



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:04 AM UTC

PDB ID : 8SCE / pdb_00008sce
Title : Crystal structure of IRAK4-HSA complexed with N-[(2R)-2-FLUORO-3-HYDROXY-3-METHYLBUTYL]-6-[(5-FLUOROPYRI-YL)AMINO]-4-[(PROPAN-2-YL)AMINO]PYRIDINE-3-CARBOXAMIDE
Authors : Muckelbauer, J.K.; Ghosh, K.
Deposited on : 2023-04-05
Resolution : 1.89 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

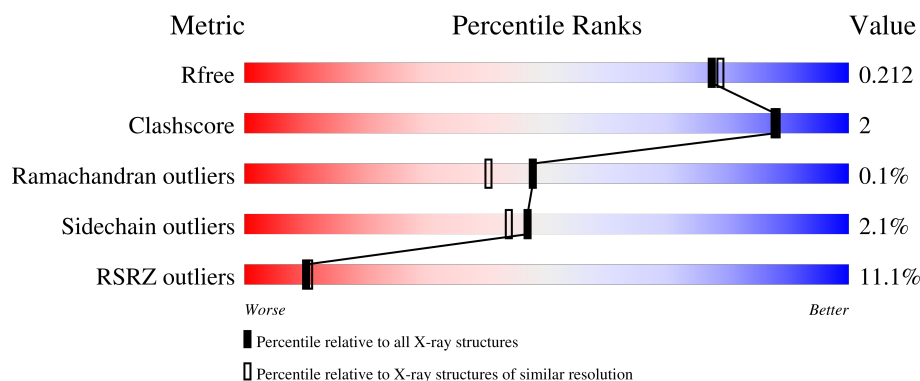
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	305	6% 88% 5% • 6%
1	B	305	10% 86% 8% 6%
1	D	305	10% 87% 7% • 5%
1	E	305	15% 87% 7% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9539 atoms, of which 96 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.

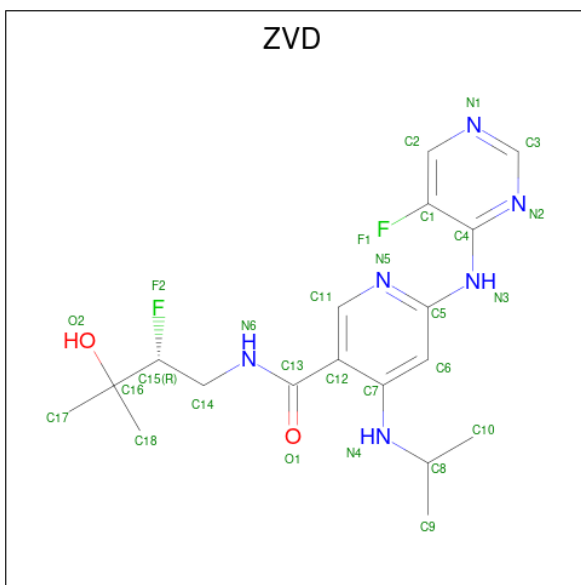
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	P	S	0	1	0
			2206	1388	375	427	2	14			
1	B	287	Total	C	N	O	P	S	0	0	0
			2201	1384	369	431	3	14			
1	D	289	Total	C	N	O	P	S	0	1	0
			2193	1377	370	428	3	15			
1	E	285	Total	C	N	O	P	S	0	1	0
			2185	1373	368	427	3	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLY	-	expression tag	UNP Q9NWZ3
A	157	ALA	-	expression tag	UNP Q9NWZ3
A	158	MET	-	expression tag	UNP Q9NWZ3
A	159	GLY	-	expression tag	UNP Q9NWZ3
B	156	GLY	-	expression tag	UNP Q9NWZ3
B	157	ALA	-	expression tag	UNP Q9NWZ3
B	158	MET	-	expression tag	UNP Q9NWZ3
B	159	GLY	-	expression tag	UNP Q9NWZ3
D	156	GLY	-	expression tag	UNP Q9NWZ3
D	157	ALA	-	expression tag	UNP Q9NWZ3
D	158	MET	-	expression tag	UNP Q9NWZ3
D	159	GLY	-	expression tag	UNP Q9NWZ3
E	156	GLY	-	expression tag	UNP Q9NWZ3
E	157	ALA	-	expression tag	UNP Q9NWZ3
E	158	MET	-	expression tag	UNP Q9NWZ3
E	159	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is N-[(2R)-2-fluoro-3-hydroxy-3-methylbutyl]-6-[(5-fluoropyrimidin-4-yl)amino]-4-[(propan-2-yl)amino]pyridine-3-carboxamide (CCD ID: ZVD) (formula: C₁₈H₂₄F₂N₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 52	C 18	F 2	H 24	N 6	O 2	0	0
2	B	1	Total 52	C 18	F 2	H 24	N 6	O 2	0	0
2	D	1	Total 52	C 18	F 2	H 24	N 6	O 2	0	0
2	E	1	Total 52	C 18	F 2	H 24	N 6	O 2	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

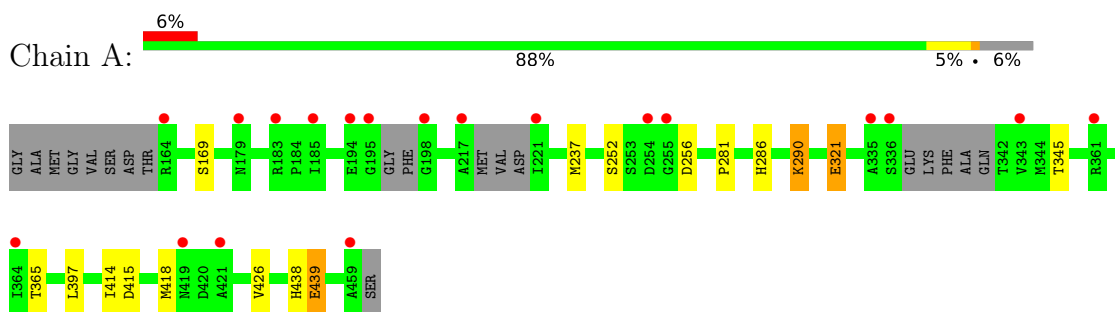
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	154	Total O 154 154	0	0
4	B	140	Total O 140 140	0	0
4	D	122	Total O 122 122	0	0
4	E	115	Total O 115 115	0	0

