



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:17 AM UTC

PDB ID : 3TCM / pdb_00003tcm
Title : Crystal Structure of Alanine Aminotransferase from Hordeum vulgare
Authors : Rydel, T.J.; Sturman, E.J.; Halls, C.; Chen, S.; Zeng, J.; Evdokimov, A.; Duff, S.M.G.
Deposited on : 2011-08-09
Resolution : 2.71 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

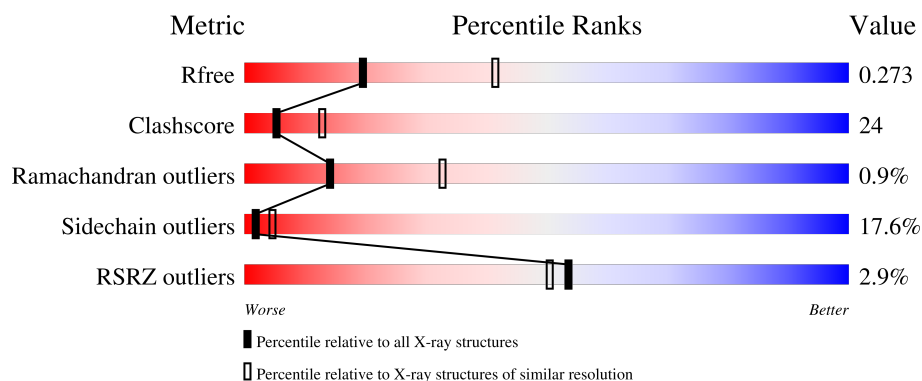
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	500	
1	B	500	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7514 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 Alanine aminotransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	1	0
			3706	2360	633	697	16			
1	B	479	Total	C	N	O	S	0	0	0
			3703	2358	633	697	15			

There are 38 discrepancies between the modelled and reference sequences:

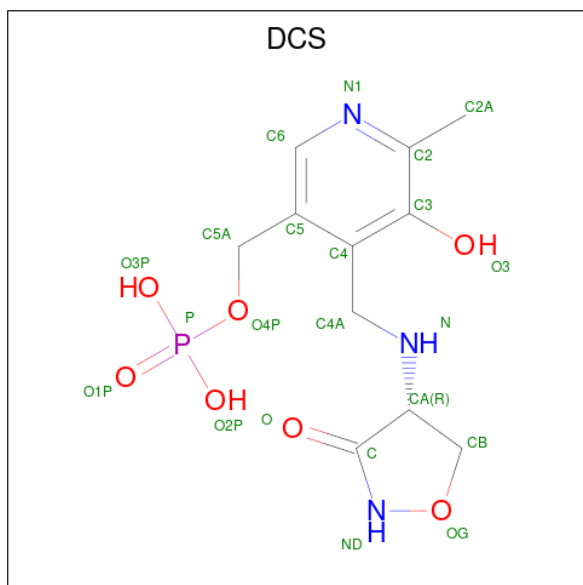
Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP P52894
A	-16	HIS	-	expression tag	UNP P52894
A	-15	HIS	-	expression tag	UNP P52894
A	-14	HIS	-	expression tag	UNP P52894
A	-13	HIS	-	expression tag	UNP P52894
A	-12	HIS	-	expression tag	UNP P52894
A	-11	HIS	-	expression tag	UNP P52894
A	-10	HIS	-	expression tag	UNP P52894
A	-9	HIS	-	expression tag	UNP P52894
A	-8	HIS	-	expression tag	UNP P52894
A	-7	HIS	-	expression tag	UNP P52894
A	-6	GLY	-	expression tag	UNP P52894
A	-5	THR	-	expression tag	UNP P52894
A	-4	ASP	-	expression tag	UNP P52894
A	-3	ASP	-	expression tag	UNP P52894
A	-2	ASP	-	expression tag	UNP P52894
A	-1	ASP	-	expression tag	UNP P52894
A	0	LYS	-	expression tag	UNP P52894
A	119	HIS	LYS	engineered mutation	UNP P52894
B	-17	MET	-	initiating methionine	UNP P52894
B	-16	HIS	-	expression tag	UNP P52894
B	-15	HIS	-	expression tag	UNP P52894
B	-14	HIS	-	expression tag	UNP P52894
B	-13	HIS	-	expression tag	UNP P52894
B	-12	HIS	-	expression tag	UNP P52894

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP P52894
B	-10	HIS	-	expression tag	UNP P52894
B	-9	HIS	-	expression tag	UNP P52894
B	-8	HIS	-	expression tag	UNP P52894
B	-7	HIS	-	expression tag	UNP P52894
B	-6	GLY	-	expression tag	UNP P52894
B	-5	THR	-	expression tag	UNP P52894
B	-4	ASP	-	expression tag	UNP P52894
B	-3	ASP	-	expression tag	UNP P52894
B	-2	ASP	-	expression tag	UNP P52894
B	-1	ASP	-	expression tag	UNP P52894
B	0	LYS	-	expression tag	UNP P52894
B	119	HIS	LYS	engineered mutation	UNP P52894

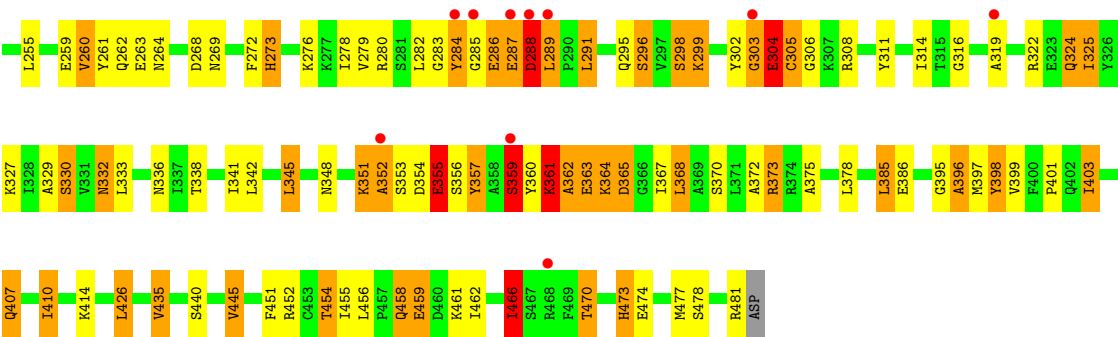
- Molecule 2 is D-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL]-N,O-CYCLOSERYLAMIDE (CCD ID: DCS) (formula: $C_{11}H_{16}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	3	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total 29	O 29	0	0
3	B	32	Total 32	O 32	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.86Å 126.97Å 75.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.16 – 2.71 87.16 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.8 (87.16-2.71) 96.8 (87.16-2.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.215 , 0.279 0.212 , 0.273	Depositor DCC
R_{free} test set	1582 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 24.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7514	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: DCS

