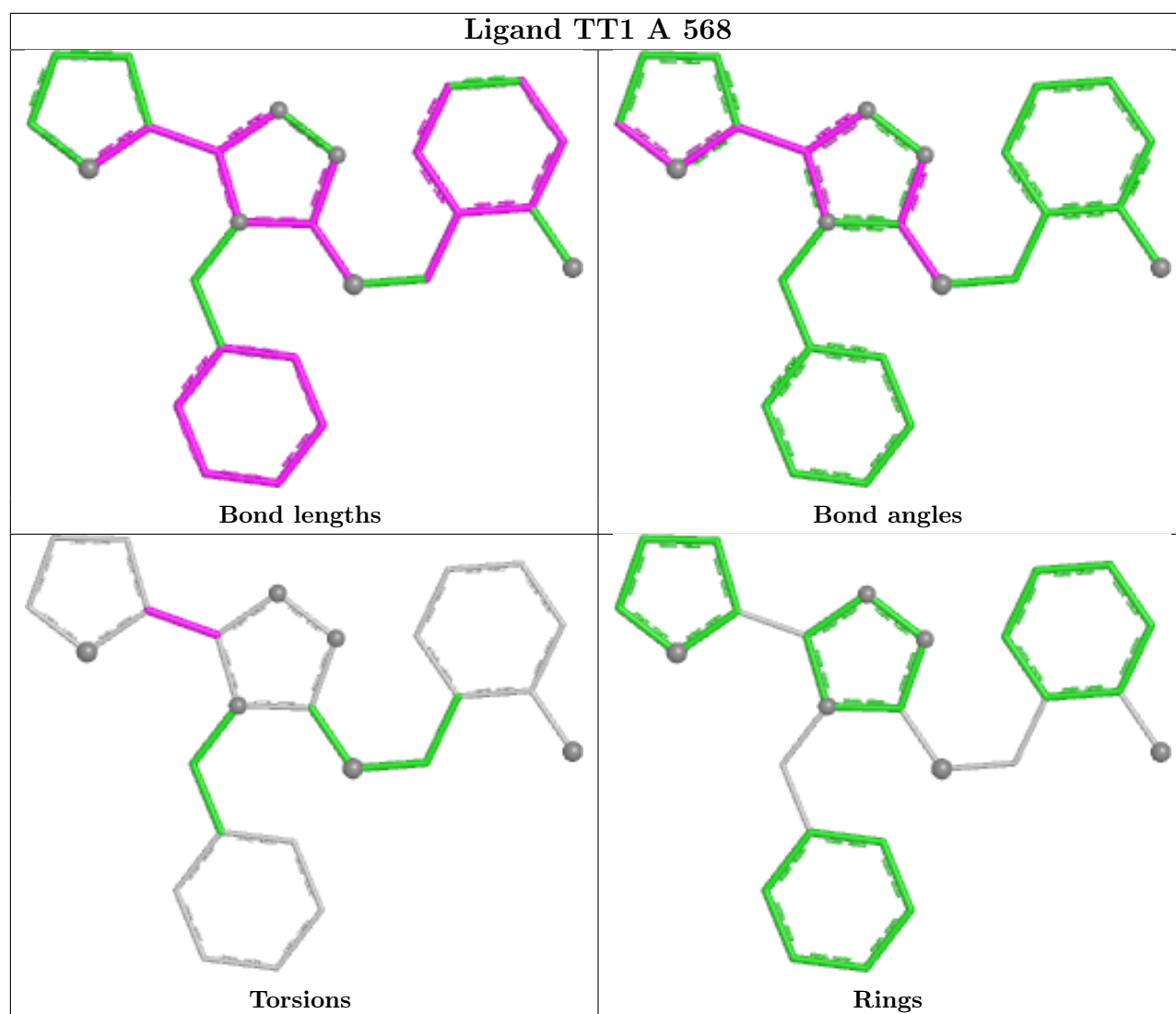
Mol	Chain	Res	Type	Atoms
3	A	568	TT1	N18-C12-C13-S14
3	A	568	TT1	N18-C12-C13-C17
3	A	568	TT1	N11-C12-C13-S14
3	A	568	TT1	N11-C12-C13-C17

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	568	TT1	2	0
4	A	569	GOL	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, 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	557/560 (99%)	0.18	11 (1%) 65 66	33, 57, 88, 117	0
2	B	402/440 (91%)	0.28	25 (6%) 26 28	34, 55, 101, 127	0
All	All	959/1000 (95%)	0.23	36 (3%) 44 46	33, 56, 95, 127	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	556	ILE	4.6
2	B	295	LEU	4.2
1	A	286	THR	4.0
2	B	429	LEU	3.9
2	B	346	PHE	3.6
2	B	24	TRP	3.4
1	A	471	ASP	3.4
2	B	213	GLY	3.3
2	B	232	TYR	3.2
2	B	214	LEU	3.2
1	A	554	ALA	3.2
2	B	362	THR	3.1
2	B	215	THR	3.0
2	B	252	TRP	2.8
2	B	426	TRP	2.8
1	A	555	GLY	2.8
2	B	282	LEU	2.7
2	B	310	LEU	2.6
1	A	462	GLY	2.5
2	B	293	ILE	2.4
1	A	402	TRP	2.4
1	A	446	ALA	2.3
2	B	355	ALA	2.3
2	B	283	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	292	VAL	2.3
1	A	357	MET	2.2
1	A	52	PRO	2.2
2	B	296	THR	2.2
2	B	14	PRO	2.1
2	B	276	VAL	2.1
2	B	87	PHE	2.1
2	B	288	ALA	2.1
1	A	551	LEU	2.0
2	B	266	TRP	2.0
2	B	216	THR	2.0
2	B	422	LEU	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, 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.