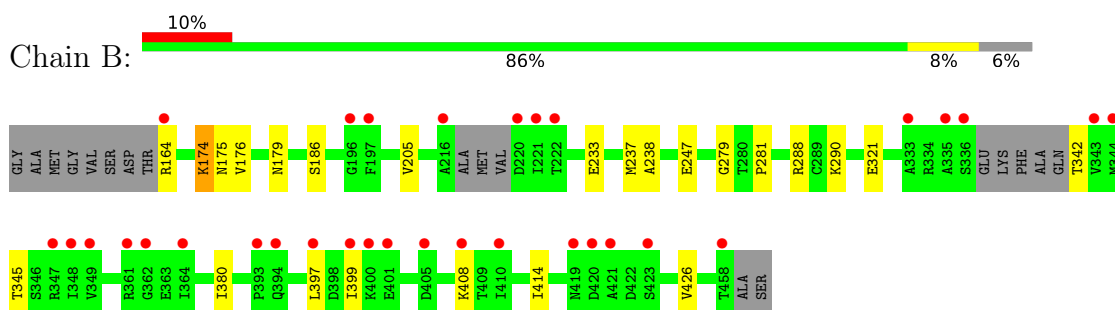
3 Residue-property plots [i](#)

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.

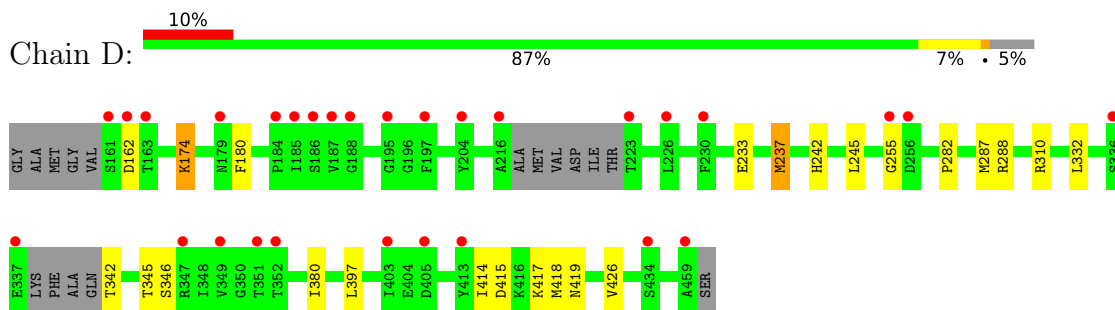
- Molecule 1: Interleukin-1 receptor-associated kinase 4



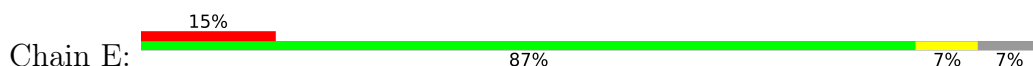
- Molecule 1: Interleukin-1 receptor-associated kinase 4

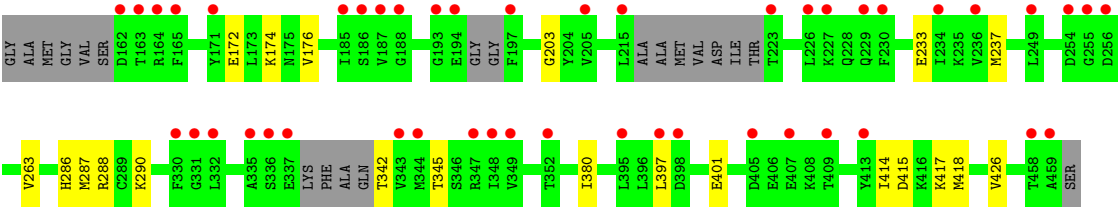


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.81Å 140.24Å 86.95Å 90.00° 126.14° 90.00°	Depositor
Resolution (Å)	43.00 – 1.89 43.00 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.00-1.89) 98.0 (43.00-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.88Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.202 , 0.228 0.212 , 0.212	Depositor DCC
R_{free} test set	5093 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9539	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3444e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TPO, ZVD, SEP, SO4

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	0.83	0/2217	1.15	4/2993 (0.1%)
1	B	0.81	0/2204	1.15	2/2978 (0.1%)
1	D	0.83	0/2199	1.20	1/2972 (0.0%)
1	E	0.80	0/2190	1.16	2/2959 (0.1%)
All	All	0.82	0/8810	1.17	9/11902 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	162	ASP	CA-CB-CG	7.77	120.37	112.60
1	E	174	LYS	N-CA-C	-6.21	104.59	111.36
1	A	169	SER	N-CA-C	-5.64	101.36	110.32
1	B	174	LYS	N-CA-C	-5.50	105.20	111.14
1	A	438	HIS	CA-C-N	5.36	129.70	121.19
1	A	438	HIS	C-N-CA	5.36	129.70	121.19
1	E	263	VAL	N-CA-C	-5.28	102.77	109.58
1	B	175	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	321	GLU	CB-CG-CD	5.20	121.43	112.60

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	2206	0	2149	8	0
1	B	2201	0	2114	12	0
1	D	2193	0	2098	11	0
1	E	2185	0	2097	9	0
2	A	28	24	0	0	0
2	B	28	24	0	0	0
2	D	28	24	0	0	0
2	E	28	24	0	0	0
3	D	5	0	0	0	0
3	E	10	0	0	0	0
4	A	154	0	0	0	0
4	B	140	0	0	0	0
4	D	122	0	0	2	0
4	E	115	0	0	1	0
All	All	9443	96	8458	34	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 2.