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	1.36	28/3788 (0.7%)	1.52	64/5135 (1.2%)
1	B	1.45	37/3782 (1.0%)	1.70	79/5127 (1.5%)
All	All	1.41	65/7570 (0.9%)	1.61	143/10262 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	363	GLU	CA-C	-9.15	1.41	1.52
1	A	299	LYS	C-O	-8.81	1.15	1.23
1	B	303	GLY	CA-C	-8.05	1.44	1.52
1	B	410	ILE	CA-CB	7.72	1.62	1.54
1	A	288	ASP	CA-C	-7.43	1.42	1.52
1	B	291	LEU	C-O	-6.81	1.16	1.23
1	A	139	ALA	CA-CB	-6.79	1.42	1.53
1	B	218	ILE	CA-CB	6.63	1.62	1.54
1	B	357	TYR	C-O	6.54	1.31	1.24
1	B	407	GLN	CD-OE1	6.44	1.35	1.23
1	B	352	ALA	CA-CB	-6.43	1.45	1.54
1	B	224	VAL	CA-CB	6.43	1.61	1.54
1	B	372	ALA	CA-CB	-6.12	1.43	1.53
1	A	374	ARG	CA-C	-6.07	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	ALA	CA-CB	-6.00	1.44	1.53
1	B	308	ARG	CA-C	-5.97	1.48	1.53
1	A	348	ASN	CG-OD1	5.97	1.34	1.23
1	B	330	SER	CA-C	-5.94	1.45	1.52
1	A	138	ASN	CG-ND2	-5.90	1.20	1.33
1	B	30	GLN	CD-OE1	5.89	1.34	1.23
1	A	28	HIS	ND1-CE1	5.88	1.38	1.32
1	A	104	ILE	CA-CB	-5.85	1.46	1.54
1	B	348	ASN	CG-OD1	5.79	1.34	1.23
1	A	303	GLY	C-O	-5.76	1.16	1.23
1	B	39	GLN	CD-OE1	5.76	1.34	1.23
1	B	305	CYS	C-O	-5.75	1.17	1.24
1	B	368	LEU	C-O	5.74	1.30	1.24
1	A	162	ASN	C-O	-5.71	1.16	1.23
1	A	358	ALA	CA-CB	-5.71	1.44	1.53
1	A	99	GLN	CD-OE1	5.70	1.34	1.23
1	B	466	ILE	CA-CB	5.62	1.61	1.54
1	B	288	ASP	N-CA	-5.59	1.39	1.46
1	A	116	GLN	CD-OE1	5.59	1.34	1.23
1	B	299	LYS	C-O	-5.59	1.18	1.23
1	B	238	GLU	CA-C	-5.57	1.45	1.52
1	A	289	LEU	C-N	-5.56	1.26	1.33
1	B	269	ASN	CG-OD1	5.54	1.34	1.23
1	B	303	GLY	C-O	-5.52	1.18	1.23
1	B	289	LEU	CA-C	-5.51	1.45	1.52
1	B	264	ASN	CG-ND2	-5.47	1.21	1.33
1	A	291	LEU	C-O	-5.47	1.17	1.23
1	A	324	GLN	CD-NE2	-5.44	1.21	1.33
1	A	273	HIS	ND1-CE1	5.43	1.38	1.32
1	A	375	ALA	CA-CB	-5.42	1.44	1.53
1	B	473	HIS	ND1-CE1	5.41	1.38	1.32
1	B	173	GLN	CD-OE1	5.36	1.33	1.23
1	B	373	ARG	CA-C	-5.30	1.46	1.52
1	A	114	HIS	ND1-CE1	5.29	1.37	1.32
1	B	114	HIS	ND1-CE1	5.29	1.37	1.32
1	B	25	ILE	CA-CB	-5.29	1.47	1.54
1	A	473	HIS	ND1-CE1	5.28	1.37	1.32
1	A	334	CYS	CA-C	-5.23	1.46	1.52
1	B	324	GLN	CD-NE2	-5.21	1.22	1.33
1	A	345	LEU	C-O	-5.21	1.18	1.24
1	A	218	ILE	CA-CB	5.17	1.60	1.54
1	A	241	GLN	CD-NE2	-5.15	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	GLN	CD-OE1	5.14	1.33	1.23
1	B	336	ASN	CG-ND2	-5.13	1.22	1.33
1	B	99	GLN	CD-OE1	5.10	1.33	1.23
1	A	369	ALA	CA-CB	-5.09	1.45	1.53
1	A	373	ARG	N-CA	-5.08	1.39	1.46
1	A	376	LYS	C-O	-5.08	1.18	1.24
1	B	273	HIS	ND1-CE1	5.07	1.37	1.32
1	B	26	VAL	CA-CB	-5.03	1.48	1.54
1	B	306	GLY	C-O	-5.01	1.17	1.23

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	LYS	N-CA-CB	-22.32	79.64	110.67
1	B	302	TYR	N-CA-C	20.15	133.32	111.36
1	B	285	GLY	N-CA-C	17.27	134.88	112.77
1	B	303	GLY	N-CA-C	17.00	131.25	111.36
1	A	373	ARG	N-CA-C	-16.21	91.75	111.69
1	B	363	GLU	CA-C-N	-15.19	99.92	120.28
1	B	363	GLU	C-N-CA	-15.19	99.92	120.28
1	B	362	ALA	N-CA-C	-13.82	96.29	111.36
1	A	287	GLU	N-CA-C	-12.99	95.61	112.24
1	B	361	LYS	N-CA-C	-12.79	97.61	113.97
1	A	303	GLY	CA-C-N	12.62	144.42	121.70
1	A	303	GLY	C-N-CA	12.62	144.42	121.70
1	B	60	GLY	N-CA-C	11.80	128.70	113.24
1	A	289	LEU	CA-C-N	-11.49	108.27	119.76
1	A	289	LEU	C-N-CA	-11.49	108.27	119.76
1	A	374	ARG	CA-C-N	-11.01	105.53	120.28
1	A	374	ARG	C-N-CA	-11.01	105.53	120.28
1	B	287	GLU	CA-C-N	-10.90	106.27	120.44
1	B	287	GLU	C-N-CA	-10.90	106.27	120.44
1	A	289	LEU	N-CA-C	-10.68	86.22	109.81
1	B	288	ASP	N-CA-C	-10.66	99.66	111.07
1	B	398	TYR	N-CA-C	10.66	125.33	109.24
1	A	269	ASN	N-CA-C	10.37	122.58	111.28
1	B	357	TYR	N-CA-C	10.01	123.12	111.11
1	A	60	GLY	N-CA-C	9.97	126.30	113.24
1	A	356	SER	N-CA-C	-9.93	99.04	111.75
1	B	319	ALA	N-CA-C	-9.75	97.36	109.65
1	B	61	GLN	N-CA-C	9.66	124.80	110.30
1	A	303	GLY	N-CA-C	9.66	136.07	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ARG	N-CA-C	-9.62	103.65	114.62
1	B	81	GLN	N-CA-C	9.16	121.26	111.28
1	B	440	SER	N-CA-C	-8.85	96.77	109.96
1	B	42	SER	N-CA-C	8.83	120.90	111.28
1	B	364	LYS	N-CA-C	8.80	120.87	111.28
1	A	299	LYS	N-CA-C	8.79	121.78	109.31
1	B	282	LEU	N-CA-C	-8.75	101.59	112.88
1	A	105	PRO	N-CA-C	8.75	125.69	113.53
1	B	351	LYS	N-CA-C	8.71	122.87	108.49
1	A	319	ALA	N-CA-C	-8.69	98.70	109.65
1	A	351	LYS	N-CA-C	8.48	123.67	113.16
