



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:26 PM UTC

PDB ID : 6VLH / pdb_00006vlh
Title : HIV Integrase Core domain (IN) in complex with dimer-spanning ligand
Authors : Gorman, M.A.; Parker, M.W.
Deposited on : 2020-01-24
Resolution : 2.04 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

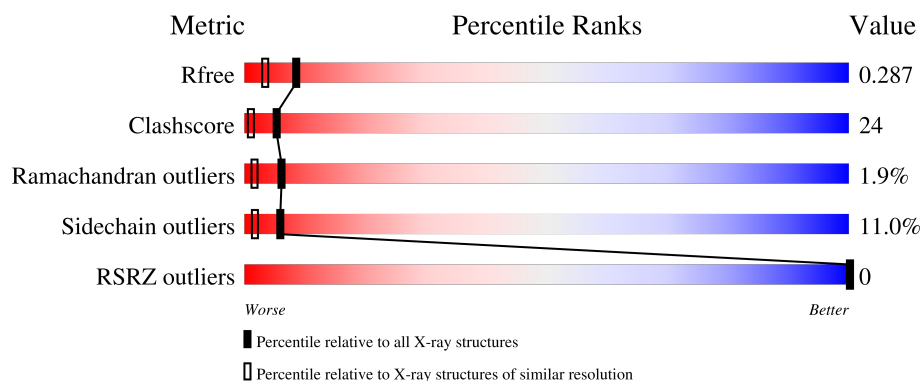
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	164	
1	B	164	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	A	301	-	-	X	-
3	SO4	B	304	-	-	X	-
3	SO4	B	305	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4413 atoms, of which 2147 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 Integrase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	137	Total	C	H	N	O	S	0	0	0
			2105	672	1051	183	195	4			
1	B	136	Total	C	H	N	O	S	0	1	0
			2109	670	1059	183	194	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLY	-	expression tag	UNP F2WR39
A	49	SER	-	expression tag	UNP F2WR39
A	53	GLU	GLN	engineered mutation	UNP F2WR39
A	56	SER	CYS	engineered mutation	UNP F2WR39
A	131	GLU	TRP	engineered mutation	UNP F2WR39
A	185	LYS	PHE	engineered mutation	UNP F2WR39
A	209	GLU	GLN	engineered mutation	UNP F2WR39
B	48	GLY	-	expression tag	UNP F2WR39
B	49	SER	-	expression tag	UNP F2WR39
B	53	GLU	GLN	engineered mutation	UNP F2WR39
B	56	SER	CYS	engineered mutation	UNP F2WR39
B	131	GLU	TRP	engineered mutation	UNP F2WR39
B	185	LYS	PHE	engineered mutation	UNP F2WR39
B	209	GLU	GLN	engineered mutation	UNP F2WR39

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

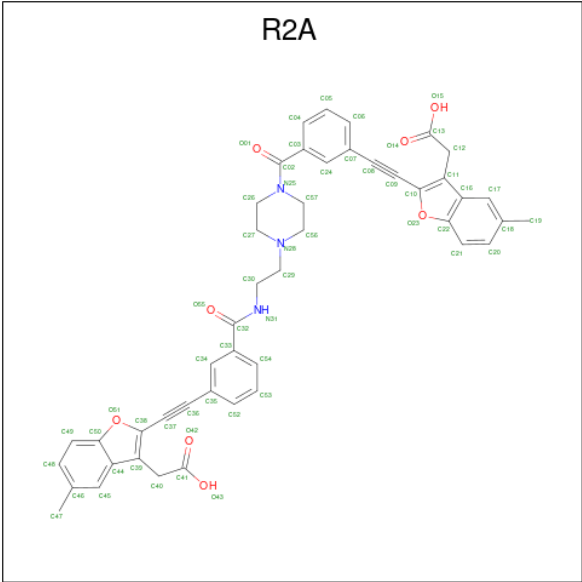
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	I	0	0
			4	4		
2	B	2	Total	I	0	0
			2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is (2-{{3-(4-{2-[(3-{[3-(carboxymethyl)-5-methyl-1-benzofuran-2-yl]ethynyl}benzene-1-carbonyl)amino]ethyl}piperazine-1-carbonyl)phenyl]ethynyl}-5-methyl-1-benzofuran-3-yl)acetic acid (CCD ID: R2A) (formula: C₄₆H₃₉N₃O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			94	46	37	3	8		

- Molecule 5 is water.

