



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:52 PM UTC

PDB ID : 3H2C / pdb_00003h2c
Title : Structural Studies of Pterin-Based Inhibitors of Dihydropteroate Synthase
Authors : Yun, M.-K.; White, S.W.
Deposited on : 2009-04-14
Resolution : 2.60 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
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

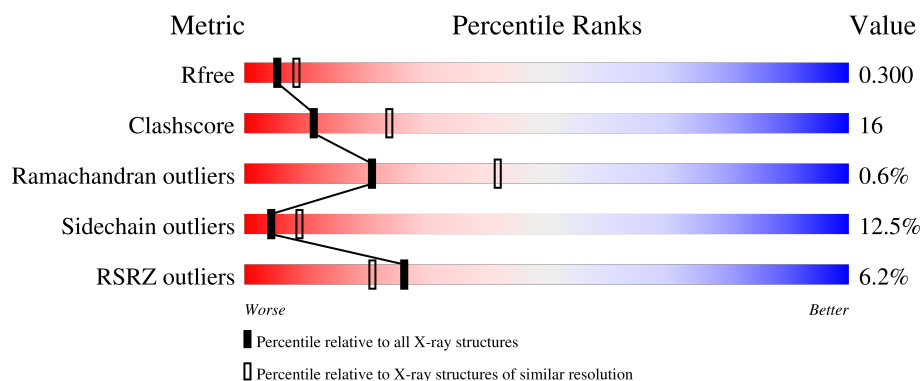
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 4132 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	257	Total	C	N	O	S	0	0	0
			1986	1249	340	381	16			
1	B	263	Total	C	N	O	S	0	2	0
			2036	1283	348	387	18			

There are 40 discrepancies between the modelled and reference sequences:

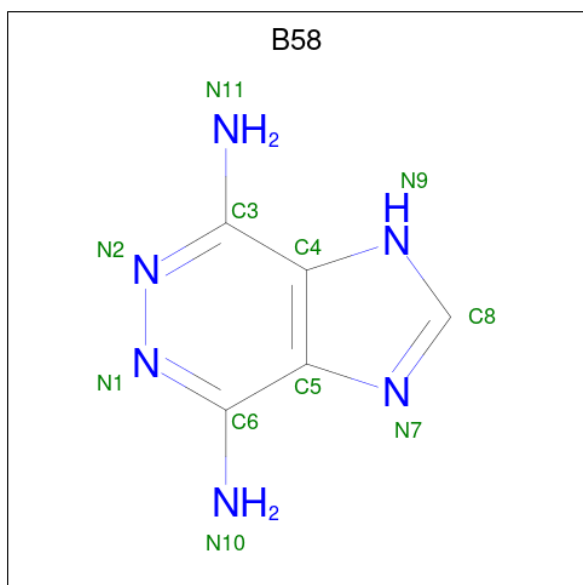
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP B1UXN2
A	-18	GLY	-	expression tag	UNP B1UXN2
A	-17	SER	-	expression tag	UNP B1UXN2
A	-16	SER	-	expression tag	UNP B1UXN2
A	-15	HIS	-	expression tag	UNP B1UXN2
A	-14	HIS	-	expression tag	UNP B1UXN2
A	-13	HIS	-	expression tag	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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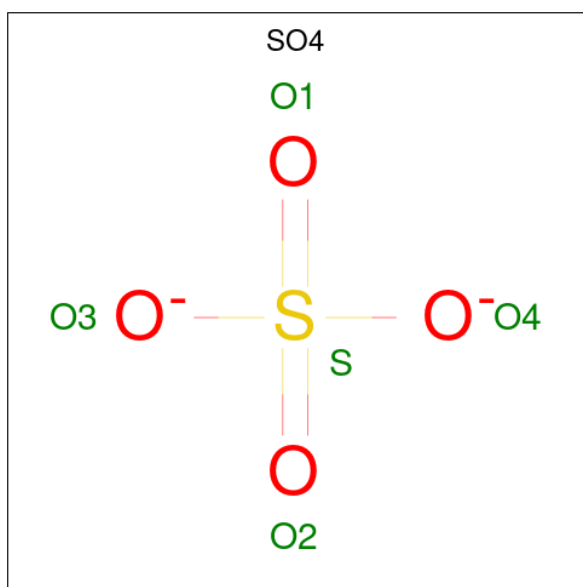
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP B1UXN2
B	-13	HIS	-	expression tag	UNP B1UXN2
B	-12	HIS	-	expression tag	UNP B1UXN2
B	-11	HIS	-	expression tag	UNP B1UXN2
B	-10	HIS	-	expression tag	UNP B1UXN2
B	-9	SER	-	expression tag	UNP B1UXN2
B	-8	SER	-	expression tag	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 1H-imidazo[4,5-d]pyridazine-4,7-diamine (CCD ID: B58) (formula: C₅H₆N₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			11	5	6		
2	B	1	Total	C	N	0	0
			11	5	6		