All (34) 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:281:PRO:HD3	1:B:321:GLU:HG3	1.62	0.79
1:D:242:HIS:HB3	1:D:245:LEU:HD13	1.72	0.71
1:B:247:GLU:OE2	1:E:286:HIS:HE1	1.76	0.66
1:B:174:LYS:HG3	1:B:179:ASN:HD22	1.68	0.58
1:A:281:PRO:HD3	1:B:321:GLU:CG	2.33	0.58
1:D:237:MET:HA	1:D:237:MET:HE2	1.87	0.57
1:E:287[B]:MET:HE2	1:E:290:LYS:HD2	1.86	0.57
1:B:237:MET:HA	1:B:237:MET:HE2	1.88	0.54
1:A:237:MET:HA	1:A:237:MET:HE2	1.89	0.53
1:E:237:MET:HA	1:E:237:MET:HE2	1.91	0.52
1:D:287[B]:MET:HA	1:D:287[B]:MET:HE2	1.91	0.51
1:D:414:ILE:HG12	1:D:426:VAL:HG11	1.92	0.51
1:E:415:ASP:HB3	1:E:418:MET:HE2	1.93	0.50
1:E:417:LYS:HE2	4:E:601:HOH:O	2.11	0.49
1:E:414:ILE:HG12	1:E:426:VAL:HG11	1.94	0.48
1:B:414:ILE:HG12	1:B:426:VAL:HG11	1.96	0.48
1:B:164:ARG:HD3	1:B:238:ALA:HA	1.97	0.47
1:E:172:GLU:O	1:E:176:VAL:HG23	2.15	0.47
1:B:176:VAL:HG11	1:B:205:VAL:HG12	1.97	0.46
1:A:415:ASP:HB3	1:A:418:MET:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:ARG:HD2	4:D:705:HOH:O	2.16	0.46
1:A:414:ILE:HG12	1:A:426:VAL:HG11	1.98	0.45
1:B:288:ARG:HB3	1:B:380:ILE:HG23	1.98	0.45
1:D:415:ASP:HB3	1:D:418:MET:HE2	1.99	0.45
1:A:439:GLU:CD	1:A:439:GLU:H	2.23	0.45
1:B:186:SER:HB2	1:D:419:ASN:HB2	2.00	0.44
1:A:286:HIS:CE1	1:A:290:LYS:HD2	2.53	0.43
1:D:417:LYS:HE2	4:D:605:HOH:O	2.20	0.42
1:E:176:VAL:HG12	1:E:203:GLY:HA3	2.00	0.42
1:E:288:ARG:HB3	1:E:380:ILE:HG23	2.03	0.41
1:A:321:GLU:HG3	1:B:281:PRO:HD3	2.03	0.41
1:B:279:GLY:HA2	1:D:282:PRO:HG2	2.02	0.41
1:D:174:LYS:HA	1:D:180:PHE:CE2	2.55	0.41
1:D:288:ARG:HB3	1:D:380:ILE:HG23	2.02	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	277/305 (91%)	272 (98%)	5 (2%)	0	100	100
1	B	279/305 (92%)	275 (99%)	4 (1%)	0	100	100
1	D	282/305 (92%)	271 (96%)	10 (4%)	1 (0%)	30	22
1	E	276/305 (90%)	269 (98%)	7 (2%)	0	100	100
All	All	1114/1220 (91%)	1087 (98%)	26 (2%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	255	GLY

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	233/260 (90%)	227 (97%)	6 (3%)	40	35
1	B	228/260 (88%)	223 (98%)	5 (2%)	45	42
1	D	225/260 (86%)	220 (98%)	5 (2%)	45	42
1	E	227/260 (87%)	224 (99%)	3 (1%)	61	61
All	All	913/1040 (88%)	894 (98%)	19 (2%)	47	44