1	B	373	ARG	N-CA-C	-8.47	102.13	111.36
1	B	86	LYS	N-CA-C	-8.32	102.21	111.28
1	A	288	ASP	N-CA-C	-8.30	103.05	113.01
1	B	365	ASP	N-CA-C	8.29	120.32	111.28
1	B	355	GLU	N-CA-C	-8.18	102.30	111.71
1	B	330	SER	O-C-N	8.17	130.48	122.07
1	A	359	SER	CA-C-N	8.05	130.91	120.44
1	A	359	SER	C-N-CA	8.05	130.91	120.44
1	B	296	SER	CA-C-N	8.02	133.45	120.30
1	B	296	SER	C-N-CA	8.02	133.45	120.30
1	A	104	ILE	N-CA-C	-7.75	92.13	108.88
1	A	442	PHE	N-CA-C	-7.75	103.97	113.50
1	A	163	GLU	N-CA-C	-7.68	102.88	111.71
1	A	298	SER	N-CA-C	7.64	119.61	111.28
1	B	40	PRO	N-CA-C	7.54	124.74	113.81
1	B	353	SER	CA-C-N	-7.49	109.64	123.05
1	B	353	SER	C-N-CA	-7.49	109.64	123.05
1	B	329	ALA	N-CA-C	7.47	121.66	112.54
1	B	397	MET	N-CA-C	7.45	122.50	112.88
1	B	299	LYS	N-CA-C	7.26	119.61	109.31
1	A	353	SER	N-CA-C	-7.12	103.52	111.28
1	B	4	THR	N-CA-C	-7.11	100.28	110.59
1	A	399	VAL	CB-CA-C	7.07	121.70	110.82
1	A	462	ILE	CA-C-N	-6.94	111.35	119.05
1	A	462	ILE	C-N-CA	-6.94	111.35	119.05
1	B	138	ASN	N-CA-C	6.82	121.16	110.32
1	A	114	HIS	CB-CG-CD2	-6.80	122.36	131.20
1	B	435	VAL	CB-CA-C	-6.80	102.73	110.96
1	B	361	LYS	CA-C-N	-6.77	110.68	120.29
1	B	361	LYS	C-N-CA	-6.77	110.68	120.29
1	B	238	GLU	CB-CA-C	-6.75	99.58	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	HIS	CA-C-N	6.70	126.29	119.19
1	B	76	HIS	C-N-CA	6.70	126.29	119.19
1	B	114	HIS	CB-CG-CD2	-6.68	122.52	131.20
1	B	473	HIS	CB-CG-CD2	-6.67	122.52	131.20
1	A	456	LEU	CA-C-N	-6.66	112.92	119.78
1	A	456	LEU	C-N-CA	-6.66	112.92	119.78
1	A	473	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	B	273	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	A	303	GLY	O-C-N	-6.53	114.21	122.70
1	A	273	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	B	319	ALA	C-N-CD	-6.44	106.43	120.60
1	B	319	ALA	CA-C-N	6.44	142.45	127.00
1	B	319	ALA	C-N-CA	6.44	142.45	127.00
1	A	162	ASN	N-CA-C	6.40	118.91	109.24
1	A	376	LYS	N-CA-C	6.40	118.34	111.36
1	B	332	ASN	N-CA-C	-6.36	105.27	113.16
1	B	359	SER	N-CA-C	-6.35	104.36	111.28
1	B	284	TYR	CA-C-N	-6.34	113.03	120.00
1	B	284	TYR	C-N-CA	-6.34	113.03	120.00
1	B	445	VAL	N-CA-CB	6.29	117.15	110.17
1	B	287	GLU	N-CA-C	-6.27	100.74	113.29
1	A	282	LEU	N-CA-C	-6.09	105.70	113.01
1	A	28	HIS	CB-CG-CD2	-6.00	123.41	131.20
1	A	88	LEU	N-CA-C	5.93	118.98	111.69
1	A	114	HIS	CB-CG-ND1	5.92	131.57	122.70
1	B	284	TYR	CB-CA-C	-5.90	98.67	110.42
1	B	352	ALA	CA-C-N	-5.87	113.02	122.24
1	B	352	ALA	C-N-CA	-5.87	113.02	122.24
1	B	289	LEU	N-CA-C	-5.85	102.95	108.22
1	B	114	HIS	CB-CG-ND1	5.77	131.35	122.70
1	A	306	GLY	CA-C-N	5.73	128.53	120.28
1	A	306	GLY	C-N-CA	5.73	128.53	120.28
1	B	233	GLY	N-CA-C	5.68	126.65	113.18
1	B	273	HIS	CB-CG-ND1	5.65	131.18	122.70
1	A	473	HIS	CB-CG-ND1	5.65	131.17	122.70
1	B	364	LYS	CA-C-N	5.62	127.81	120.28
1	B	364	LYS	C-N-CA	5.62	127.81	120.28
1	B	473	HIS	CB-CG-ND1	5.62	131.13	122.70
1	A	273	HIS	CB-CG-ND1	5.61	131.12	122.70
1	B	363	GLU	N-CA-C	-5.60	105.26	111.36
1	B	77	PRO	N-CA-C	5.54	120.83	113.57
1	A	61	GLN	N-CA-C	5.52	118.48	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	GLY	CA-C-O	-5.51	110.97	120.57
1	B	142	ILE	N-CA-C	5.51	116.92	108.71
1	A	480	TYR	N-CA-C	5.51	120.88	113.72
1	A	305	CYS	N-CA-C	5.50	117.28	111.28
1	A	28	HIS	CB-CG-ND1	5.49	130.93	122.70
1	A	157	GLN	N-CA-C	5.48	118.01	111.71
1	B	302	TYR	CA-C-N	5.43	125.14	119.92
1	B	302	TYR	C-N-CA	5.43	125.14	119.92
1	A	354	ASP	N-CA-C	5.41	118.38	109.72
1	B	435	VAL	N-CA-C	5.40	116.49	108.23
1	A	260	VAL	N-CA-C	5.39	117.78	111.05
1	A	403	ILE	CB-CA-C	-5.38	102.63	110.81
1	A	51[A]	CYS	N-CA-C	-5.33	106.08	112.59
1	A	51[B]	CYS	N-CA-C	-5.33	106.08	112.59
1	A	290	PRO	N-CA-C	-5.27	102.92	111.19
1	A	355	GLU	CA-C-N	-5.25	112.71	120.38
1	A	355	GLU	C-N-CA	-5.25	112.71	120.38
1	A	421	ASP	CB-CA-C	-5.24	102.43	110.81
1	A	422	ALA	N-CA-C	-5.24	105.63	112.23
1	A	304	GLU	CB-CA-C	5.23	120.05	110.10
1	B	43	LEU	CA-CB-CG	-5.22	98.01	116.30
1	B	298	SER	N-CA-C	5.22	116.97	111.28
1	A	106	GLY	N-CA-C	-5.19	100.88	113.18
1	B	284	TYR	N-CA-C	5.18	121.84	110.80
1	B	305	CYS	CA-C-N	5.17	125.72	119.98
1	B	305	CYS	C-N-CA	5.17	125.72	119.98
1	A	162	ASN	N-CA-CB	-5.17	102.70	111.69
1	B	83	GLU	N-CA-C	5.13	119.54	113.28
1	B	302	TYR	CB-CA-C	-5.12	102.14	110.85
1	B	403	ILE	CB-CA-C	-5.05	103.13	110.81

