



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:15 PM UTC

PDB ID : 3H2O / pdb_00003h2o
Title : Structural Studies of Pterin-Based Inhibitors of Dihydropteroate Synthase
Authors : Yun, M.-K.; White, S.W.
Deposited on : 2009-04-14
Resolution : 2.70 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

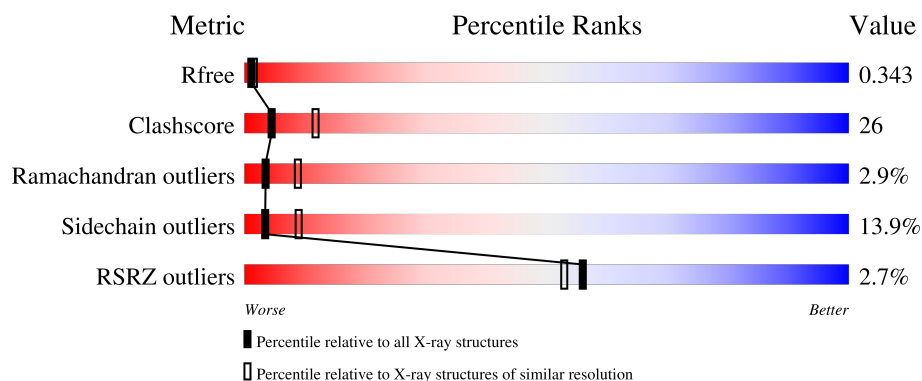
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	297	
1	B	297	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4069 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 Dihydropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2000	1257	345	382	16			
1	B	262	Total	C	N	O	S	0	0	0
			1996	1256	344	380	16			

There are 40 discrepancies between the modelled and reference sequences:

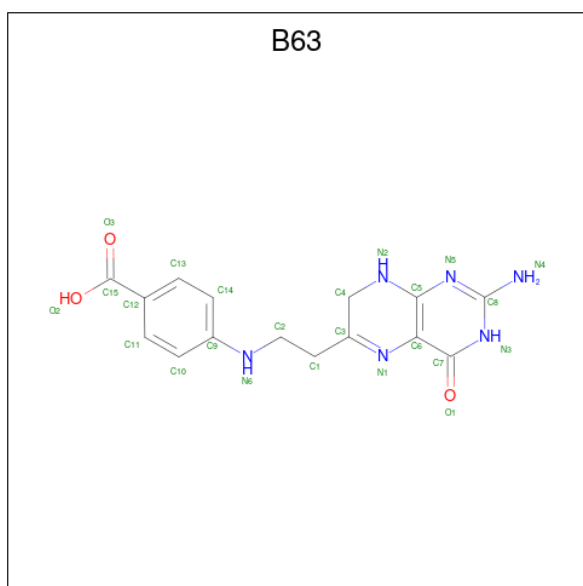
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP B1UXN2
A	-18	GLY	-	expression tag	UNP B1UXN2
A	-17	SER	-	expression tag	UNP B1UXN2
A	-16	SER	-	expression tag	UNP B1UXN2
A	-15	HIS	-	expression tag	UNP B1UXN2
A	-14	HIS	-	expression tag	UNP B1UXN2
A	-13	HIS	-	expression tag	UNP B1UXN2
A	-12	HIS	-	expression tag	UNP B1UXN2
A	-11	HIS	-	expression tag	UNP B1UXN2
A	-10	HIS	-	expression tag	UNP B1UXN2
A	-9	SER	-	expression tag	UNP B1UXN2
A	-8	SER	-	expression tag	UNP B1UXN2
A	-7	GLY	-	expression tag	UNP B1UXN2
A	-6	LEU	-	expression tag	UNP B1UXN2
A	-5	VAL	-	expression tag	UNP B1UXN2
A	-4	PRO	-	expression tag	UNP B1UXN2
A	-3	ARG	-	expression tag	UNP B1UXN2
A	-2	GLY	-	expression tag	UNP B1UXN2
A	-1	SER	-	expression tag	UNP B1UXN2
A	0	HIS	-	expression tag	UNP B1UXN2
B	-19	MET	-	expression tag	UNP B1UXN2
B	-18	GLY	-	expression tag	UNP B1UXN2
B	-17	SER	-	expression tag	UNP B1UXN2
B	-16	SER	-	expression tag	UNP B1UXN2
B	-15	HIS	-	expression tag	UNP B1UXN2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP B1UXN2
B	-13	HIS	-	expression tag	UNP B1UXN2
B	-12	HIS	-	expression tag	UNP B1UXN2
B	-11	HIS	-	expression tag	UNP B1UXN2
B	-10	HIS	-	expression tag	UNP B1UXN2
B	-9	SER	-	expression tag	UNP B1UXN2
B	-8	SER	-	expression tag	UNP B1UXN2
B	-7	GLY	-	expression tag	UNP B1UXN2
B	-6	LEU	-	expression tag	UNP B1UXN2
B	-5	VAL	-	expression tag	UNP B1UXN2
B	-4	PRO	-	expression tag	UNP B1UXN2
B	-3	ARG	-	expression tag	UNP B1UXN2
B	-2	GLY	-	expression tag	UNP B1UXN2
B	-1	SER	-	expression tag	UNP B1UXN2
B	0	HIS	-	expression tag	UNP B1UXN2

- Molecule 2 is 4-{[2-(2-amino-4-oxo-3,4,7,8-tetrahydropteridin-6-yl)ethyl]amino}benzoic acid (CCD ID: B63) (formula: C₁₅H₁₆N₆O₃).