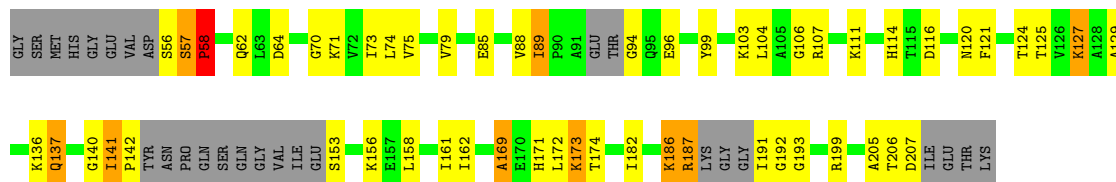
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	23	Total O	0	0
			23 23		
5	B	31	Total O	0	0
			31 31		

3 Residue-property plots [i](#)

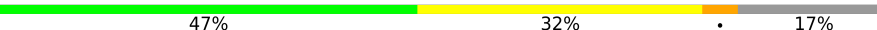
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

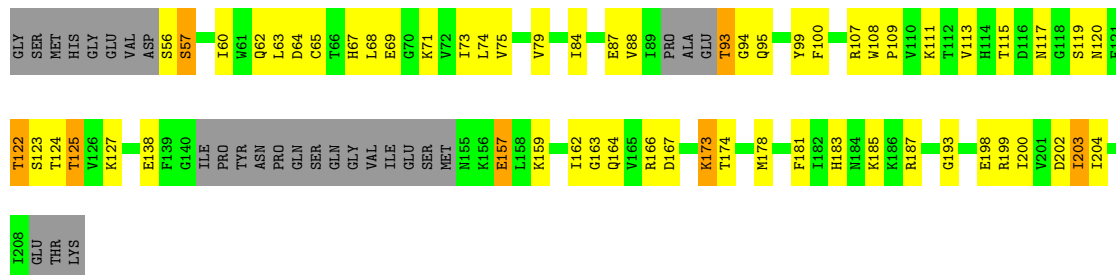
• Molecule 1: Integrase

Chain A: 



• Molecule 1: Integrase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	46.31Å 46.31Å 139.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.31 – 2.04 46.31 – 2.04	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.31-2.04) 94.5 (46.31-2.04)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.03Å)	Xtriage
Refinement program	PHENIX (1.13_2998-000)	Depositor
R, R_{free}	0.209 , 0.298 0.209 , 0.287	Depositor DCC
R_{free} test set	1851 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.480 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4413	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.71% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, CSO, SO4, R2A

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	0.75	2/1064 (0.2%)	0.80	0/1434
1	B	0.63	0/1062	0.77	0/1430
All	All	0.69	2/2126 (0.1%)	0.78	0/2864

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	LEU	C-O	-6.68	1.15	1.24
1	A	169	ALA	C-O	-5.52	1.16	1.23

There are no bond angle outliers.

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	1054	1051	1063	50	0
1	B	1050	1059	1068	58	1
2	A	4	0	0	4	0
2	B	2	0	0	1	0
3	A	20	0	0	0	1
3	B	25	0	0	10	0
4	B	57	37	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	23	0	0	5	0
5	B	31	0	0	3	1
All	All	2266	2147	2131	105	2

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 24.