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		

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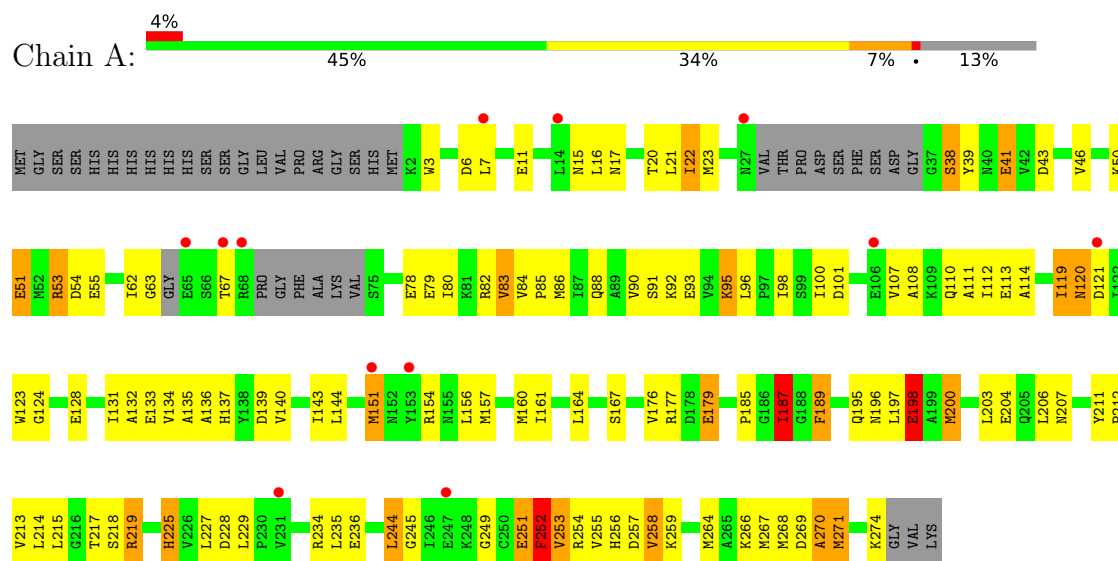
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	16	Total	O	0	0
			16	16		

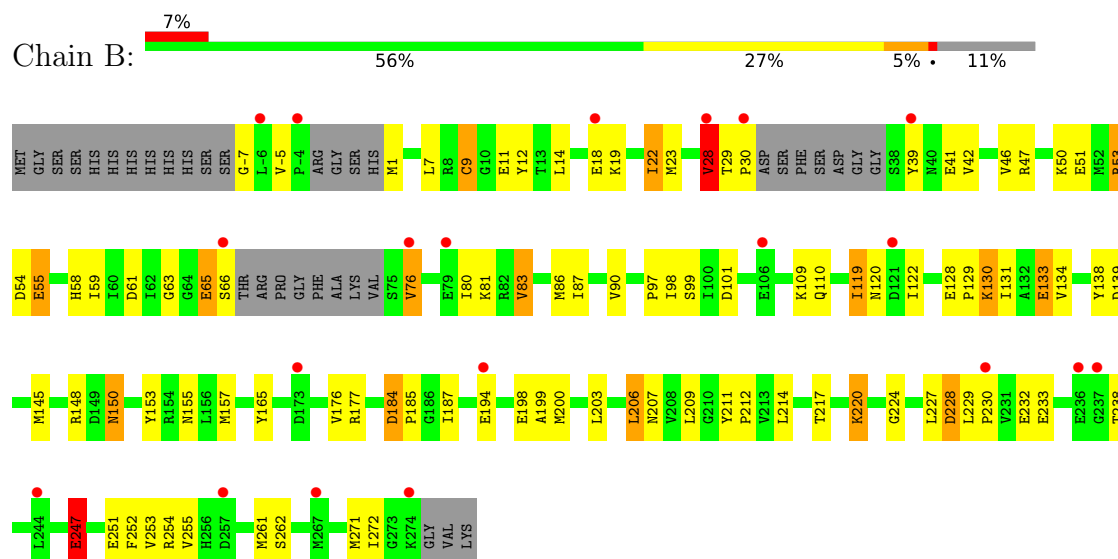
3 Residue-property plots [i](#)