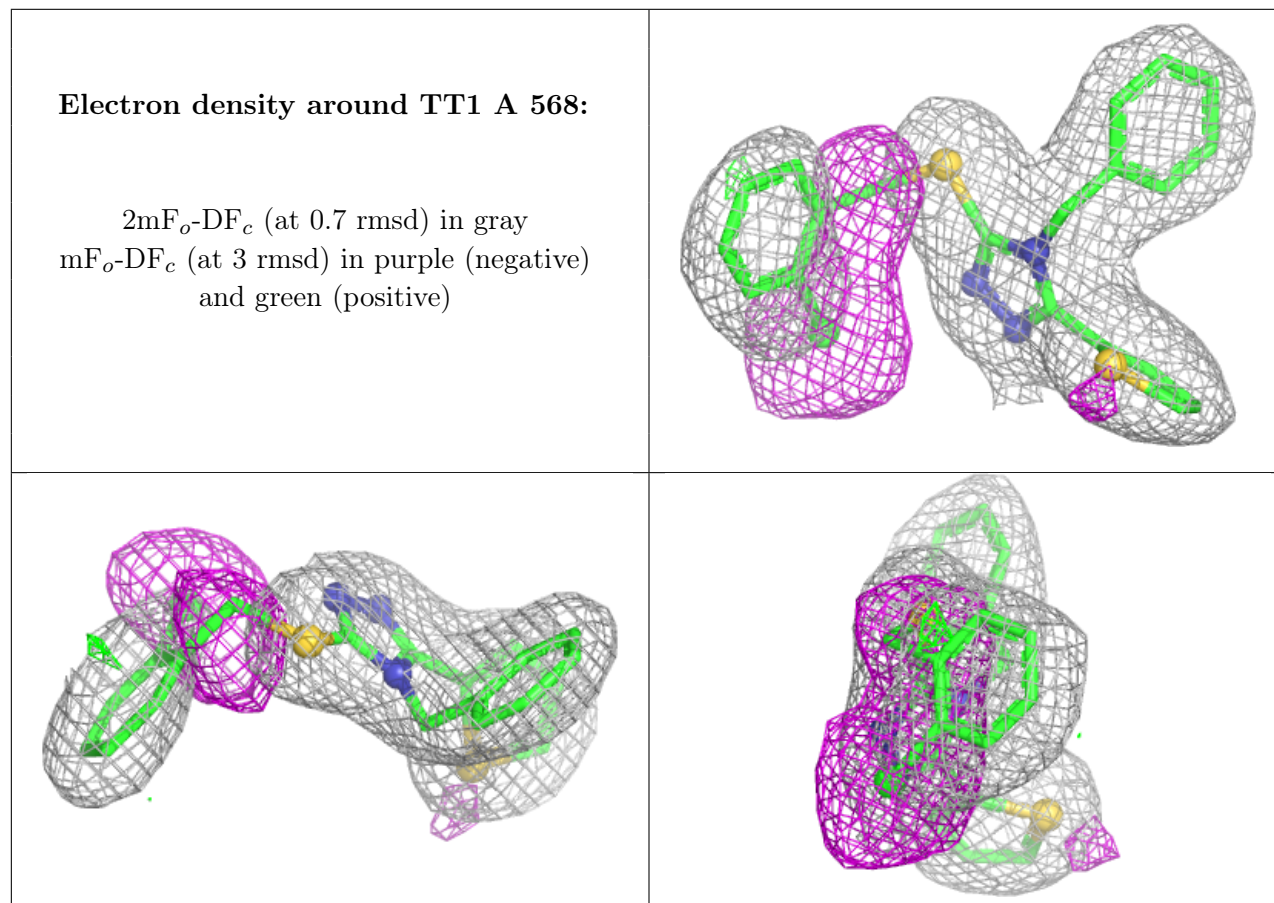
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	569	6/6	0.65	0.21	98,100,101,101	0
7	MG	A	567	1/1	0.79	0.31	82,82,82,82	0
5	SO4	A	565	5/5	0.82	0.10	90,91,91,92	0
5	SO4	A	564	5/5	0.82	0.08	117,118,118,118	0
5	SO4	A	563	5/5	0.83	0.18	159,159,159,159	0
3	TT1	A	568	26/26	0.83	0.13	39,44,58,59	0
5	SO4	A	561	5/5	0.84	0.15	95,95,96,98	0
6	CL	B	442	1/1	0.85	0.25	96,96,96,96	0
5	SO4	A	562	5/5	0.86	0.11	81,82,83,84	0
6	CL	B	444	1/1	0.91	0.13	80,80,80,80	0
6	CL	B	443	1/1	0.93	0.19	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CL	A	566	1/1	0.96	0.14	83,83,83,83	0
6	CL	B	441	1/1	0.97	0.14	73,73,73,73	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.