All (105) 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:57:SER:HB2	1:A:58:PRO:HD3	1.47	0.96
1:A:173:LYS:HE2	2:A:301:IOD:I	2.40	0.92
1:A:99:TYR:OH	1:B:87:GLU:OE2	1.91	0.86
1:A:85:GLU:OE1	1:A:107:ARG:NH1	2.12	0.82
1:A:96:GLU:N	1:A:96:GLU:OE1	2.13	0.81
1:B:93:THR:OG1	1:B:94:GLY:N	2.15	0.78
1:A:103:LYS:O	5:A:401:HOH:O	2.01	0.78
1:A:114:HIS:ND1	1:A:140:GLY:O	2.17	0.78
1:A:199:ARG:NH2	5:A:402:HOH:O	2.19	0.75
1:A:57:SER:CB	1:A:58:PRO:HD3	2.18	0.74
1:A:57:SER:CB	1:A:58:PRO:CD	2.66	0.73
1:A:57:SER:HB2	1:A:58:PRO:CD	2.19	0.72
1:B:107:ARG:O	5:B:401:HOH:O	2.09	0.70
1:A:187:ARG:HD3	2:A:303:IOD:I	2.62	0.69
1:A:120:ASN:ND2	1:A:137:GLN:OE1	2.24	0.67
1:B:64:ASP:OD1	1:B:65:CSO:N	2.33	0.62
1:B:187:ARG:NH2	1:B:198:GLU:OE1	2.33	0.61
1:B:67:HIS:ND1	3:B:303:SO4:O1	2.30	0.61
1:B:115:THR:HG21	1:B:120:ASN:HD22	1.65	0.60
1:B:117:ASN:ND2	1:B:119:SER:OG	2.36	0.58
1:B:56:SER:O	1:B:57:SER:CB	2.51	0.58
1:B:57:SER:HB3	3:B:305:SO4:S	2.45	0.57
1:A:74:LEU:HD11	1:A:89:ILE:HD13	1.86	0.57
1:B:164:GLN:NE2	5:B:406:HOH:O	2.38	0.56
1:A:99:TYR:O	1:A:103:LYS:HG3	2.06	0.55
1:B:56:SER:O	1:B:57:SER:OG	2.24	0.55
1:B:124:THR:O	5:B:402:HOH:O	2.18	0.55
1:B:57:SER:HB3	3:B:305:SO4:O4	2.05	0.55
1:B:108:TRP:HB3	1:B:109:PRO:HD2	1.88	0.55
1:B:166:ARG:HB2	3:B:304:SO4:O4	2.08	0.54
1:B:57:SER:HB2	1:B:60:ILE:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ARG:NH1	1:B:202:ASP:OD2	2.39	0.54
1:B:73:ILE:HG22	1:B:75:VAL:CG2	2.38	0.54
1:B:57:SER:OG	3:B:305:SO4:O1	2.16	0.53
1:A:74:LEU:CD1	1:A:89:ILE:HD13	2.39	0.53
1:A:58:PRO:O	5:A:403:HOH:O	2.19	0.52
1:B:99:TYR:HB2	4:B:308:R2A:C08	2.41	0.51
1:A:121:PHE:CD2	1:A:121:PHE:N	2.78	0.51
1:A:64:ASP:OD2	1:A:141:ILE:CD1	2.58	0.51
1:A:71:LYS:NZ	2:A:301:IOD:I	3.14	0.50
1:B:74:LEU:N	1:B:87:GLU:O	2.40	0.50
1:B:95:GLN:HG2	1:B:125:THR:HG21	1.93	0.50
1:A:120:ASN:HB3	1:A:137:GLN:HE22	1.78	0.49
1:B:162:ILE:HG22	3:B:304:SO4:O4	2.12	0.49
1:A:107:ARG:HD3	1:B:107:ARG:HD3	1.95	0.49
1:A:141:ILE:CG2	1:A:141:ILE:O	2.60	0.49
1:A:104:LEU:O	1:A:107:ARG:N	2.44	0.49
1:B:162:ILE:O	1:B:166:ARG:N	2.45	0.49
1:B:187:ARG:HH22	1:B:198:GLU:CD	2.21	0.48
1:B:74:LEU:HD21	1:B:100:PHE:CD2	2.48	0.48
1:B:123:SER:OG	3:B:306:SO4:O1	2.21	0.48
1:B:166:ARG:NH1	1:B:166:ARG:O	2.44	0.48