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: 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	97.67Å 97.67Å 263.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.02 – 2.60 48.02 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.02-2.60) 94.8 (48.02-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.246 , 0.298 0.263 , 0.300	Depositor DCC
R_{free} test set	1336 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.915	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 74.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4132	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 47.68 % 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 9.5856e-05. 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: B58, 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	1.59	24/2012 (1.2%)	1.50	21/2711 (0.8%)
1	B	1.34	16/2071 (0.8%)	1.31	14/2794 (0.5%)
All	All	1.47	40/4083 (1.0%)	1.41	35/5505 (0.6%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	LYS	CE-NZ	11.11	1.82	1.49
1	A	213	VAL	CA-CB	-8.47	1.44	1.54
1	A	245	GLY	N-CA	7.57	1.56	1.45
1	B	50	LYS	CA-CB	7.46	1.65	1.53
1	B	251	GLU	N-CA	-7.03	1.36	1.46
1	A	249	GLY	C-O	-7.00	1.15	1.24
1	A	196	ASN	N-CA	6.42	1.54	1.46
1	A	62	ILE	CA-CB	-6.25	1.46	1.54
1	A	119	ILE	CA-CB	-6.14	1.44	1.55
1	B	28	VAL	CA-CB	6.02	1.60	1.53
1	A	16	LEU	C-O	-6.01	1.15	1.24
1	A	251	GLU	C-O	-6.00	1.15	1.23
1	A	252	PHE	CA-C	5.75	1.59	1.52
1	B	262	SER	C-O	-5.67	1.17	1.24
1	A	67	THR	CA-CB	5.56	1.62	1.53
1	A	187	ILE	CA-CB	5.54	1.59	1.54
1	A	46	VAL	CA-CB	5.51	1.61	1.54
1	B	207	ASN	C-O	-5.48	1.17	1.24
1	B	200	MET	C-O	-5.47	1.17	1.24
1	A	251	GLU	N-CA	5.39	1.53	1.46
1	B	-7	GLY	N-CA	5.33	1.54	1.45
1	B	199	ALA	N-CA	-5.32	1.39	1.46
1	A	270	ALA	CA-CB	-5.31	1.45	1.53
1	B	39	TYR	C-N	5.30	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	GLU	C-O	5.27	1.30	1.24
1	B	76	VAL	CA-CB	5.23	1.60	1.54
1	A	249	GLY	N-CA	5.22	1.53	1.45
1	A	120	ASN	N-CA	-5.20	1.40	1.46
1	A	176	VAL	CA-CB	5.19	1.60	1.53
1	B	198	GLU	CA-C	5.18	1.59	1.52
1	B	-5	VAL	CA-C	5.16	1.58	1.52
1	A	189	PHE	CA-C	-5.15	1.46	1.52
1	B	253	VAL	C-O	-5.13	1.18	1.24
1	A	264	MET	CB-CG	-5.11	1.37	1.52
1	A	195	GLN	C-O	-5.11	1.18	1.24
1	B	41	GLU	C-N	5.10	1.39	1.34
1	B	119	ILE	CA-CB	-5.09	1.48	1.54
1	A	234	ARG	CA-C	-5.08	1.46	1.53
1	A	38	SER	CB-OG	5.08	1.52	1.42
1	A	271	MET	N-CA	-5.07	1.40	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	MET	N-CA-C	-8.65	101.05	111.69
1	A	3	TRP	N-CA-C	-7.33	99.05	110.42
1	A	154	ARG	N-CA-C	-7.31	103.25	111.07
1	A	249	GLY	O-C-N	-7.20	115.19	122.54
1	B	211	TYR	CA-C-N	6.71	127.11	119.93
1	B	211	TYR	C-N-CA	6.71	127.11	119.93
1	A	20	THR	CA-C-N	6.51	130.00	120.82
1	A	20	THR	C-N-CA	6.51	130.00	120.82
1	A	258	VAL	N-CA-C	6.46	116.62	110.42
1	A	198	GLU	N-CA-C	-6.41	104.50	112.90
1	B	228	ASP	N-CA-C	6.39	119.01	111.02
1	A	51	GLU	N-CA-C	-6.24	105.16	112.89
1	B	128	GLU	CA-C-N	6.11	125.59	119.24
1	B	128	GLU	C-N-CA	6.11	125.59	119.24
1	B	247	GLU	N-CA-C	-6.03	104.27	111.69
1	B	194	GLU	N-CA-C	5.93	119.34	111.75
1	A	53	ARG	N-CA-C	-5.93	104.90	111.36
1	B	272	ILE	N-CA-C	-5.81	105.17	113.07
1	B	157	MET	N-CA-C	5.78	117.58	111.28
1	A	21	LEU	N-CA-C	5.69	118.58	110.10
1	A	93	GLU	N-CA-C	5.65	120.67	113.55
1	A	137	HIS	N-CA-C	5.47	117.68	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	VAL	N-CA-C	5.45	117.94	108.90
1	B	238	THR	N-CA-C	-5.44	105.43	111.36
1	B	255	VAL	N-CA-C	5.44	116.87	108.44
1	A	128	GLU	CA-C-N	5.40	125.48	119.32
1	A	128	GLU	C-N-CA	5.40	125.48	119.32
1	A	111	ALA	N-CA-C	5.39	116.96	111.14
1	B	9	CYS	CB-CA-C	-5.36	104.40	111.42
1	A	151	MET	N-CA-C	5.27	119.20	109.24
1	A	164	LEU	N-CA-C	-5.26	105.63	111.36
1	A	107	VAL	N-CA-C	-5.23	105.50	110.42
1	B	184	ASP	CA-C-N	5.22	124.89	119.56
1	B	184	ASP	C-N-CA	5.22	124.89	119.56
1	A	20	THR	CB-CA-C	-5.11	102.91	110.67