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	SER
1	A	256	ASP
1	A	290	LYS
1	A	365	THR
1	A	397	LEU
1	A	439	GLU
1	B	233	GLU
1	B	290	LYS
1	B	397	LEU
1	B	399	ILE
1	B	408	LYS
1	D	174	LYS
1	D	233	GLU
1	D	237	MET
1	D	332	LEU
1	D	397	LEU
1	E	233	GLU
1	E	397	LEU
1	E	401	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	HIS
1	A	435	GLN
1	A	442	ASN
1	B	179	ASN
1	B	206	ASN
1	D	166	HIS
1	D	232	GLN
1	D	419	ASN
1	E	166	HIS
1	E	175	ASN
1	E	190	ASN
1	E	286	HIS
1	E	455	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	SEP	E	346	1	8,9,10	0.93	0	7,12,14	0.87	0
1	TPO	E	345	1	8,10,11	1.22	1 (12%)	10,14,16	1.50	2 (20%)
1	TPO	E	342	1	8,10,11	1.31	1 (12%)	10,14,16	1.15	0
1	SEP	B	346	1	8,9,10	0.85	0	7,12,14	0.96	0
1	TPO	A	345	1	8,10,11	1.30	1 (12%)	10,14,16	1.22	1 (10%)
1	TPO	D	342	1	8,10,11	1.27	1 (12%)	10,14,16	1.16	0
1	SEP	A	346	1	8,9,10	0.92	0	7,12,14	0.95	0
1	SEP	D	346	1	8,9,10	0.94	1 (12%)	7,12,14	1.08	0
1	TPO	D	345	1	8,10,11	1.47	2 (25%)	10,14,16	1.46	1 (10%)
1	TPO	B	345	1	8,10,11	1.03	0	10,14,16	1.26	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	B	342	1	8,10,11	1.28	1 (12%)	10,14,16	1.15	0
1	TPO	A	342	1	3,4,11	0.84	0	2,4,16	0.85	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	SEP	E	346	1	-	0/6/8/10	-
1	TPO	E	345	1	-	3/9/11/13	-
1	TPO	E	342	1	-	2/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-
1	TPO	A	345	1	-	2/9/11/13	-
1	TPO	D	342	1	-	1/9/11/13	-
1	SEP	A	346	1	-	0/6/8/10	-
1	SEP	D	346	1	-	0/6/8/10	-
1	TPO	D	345	1	-	3/9/11/13	-
1	TPO	B	345	1	-	4/9/11/13	-
1	TPO	B	342	1	-	2/9/11/13	-
1	TPO	A	342	1	-	0/1/2/13	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	342	TPO	P-OG1	-2.74	1.54	1.59
1	B	342	TPO	P-OG1	-2.57	1.55	1.59
1	D	345	TPO	CB-CA	2.42	1.58	1.53
1	E	345	TPO	P-OG1	-2.40	1.55	1.59
1	D	345	TPO	CG2-CB	2.35	1.57	1.51
1	D	342	TPO	P-OG1	-2.29	1.55	1.59
1	A	345	TPO	CG2-CB	2.19	1.56	1.51
1	D	346	SEP	P-OG	-2.01	1.54	1.60

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	345	TPO	O3P-P-OG1	3.46	119.33	105.85
1	D	345	TPO	O3P-P-OG1	3.12	118.01	105.85
1	A	345	TPO	OG1-P-O1P	2.49	118.22	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	345	TPO	OG1-P-O1P	-2.14	101.70	109.33
1	B	345	TPO	O3P-P-OG1	2.06	113.87	105.85

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	B	345	TPO	N-CA-CB-OG1
1	D	345	TPO	N-CA-CB-OG1
1	E	345	TPO	N-CA-CB-OG1
1	E	345	TPO	CB-OG1-P-O1P
1	B	342	TPO	C-CA-CB-CG2
1	D	342	TPO	C-CA-CB-CG2
1	E	342	TPO	C-CA-CB-CG2
1	B	342	TPO	CA-CB-OG1-P
1	E	342	TPO	CA-CB-OG1-P
1	B	345	TPO	CB-OG1-P-O1P
1	D	345	TPO	CB-OG1-P-O2P
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	O-C-CA-CB
1	D	345	TPO	O-C-CA-CB
1	E	345	TPO	O-C-CA-CB
1	B	345	TPO	CG2-CB-OG1-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands 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	$\# Z > 2$
2	ZVD	E	503	-	27,29,29	1.31	3 (11%)	35,41,41	1.17	3 (8%)
3	SO4	E	501	-	4,4,4	0.44	0	6,6,6	0.16	0
3	SO4	E	502	-	4,4,4	0.20	0	6,6,6	0.16	0
2	ZVD	A	501	-	27,29,29	1.51	7 (25%)	35,41,41	1.06	1 (2%)
2	ZVD	D	502	-	27,29,29	1.40	5 (18%)	35,41,41	1.20	2 (5%)
2	ZVD	B	501	-	27,29,29	1.45	6 (22%)	35,41,41	1.10	2 (5%)
3	SO4	D	501	-	4,4,4	0.23	0	6,6,6	0.12	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
2	ZVD	B	501	-	-	2/20/23/23	0/2/2/2
2	ZVD	A	501	-	-	1/20/23/23	0/2/2/2
2	ZVD	D	502	-	-	0/20/23/23	0/2/2/2
2	ZVD	E	503	-	-	1/20/23/23	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ZVD	F2-C15	-3.59	1.33	1.40
2	D	502	ZVD	F2-C15	-3.43	1.33	1.40
2	E	503	ZVD	O2-C16	-2.95	1.39	1.44
2	B	501	ZVD	O2-C16	-2.94	1.39	1.44
2	E	503	ZVD	C6-C7	2.65	1.43	1.39
2	B	501	ZVD	C13-N6	2.51	1.39	1.33
2	A	501	ZVD	C13-N6	2.46	1.39	1.33
2	A	501	ZVD	C18-C16	2.43	1.56	1.52
2	E	503	ZVD	F2-C15	-2.37	1.36	1.40
2	B	501	ZVD	F1-C1	-2.34	1.29	1.35
2	B	501	ZVD	C2-C1	2.33	1.41	1.37
2	A	501	ZVD	O2-C16	-2.30	1.40	1.44
2	A	501	ZVD	C6-C7	2.24	1.43	1.39
2	D	502	ZVD	C18-C16	2.23	1.56	1.52
2	A	501	ZVD	C4-N2	2.23	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ZVD	C3-N2	2.21	1.37	1.33
2	A	501	ZVD	C12-C7	2.20	1.44	1.41
2	D	502	ZVD	C3-N1	2.19	1.37	1.33
2	D	502	ZVD	O2-C16	-2.17	1.40	1.44
2	D	502	ZVD	F1-C1	-2.08	1.29	1.35
2	A	501	ZVD	F1-C1	-2.07	1.30	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	ZVD	N3-C4-N2	3.68	122.83	118.38
2	D	502	ZVD	N3-C4-N2	3.60	122.73	118.38
2	E	503	ZVD	N3-C4-N2	3.12	122.15	118.38
2	D	502	ZVD	C11-N5-C5	-2.47	115.51	117.83
2	A	501	ZVD	O2-C16-C18	2.47	113.32	107.90
2	E	503	ZVD	C17-C16-C18	-2.25	107.23	110.52
2	E	503	ZVD	C9-C8-N4	-2.11	105.81	109.95
2	B	501	ZVD	C9-C8-N4	-2.08	105.86	109.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