1:A:62:GLN:HG3	1:A:79:VAL:CG2	2.44	0.47
1:B:174:THR:HG22	1:B:178:MET:HE3	1.96	0.47
1:B:123:SER:N	1:B:127:LYS:HE2	2.29	0.47
1:A:62:GLN:NE2	1:A:142:PRO:O	2.47	0.47
1:A:187:ARG:HG3	1:A:192:GLY:HA3	1.97	0.47
1:A:158:LEU:O	1:A:162:ILE:HG13	2.15	0.47
1:A:153:SER:O	1:A:156:LYS:HB3	2.15	0.46
1:B:122:THR:O	1:B:122:THR:HG23	2.14	0.46
1:B:173:LYS:HD3	2:B:301:IOD:I	2.84	0.46
1:B:187:ARG:NH1	1:B:198:GLU:OE2	2.45	0.46
1:A:161:ILE:O	1:A:162:ILE:C	2.55	0.46
1:B:163:GLY:HA2	3:B:304:SO4:O3	2.15	0.46
1:A:106:GLY:HA3	5:A:401:HOH:O	2.16	0.46
1:A:94:GLY:O	1:A:125:THR:HB	2.16	0.46
1:B:99:TYR:HB2	4:B:308:R2A:C09	2.47	0.45
1:A:107:ARG:HD3	1:B:107:ARG:CD	2.46	0.45
1:A:141:ILE:O	1:A:141:ILE:HG22	2.16	0.45
1:B:178:MET:O	1:B:181:PHE:HB3	2.17	0.45
1:A:96:GLU:HB2	4:B:308:R2A:O55	2.17	0.45
1:B:167:ASP:OD1	1:B:167:ASP:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:SER:OG	1:A:58:PRO:HD2	2.17	0.44
1:A:121:PHE:O	1:A:127:LYS:NZ	2.40	0.44
1:B:181:PHE:O	1:B:185:LYS:HG2	2.17	0.44
1:B:202:ASP:OD1	1:B:202:ASP:C	2.59	0.44
1:B:57:SER:CB	3:B:305:SO4:O1	2.66	0.44
1:B:69:GLU:OE1	1:B:71:LYS:NZ	2.51	0.44
1:B:73:ILE:HG22	1:B:75:VAL:HG23	1.99	0.44
1:A:205:ALA:O	1:A:206:THR:C	2.61	0.43
1:B:63:LEU:HD12	1:B:63:LEU:HA	1.92	0.43
1:B:73:ILE:HG12	1:B:88:VAL:HG22	2.01	0.43
1:B:157:GLU:OE2	1:B:183:HIS:HD2	2.02	0.43
1:A:129:ALA:HB2	4:B:308:R2A:C48	2.48	0.43
1:B:63:LEU:HD22	1:B:113:VAL:HG11	1.99	0.43
1:B:119:SER:O	1:B:122:THR:HG22	2.18	0.43
1:A:174:THR:OG1	4:B:308:R2A:C10	2.67	0.43
1:A:88:VAL:HG11	2:A:301:IOD:I	2.89	0.42
1:A:70:GLY:O	1:A:71:LYS:HG3	2.19	0.42
1:A:89:ILE:HG23	1:A:96:GLU:HG3	2.01	0.42
1:A:57:SER:OG	1:A:58:PRO:CD	2.68	0.42
1:B:60:ILE:HG13	3:B:305:SO4:O4	2.20	0.42
1:B:199:ARG:HA	1:B:199:ARG:HD2	1.78	0.42
1:B:203:ILE:O	1:B:204:ILE:C	2.62	0.42
1:B:68:LEU:HD13	1:B:159:LYS:HE2	2.02	0.41
1:B:187:ARG:HD3	1:B:193:GLY:O	2.20	0.41
1:B:123:SER:O	1:B:127:LYS:HG3	2.20	0.41
1:A:73:ILE:HG22	1:A:75:VAL:HG22	2.02	0.41
1:B:200:ILE:O	1:B:204:ILE:HD12	2.20	0.41
1:A:116:ASP:HB3	1:A:141:ILE:HB	2.03	0.41
1:A:182:ILE:O	1:A:186:LYS:HB3	2.21	0.41
1:B:99:TYR:O	1:B:100:PHE:C	2.63	0.41
1:A:191:ILE:O	1:A:192:GLY:C	2.64	0.40
1:A:127:LYS:HA	5:A:422:HOH:O	2.22	0.40
1:A:169:ALA:HB1	1:A:174:THR:HG21	2.03	0.40