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	1986	0	1981	74	0
1	B	2036	0	2039	58	0
2	A	11	0	6	0	0
2	B	11	0	6	1	0
3	A	25	0	0	1	0
3	B	30	0	0	0	0
4	A	17	0	0	0	0
4	B	16	0	0	0	0
All	All	4132	0	4032	131	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 16.

All (131) 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:95:LYS:CE	1:A:95:LYS:NZ	1.82	1.41
1:B:23:MET:HE2	1:B:254:ARG:HD2	1.33	1.06
1:A:212:PRO:HA	1:A:251:GLU:OE2	1.65	0.96
1:B:165[A]:TYR:CE1	1:B:209:LEU:HD22	2.05	0.91
1:B:214:LEU:HD12	1:B:252:PHE:CB	2.02	0.90
1:A:119:ILE:HG22	1:A:120:ASN:N	1.87	0.90
1:A:177:ARG:NH1	1:A:179:GLU:HG3	1.94	0.82
1:A:119:ILE:HG22	1:A:120:ASN:H	1.45	0.80
1:B:214:LEU:HD12	1:B:252:PHE:HB3	1.66	0.78
1:B:214:LEU:HD12	1:B:252:PHE:HB2	1.64	0.78
1:B:247:GLU:OE1	1:B:247:GLU:C	2.29	0.76
1:B:28:VAL:O	1:B:30:PRO:HD3	1.89	0.72
1:A:144:LEU:HD13	1:A:167:SER:HB3	1.70	0.72
1:B:63:GLY:HA2	1:B:101:ASP:HB3	1.73	0.69
1:A:119:ILE:CG2	1:A:120:ASN:H	2.06	0.69
1:A:156:LEU:HG	1:A:160:MET:CE	2.24	0.68
1:B:14:LEU:HD21	1:B:97:PRO:HG2	1.76	0.68
1:A:119:ILE:CG2	1:A:120:ASN:N	2.55	0.67
1:A:252:PHE:CD1	1:A:252:PHE:N	2.61	0.67
1:B:18:GLU:HG3	1:B:19:LYS:HG2	1.75	0.66
1:A:225:HIS:HD1	1:A:225:HIS:C	2.03	0.66
1:B:227:LEU:HB3	1:B:229:LEU:HD12	1.79	0.65
1:B:220:LYS:NZ	2:B:902:B58:HN9	1.95	0.65
1:B:22:ILE:H	1:B:58:HIS:HD1	1.43	0.64
1:A:110:GLN:O	1:A:113:GLU:HB3	1.97	0.64
1:B:214:LEU:CD1	1:B:252:PHE:HB3	2.29	0.63
1:B:23:MET:HB2	1:B:59:ILE:HB	1.81	0.63
1:B:23:MET:HE3	1:B:61:ASP:CG	2.23	0.63
1:B:145:MET:HA	1:B:184:ASP:HB3	1.81	0.62
1:B:247:GLU:OE1	1:B:247:GLU:O	2.17	0.62
1:B:23:MET:HE2	1:B:254:ARG:CD	2.20	0.61
1:A:39:TYR:CD1	1:B:42:VAL:HB	2.36	0.61
1:A:23:MET:HB3	1:A:254:ARG:HA	1.82	0.60
1:B:214:LEU:CD1	1:B:252:PHE:CB	2.79	0.60
1:B:65:GLU:HG2	1:B:66:SER:N	2.18	0.59
1:A:91:SER:HB3	1:A:98:ILE:HD13	1.84	0.59
1:A:214:LEU:HD11	1:A:254:ARG:HB2	1.85	0.59
1:A:206:LEU:HD12	1:A:206:LEU:N	2.19	0.57
1:A:63:GLY:HA2	1:A:101:ASP:HB3	1.87	0.57
1:A:236:GLU:H	1:A:236:GLU:CD	2.13	0.57
1:B:23:MET:CE	1:B:254:ARG:HD2	2.23	0.56