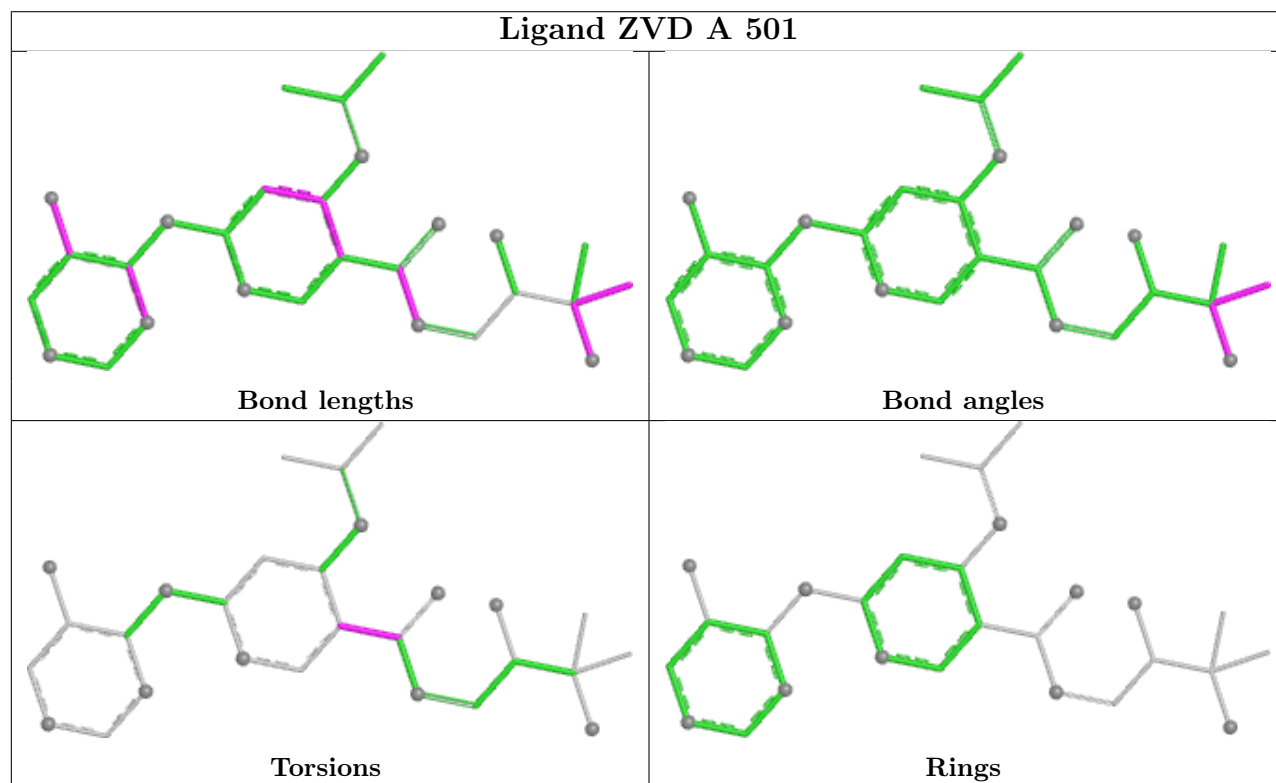
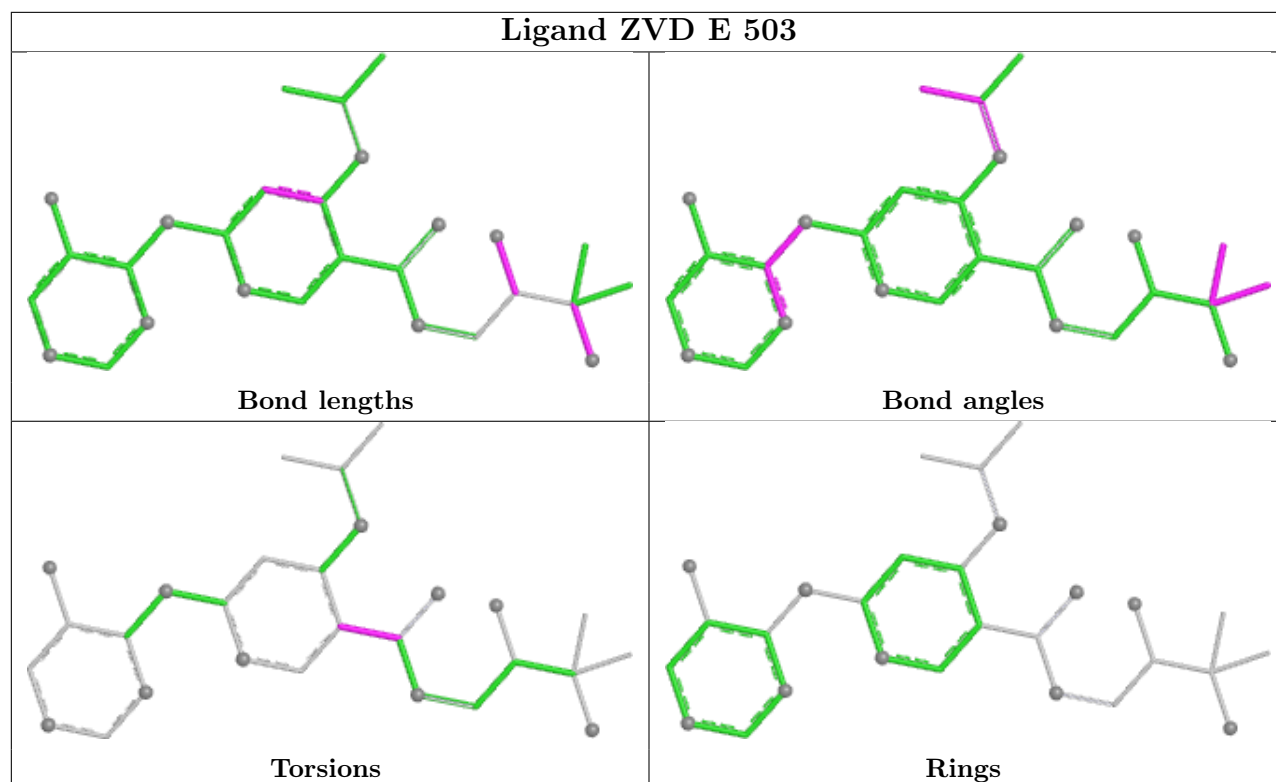
Mol	Chain	Res	Type	Atoms
2	A	501	ZVD	C11-C12-C13-O1
2	B	501	ZVD	C11-C12-C13-O1
2	E	503	ZVD	C11-C12-C13-O1
2	B	501	ZVD	C11-C12-C13-N6