All (2) 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)
5:B:425:HOH:O	5:B:426:HOH:O[4_555]	1.91	0.29
1:B:122:THR:OG1	3:A:308:SO4:O3[3_554]	2.06	0.14

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	128/164 (78%)	112 (88%)	13 (10%)	3 (2%)	5	1
1	B	130/164 (79%)	119 (92%)	9 (7%)	2 (2%)	8	2
All	All	258/328 (79%)	231 (90%)	22 (8%)	5 (2%)	6	2

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	58	PRO
1	B	57	SER
1	A	193	GLY
1	B	203	ILE

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	110/132 (83%)	96 (87%)	14 (13%)	4	1
1	B	109/132 (83%)	99 (91%)	10 (9%)	8	4
All	All	219/264 (83%)	195 (89%)	24 (11%)	6	2

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	SER

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Mol	Chain	Res	Type
1	A	58	PRO
1	A	89	ILE
1	A	111	LYS
1	A	124	THR
1	A	127	LYS
1	A	136	LYS
1	A	137	GLN
1	A	141	ILE
1	A	171	HIS
1	A	173	LYS
1	A	186	LYS
1	A	187	ARG
1	A	207	ASP
1	B	62	GLN
1	B	79	VAL
1	B	84	ILE
1	B	93	THR
1	B	111	LYS
1	B	122	THR
1	B	125	THR
1	B	138	GLU
1	B	157	GLU
1	B	173	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	120	ASN
1	A	137	GLN
1	A	164	GLN
1	B	120	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
1	CSO	B	65	1	3,6,7	0.89	0	1,6,8	1.12	0
1	CSO	A	65	1	3,6,7	0.68	0	1,6,8	0.90	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
1	CSO	B	65	1	-	0/1/5/7	-
1	CSO	A	65	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	65	CSO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	$\# Z > 2$
3	SO4	A	308	-	4,4,4	0.41	0	6,6,6	0.31	0
3	SO4	B	305	-	4,4,4	0.26	0	6,6,6	0.47	0
3	SO4	B	304	-	4,4,4	0.32	0	6,6,6	0.13	0
4	R2A	B	308	-	61,63,63	2.54	17 (27%)	81,89,89	1.95	25 (30%)
3	SO4	B	303	-	4,4,4	0.26	0	6,6,6	0.18	0
3	SO4	B	307	-	4,4,4	0.23	0	6,6,6	0.38	0
3	SO4	A	307	-	4,4,4	0.27	0	6,6,6	0.21	0
3	SO4	A	305	-	4,4,4	0.28	0	6,6,6	0.20	0
3	SO4	A	306	-	4,4,4	0.32	0	6,6,6	0.51	0
3	SO4	B	306	-	4,4,4	0.26	0	6,6,6	0.22	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
4	R2A	B	308	-	-	5/32/46/46	0/7/7/7

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	308	R2A	C37-C38	7.25	1.53	1.42
4	B	308	R2A	C32-N31	7.08	1.49	1.33
4	B	308	R2A	C02-N25	6.64	1.48	1.34
4	B	308	R2A	O51-C38	-5.57	1.30	1.38
4	B	308	R2A	O23-C10	-5.33	1.31	1.38
4	B	308	R2A	C16-C22	-4.89	1.33	1.39
4	B	308	R2A	C35-C36	4.61	1.55	1.44
4	B	308	R2A	O23-C22	-4.32	1.31	1.38
4	B	308	R2A	C09-C10	3.70	1.48	1.42
4	B	308	R2A	C33-C32	3.46	1.57	1.50
4	B	308	R2A	C09-C08	-3.29	1.15	1.20
4	B	308	R2A	C40-C41	2.95	1.55	1.51
4	B	308	R2A	C12-C13	2.88	1.55	1.51
4	B	308	R2A	O51-C50	-2.77	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	308	R2A	C40-C39	2.40	1.55	1.50
4	B	308	R2A	C03-C02	2.31	1.53	1.50
4	B	308	R2A	C07-C08	2.23	1.49	1.44