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	SER	Peptide
1	A	441	GLY	Peptide
1	B	161	ARG	Peptide

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	3706	0	3697	185	0
1	B	3703	0	3694	190	0
2	A	22	0	13	6	0
2	B	22	0	14	3	0
3	A	29	0	0	3	0
3	B	32	0	0	2	0
All	All	7514	0	7418	361	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 24.

All (361) 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:B:82:ARG:HH11	1:B:82:ARG:CB	1.43	1.29
1:B:284:TYR:CG	1:B:288:ASP:CG	2.12	1.28
1:B:284:TYR:CD1	1:B:288:ASP:OD1	1.90	1.24
1:B:303:GLY:HA2	1:B:304:GLU:CB	1.56	1.21
1:B:92:ASP:OD1	1:B:356:SER:HB2	1.42	1.18
1:A:354:ASP:OD1	1:A:355:GLU:N	1.76	1.18
1:B:84:GLU:O	1:B:87:THR:HG23	1.48	1.14
1:B:284:TYR:CD1	1:B:288:ASP:CG	2.29	1.11
1:B:82:ARG:HH11	1:B:82:ARG:HB2	0.97	1.07
1:B:82:ARG:HB2	1:B:82:ARG:NH1	1.70	1.05
1:B:303:GLY:HA2	1:B:304:GLU:HB2	1.09	1.05
1:B:141:ASP:OD1	1:B:322:ARG:NH1	1.90	1.04
1:B:284:TYR:CG	1:B:288:ASP:OD2	2.11	1.04
1:B:284:TYR:HB3	1:B:288:ASP:CB	1.88	1.03
1:A:49:LEU:CD2	1:A:51[B]:CYS:SG	2.49	1.01
1:A:354:ASP:O	1:A:357:TYR:HB3	1.60	1.01
1:A:373:ARG:HD2	1:A:459:GLU:OE2	1.59	1.01
1:B:303:GLY:CA	1:B:304:GLU:HB2	1.89	0.99
1:B:284:TYR:HB3	1:B:288:ASP:CG	1.88	0.98
1:B:238:GLU:OE2	1:B:273:HIS:CG	2.18	0.96
1:B:284:TYR:CB	1:B:288:ASP:OD2	2.14	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:TYR:CE1	1:B:288:ASP:OD1	2.20	0.94
1:B:378:LEU:HD12	1:B:455:ILE:HD12	1.49	0.93
1:B:284:TYR:CB	1:B:288:ASP:CG	2.40	0.93
1:B:82:ARG:CB	1:B:82:ARG:NH1	2.29	0.93
1:B:82:ARG:HH11	1:B:82:ARG:CG	1.81	0.92
1:A:407:GLN:HA	1:A:410:ILE:HG12	1.52	0.92
1:A:43:LEU:HD12	1:A:44:PRO:HD2	1.50	0.92
1:A:49:LEU:HD21	1:A:51[B]:CYS:SG	2.10	0.92
1:B:238:GLU:OE2	1:B:273:HIS:CD2	2.23	0.91
1:B:466:ILE:O	1:B:470:THR:HG22	1.73	0.89
1:B:49:LEU:HD23	1:B:51:CYS:SG	2.13	0.89
1:A:320:PRO:HB3	3:A:489:HOH:O	1.71	0.89
1:A:466:ILE:O	1:A:470:THR:HG23	1.74	0.88
1:B:260:VAL:HG22	1:B:296:SER:HB3	1.56	0.88
1:B:373:ARG:NH1	1:B:459:GLU:OE2	2.06	0.88
1:A:355:GLU:OE2	1:A:355:GLU:HA	1.73	0.88
1:B:92:ASP:OD1	1:B:354:ASP:HB3	1.74	0.87
1:A:288:ASP:O	1:A:289:LEU:HD23	1.76	0.85
1:A:349:PRO:O	1:A:351:LYS:HE2	1.76	0.85
1:B:284:TYR:HB3	1:B:288:ASP:HB2	1.59	0.85
1:B:466:ILE:O	1:B:470:THR:CG2	2.24	0.84
1:B:83:GLU:O	1:B:86:LYS:HG3	1.79	0.83
1:A:174:TYR:CE2	2:A:501:DCS:HA	2.13	0.83
1:A:454:THR:HG23	1:A:456:LEU:H	1.43	0.83
1:B:218:ILE:HD11	1:B:220:VAL:HG22	1.59	0.83
1:B:49:LEU:CD2	1:B:51:CYS:SG	2.67	0.83
1:A:68:ARG:HH21	1:B:109:THR:HG23	1.44	0.82
1:A:68:ARG:HH11	1:A:68:ARG:HG2	1.43	0.82
1:A:288:ASP:O	1:A:289:LEU:CG	2.27	0.81
1:A:354:ASP:O	1:A:357:TYR:CB	2.28	0.81
1:B:259:GLU:O	1:B:262:GLN:HG3	1.81	0.81
1:A:288:ASP:O	1:A:289:LEU:HG	1.80	0.80
1:A:68:ARG:HH11	1:A:68:ARG:CG	1.94	0.80
1:A:304:GLU:HG3	1:A:342:LEU:HD21	1.62	0.80
1:A:288:ASP:O	1:A:289:LEU:CD2	2.30	0.79
1:B:284:TYR:HB3	1:B:288:ASP:OD2	1.81	0.79
1:B:284:TYR:CD2	1:B:288:ASP:OD2	2.36	0.78
1:A:71:LEU:HD11	1:A:342:LEU:HD13	1.64	0.78
1:A:366:GLY:O	1:A:370:SER:HB2	1.83	0.78
1:A:351:LYS:O	1:A:352:ALA:HB3	1.81	0.78
1:B:92:ASP:CG	1:B:354:ASP:HB3	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:TYR:CD1	1:A:282:LEU:HD13	2.17	0.78
1:A:249:LYS:HD2	1:A:284:TYR:CE1	2.19	0.78
1:A:288:ASP:C	1:A:289:LEU:HD23	2.08	0.78
1:B:245:VAL:HG21	1:B:278:ILE:HG22	1.65	0.77
1:A:351:LYS:O	1:A:352:ALA:CB	2.30	0.77
1:B:82:ARG:NH1	1:B:82:ARG:CG	2.43	0.77
1:B:407:GLN:O	1:B:410:ILE:HG12	1.84	0.76
1:A:269:ASN:OD1	1:A:269:ASN:C	2.29	0.76
1:B:286:GLU:O	1:B:287:GLU:CB	2.30	0.76
1:B:68:ARG:HG2	1:B:68:ARG:HH11	1.52	0.75
1:A:275:PHE:O	1:A:279:VAL:HG23	1.87	0.75
1:B:303:GLY:HA2	1:B:304:GLU:HB3	1.61	0.74
1:A:355:GLU:O	1:A:356:SER:C	2.30	0.74
1:A:354:ASP:OD1	1:A:354:ASP:C	2.30	0.73
1:A:290:PRO:HB3	1:A:317:PHE:CZ	2.23	0.73
1:B:330:SER:O	1:B:333:LEU:HA	1.89	0.73
1:B:238:GLU:OE2	1:B:273:HIS:CE1	2.41	0.73
1:A:83:GLU:CD	1:A:83:GLU:H	1.96	0.72
1:B:63:PRO:HB2	1:B:68:ARG:HD2	1.72	0.72
1:B:83:GLU:HB3	1:B:86:LYS:HE3	1.70	0.72
1:A:68:ARG:HG2	1:A:68:ARG:NH1	2.04	0.72
1:A:286:GLU:C	1:A:288:ASP:N	2.41	0.71
1:A:354:ASP:OD1	1:A:356:SER:N	2.23	0.71
1:B:261:TYR:CE1	1:B:299:LYS:HG2	2.25	0.71
1:B:68:ARG:HG2	1:B:68:ARG:NH1	2.05	0.70
1:A:454:THR:HG22	1:A:457:PRO:HD3	1.72	0.70
1:A:197:THR:HG22	1:A:197:THR:O	1.91	0.70
1:A:421:ASP:HB3	1:A:438:PRO:HB2	1.73	0.70
1:B:351:LYS:O	1:B:352:ALA:HB3	1.90	0.70
1:A:173:GLN:NE2	1:A:178:SER:HB3	2.07	0.69
1:A:282:LEU:HD23	1:A:284:TYR:HE2	1.56	0.69
1:A:302:TYR:N	1:A:302:TYR:CD1	2.61	0.69
1:B:287:GLU:O	1:B:288:ASP:C	2.30	0.69
1:A:38:THR:HG22	1:A:39:GLN:HG3	1.75	0.69
1:A:218:ILE:HD11	1:A:220:VAL:HG22	1.76	0.67
1:A:466:ILE:HD11	3:A:506:HOH:O	1.94	0.67
1:A:290:PRO:HB3	1:A:317:PHE:CE2	2.29	0.67
1:B:28:HIS:HD2	1:B:426:LEU:HD21	1.58	0.67
1:B:284:TYR:CG	1:B:288:ASP:OD1	2.32	0.67
1:B:78:ASP:O	1:B:81:GLN:HB2	1.95	0.67
1:B:68:ARG:HH11	1:B:68:ARG:CG	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD12	1:A:456:LEU:HB2	1.77	0.67
1:B:373:ARG:NH1	1:B:459:GLU:CD	2.53	0.66
1:A:268:ASP:N	1:A:268:ASP:OD1	2.29	0.66
1:A:242:TYR:CD1	1:A:282:LEU:CD1	2.78	0.66
1:B:303:GLY:CA	1:B:304:GLU:CB	2.49	0.66
1:A:205:ASP:O	1:A:209:GLN:HG2	1.96	0.65
1:A:288:ASP:C	1:A:289:LEU:O	2.34	0.65
1:B:473:HIS:CE1	1:B:477:MET:HE3	2.32	0.65
1:B:84:GLU:OE2	1:B:84:GLU:N	2.29	0.64
1:B:454:THR:HG23	1:B:456:LEU:H	1.62	0.64
1:B:298:SER:HB3	1:B:305:CYS:SG	2.38	0.64
1:B:401:PRO:HD2	1:B:451:PHE:O	1.98	0.64