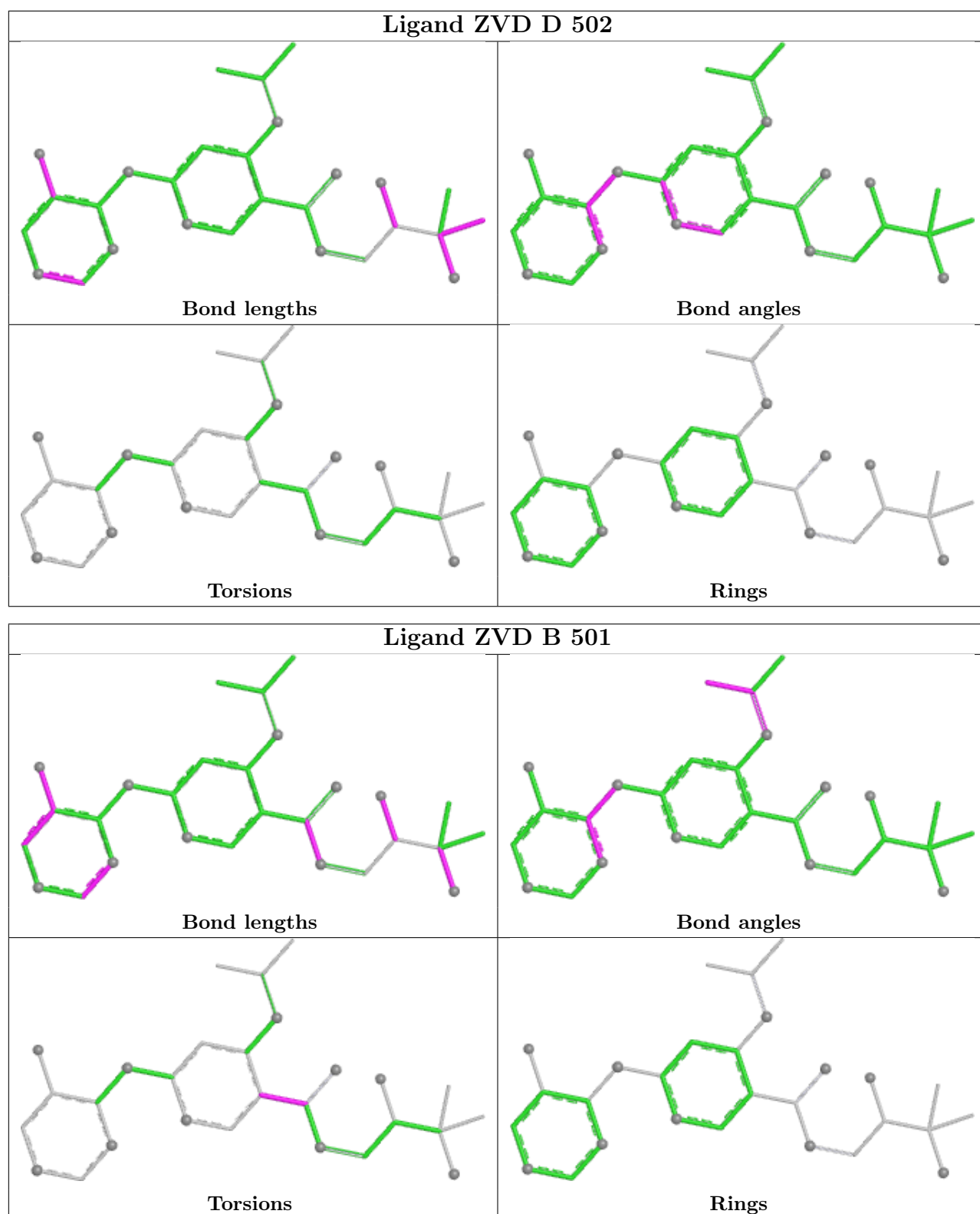
There are no ring outliers.

No monomer is involved in short contacts.