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	308	R2A	C50-O51-C38	6.01	111.62	105.68
4	B	308	R2A	C29-C30-N31	4.57	120.39	111.56
4	B	308	R2A	C17-C16-C22	4.56	123.75	119.28
4	B	308	R2A	C16-C17-C18	-4.50	114.83	121.65
4	B	308	R2A	C56-C57-N25	4.09	118.55	110.42
4	B	308	R2A	C27-C26-N25	3.68	117.73	110.42
4	B	308	R2A	C29-N28-C56	3.59	120.81	111.24
4	B	308	R2A	C49-C50-C44	-3.49	119.56	123.58
4	B	308	R2A	O23-C22-C16	3.27	114.04	110.84
4	B	308	R2A	O23-C10-C09	3.10	120.80	116.84
4	B	308	R2A	O51-C38-C37	3.08	120.78	116.84
4	B	308	R2A	C12-C11-C16	3.02	129.99	124.80
4	B	308	R2A	C03-C02-N25	2.96	122.36	118.66
4	B	308	R2A	C33-C32-N31	2.60	122.53	117.12
4	B	308	R2A	O43-C41-O42	-2.36	117.26	123.33
4	B	308	R2A	C30-C29-N28	2.27	118.38	112.84
4	B	308	R2A	O51-C50-C49	2.26	131.25	126.49
4	B	308	R2A	C20-C21-C22	-2.24	115.81	120.06
4	B	308	R2A	O15-C13-C12	2.22	121.38	114.51
4	B	308	R2A	O43-C41-C40	2.20	121.32	114.51
4	B	308	R2A	C20-C18-C17	2.14	121.11	117.96
4	B	308	R2A	O15-C13-O14	-2.08	117.99	123.33
4	B	308	R2A	O01-C02-N25	-2.07	119.09	122.35
4	B	308	R2A	C54-C33-C34	-2.05	116.88	119.25
4	B	308	R2A	C30-N31-C32	2.03	126.69	122.11

There are no chirality outliers.

All (5) torsion outliers are listed below:

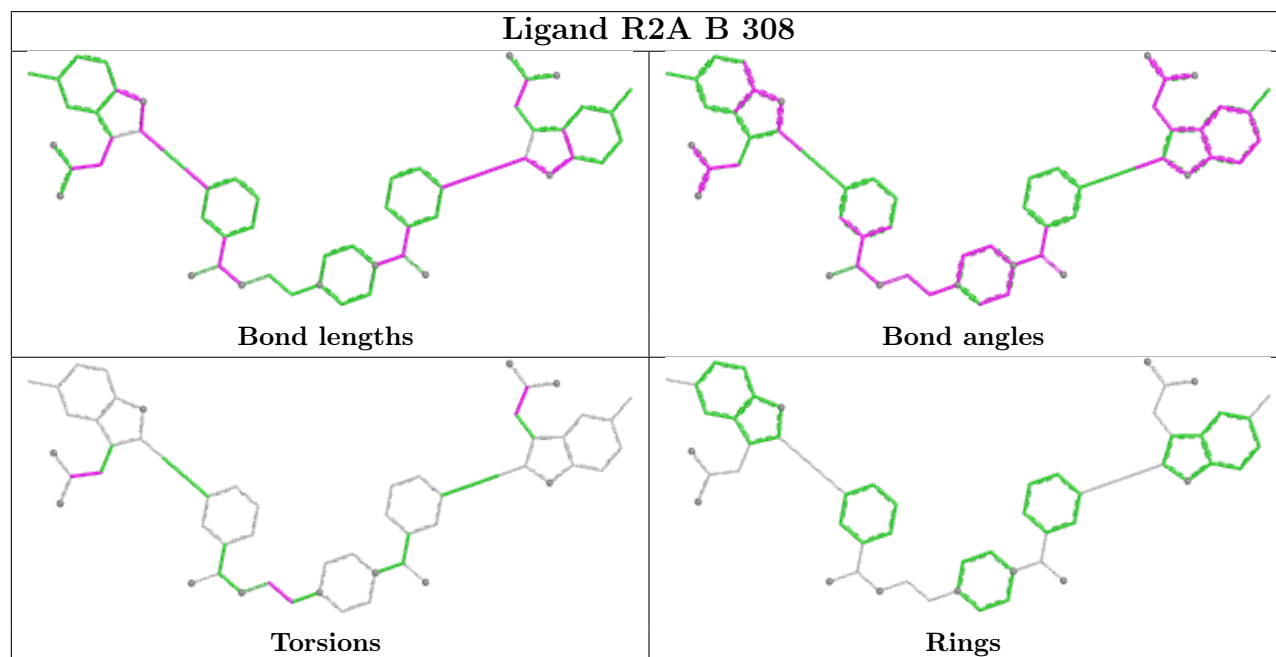
Mol	Chain	Res	Type	Atoms
4	B	308	R2A	N28-C29-C30-N31
4	B	308	R2A	C39-C40-C41-O43
4	B	308	R2A	C39-C40-C41-O42
4	B	308	R2A	C11-C12-C13-O14
4	B	308	R2A	C11-C12-C13-O15