1:A:156:LEU:CD2	1:A:198:GLU:HG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLU:O	1:A:207:ASN:HB2	2.04	0.56
1:A:227:LEU:HB3	1:A:229:LEU:HD12	1.88	0.56
1:A:51:GLU:O	1:A:55:GLU:HG2	2.06	0.55
1:B:51:GLU:O	1:B:55:GLU:HG2	2.06	0.54
1:B:53:ARG:NH1	1:B:54:ASP:OD1	2.40	0.54
1:A:121:ASP:C	1:A:121:ASP:OD2	2.50	0.54
1:B:51:GLU:O	1:B:55:GLU:CG	2.56	0.54
1:A:95:LYS:NZ	1:A:95:LYS:CD	2.68	0.53
1:A:22:ILE:HD12	1:A:253:VAL:HG22	1.91	0.53
1:A:187:ILE:HG21	1:A:217:THR:HG22	1.91	0.53
1:A:86:MET:O	1:A:90:VAL:HG23	2.08	0.52
1:A:214:LEU:HD13	1:A:252:PHE:HB2	1.90	0.52
1:A:108:ALA:O	1:A:112:ILE:HD12	2.09	0.52
1:A:225:HIS:C	1:A:225:HIS:ND1	2.64	0.51
1:A:41:GLU:HB2	1:A:86:MET:HE1	1.93	0.51
1:A:211:TYR:HB3	1:A:212:PRO:HD2	1.91	0.51
1:A:204:GLU:OE2	1:A:204:GLU:N	2.36	0.51
1:B:12:TYR:CB	1:B:97:PRO:HG3	2.41	0.51
1:A:95:LYS:O	1:A:96:LEU:HD23	2.10	0.51
1:B:165[A]:TYR:CZ	1:B:209:LEU:HD22	2.45	0.50
1:A:6:ASP:OD1	1:A:15:ASN:HA	2.11	0.49
1:B:61:ASP:OD2	1:B:99:SER:OG	2.31	0.49
1:A:38:SER:OG	1:A:41:GLU:HG3	2.13	0.49
1:A:156:LEU:HG	1:A:160:MET:HE3	1.93	0.49
1:A:53:ARG:NH1	1:A:54:ASP:OD1	2.46	0.49
1:A:120:ASN:HA	1:A:143:ILE:HB	1.95	0.48
1:A:228:ASP:OD1	1:A:228:ASP:C	2.56	0.48
1:A:206:LEU:HD12	1:A:206:LEU:H	1.79	0.48
1:A:268:MET:HA	1:A:271:MET:CE	2.42	0.48
1:B:80:ILE:O	1:B:81:LYS:C	2.58	0.47
1:A:225:HIS:ND1	1:A:225:HIS:O	2.47	0.47
1:A:271:MET:HB2	1:A:271:MET:HE3	1.49	0.47
1:B:187:ILE:HG21	1:B:217:THR:HG22	1.97	0.47
1:A:228:ASP:O	1:A:229:LEU:HG	2.14	0.47
1:B:129:PRO:O	1:B:131:ILE:N	2.48	0.47
1:B:83:VAL:O	1:B:87:ILE:HG13	2.15	0.47
1:B:83:VAL:O	1:B:86:MET:HB2	2.15	0.46
1:A:259:LYS:HB3	1:A:259:LYS:HE2	1.75	0.46
1:A:200:MET:HE1	1:A:215:LEU:HD21	1.97	0.46
1:A:110:GLN:O	1:A:114:ALA:N	2.49	0.45
1:A:135:ALA:O	1:A:136:ALA:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:GLY:O	1:B:228:ASP:HA	2.17	0.45
1:A:131:ILE:CG2	1:A:132:ALA:N	2.80	0.45
1:B:165[A]:TYR:HE1	1:B:209:LEU:HD22	1.72	0.45
1:A:131:ILE:O	1:A:134:VAL:HB	2.17	0.44
1:B:119:ILE:HG22	1:B:120:ASN:N	2.31	0.44
1:A:218:SER:HB3	1:A:256:HIS:ND1	2.31	0.44