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	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

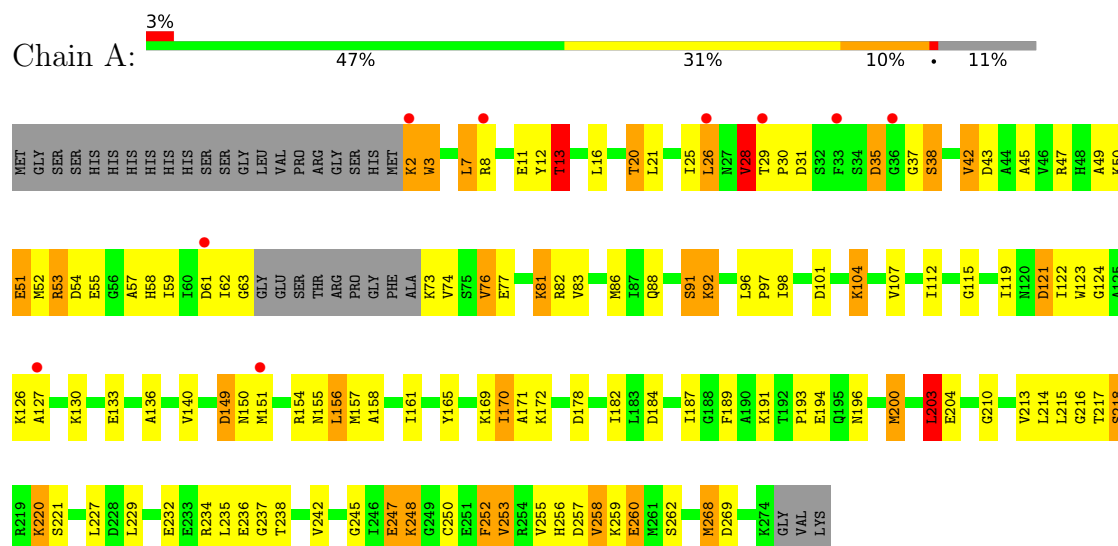
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	3	Total	O	0	0
			3	3		

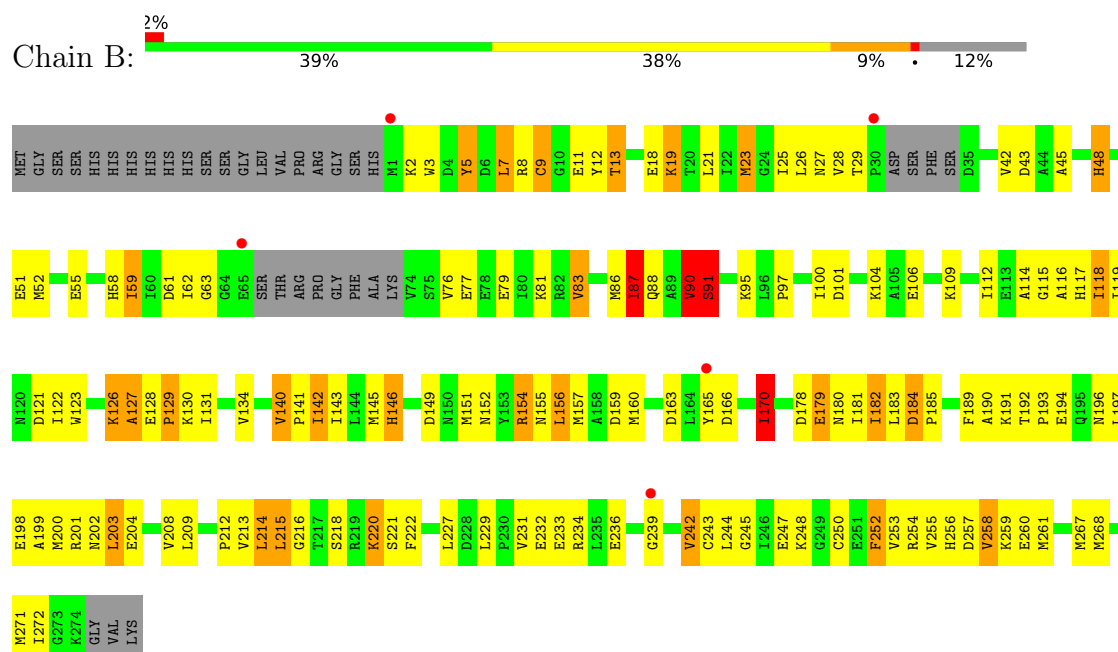
3 Residue-property plots

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: Dihydropteroate synthase



• Molecule 1: Dihydropteroate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	99.29Å 99.29Å 263.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.78 – 2.70 48.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.78-2.70) 97.2 (48.78-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.64 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.271 , 0.311 0.301 , 0.343	Depositor DCC
R_{free} test set	1158 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.930	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4069	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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 46.76 % 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 1.0926e-04. 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: SO4, B63