1:B:322:ARG:HA	1:B:325:ILE:HG13	1.79	0.64
1:B:238:GLU:OE2	1:B:273:HIS:ND1	2.30	0.63
1:A:332:ASN:O	1:A:333:LEU:HB2	1.97	0.63
1:A:373:ARG:HH11	1:A:459:GLU:CD	2.07	0.63
1:B:284:TYR:CB	1:B:288:ASP:CB	2.74	0.62
1:A:305:CYS:HB3	1:B:112:TYR:CE2	2.34	0.62
1:B:55:ASN:O	1:B:58:SER:HB2	1.98	0.62
1:B:357:TYR:O	1:B:361:LYS:HB2	2.00	0.62
1:A:174:TYR:CE1	1:A:176:LEU:HB3	2.34	0.62
1:A:249:LYS:CD	1:A:284:TYR:CE1	2.83	0.62
1:A:298:SER:HB3	1:A:305:CYS:SG	2.39	0.62
1:A:174:TYR:CZ	2:A:501:DCS:HA	2.35	0.61
1:B:332:ASN:O	1:B:333:LEU:HB2	2.00	0.61
1:A:54:GLY:H	2:A:501:DCS:HND	1.48	0.61
1:B:260:VAL:HG22	1:B:296:SER:CB	2.30	0.61
1:B:85:ILE:HG13	1:B:86:LYS:N	2.14	0.60
1:A:454:THR:CG2	1:A:456:LEU:H	2.14	0.60
1:B:327:LYS:O	1:B:330:SER:OG	2.20	0.60
1:B:49:LEU:HD21	1:B:51:CYS:SG	2.42	0.59
1:A:349:PRO:O	1:A:351:LYS:CE	2.48	0.59
1:A:371:LEU:O	1:A:375:ALA:N	2.35	0.59
1:A:242:TYR:CE1	1:A:282:LEU:HD13	2.36	0.59
1:B:354:ASP:OD1	1:B:355:GLU:N	2.29	0.59
1:A:132:ARG:HD2	1:A:133:ASP:OD1	2.03	0.59
1:A:49:LEU:HD22	1:A:51[B]:CYS:SG	2.38	0.59
1:A:261:TYR:CE1	1:A:299:LYS:HG3	2.37	0.58
1:A:432:THR:OG1	1:A:434:ILE:HG13	2.03	0.58
1:B:84:GLU:O	1:B:87:THR:CG2	2.39	0.58
1:A:242:TYR:HD1	1:A:282:LEU:HD13	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:VAL:HB	1:B:188:LEU:CD1	2.33	0.58
1:B:286:GLU:O	1:B:287:GLU:HB3	2.03	0.58
1:A:286:GLU:O	1:A:287:GLU:C	2.44	0.58
1:A:298:SER:C	1:A:299:LYS:HD3	2.29	0.58
1:B:218:ILE:C	1:B:218:ILE:HD12	2.29	0.58
1:B:261:TYR:CE1	1:B:299:LYS:CG	2.87	0.58
1:B:22:ARG:HA	1:B:26:VAL:HG21	1.86	0.57
1:B:407:GLN:HB2	1:B:410:ILE:HD11	1.86	0.57
1:A:249:LYS:HD2	1:A:284:TYR:HE1	1.69	0.57
1:A:112:TYR:CZ	1:B:305:CYS:HB3	2.40	0.57
1:A:295:GLN:OE1	1:A:296:SER:N	2.34	0.57
1:B:48:ILE:CG2	1:B:48:ILE:O	2.52	0.57
1:B:311:TYR:C	1:B:311:TYR:CD2	2.83	0.57
1:B:132:ARG:HD2	1:B:133:ASP:OD1	2.04	0.57
1:A:109:THR:CG2	1:B:68:ARG:HH21	2.17	0.57
1:A:112:TYR:CE2	1:B:305:CYS:HB3	2.40	0.57
1:B:82:ARG:NH1	1:B:82:ARG:HG3	2.19	0.56
1:A:297:VAL:HG11	1:A:342:LEU:HD23	1.87	0.56
1:B:201:LEU:O	1:B:201:LEU:HD23	2.06	0.56
1:A:231:PRO:HB3	1:A:452:ARG:HD3	1.88	0.56
1:A:354:ASP:OD1	1:A:355:GLU:CA	2.52	0.56
1:B:209:GLN:OE1	3:B:497:HOH:O	2.17	0.56
1:B:361:LYS:O	1:B:362:ALA:C	2.45	0.56
1:B:238:GLU:OE2	1:B:273:HIS:NE2	2.39	0.56
1:A:109:THR:HG22	1:B:68:ARG:HH21	1.70	0.56
1:A:298:SER:O	1:A:303:GLY:HA2	2.05	0.56
1:A:333:LEU:O	1:A:334:CYS:HB3	2.06	0.55
1:B:92:ASP:CG	1:B:354:ASP:CB	2.79	0.55
1:B:298:SER:O	1:B:303:GLY:HA3	2.07	0.55
1:B:210:LEU:HD21	1:B:251:GLU:HG3	1.88	0.55
1:B:361:LYS:HA	1:B:364:LYS:HB3	1.88	0.55
1:B:375:ALA:HA	1:B:455:ILE:HD11	1.88	0.54
1:B:378:LEU:HD12	1:B:455:ILE:CD1	2.30	0.54
1:B:144:LEU:CD1	1:B:144:LEU:N	2.71	0.54
1:A:357:TYR:C	1:A:357:TYR:CD2	2.85	0.54
1:A:280:ARG:HH22	1:A:315:THR:HG21	1.72	0.54
1:A:354:ASP:O	1:A:357:TYR:N	2.40	0.54
1:A:354:ASP:CG	1:A:355:GLU:N	2.58	0.54
1:A:49:LEU:C	1:A:49:LEU:HD23	2.33	0.54
1:A:144:LEU:HD12	1:A:311:TYR:HB3	1.90	0.54
1:A:82:ARG:HD2	1:B:88:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:TYR:CB	1:B:288:ASP:HB2	2.33	0.53
1:B:360:TYR:CG	1:B:360:TYR:O	2.61	0.53
1:A:297:VAL:O	1:A:297:VAL:CG1	2.55	0.53
1:A:352:ALA:HA	1:A:357:TYR:CG	2.43	0.53
1:B:48:ILE:O	1:B:48:ILE:HG23	2.08	0.53
1:B:357:TYR:O	1:B:360:TYR:HB3	2.08	0.53
1:A:355:GLU:C	1:A:357:TYR:N	2.60	0.53
1:B:341:ILE:HG22	1:B:345:LEU:CD2	2.39	0.53
1:A:218:ILE:C	1:A:218:ILE:HD12	2.34	0.53
1:A:305:CYS:O	1:A:308:ARG:HD2	2.09	0.52
1:B:478:SER:HA	1:B:481:ARG:HG3	1.91	0.52
1:B:226:ILE:HG22	1:B:229:GLY:HA2	1.91	0.52
1:B:115:SER:OG	1:B:330:SER:HA	2.10	0.52
1:B:154:LEU:HD11	1:B:325:ILE:HG23	1.92	0.52
1:A:373:ARG:NH1	1:A:459:GLU:OE1	2.42	0.52
1:A:254:VAL:HG13	1:A:290:PRO:HB2	1.91	0.52
1:B:169:VAL:HG13	1:B:170:PRO:HD2	1.92	0.52
1:B:407:GLN:HA	1:B:410:ILE:HG12	1.92	0.52
1:A:76:HIS:HB3	1:A:79:LEU:HD22	1.91	0.52
1:B:304:GLU:OE2	1:B:304:GLU:HA	2.09	0.52
1:B:385:LEU:HD11	1:B:470:THR:HB	1.92	0.51
1:B:286:GLU:O	1:B:287:GLU:HB2	2.07	0.51
1:B:279:VAL:HG13	1:B:288:ASP:OD2	2.10	0.51
1:A:282:LEU:HD23	1:A:284:TYR:CE2	2.44	0.51
1:A:88:LEU:HD23	1:A:88:LEU:H	1.75	0.51
1:B:218:ILE:HD11	1:B:220:VAL:CG2	2.38	0.51
1:B:367:ILE:O	1:B:368:LEU:C	2.50	0.51
1:A:9:ASN:O	1:B:221:ARG:NH2	2.44	0.51
1:A:113:SER:HB2	1:A:118:ILE:HG13	1.92	0.50
1:B:466:ILE:O	1:B:470:THR:HG23	2.06	0.50
1:A:287:GLU:C	1:A:289:LEU:N	2.68	0.50
1:A:269:ASN:OD1	1:A:269:ASN:O	2.29	0.50
1:A:304:GLU:CG	1:A:342:LEU:HD21	2.37	0.50
1:B:351:LYS:O	1:B:352:ALA:CB	2.56	0.50
1:A:158:LEU:HD13	1:A:325:ILE:HD13	1.93	0.50
1:B:166:GLY:HA3	1:B:218:ILE:HD13	1.94	0.50
1:B:174:TYR:CZ	2:B:502:DCS:HA	2.46	0.50
1:B:245:VAL:HG21	1:B:278:ILE:CG2	2.40	0.50
1:A:83:GLU:CD	1:A:83:GLU:N	2.65	0.50
1:B:53:ILE:HG13	2:B:502:DCS:OG	2.11	0.50
1:B:144:LEU:N	1:B:144:LEU:HD12	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:GLU:O	1:B:287:GLU:OE1	2.30	0.49
1:A:299:LYS:HD3	1:A:299:LYS:N	2.26	0.49
1:A:170:PRO:O	1:A:173:GLN:HB3	2.13	0.49
1:A:88:LEU:H	1:A:88:LEU:CD2	2.26	0.49
1:A:154:LEU:HD11	1:A:325:ILE:HG23	1.94	0.48
1:B:43:LEU:HD23	1:B:43:LEU:HA	1.58	0.48
1:B:78:ASP:O	1:B:81:GLN:CB	2.60	0.48
1:B:81:GLN:OE1	1:B:81:GLN:HA	2.12	0.48
1:B:81:GLN:OE1	1:B:81:GLN:CA	2.57	0.48
1:A:173:GLN:HG2	1:A:174:TYR:O	2.13	0.48
1:B:169:VAL:HB	1:B:188:LEU:HD13	1.94	0.48
1:A:55:ASN:O	1:A:58:SER:HB2	2.14	0.48
1:B:330:SER:O	1:B:333:LEU:CA	2.62	0.48
1:B:148:ALA:HB2	1:B:296:SER:HB2	1.96	0.48