1:A:254:ARG:NH2	3:A:278:SO4:O3	2.42	0.44
1:B:214:LEU:CD1	1:B:252:PHE:HB2	2.42	0.44
1:A:131:ILE:HG23	1:A:132:ALA:N	2.32	0.44
1:A:157:MET:HE1	1:A:206:LEU:HD11	2.00	0.44
1:B:28:VAL:O	1:B:30:PRO:CD	2.63	0.44
1:B:86:MET:O	1:B:90:VAL:HG23	2.18	0.44
1:B:176:VAL:HG12	1:B:177:ARG:O	2.18	0.43
1:A:185:PRO:HG3	1:A:203:LEU:HD21	2.01	0.43
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.76	0.43
1:A:258:VAL:O	1:A:259:LYS:C	2.62	0.43
1:B:129:PRO:C	1:B:131:ILE:N	2.77	0.43
1:B:134:VAL:HG12	1:B:138:TYR:HD2	1.83	0.43
1:B:227:LEU:HD23	1:B:227:LEU:HA	1.80	0.43
1:A:23:MET:SD	1:A:254:ARG:HG3	2.59	0.43
1:A:123:TRP:O	1:A:124:GLY:C	2.62	0.43
1:A:211:TYR:HB3	1:A:212:PRO:CD	2.48	0.43
1:A:41:GLU:C	1:A:43:ASP:H	2.25	0.43
1:A:189:PHE:CD1	1:A:189:PHE:N	2.86	0.43
1:A:269:ASP:O	1:A:270:ALA:C	2.57	0.43
1:B:148:ARG:HD2	1:B:153:TYR:CZ	2.53	0.42
1:B:185:PRO:HD2	1:B:214:LEU:O	2.19	0.42
1:B:28:VAL:HG21	1:B:63:GLY:O	2.19	0.42
1:B:130:LYS:HA	1:B:133:GLU:HG3	2.01	0.42
1:B:206:LEU:HD23	1:B:206:LEU:HA	1.77	0.42
1:B:129:PRO:C	1:B:131:ILE:H	2.28	0.42
1:A:84:VAL:HB	1:A:85:PRO:HD3	2.02	0.42
1:A:91:SER:HA	1:A:98:ILE:HD11	2.02	0.41
1:A:17:ASN:O	1:A:274:LYS:HG3	2.20	0.41
1:A:156:LEU:HD23	1:A:198:GLU:HG2	2.02	0.41
1:A:79:GLU:O	1:A:83:VAL:HB	2.20	0.41
1:B:86:MET:H	1:B:86:MET:HG2	1.68	0.41
1:B:230:PRO:HD2	1:B:233:GLU:HG3	2.02	0.41
1:B:232:GLU:OE1	1:B:232:GLU:N	2.51	0.41
1:A:266:LYS:O	1:A:267:MET:C	2.63	0.40
1:B:53:ARG:NH1	1:B:53:ARG:HB3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:HD22	1:A:198:GLU:HG2	2.02	0.40
1:A:244:LEU:O	1:A:244:LEU:HG	2.21	0.40
1:B:46:VAL:O	1:B:47:ARG:C	2.62	0.40
1:B:53:ARG:HB3	1:B:53:ARG:HH11	1.85	0.40
1:A:206:LEU:N	1:A:206:LEU:CD1	2.84	0.40
1:B:150:ASN:ND2	1:B:150:ASN:C	2.79	0.40
1:B:109:LYS:O	1:B:110:GLN:C	2.64	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	249/297 (84%)	224 (90%)	24 (10%)	1 (0%)	30	51
1	B	257/297 (86%)	230 (90%)	25 (10%)	2 (1%)	16	34
All	All	506/594 (85%)	454 (90%)	49 (10%)	3 (1%)	21	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	130	LYS
1	A	219	ARG
1	B	29	THR