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	1.34	12/2029 (0.6%)	1.45	17/2744 (0.6%)
1	B	1.18	5/2024 (0.2%)	1.43	20/2733 (0.7%)
All	All	1.26	17/4053 (0.4%)	1.44	37/5477 (0.7%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	LYS	N-CA	8.58	1.62	1.46
1	A	73	LYS	CA-CB	8.31	1.70	1.53
1	A	81	LYS	CE-NZ	6.74	1.69	1.49
1	A	248	LYS	CE-NZ	6.26	1.68	1.49
1	A	203	LEU	CA-C	-6.00	1.45	1.52
1	A	258	VAL	CA-CB	-5.97	1.47	1.54
1	A	220	LYS	N-CA	-5.64	1.38	1.45
1	A	42	VAL	CA-CB	-5.44	1.48	1.54
1	B	202	ASN	CA-CB	-5.34	1.46	1.53
1	A	210	GLY	N-CA	5.33	1.53	1.45
1	A	248	LYS	CA-C	-5.22	1.45	1.52
1	B	146	HIS	CA-C	-5.21	1.46	1.52
1	B	83	VAL	CA-CB	5.21	1.60	1.54
1	A	234	ARG	CA-C	-5.15	1.46	1.52
1	B	199	ALA	CA-CB	-5.12	1.45	1.53
1	B	220	LYS	N-CA	-5.11	1.39	1.46
1	A	165	TYR	CA-C	5.04	1.59	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ASP	CA-C-N	12.52	135.49	119.84
1	B	184	ASP	C-N-CA	12.52	135.49	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ARG	N-CA-C	-9.32	100.68	111.03
1	A	194	GLU	N-CA-C	-8.58	102.74	113.55
1	A	88	GLN	OE1-CD-NE2	-8.22	114.38	122.60
1	A	184	ASP	CA-C-N	6.76	126.71	119.28
1	A	184	ASP	C-N-CA	6.76	126.71	119.28
1	A	258	VAL	N-CA-C	6.66	117.35	110.36
1	B	199	ALA	N-CA-C	-6.53	104.16	111.28
1	B	222	PHE	CA-C-N	-6.52	112.35	120.56
1	B	222	PHE	C-N-CA	-6.52	112.35	120.56
1	A	140	VAL	N-CA-C	6.48	114.50	109.19
1	B	2	LYS	CA-C-N	-6.23	114.41	123.00
1	B	2	LYS	C-N-CA	-6.23	114.41	123.00
1	B	87	ILE	CB-CA-C	-6.19	104.07	111.81
1	A	200	MET	N-CA-C	-6.16	104.47	112.23
1	B	90	VAL	N-CA-C	-6.14	104.65	110.42
1	B	247	GLU	N-CA-C	-6.01	105.21	112.54
1	A	150	ASN	N-CA-C	-6.00	100.32	108.24
1	A	121	ASP	N-CA-C	5.83	118.45	109.07
1	B	243	CYS	N-CA-C	5.75	117.22	111.07
1	A	91	SER	N-CA-C	-5.74	105.16	111.82
1	A	203	LEU	CB-CA-C	-5.74	101.27	110.79
1	B	48	HIS	N-CA-C	-5.68	105.17	111.36
1	A	3	TRP	N-CA-C	-5.52	101.48	110.20
1	A	13	THR	CB-CA-C	-5.47	100.64	109.89
1	A	237	GLY	N-CA-C	-5.45	106.17	112.50
1	B	5	TYR	N-CA-C	5.42	117.30	109.07
1	B	170	ILE	N-CA-C	-5.39	105.35	110.42
1	B	118	ILE	CA-C-N	-5.34	116.20	122.93
1	B	118	ILE	C-N-CA	-5.34	116.20	122.93
1	A	53	ARG	N-CA-C	-5.21	104.86	111.11
1	B	182	ILE	N-CA-C	5.15	117.26	108.86
1	A	61	ASP	N-CA-C	5.15	117.14	108.96
1	B	28	VAL	N-CA-C	5.08	117.27	111.88
1	B	9	CYS	CB-CA-C	-5.05	103.43	111.86
1	B	126	LYS	CG-CD-CE	-5.04	99.71	111.30

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	2000	0	1974	94	0
1	B	1996	0	1984	116	0
2	A	24	0	15	4	0
2	B	24	0	15	2	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
All	All	4069	0	3988	212	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 26.