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	308	SO4	0	1
3	B	305	SO4	5	0
3	B	304	SO4	3	0
4	B	308	R2A	5	0
3	B	303	SO4	1	0
3	B	306	SO4	1	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 ⓘ

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 [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	136/164 (82%)	-0.91	0 100 100	20, 38, 63, 74	0
1	B	135/164 (82%)	-0.99	0 100 100	18, 36, 61, 77	1 (0%)
All	All	271/328 (82%)	-0.95	0 100 100	18, 37, 62, 77	1 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSO	A	65	7/8	0.97	0.06	40,43,51,58	0
1	CSO	B	65	7/8	0.97	0.05	33,40,48,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

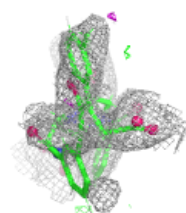
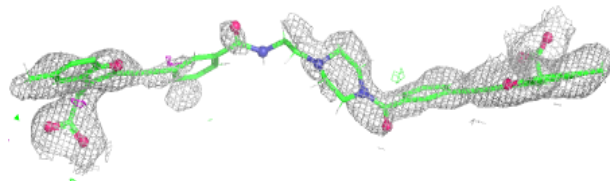
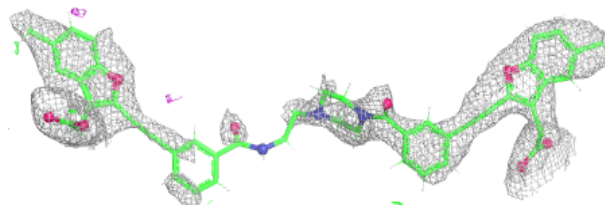
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	306	5/5	0.97	0.07	53,60,72,80	0
3	SO4	B	304	5/5	0.97	0.09	49,51,67,75	0
3	SO4	A	307	5/5	0.98	0.05	48,49,56,63	0
3	SO4	A	305	5/5	0.98	0.05	46,55,59,67	0
3	SO4	B	305	5/5	0.98	0.06	33,35,44,47	0
3	SO4	B	306	5/5	0.98	0.04	35,38,44,47	0
4	R2A	B	308	57/57	0.98	0.06	27,49,64,73	0
3	SO4	A	308	5/5	0.99	0.05	29,31,40,54	0
3	SO4	B	303	5/5	0.99	0.05	49,50,53,72	0
2	IOD	B	302	1/1	0.99	0.03	58,58,58,58	0
2	IOD	A	301	1/1	1.00	0.03	57,57,57,57	0
2	IOD	A	302	1/1	1.00	0.04	46,46,46,46	0
2	IOD	A	303	1/1	1.00	0.03	56,56,56,56	0
2	IOD	A	304	1/1	1.00	0.08	78,78,78,78	0
3	SO4	B	307	5/5	1.00	0.03	33,33,43,46	0
2	IOD	B	301	1/1	1.00	0.04	52,52,52,52	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.

Electron density around R2A B 308:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.