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/247 (85%)	181 (86%)	29 (14%)	3	7
1	B	216/247 (87%)	192 (89%)	24 (11%)	6	12
All	All	426/494 (86%)	373 (88%)	53 (12%)	4	9

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	GLU
1	A	22	ILE
1	A	41	GLU
1	A	50	LYS
1	A	78	GLU
1	A	80	ILE
1	A	82	ARG
1	A	83	VAL
1	A	88	GLN
1	A	92	LYS
1	A	100	ILE
1	A	133	GLU
1	A	139	ASP
1	A	140	VAL
1	A	151	MET
1	A	161	ILE
1	A	179	GLU
1	A	187	ILE
1	A	197	LEU
1	A	198	GLU
1	A	200	MET
1	A	219	ARG
1	A	225	HIS
1	A	235	LEU
1	A	244	LEU
1	A	252	PHE
1	A	253	VAL
1	A	257	ASP
1	B	1	MET
1	B	7	LEU
1	B	9	CYS
1	B	11	GLU
1	B	22	ILE

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Mol	Chain	Res	Type
1	B	28	VAL
1	B	53	ARG
1	B	55	GLU
1	B	65	GLU
1	B	76	VAL
1	B	83	VAL
1	B	98	ILE
1	B	122	ILE
1	B	133	GLU
1	B	139	ASP
1	B	150	ASN
1	B	155	ASN
1	B	203	LEU
1	B	206	LEU
1	B	212	PRO
1	B	220	LYS
1	B	247	GLU
1	B	261	MET
1	B	271	MET

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	110	GLN
1	B	15	ASN
1	B	48	HIS
1	B	137	HIS
1	B	150	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