All (212) 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:81:LYS:CE	1:A:81:LYS:NZ	1.69	1.52
1:A:248:LYS:NZ	1:A:248:LYS:CE	1.68	1.51
1:B:9:CYS:HB2	1:B:12:TYR:O	1.65	0.96
1:A:2:LYS:C	1:A:2:LYS:HD3	1.95	0.90
1:A:242:VAL:HG13	1:A:253:VAL:HG11	1.59	0.84
1:B:214:LEU:HD23	1:B:215:LEU:N	1.91	0.84
1:B:79:GLU:O	1:B:83:VAL:HG12	1.78	0.83
1:A:121:ASP:OD2	1:A:123:TRP:N	2.11	0.82
1:A:2:LYS:HD3	1:A:2:LYS:O	1.80	0.81
1:A:2:LYS:C	1:A:2:LYS:CD	2.51	0.79
1:B:51:GLU:O	1:B:55:GLU:HG2	1.84	0.78
1:B:227:LEU:HB3	1:B:229:LEU:HD12	1.65	0.78
1:A:227:LEU:HB3	1:A:229:LEU:CD1	2.13	0.78
1:A:227:LEU:C	1:A:229:LEU:HD12	2.11	0.76
1:B:216:GLY:O	1:B:220:LYS:NZ	2.19	0.76
1:A:227:LEU:O	1:A:229:LEU:CD1	2.36	0.73
1:A:133:GLU:O	1:A:136:ALA:HB3	1.90	0.71
1:A:227:LEU:O	1:A:229:LEU:HD11	1.92	0.70
1:A:172:LYS:HD2	1:A:178:ASP:OD1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLY:C	1:A:250:CYS:HG	2.02	0.66
1:A:216:GLY:O	1:A:220:LYS:NZ	2.28	0.66
1:A:112:ILE:HD11	1:A:119:ILE:HD11	1.77	0.66
1:A:121:ASP:OD2	1:A:121:ASP:C	2.39	0.66
1:B:8:ARG:HH11	1:B:8:ARG:HA	1.61	0.66
1:A:218:SER:HB2	1:A:255:VAL:HA	1.78	0.65
1:B:59:ILE:HG23	1:B:97:PRO:HG2	1.79	0.64
1:B:221:SER:H	2:B:502:B63:C15	2.10	0.64
1:B:26:LEU:HD21	1:B:45:ALA:HB1	1.78	0.64
1:B:117:HIS:O	1:B:140:VAL:HB	1.98	0.64
1:B:149:ASP:OD1	1:B:149:ASP:N	2.30	0.64
1:B:156:LEU:HD23	1:B:198:GLU:HG3	1.79	0.64
1:B:201:ARG:O	1:B:248:LYS:HE3	1.97	0.63
1:B:123:TRP:HB2	1:B:127:ALA:HB2	1.81	0.62
1:B:178:ASP:HA	1:B:181:ILE:HD12	1.81	0.62
1:A:104:LYS:HB3	1:A:107:VAL:HG23	1.81	0.62
1:B:267:MET:HG3	1:B:271:MET:HE2	1.80	0.62
1:A:235:LEU:HD11	1:A:260:GLU:HG3	1.81	0.61
1:B:245:GLY:C	1:B:250:CYS:HG	2.09	0.60
1:A:123:TRP:CB	1:A:127:ALA:HB2	2.32	0.60
1:B:27:ASN:HB2	1:B:48:HIS:ND1	2.17	0.59
1:B:214:LEU:HD23	1:B:214:LEU:C	2.27	0.59
1:B:145:MET:HA	1:B:184:ASP:O	2.02	0.59
1:B:87:ILE:O	1:B:91:SER:HB3	2.03	0.59
1:B:215:LEU:HD23	1:B:253:VAL:HG12	1.84	0.59
1:B:83:VAL:O	1:B:86:MET:HB2	2.03	0.58
1:B:257:ASP:O	1:B:258:VAL:C	2.44	0.58
1:A:123:TRP:HB2	1:A:127:ALA:HB2	1.85	0.58
1:A:227:LEU:O	1:A:229:LEU:HD12	2.03	0.58
1:A:104:LYS:HE3	1:A:104:LYS:HA	1.86	0.58
1:A:51:GLU:O	1:A:55:GLU:HG2	2.04	0.57
1:B:182:ILE:HG22	1:B:183:LEU:N	2.18	0.57
1:A:28:VAL:CG1	1:A:86:MET:HE1	2.34	0.57
1:B:146:HIS:HB3	1:B:185:PRO:O	2.04	0.57
1:B:218:SER:HB2	1:B:255:VAL:HA	1.86	0.57
1:A:204:GLU:OE2	1:A:248:LYS:HD3	2.05	0.57
1:B:232:GLU:H	1:B:232:GLU:CD	2.13	0.57
1:B:87:ILE:HD12	1:B:114:ALA:HB3	1.86	0.56
1:B:214:LEU:HG	1:B:252:PHE:HB2	1.88	0.56
1:B:166:ASP:O	1:B:170:ILE:HG13	2.06	0.56
1:B:123:TRP:CB	1:B:127:ALA:HB2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:THR:HB	1:B:193:PRO:CD	2.36	0.56
1:B:259:LYS:HB3	1:B:260:GLU:OE1	2.06	0.56
1:B:128:GLU:O	1:B:129:PRO:C	2.48	0.55
1:A:55:GLU:HB2	1:A:258:VAL:CG1	2.37	0.55
1:A:96:LEU:HB3	1:A:97:PRO:HD2	1.87	0.55
1:B:208:VAL:HG23	1:B:209:LEU:HD23	1.87	0.55
1:A:259:LYS:HB3	1:A:260:GLU:OE2	2.07	0.55
1:B:25:ILE:HD12	1:B:255:VAL:C	2.31	0.55
1:A:214:LEU:HG	1:A:252:PHE:HB2	1.88	0.55
1:A:43:ASP:O	1:A:47:ARG:HG3	2.07	0.54
1:A:236:GLU:CD	1:A:236:GLU:H	2.16	0.54
1:B:5:TYR:CE1	1:B:179:GLU:HA	2.43	0.54
1:B:182:ILE:CG2	1:B:183:LEU:N	2.71	0.54
1:B:104:LYS:HB3	1:B:128:GLU:OE2	2.08	0.53
1:A:57:ALA:HB2	1:A:258:VAL:HG11	1.89	0.53
1:A:20:THR:OG1	1:A:269:ASP:OD2	2.26	0.53
1:A:193:PRO:HA	1:A:196:ASN:HD22	1.72	0.53
1:B:8:ARG:HD2	1:B:13:THR:HG23	1.89	0.53
1:A:121:ASP:OD2	1:A:124:GLY:N	2.41	0.53
1:A:227:LEU:HB3	1:A:229:LEU:HD13	1.90	0.52
1:A:155:ASN:HB3	1:A:158:ALA:HB3	1.90	0.52
1:A:157:MET:O	1:A:158:ALA:C	2.52	0.52
1:B:130:LYS:H	1:B:130:LYS:HD2	1.73	0.52
1:B:165:TYR:HE1	1:B:209:LEU:HD22	1.75	0.52
1:A:221:SER:N	2:A:501:B63:O2	2.34	0.52
1:B:236:GLU:H	1:B:236:GLU:CD	2.17	0.52
1:B:156:LEU:HD23	1:B:198:GLU:CG	2.40	0.52
1:A:149:ASP:OD1	1:A:149:ASP:N	2.43	0.51
1:A:252:PHE:CD1	1:A:252:PHE:N	2.77	0.51
1:B:151:MET:HG2	1:B:190:ALA:O	2.10	0.51
1:B:252:PHE:CD1	1:B:252:PHE:N	2.79	0.51
1:B:86:MET:O	1:B:90:VAL:HG23	2.10	0.51
1:A:200:MET:SD	1:A:215:LEU:HD11	2.51	0.51
1:B:140:VAL:HG23	1:B:141:PRO:O	2.09	0.51
1:A:42:VAL:O	1:A:43:ASP:C	2.52	0.51
1:A:53:ARG:NH1	1:A:54:ASP:OD1	2.44	0.51
1:B:18:GLU:HG3	1:B:19:LYS:HG2	1.92	0.51
1:B:142:ILE:CG1	1:B:143:ILE:N	2.74	0.51
1:B:25:ILE:HD12	1:B:256:HIS:N	2.25	0.50
1:A:232:GLU:CD	1:A:232:GLU:H	2.19	0.50
1:B:245:GLY:O	1:B:250:CYS:SG	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ARG:O	1:B:254:ARG:HG2	2.10	0.50
1:A:28:VAL:HG21	1:A:63:GLY:C	2.37	0.50
1:B:214:LEU:HD23	1:B:215:LEU:H	1.73	0.50
1:A:104:LYS:HB3	1:A:107:VAL:CG2	2.41	0.49
1:A:258:VAL:O	1:A:262:SER:HB2	2.13	0.49
1:B:231:VAL:C	1:B:233:GLU:H	2.20	0.49