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

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	283/305 (92%)	0.43	19 (6%)	24	25	15, 30, 59, 74	1 (0%)
1	B	284/305 (93%)	0.60	32 (11%)	10	10	17, 33, 64, 82	0
1	D	286/305 (93%)	0.72	29 (10%)	12	13	13, 37, 63, 82	1 (0%)
1	E	282/305 (92%)	0.84	46 (16%)	4	4	15, 36, 71, 92	1 (0%)
All	All	1135/1220 (93%)	0.65	126 (11%)	10	11	13, 33, 65, 92	3 (0%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	SER	6.7
1	A	336	SER	6.1
1	E	335	ALA	5.6
1	E	459	ALA	5.2
1	D	185	ILE	5.1
1	A	343	VAL	4.9
1	A	217	ALA	4.7
1	D	216	ALA	4.6
1	A	195	GLY	4.5
1	D	162	ASP	4.3
1	E	336	SER	4.2
1	B	399	ILE	4.1
1	E	223	THR	4.1
1	D	197	PHE	4.0
1	E	185	ILE	4.0
1	B	343	VAL	3.9
1	E	163	THR	3.9
1	D	186	SER	3.8
1	B	222	THR	3.8
1	D	161	SER	3.8
1	E	187	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	162	ASP	3.7
1	E	236	VAL	3.7
1	E	343	VAL	3.7
1	E	349	VAL	3.6
1	B	197	PHE	3.6
1	E	215	LEU	3.6
1	D	337	GLU	3.6
1	B	221	ILE	3.4
1	A	459	ALA	3.4
1	D	204	TYR	3.3
1	E	186	SER	3.3
1	E	347	ARG	3.3
1	A	361[A]	ARG	3.3
1	D	405	ASP	3.2
1	D	163	THR	3.2
1	D	195	GLY	3.2
1	A	198	GLY	3.2
1	E	230	PHE	3.2
1	D	256	ASP	3.1
1	B	216	ALA	3.1
1	E	330	PHE	3.1
1	E	164	ARG	3.0
1	A	335	ALA	3.0
1	E	197	PHE	3.0
1	B	196	GLY	3.0
1	B	400	LYS	2.9
1	E	344	MET	2.9
1	B	220	ASP	2.9
1	B	405	ASP	2.9
1	E	332	LEU	2.9
1	A	164	ARG	2.9
1	A	221	ILE	2.9
1	B	419	ASN	2.8
1	B	458	THR	2.8
1	E	254	ASP	2.8
1	E	171	TYR	2.8
1	E	226	LEU	2.8
1	E	255	GLY	2.7
1	D	187	VAL	2.7
1	E	337	GLU	2.7
1	D	226	LEU	2.7
1	B	361	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	254	ASP	2.7
1	E	194	GLU	2.7
1	E	348	ILE	2.6
1	E	188	GLY	2.6
1	B	335	ALA	2.6
1	B	333	ALA	2.6
1	D	459	ALA	2.6
1	B	348	ILE	2.5
1	B	347	ARG	2.5
1	E	405	ASP	2.5
1	D	403	ILE	2.5
1	B	349	VAL	2.5
1	D	223	THR	2.5
1	E	249	LEU	2.5
1	A	364	ILE	2.4
1	B	364	ILE	2.4
1	D	352	THR	2.4
1	B	423	SER	2.4
1	E	458	THR	2.4
1	E	227	LYS	2.4
1	D	179	ASN	2.4
1	E	395	LEU	2.3
1	E	397	LEU	2.3
1	B	393	PRO	2.3
1	B	401	GLU	2.3
1	B	408	LYS	2.3
1	D	188	GLY	2.3
1	D	336	SER	2.2
1	E	398	ASP	2.2
1	A	194	GLU	2.2
1	A	421	ALA	2.2
1	E	407	GLU	2.2
1	E	352	THR	2.2
1	E	165	PHE	2.2
1	A	419	ASN	2.2
1	D	434	SER	2.2
1	A	255	GLY	2.2
1	D	184	PRO	2.2
1	B	421	ALA	2.2
1	D	347	ARG	2.2
1	A	179	ASN	2.1
1	B	344	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	234	ILE	2.1
1	A	185	ILE	2.1
1	B	410	ILE	2.1
1	B	164	ARG	2.1
1	E	409	THR	2.1
1	D	255	GLY	2.1
1	E	331	GLY	2.1
1	D	349	VAL	2.1
1	B	397	LEU	2.1
1	D	230	PHE	2.0
1	D	413	TYR	2.0
1	E	413	TYR	2.0
1	D	351	THR	2.0
1	E	193	GLY	2.0
1	E	205	VAL	2.0
1	A	183	ARG	2.0
1	B	420	ASP	2.0
1	E	256	ASP	2.0
1	B	362	GLY	2.0
1	B	394	GLN	2.0
1	E	229	GLN	2.0

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

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	TPO	A	342	5/12	0.38	0.19	56,56,59,60	0
1	SEP	E	346	10/11	0.62	0.17	77,80,86,86	0
1	SEP	D	346	10/11	0.65	0.16	60,68,77,77	0
1	TPO	B	342	11/12	0.71	0.19	75,77,81,82	0
1	TPO	E	342	11/12	0.72	0.18	83,85,86,87	0
1	SEP	B	346	10/11	0.74	0.16	66,71,78,78	0
1	SEP	A	346	10/11	0.74	0.14	59,64,72,73	0
1	TPO	D	342	11/12	0.84	0.13	59,60,66,67	0
1	TPO	E	345	11/12	0.88	0.13	74,74,78,79	0
1	TPO	A	345	11/12	0.88	0.12	54,58,60,61	0
1	TPO	B	345	11/12	0.89	0.12	60,61,66,67	0
1	TPO	D	345	11/12	0.94	0.08	47,49,58,59	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