1:A:59:LEU:CD1	1:A:456:LEU:HB2	2.43	0.48
1:A:260:VAL:HG22	1:A:296:SER:HB3	1.96	0.48
1:B:361:LYS:CA	1:B:364:LYS:H	2.26	0.48
1:B:395:GLY:O	1:B:396:ALA:HB3	2.13	0.48
1:A:407:GLN:H	1:A:407:GLN:HG2	1.59	0.47
1:B:363:GLU:O	1:B:364:LYS:C	2.54	0.47
1:A:466:ILE:CD1	3:A:506:HOH:O	2.57	0.47
1:A:287:GLU:C	1:A:289:LEU:H	2.17	0.47
1:A:399:VAL:HG13	1:A:401:PRO:HD3	1.96	0.47
1:B:360:TYR:O	1:B:364:LYS:N	2.47	0.47
1:A:221:ARG:NH2	1:B:9:ASN:O	2.48	0.47
1:A:308:ARG:NH2	2:A:501:DCS:O2P	2.48	0.47
1:B:284:TYR:CD2	1:B:288:ASP:CG	2.80	0.46
1:A:214:ARG:NH2	1:A:251:GLU:OE1	2.46	0.46
1:B:174:TYR:CD2	1:B:175:PRO:HD2	2.50	0.46
1:A:288:ASP:HB3	1:A:289:LEU:O	2.16	0.46
1:B:473:HIS:HE1	1:B:477:MET:HE3	1.75	0.46
1:A:274:SER:HB2	1:A:277:LYS:H	1.80	0.46
1:A:11:ASN:HA	1:B:161:ARG:HG2	1.98	0.46
1:A:218:ILE:HD11	1:A:220:VAL:CG2	2.44	0.46
1:A:355:GLU:O	1:A:358:ALA:N	2.48	0.46
1:B:201:LEU:HD23	1:B:201:LEU:C	2.40	0.46
1:A:197:THR:O	1:A:197:THR:CG2	2.62	0.46
1:B:138:ASN:HB3	3:B:509:HOH:O	2.16	0.45
1:B:240:ASN:OD1	1:B:240:ASN:O	2.34	0.45
1:A:369:ALA:O	1:A:373:ARG:HB2	2.16	0.45
1:A:395:GLY:O	1:A:396:ALA:HB3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:GLN:HB2	1:B:410:ILE:CD1	2.46	0.45
1:A:304:GLU:OE2	1:A:304:GLU:HA	2.16	0.45
1:B:399:VAL:HG13	1:B:455:ILE:HD13	1.98	0.45
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.46	0.45
1:A:407:GLN:O	1:A:408:LYS:C	2.59	0.45
1:A:96:ARG:HG3	1:A:100:ILE:HD12	1.98	0.45
1:A:49:LEU:HD23	1:A:49:LEU:O	2.17	0.44
1:A:63:PRO:HB2	1:A:68:ARG:HD2	1.97	0.44
1:B:407:GLN:O	1:B:410:ILE:CG1	2.58	0.44
1:A:85:ILE:HA	1:A:88:LEU:CD2	2.47	0.44
1:B:77:PRO:HB3	1:B:101:LEU:HD11	1.98	0.44
1:A:239:GLU:O	1:A:243:ASP:OD1	2.35	0.44
1:B:240:ASN:OD1	1:B:240:ASN:C	2.59	0.44
1:A:249:LYS:HD3	1:A:284:TYR:OH	2.17	0.44
1:B:458:GLN:CG	1:B:461:LYS:HD3	2.48	0.44
1:A:82:ARG:NH1	1:A:82:ARG:HB2	2.33	0.44
1:A:362:ALA:O	1:A:365:ASP:O	2.35	0.44
1:B:287:GLU:O	1:B:288:ASP:O	2.35	0.44
1:A:242:TYR:HD1	1:A:282:LEU:CD1	2.27	0.44
1:A:336:ASN:OD1	1:A:338:THR:HG23	2.17	0.44
1:B:170:PRO:O	1:B:171:ILE:HD12	2.17	0.44
1:A:231:PRO:HG3	1:A:442:PHE:CD2	2.52	0.44
1:A:281:SER:OG	1:A:282:LEU:N	2.47	0.44
1:B:330:SER:O	1:B:333:LEU:N	2.50	0.44
1:B:360:TYR:C	1:B:364:LYS:H	2.26	0.44
1:A:297:VAL:O	1:A:302:TYR:HD2	2.01	0.44
1:B:215:SER:C	1:B:217:GLY:H	2.23	0.44
1:B:262:GLN:HG2	1:B:272:PHE:CZ	2.53	0.44
1:A:112:TYR:CE1	1:B:305:CYS:SG	3.11	0.44
1:A:237:ALA:HB2	1:A:270:LYS:HE3	2.00	0.44
1:A:466:ILE:HD12	1:A:470:THR:CG2	2.48	0.44
1:B:85:ILE:O	1:B:86:LYS:C	2.58	0.44
1:B:210:LEU:CD2	1:B:251:GLU:HG3	2.47	0.43
1:A:308:ARG:HE	1:A:308:ARG:HA	1.84	0.43
1:A:49:LEU:CD2	1:A:51[A]:CYS:HB2	2.48	0.43
1:B:361:LYS:HD2	1:B:365:ASP:OD2	2.19	0.43
1:A:212:ASP:OD1	1:A:216:ARG:NH2	2.46	0.43
1:A:228:PRO:HG2	1:A:261:TYR:O	2.19	0.43
1:A:84:GLU:OE2	1:A:84:GLU:N	2.51	0.43
1:A:263:GLU:HG3	1:A:302:TYR:OH	2.19	0.43
1:B:255:LEU:O	1:B:291:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:LEU:HD12	1:B:385:LEU:HA	1.74	0.43
1:A:85:ILE:HA	1:A:88:LEU:HD23	2.00	0.43
1:A:304:GLU:HG3	1:A:342:LEU:CD2	2.42	0.43
1:B:38:THR:HG22	1:B:39:GLN:HG2	2.00	0.43
1:B:78:ASP:OD1	1:B:78:ASP:N	2.50	0.43
1:B:141:ASP:HB3	1:B:314:ILE:O	2.18	0.43
1:B:191:TYR:O	1:B:191:TYR:CD1	2.71	0.43
1:A:158:LEU:CD1	1:A:325:ILE:HD13	2.48	0.43
1:A:299:LYS:HZ1	2:A:501:DCS:H4A2	1.83	0.43
1:B:295:GLN:HB3	1:B:311:TYR:CZ	2.54	0.43
1:B:454:THR:HG23	1:B:456:LEU:HB2	2.00	0.43
1:B:359:SER:O	1:B:363:GLU:HB2	2.18	0.43
1:B:218:ILE:HD12	1:B:219:ASN:N	2.33	0.43
1:B:470:THR:O	1:B:474:GLU:HG2	2.19	0.43
1:A:408:LYS:HE2	1:A:408:LYS:HB3	1.70	0.42
1:A:345:LEU:HA	1:A:345:LEU:HD12	1.86	0.42
1:B:143:PHE:O	1:B:311:TYR:HA	2.19	0.42
1:A:307:LYS:HA	1:A:307:LYS:HD3	1.69	0.42
1:A:280:ARG:HD3	1:A:280:ARG:HA	1.55	0.42
1:A:381:ALA:HB1	1:A:466:ILE:HD13	2.01	0.42
1:B:215:SER:C	1:B:217:GLY:N	2.78	0.42
1:B:296:SER:OG	2:B:502:DCS:O1P	2.26	0.42
1:A:166:GLY:HA3	1:A:218:ILE:CD1	2.49	0.42
1:A:281:SER:C	1:A:283:GLY:N	2.77	0.41
1:B:13:LYS:HE2	1:B:185:GLY:HA3	2.01	0.41
1:B:170:PRO:HD3	1:B:224:VAL:O	2.20	0.41
1:A:258:ASP:OD2	2:A:501:DCS:N1	2.52	0.41
1:A:305:CYS:HB3	1:B:112:TYR:CD2	2.55	0.41
1:A:363:GLU:O	1:A:367:ILE:HB	2.20	0.41
1:A:171:ILE:HG13	1:A:190:PRO:HB3	2.03	0.41
1:A:28:HIS:CG	1:A:31:ARG:HH12	2.39	0.41
1:A:293:SER:O	1:A:312:PHE:HA	2.20	0.41
1:A:426:LEU:HD23	1:A:426:LEU:HA	1.81	0.41
1:B:231:PRO:HB3	1:B:452:ARG:HD3	2.02	0.41
1:A:76:HIS:HB3	1:A:79:LEU:CD2	2.51	0.41
1:A:445:VAL:O	1:A:446:PRO:C	2.63	0.41
1:B:218:ILE:HD12	1:B:219:ASN:C	2.46	0.41
1:B:455:ILE:HD12	1:B:455:ILE:HA	1.93	0.41
1:A:68:ARG:NH2	1:B:109:THR:HG23	2.24	0.41
1:A:466:ILE:HD12	1:A:470:THR:HG23	2.03	0.41
1:B:188:LEU:HD12	1:B:189:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.98	0.41
1:A:43:LEU:HD13	1:A:43:LEU:HA	1.68	0.40
1:A:84:GLU:O	1:A:85:ILE:C	2.64	0.40
1:A:462:ILE:O	1:A:463:PRO:C	2.60	0.40
1:A:72:ALA:HB2	1:B:76:HIS:HB2	2.03	0.40
1:A:371:LEU:HD23	1:A:374:ARG:NH2	2.37	0.40
1:B:71:LEU:O	1:B:72:ALA:C	2.63	0.40
1:A:85:ILE:HG13	1:A:86:LYS:N	2.37	0.40
1:A:212:ASP:CG	1:A:216:ARG:HH21	2.26	0.40
1:A:473:HIS:CE1	1:A:477:MET:HE3	2.57	0.40
1:A:249:LYS:HD3	1:A:284:TYR:CZ	2.57	0.40
1:B:287:GLU:H	1:B:316:GLY:HA2	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	478/500 (96%)	450 (94%)	24 (5%)	4 (1%)	16	35
1	B	477/500 (95%)	446 (94%)	26 (6%)	5 (1%)	12	30
All	All	955/1000 (96%)	896 (94%)	50 (5%)	9 (1%)	14	33