1:B:42:VAL:O	1:B:43:ASP:C	2.55	0.49
1:B:214:LEU:C	1:B:214:LEU:CD2	2.85	0.49
1:A:247:GLU:C	1:A:247:GLU:CD	2.81	0.49
1:B:63:GLY:HA2	1:B:101:ASP:HB3	1.94	0.49
1:B:221:SER:N	2:B:502:B63:O2	2.40	0.49
1:B:3:TRP:CH2	1:B:212:PRO:HD3	2.48	0.49
1:A:227:LEU:C	1:A:229:LEU:CD1	2.82	0.49
1:A:221:SER:H	2:A:501:B63:C15	2.26	0.48
1:B:131:ILE:O	1:B:134:VAL:HB	2.13	0.48
1:A:26:LEU:HD21	1:A:45:ALA:HB1	1.96	0.48
1:A:81:LYS:NZ	1:A:81:LYS:CD	2.69	0.48
1:B:242:VAL:HG22	1:B:253:VAL:HG11	1.95	0.48
1:A:189:PHE:O	1:A:191:LYS:HG3	2.14	0.47
1:A:203:LEU:HD21	1:A:215:LEU:HD13	1.96	0.47
1:B:121:ASP:OD2	1:B:123:TRP:N	2.36	0.47
1:A:91:SER:HA	1:A:98:ILE:CD1	2.44	0.47
1:B:55:GLU:HB3	1:B:258:VAL:CG1	2.44	0.47
1:A:12:TYR:CE1	1:A:96:LEU:C	2.93	0.47
1:A:42:VAL:O	1:A:45:ALA:N	2.45	0.47
1:B:48:HIS:ND1	1:B:52:MET:HE2	2.29	0.47
1:B:7:LEU:HD23	1:B:7:LEU:HA	1.39	0.47
1:B:156:LEU:O	1:B:159:ASP:N	2.46	0.47
1:A:123:TRP:O	1:A:126:LYS:HB2	2.15	0.47
1:B:58:HIS:O	1:B:97:PRO:HD2	2.15	0.47
1:B:104:LYS:CB	1:B:128:GLU:OE2	2.63	0.46
1:B:156:LEU:O	1:B:159:ASP:HB2	2.15	0.46
1:A:58:HIS:C	1:A:59:ILE:HG13	2.40	0.46
1:B:214:LEU:HA	1:B:252:PHE:O	2.15	0.46
1:B:23:MET:HB3	1:B:254:ARG:HB2	1.97	0.46
1:B:48:HIS:CE1	1:B:52:MET:HE2	2.51	0.46
1:B:26:LEU:HA	1:B:52:MET:HE1	1.97	0.46
1:A:227:LEU:HB3	1:A:229:LEU:HD12	1.96	0.46
1:B:123:TRP:O	1:B:126:LYS:HB2	2.15	0.46
1:B:255:VAL:HG11	1:B:261:MET:HG3	1.98	0.46
1:A:257:ASP:HB3	1:A:260:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:MET:HE2	1:A:268:MET:HB3	1.75	0.45
1:B:141:PRO:HA	1:B:180:ASN:HB3	1.99	0.45
1:B:268:MET:O	1:B:271:MET:N	2.48	0.45
1:B:81:LYS:HE3	1:B:81:LYS:HB2	1.75	0.45
1:A:200:MET:O	1:A:203:LEU:HD12	2.16	0.45
1:B:231:VAL:HA	1:B:234:ARG:HD2	1.97	0.45
1:A:52:MET:O	1:A:53:ARG:C	2.59	0.45
1:A:155:ASN:O	1:A:156:LEU:C	2.59	0.45
1:A:52:MET:HA	1:A:55:GLU:CG	2.47	0.45
1:B:27:ASN:HB2	1:B:48:HIS:CE1	2.51	0.45
1:B:5:TYR:CZ	1:B:179:GLU:HA	2.52	0.45
1:A:112:ILE:CD1	1:A:119:ILE:HD11	2.46	0.44
1:B:184:ASP:OD2	1:B:184:ASP:C	2.60	0.44
1:A:29:THR:HA	1:A:30:PRO:HD3	1.88	0.44
1:B:55:GLU:HB3	1:B:258:VAL:HG12	1.98	0.44
1:B:192:THR:HB	1:B:193:PRO:HD2	1.99	0.44
1:A:2:LYS:HD2	1:A:3:TRP:CD1	2.53	0.44
1:B:3:TRP:CZ3	1:B:212:PRO:HD3	2.53	0.44
1:B:192:THR:C	1:B:194:GLU:H	2.24	0.44
1:A:25:ILE:HD12	1:A:256:HIS:CD2	2.53	0.44
1:A:203:LEU:HB2	1:A:248:LYS:HD2	1.99	0.44
1:B:26:LEU:HB2	1:B:61:ASP:O	2.17	0.44
1:B:157:MET:HA	1:B:160:MET:HG3	1.99	0.44
1:A:92:LYS:O	1:A:92:LYS:HG3	2.16	0.44
1:B:258:VAL:O	1:B:259:LYS:C	2.61	0.44
1:A:170:ILE:O	1:A:171:ALA:C	2.60	0.43
1:B:90:VAL:O	1:B:91:SER:C	2.61	0.43
1:B:181:ILE:C	1:B:182:ILE:HG13	2.43	0.43
1:A:7:LEU:HD21	1:A:182:ILE:HD11	2.01	0.43
1:B:21:LEU:HA	1:B:21:LEU:HD23	1.68	0.43
1:A:16:LEU:HA	1:A:16:LEU:HD23	1.71	0.43
1:A:63:GLY:HA2	1:A:101:ASP:HB3	2.00	0.43
1:A:187:ILE:HG21	1:A:217:THR:HG22	2.01	0.43
1:B:203:LEU:HA	1:B:203:LEU:HD22	1.70	0.43
1:B:130:LYS:O	1:B:131:ILE:C	2.62	0.42
1:A:28:VAL:HG12	1:A:86:MET:HE1	2.01	0.42
1:A:218:SER:HA	1:A:238:THR:CG2	2.50	0.42
2:A:501:B63:H1A	3:A:279:SO4:O4	2.19	0.42
1:B:112:ILE:HG23	1:B:116:ALA:O	2.19	0.42
1:B:271:MET:HE3	1:B:271:MET:HB2	1.88	0.42
1:A:49:ALA:O	1:A:52:MET:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ILE:HG21	1:B:118:ILE:HD12	2.02	0.42
1:A:49:ALA:O	1:A:50:LYS:C	2.62	0.42
1:A:218:SER:HA	1:A:238:THR:HG23	2.01	0.42
1:A:121:ASP:OD2	1:A:122:ILE:N	2.53	0.42
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.80	0.42
1:B:122:ILE:HA	1:B:145:MET:HB3	2.01	0.41
1:B:146:HIS:HD2	1:B:163:ASP:HB2	1.84	0.41
1:B:192:THR:O	1:B:196:ASN:ND2	2.53	0.41
1:B:204:GLU:OE2	1:B:204:GLU:N	2.45	0.41
1:B:178:ASP:C	1:B:180:ASN:N	2.79	0.41
1:A:8:ARG:HA	1:A:13:THR:HG23	2.01	0.41
2:A:501:B63:H16	2:A:501:B63:H2A	1.79	0.41
1:B:244:LEU:O	1:B:245:GLY:C	2.63	0.41
1:B:245:GLY:C	1:B:250:CYS:SG	3.03	0.41
1:A:76:VAL:O	1:A:77:GLU:C	2.64	0.41
1:A:236:GLU:CD	1:A:236:GLU:N	2.79	0.41
1:B:142:ILE:HG13	1:B:143:ILE:N	2.36	0.41
1:B:154:ARG:HE	1:B:154:ARG:HB3	1.62	0.41
1:B:165:TYR:O	1:B:166:ASP:C	2.63	0.41
1:B:197:LEU:O	1:B:200:MET:HB2	2.21	0.40
1:A:35:ASP:O	1:A:82:ARG:NH1	2.54	0.40
1:B:3:TRP:C	1:B:5:TYR:H	2.30	0.40
1:B:26:LEU:HD22	1:B:62:ILE:HG12	2.02	0.40
1:B:112:ILE:HD11	1:B:119:ILE:HD11	2.04	0.40
1:B:155:ASN:O	1:B:156:LEU:C	2.65	0.40
1:B:189:PHE:C	1:B:191:LYS:H	2.30	0.40
1:A:2:LYS:CD	1:A:3:TRP:N	2.83	0.40
1:A:155:ASN:HD22	1:A:158:ALA:HB2	1.85	0.40
1:A:30:PRO:HB3	1:A:82:ARG:HH21	1.86	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	260/297 (88%)	221 (85%)	33 (13%)	6 (2%)	5	13
1	B	256/297 (86%)	222 (87%)	25 (10%)	9 (4%)	3	6
All	All	516/594 (87%)	443 (86%)	58 (11%)	15 (3%)	3	9