13 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	278	-	4,4,4	0.70	0	6,6,6	0.80	0
3	SO4	A	281	-	4,4,4	0.54	0	6,6,6	0.56	0
2	B58	B	902	-	12,12,12	2.51	4 (33%)	13,17,17	1.90	4 (30%)
3	SO4	B	280	-	4,4,4	0.34	0	6,6,6	0.25	0
3	SO4	B	282	-	4,4,4	0.43	0	6,6,6	0.76	0
3	SO4	A	279	-	4,4,4	0.25	0	6,6,6	0.76	0
2	B58	A	901	-	12,12,12	2.36	4 (33%)	13,17,17	2.48	5 (38%)
3	SO4	B	283	-	4,4,4	0.37	0	6,6,6	0.84	0
3	SO4	A	280	-	4,4,4	0.37	0	6,6,6	0.69	0
3	SO4	A	282	-	4,4,4	0.50	0	6,6,6	0.50	0
3	SO4	B	278	-	4,4,4	0.20	0	6,6,6	0.86	0
3	SO4	B	279	-	4,4,4	0.47	0	6,6,6	0.52	0
3	SO4	B	281	-	4,4,4	0.23	0	6,6,6	0.55	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	B58	B	902	-	-	-	0/2/2/2
2	B58	A	901	-	-	-	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	B58	C4-C5	5.00	1.47	1.40
2	B	902	B58	C4-C5	4.54	1.46	1.40
2	B	902	B58	C5-N7	-4.10	1.31	1.39
2	A	901	B58	N2-N1	3.59	1.43	1.34
2	B	902	B58	N2-N1	3.31	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	B58	C4-N9	-3.28	1.32	1.37
2	A	901	B58	C5-C6	2.67	1.48	1.41
2	A	901	B58	C4-C3	2.63	1.50	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	B58	C4-C5-N7	-4.80	106.12	109.64
2	A	901	B58	C5-N7-C8	4.79	108.88	103.48
2	B	902	B58	C4-C5-N7	-3.55	107.04	109.64
2	B	902	B58	C5-N7-C8	3.34	107.24	103.48
2	A	901	B58	C4-N9-C8	3.21	108.96	106.27
2	B	902	B58	C5-C4-N9	2.86	107.76	105.74
2	A	901	B58	N9-C8-N7	-2.73	109.72	113.87
2	A	901	B58	C4-C3-N11	-2.43	117.96	123.49
2	B	902	B58	C5-C6-N1	-2.04	115.71	118.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	278	SO4	1	0
2	B	902	B58	1	0

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	257/297 (86%)	0.69	12 (4%) 36 30	30, 57, 69, 93	0
1	B	263/297 (88%)	0.79	20 (7%) 20 16	32, 61, 74, 97	2 (0%)
All	All	520/594 (87%)	0.74	32 (6%) 26 21	30, 59, 74, 97	2 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	SER	4.6
1	A	67	THR	4.3
1	B	106	GLU	3.9
1	B	30	PRO	3.4
1	B	28	VAL	3.1
1	B	173	ASP	3.1
1	A	27	ASN	3.0
1	B	-4	PRO	2.9
1	B	76	VAL	2.8
1	B	39	TYR	2.8
1	A	247	GLU	2.7
1	B	237	GLY	2.7
1	A	106	GLU	2.7
1	B	18	GLU	2.5
1	B	267	MET	2.5
1	A	121	ASP	2.5
1	A	65	GLU	2.5
1	A	153	TYR	2.5
1	B	-6	LEU	2.4
1	B	244	LEU	2.4
1	B	236	GLU	2.4
1	A	151	MET	2.3
1	B	257	ASP	2.2
1	A	231	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	68	ARG	2.2
1	B	230	PRO	2.2
1	B	121	ASP	2.2
1	B	79	GLU	2.1
1	A	7	LEU	2.1
1	A	14	LEU	2.1
1	B	274	LYS	2.1
1	B	194	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

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	282	5/5	0.55	0.14	101,101,102,104	0
3	SO4	B	283	5/5	0.60	0.13	98,98,99,101	0
3	SO4	B	280	5/5	0.63	0.14	106,107,107,108	0
3	SO4	B	281	5/5	0.68	0.13	99,99,99,100	0
3	SO4	B	282	5/5	0.74	0.22	95,97,97,99	0
3	SO4	A	281	5/5	0.75	0.28	84,85,87,88	0
3	SO4	B	279	5/5	0.83	0.12	88,89,90,91	0
3	SO4	A	280	5/5	0.84	0.28	84,85,86,88	0
3	SO4	A	279	5/5	0.85	0.16	86,87,88,90	0
3	SO4	B	278	5/5	0.86	0.22	68,69,69,70	0
2	B58	A	901	11/11	0.87	0.12	47,48,48,49	0
2	B58	B	902	11/11	0.89	0.10	47,49,50,52	0
3	SO4	A	278	5/5	0.89	0.19	57,58,60,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.