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	GLU
1	B	283	GLY
1	B	304	GLU
1	A	352	ALA
1	A	396	ALA
1	B	105	PRO

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Mol	Chain	Res	Type
1	B	396	ALA
1	B	233	GLY
1	A	456	LEU

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	396/414 (96%)	324 (82%)	72 (18%)	2	4
1	B	395/414 (95%)	328 (83%)	67 (17%)	2	5
All	All	791/828 (96%)	652 (82%)	139 (18%)	2	4

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	8	ASP
1	A	32	LEU
1	A	36	LEU
1	A	37	LYS
1	A	43	LEU
1	A	46	ASP
1	A	47	GLU
1	A	58	SER
1	A	65	THR
1	A	68	ARG
1	A	78	ASP
1	A	79	LEU
1	A	80	LEU
1	A	88	LEU
1	A	90	SER
1	A	103	MET
1	A	104	ILE
1	A	109	THR
1	A	116	GLN

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Mol	Chain	Res	Type
1	A	118	ILE
1	A	132	ARG
1	A	144	LEU
1	A	154	LEU
1	A	155	MET
1	A	159	LEU
1	A	163	GLU
1	A	167	ILE
1	A	168	LEU
1	A	176	LEU
1	A	196	SER
1	A	203	THR
1	A	204	SER
1	A	207	LYS
1	A	218	ILE
1	A	236	LEU
1	A	250	ASN
1	A	263	GLU
1	A	268	ASP
1	A	278	ILE
1	A	282	LEU
1	A	287	GLU
1	A	288	ASP
1	A	289	LEU
1	A	290	PRO
1	A	295	GLN
1	A	302	TYR
1	A	304	GLU
1	A	308	ARG
1	A	313	GLU
1	A	315	THR
1	A	323	GLU
1	A	324	GLN
1	A	336	ASN
1	A	338	THR
1	A	345	LEU
1	A	355	GLU
1	A	367	ILE
1	A	385	LEU
1	A	392	GLU
1	A	399	VAL
1	A	403	ILE

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Mol	Chain	Res	Type
1	A	407	GLN
1	A	408	LYS
1	A	426	LEU
1	A	445	VAL
1	A	453	CYS
1	A	454	THR
1	A	455	ILE
1	A	461	LYS
1	A	465	VAL
1	A	466	ILE
1	B	8	ASP
1	B	17	CYS
1	B	21	VAL
1	B	25	ILE
1	B	30	GLN
1	B	32	LEU
1	B	38	THR
1	B	39	GLN
1	B	48	ILE
1	B	58	SER
1	B	68	ARG
1	B	78	ASP
1	B	79	LEU
1	B	80	LEU
1	B	81	GLN
1	B	82	ARG
1	B	87	THR
1	B	101	LEU
1	B	104	ILE
1	B	105	PRO
1	B	123	ASP
1	B	154	LEU
1	B	159	LEU
1	B	173	GLN
1	B	188	LEU
1	B	193	LEU
1	B	201	LEU
1	B	202	GLU
1	B	204	SER
1	B	207	LYS
1	B	215	SER
1	B	218	ILE

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Mol	Chain	Res	Type
1	B	224	VAL
1	B	236	LEU
1	B	251	GLU
1	B	260	VAL
1	B	263	GLU
1	B	268	ASP
1	B	276	LYS
1	B	280	ARG
1	B	286	GLU
1	B	288	ASP
1	B	289	LEU
1	B	304	GLU
1	B	324	GLN
1	B	325	ILE
1	B	338	THR
1	B	342	LEU
1	B	345	LEU
1	B	355	GLU
1	B	359	SER
1	B	361	LYS
1	B	370	SER
1	B	385	LEU
1	B	386	GLU
1	B	398	TYR
1	B	403	ILE
1	B	414	LYS
1	B	426	LEU
1	B	435	VAL
1	B	445	VAL
1	B	454	THR
1	B	458	GLN
1	B	459	GLU
1	B	462	ILE
1	B	466	ILE
1	B	470	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	B	35	GLN
1	B	116	GLN

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 ⓘ

2 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	DCS	A	501	-	22,23,23	2.71	6 (27%)	27,33,33	1.80	6 (22%)
2	DCS	B	502	-	22,23,23	2.72	4 (18%)	27,33,33	2.62	12 (44%)

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	DCS	A	501	-	-	6/11/21/21	0/2/2/2
2	DCS	B	502	-	-	6/11/21/21	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	DCS	CA-C	-7.59	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	DCS	C3-C2	7.54	1.48	1.41
2	B	502	DCS	C5-C4	6.70	1.49	1.40
2	B	502	DCS	C3-C4	6.67	1.49	1.40
2	A	501	DCS	C3-C2	6.30	1.47	1.41
2	A	501	DCS	C5-C4	5.05	1.47	1.40
2	A	501	DCS	C3-C4	4.51	1.46	1.40
2	B	502	DCS	C-ND	-2.68	1.31	1.34
2	A	501	DCS	C-ND	-2.67	1.31	1.34
2	A	501	DCS	O-C	-2.36	1.18	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	DCS	C4A-N-CA	5.91	124.93	113.84
2	B	502	DCS	CB-OG-ND	5.56	115.61	105.92
2	B	502	DCS	CA-C-ND	5.06	110.73	107.63
2	A	501	DCS	O-C-CA	-4.31	123.09	126.19
2	A	501	DCS	C4A-C4-C3	3.73	124.94	119.98
2	B	502	DCS	C6-C5-C4	3.61	120.79	118.06
2	B	502	DCS	OG-CB-CA	-3.59	99.67	104.80
2	A	501	DCS	CA-C-ND	3.30	109.65	107.63
2	B	502	DCS	C4-C3-C2	-3.02	115.35	119.91
2	B	502	DCS	O3P-P-O4P	-2.98	98.90	106.67
2	A	501	DCS	CB-OG-ND	2.55	110.36	105.92
2	A	501	DCS	O3P-P-O2P	2.43	116.91	107.80
2	B	502	DCS	O-C-CA	-2.42	124.45	126.19
2	B	502	DCS	C3-C4-C5	-2.39	116.56	118.73
2	B	502	DCS	O3-C3-C4	2.32	124.91	118.18
2	A	501	DCS	C3-C4-C5	-2.32	116.63	118.73
2	B	502	DCS	C6-N1-C2	2.28	123.34	119.20
2	B	502	DCS	O3P-P-O2P	2.26	116.27	107.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	DCS	C3-C4-C4A-N
2	A	501	DCS	C5-C4-C4A-N
2	A	501	DCS	C5A-O4P-P-O2P
2	A	501	DCS	C5A-O4P-P-O3P
2	B	502	DCS	C3-C4-C4A-N
2	B	502	DCS	C5-C4-C4A-N

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Mol	Chain	Res	Type	Atoms
2	B	502	DCS	C5A-O4P-P-O1P
2	B	502	DCS	C5A-O4P-P-O2P
2	B	502	DCS	C5A-O4P-P-O3P
2	B	502	DCS	C4-C4A-N-CA
2	A	501	DCS	C4-C4A-N-CA
2	A	501	DCS	C5A-O4P-P-O1P

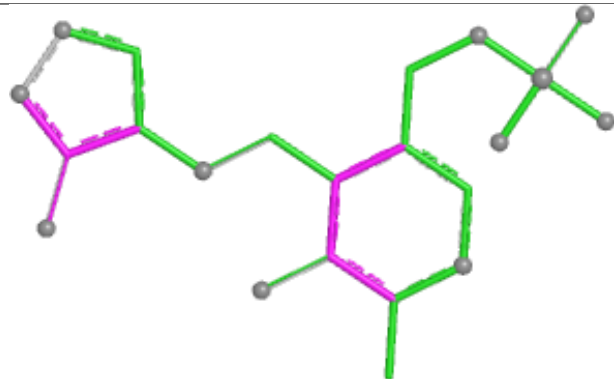
There are no ring outliers.

2 monomers are involved in 9 short contacts:

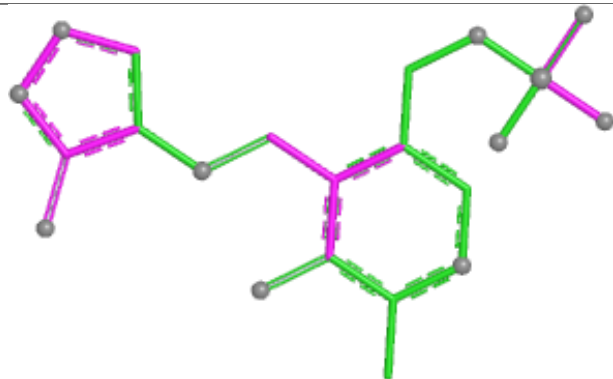
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	DCS	6	0
2	B	502	DCS	3	0

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.