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	LEU
1	B	179	GLU
1	B	239	GLY
1	B	258	VAL
1	A	37	GLY
1	A	115	GLY
1	A	156	LEU
1	B	91	SER
1	A	38	SER
1	B	127	ALA
1	A	31	ASP
1	B	115	GLY
1	A	28	VAL
1	B	29	THR
1	B	129	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/247 (84%)	178 (86%)	30 (14%)	3	8
1	B	208/247 (84%)	180 (86%)	28 (14%)	4	9
All	All	416/494 (84%)	358 (86%)	58 (14%)	3	9

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS

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Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	GLU
1	A	13	THR
1	A	20	THR
1	A	26	LEU
1	A	28	VAL
1	A	35	ASP
1	A	38	SER
1	A	51	GLU
1	A	62	ILE
1	A	74	VAL
1	A	76	VAL
1	A	83	VAL
1	A	92	LYS
1	A	104	LYS
1	A	130	LYS
1	A	149	ASP
1	A	151	MET
1	A	161	ILE
1	A	169	LYS
1	A	170	ILE
1	A	203	LEU
1	A	213	VAL
1	A	218	SER
1	A	247	GLU
1	A	252	PHE
1	A	253	VAL
1	A	260	GLU
1	A	268	MET
1	B	7	LEU
1	B	11	GLU
1	B	13	THR
1	B	19	LYS
1	B	23	MET
1	B	59	ILE
1	B	76	VAL
1	B	77	GLU
1	B	87	ILE
1	B	88	GLN
1	B	90	VAL
1	B	91	SER
1	B	95	LYS

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Mol	Chain	Res	Type
1	B	100	ILE
1	B	106	GLU
1	B	109	LYS
1	B	140	VAL
1	B	142	ILE
1	B	152	ASN
1	B	154	ARG
1	B	170	ILE
1	B	203	LEU
1	B	213	VAL
1	B	214	LEU
1	B	215	LEU
1	B	242	VAL
1	B	252	PHE
1	B	272	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	180	ASN
1	A	225	HIS
1	B	88	GLN
1	B	146	HIS
1	B	152	ASN
1	B	180	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