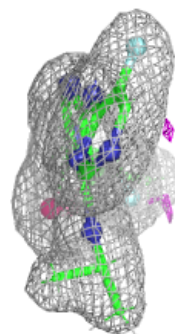
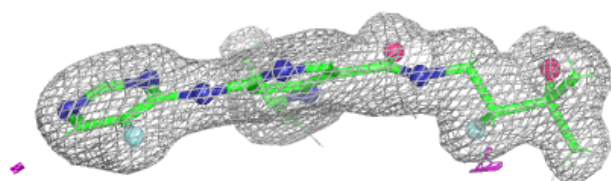
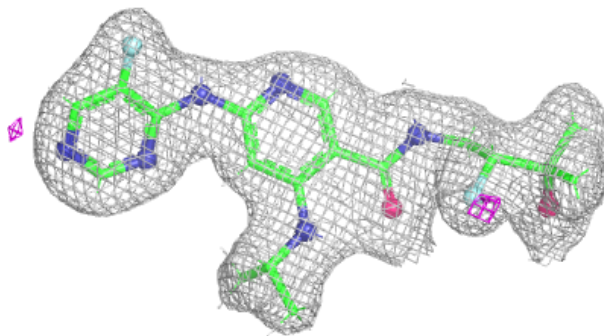
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	E	502	5/5	0.87	0.12	53,53,55,56	0
3	SO4	E	501	5/5	0.91	0.09	46,54,55,55	0
2	ZVD	D	502	28/28	0.94	0.07	20,24,28,31	0
3	SO4	D	501	5/5	0.94	0.07	52,52,54,55	0
2	ZVD	E	503	28/28	0.95	0.07	21,27,35,35	0
2	ZVD	A	501	28/28	0.96	0.05	15,23,28,29	0
2	ZVD	B	501	28/28	0.97	0.04	16,22,26,27	0

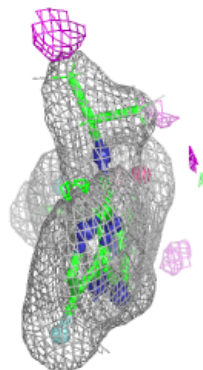
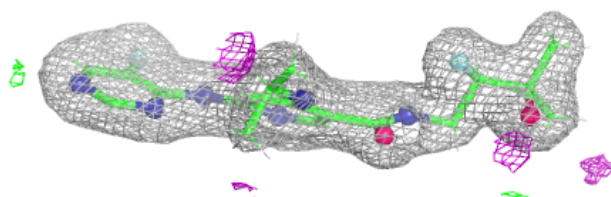
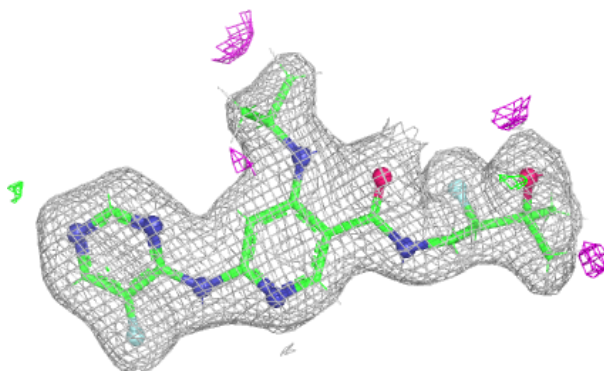
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZVD D 502:

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

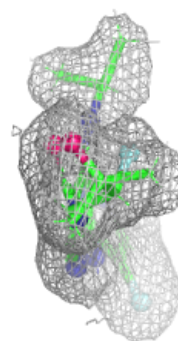
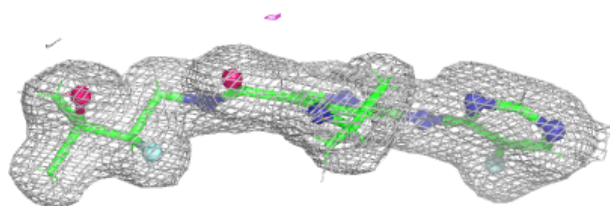
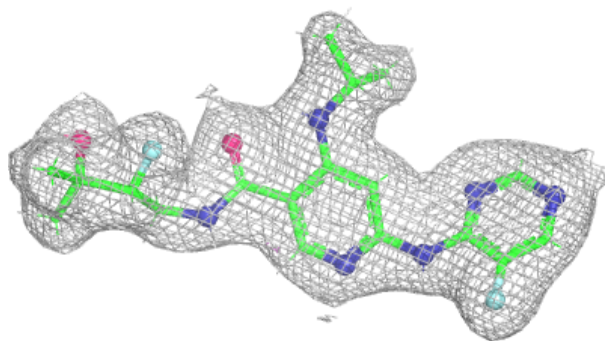
**Electron density around ZVD E 503:**

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

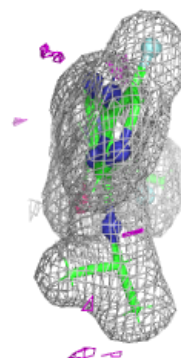
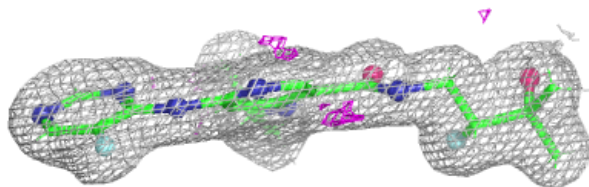
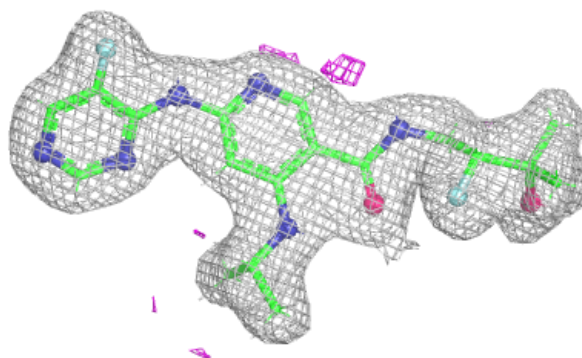


Electron density around ZVD A 501:

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

**Electron density around ZVD B 501:**

$2mF_o-DF_c$ (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.