6 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
3	SO4	A	279	-	4,4,4	0.65	0	6,6,6	0.31	0
3	SO4	B	278	-	4,4,4	0.51	0	6,6,6	1.09	0
2	B63	A	501	-	24,26,26	1.41	3 (12%)	26,36,36	1.41	3 (11%)
2	B63	B	502	-	24,26,26	1.15	3 (12%)	26,36,36	1.84	6 (23%)
3	SO4	B	279	-	4,4,4	0.44	0	6,6,6	0.60	0
3	SO4	A	278	-	4,4,4	0.60	0	6,6,6	0.82	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	B63	A	501	-	-	5/10/19/19	0/3/3/3
2	B63	B	502	-	-	5/10/19/19	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	B63	C6-C5	4.58	1.51	1.40
2	B	502	B63	C6-C5	2.94	1.47	1.40
2	A	501	B63	C7-N3	-2.39	1.34	1.38
2	A	501	B63	C8-N5	2.16	1.38	1.33
2	B	502	B63	O2-C15	-2.08	1.24	1.30
2	B	502	B63	C8-N4	2.03	1.38	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	B63	C8-N5-C5	6.37	124.60	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	B63	C8-N5-C5	3.37	119.31	113.36
2	A	501	B63	C2-C1-C3	-2.93	107.20	112.36
2	B	502	B63	N4-C8-N3	2.85	122.79	116.76
2	B	502	B63	C6-N1-C3	2.71	121.61	116.24
2	B	502	B63	O1-C7-C6	-2.55	119.80	126.53
2	A	501	B63	C6-N1-C3	2.50	121.20	116.24
2	B	502	B63	N3-C8-N5	-2.36	119.01	123.32
2	B	502	B63	C6-C7-N3	2.22	118.90	113.25

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	B63	C3-C1-C2-N6
2	A	501	B63	C2-C1-C3-N1
2	B	502	B63	C3-C1-C2-N6
2	B	502	B63	C1-C2-N6-C9
2	A	501	B63	C1-C2-N6-C9
2	B	502	B63	C10-C9-N6-C2
2	A	501	B63	C14-C9-N6-C2
2	B	502	B63	C2-C1-C3-N1
2	A	501	B63	C10-C9-N6-C2
2	B	502	B63	C14-C9-N6-C2

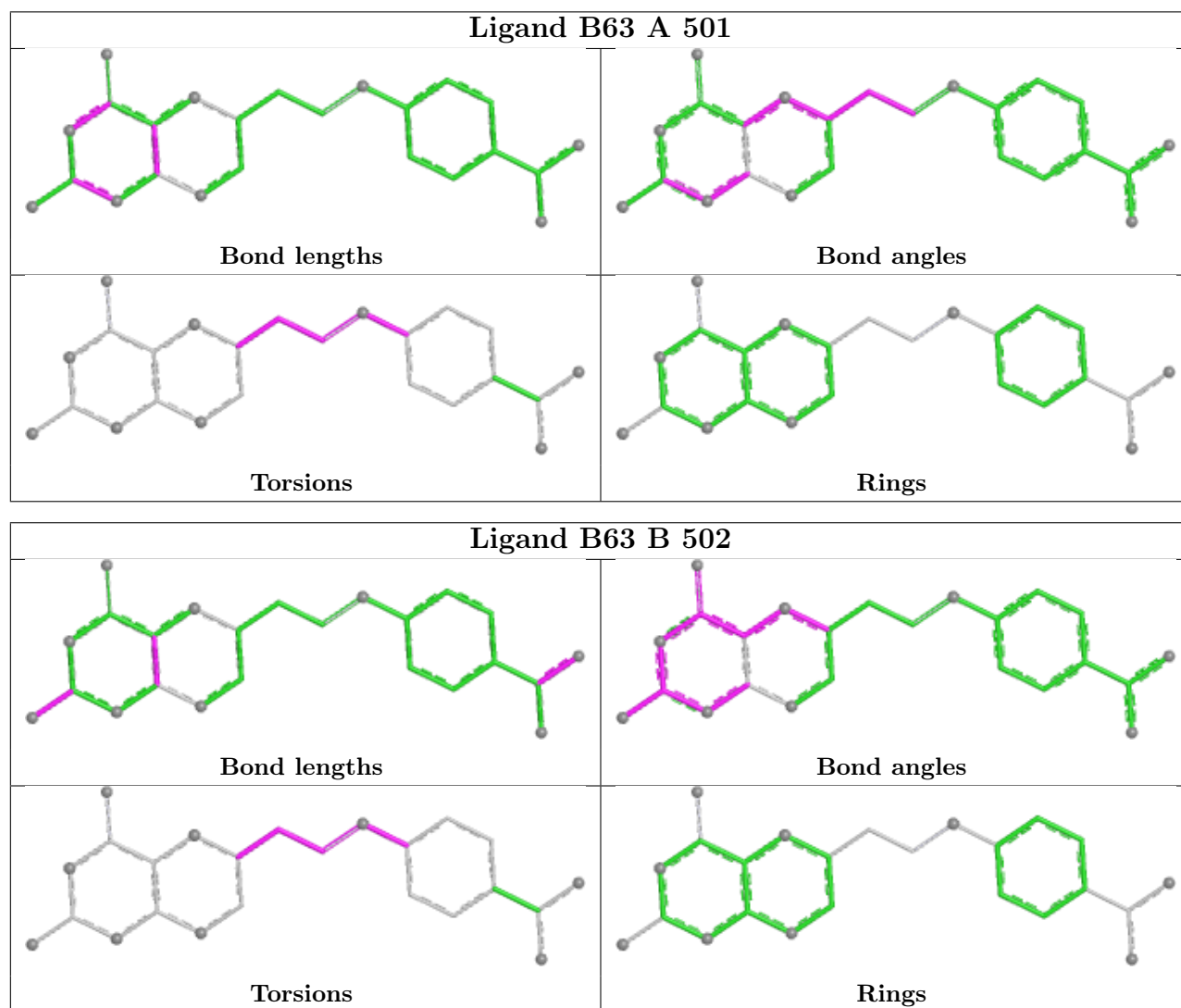
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	279	SO4	1	0
2	A	501	B63	4	0
2	B	502	B63	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 [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	264/297 (88%)	0.36	9 (3%)	48 44	31, 48, 68, 76	0
1	B	262/297 (88%)	0.20	5 (1%)	66 63	34, 49, 60, 69	0
All	All	526/594 (88%)	0.28	14 (2%)	56 53	31, 48, 63, 76	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65	GLU	3.3
1	B	165	TYR	3.2
1	A	8	ARG	3.0
1	A	36	GLY	2.7
1	A	33	PHE	2.6
1	B	1	MET	2.6
1	B	30	PRO	2.4
1	A	61	ASP	2.3
1	A	29	THR	2.3
1	A	26	LEU	2.3
1	A	2	LYS	2.2
1	A	151	MET	2.2
1	A	127	ALA	2.1
1	B	239	GLY	2.1

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 ⓘ

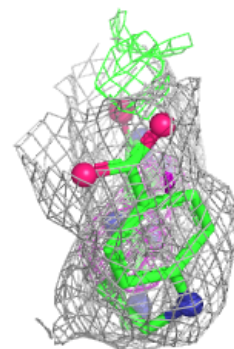
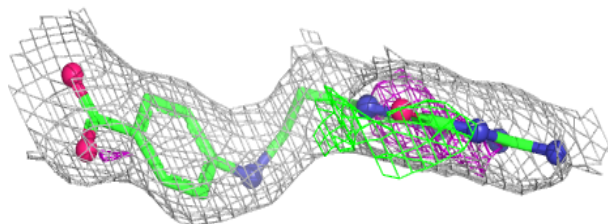
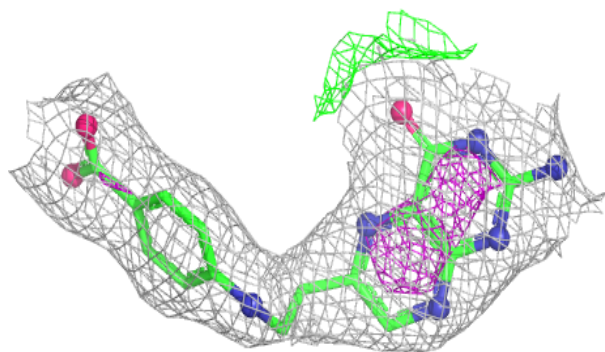
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

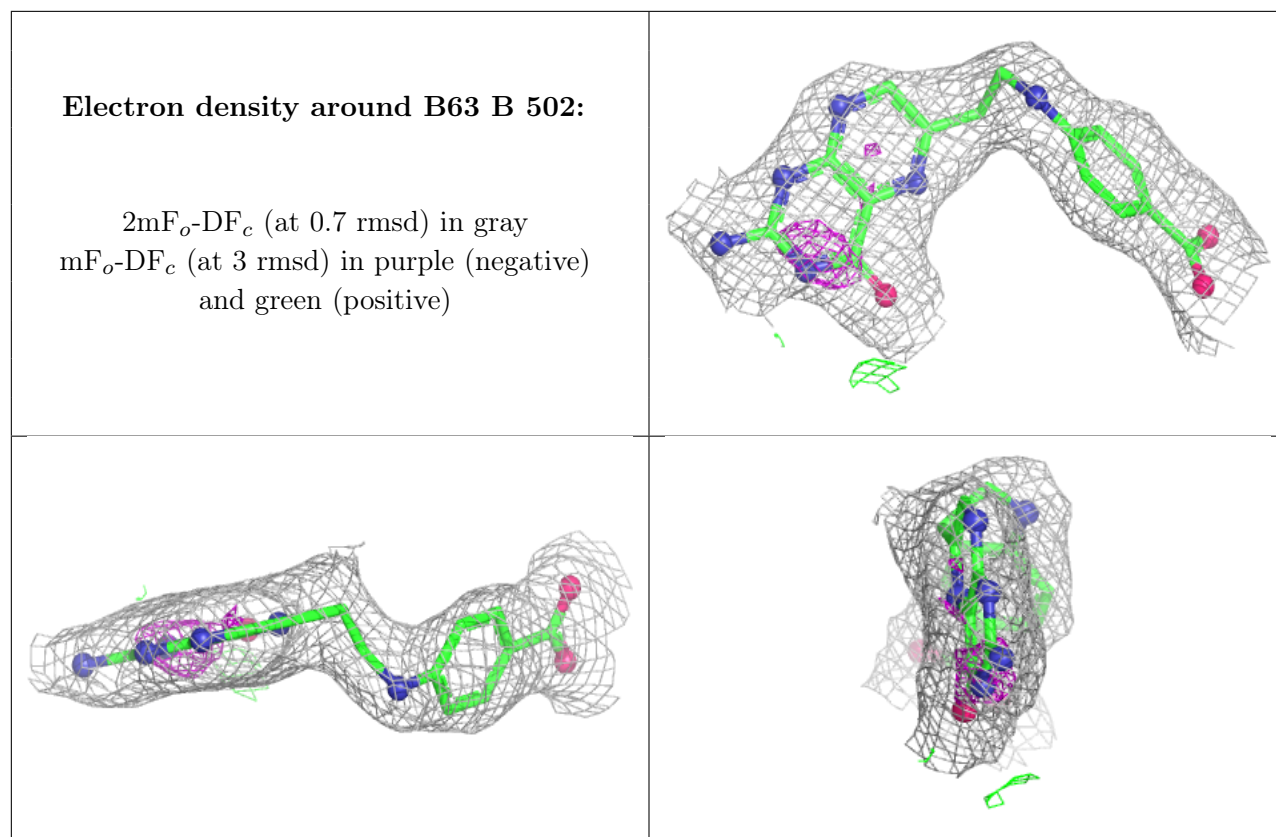
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	278	5/5	0.63	0.18	90,90,90,90	0
3	SO4	B	278	5/5	0.64	0.21	92,95,96,97	0
3	SO4	B	279	5/5	0.68	0.17	89,89,90,90	0
3	SO4	A	279	5/5	0.79	0.13	92,93,95,96	0
2	B63	A	501	24/24	0.90	0.08	39,41,42,43	0
2	B63	B	502	24/24	0.90	0.09	36,42,44,44	0

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 B63 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.