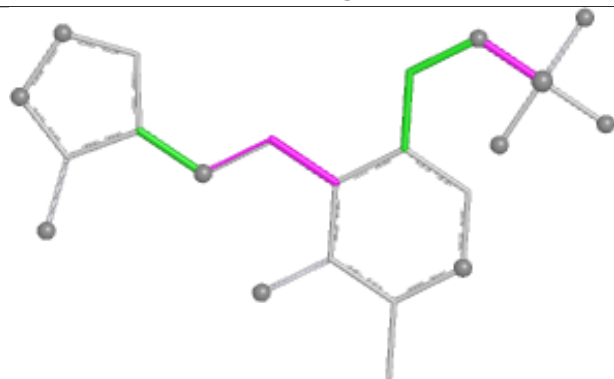
Ligand DCS A 501



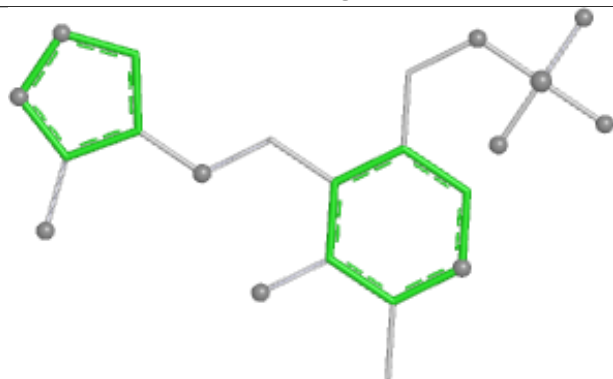
Bond lengths



Bond angles

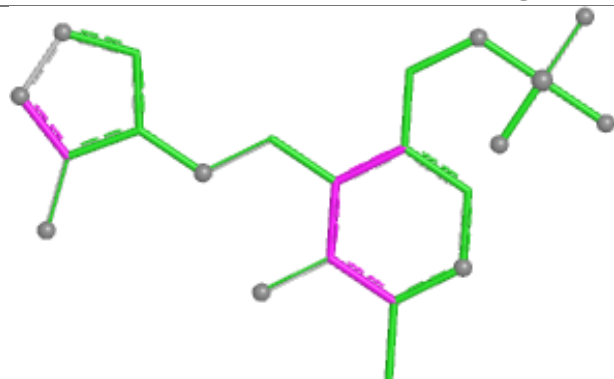


Torsions

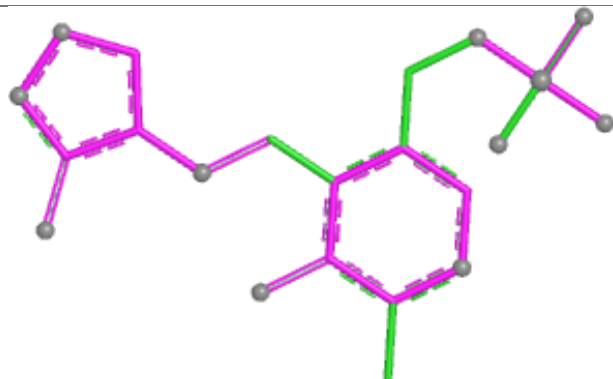


Rings

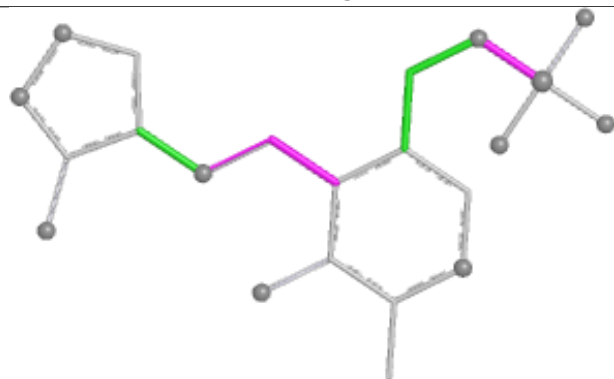
Ligand DCS B 502



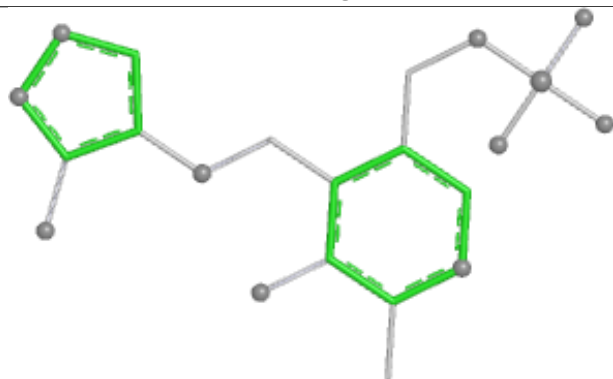
Bond lengths



Bond angles



Torsions



Rings

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	479/500 (95%)	0.04	14 (2%)	53	50	24, 39, 61, 76	1 (0%)
1	B	479/500 (95%)	0.07	14 (2%)	53	50	24, 39, 61, 76	0
All	All	958/1000 (95%)	0.06	28 (2%)	53	50	24, 40, 61, 76	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	ASP	9.8
1	A	355	GLU	4.9
1	A	288	ASP	4.4
1	B	287	GLU	3.6
1	A	352	ALA	3.5
1	B	303	GLY	3.4
1	B	284	TYR	3.4
1	B	285	GLY	3.1
1	A	305	CYS	3.0
1	A	392	GLU	2.9
1	A	375	ALA	2.7
1	B	319	ALA	2.6
1	B	51	CYS	2.5
1	B	468	ARG	2.4
1	A	74	CYS	2.4
1	A	197	THR	2.4
1	B	74	CYS	2.3
1	B	248	CYS	2.2
1	A	46	ASP	2.2
1	A	290	PRO	2.1
1	A	268	ASP	2.1
1	A	75	ASP	2.1
1	A	163	GLU	2.0
1	B	352	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	359	SER	2.0
1	B	289	LEU	2.0
1	A	303	GLY	2.0
1	B	3	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

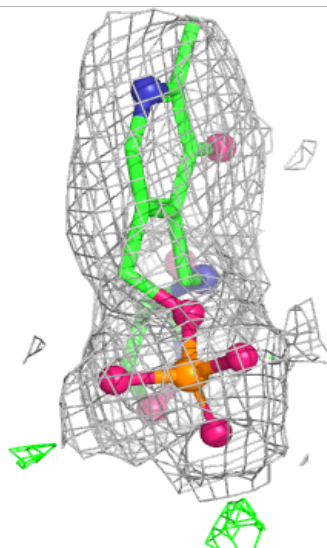
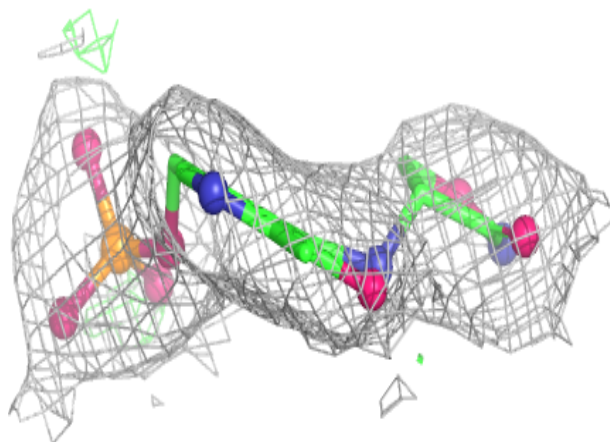
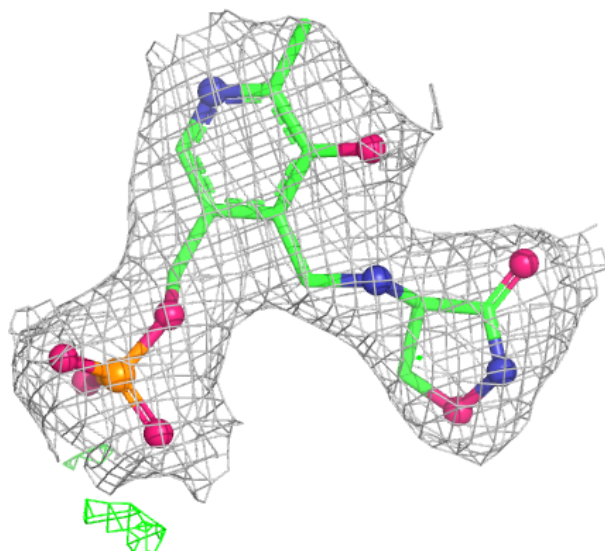
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DCS	A	501	22/22	0.97	0.06	27,32,38,39	0
2	DCS	B	502	22/22	0.97	0.07	26,33,42,44	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.

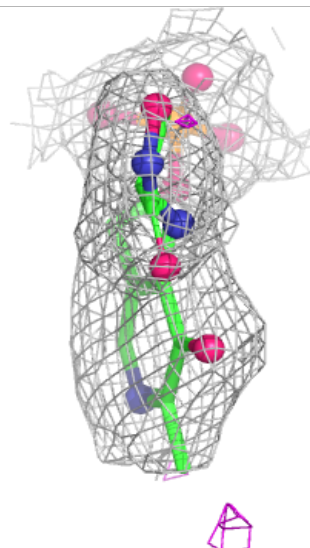
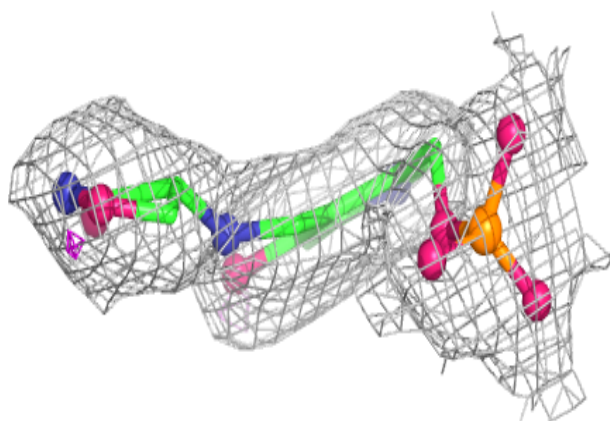
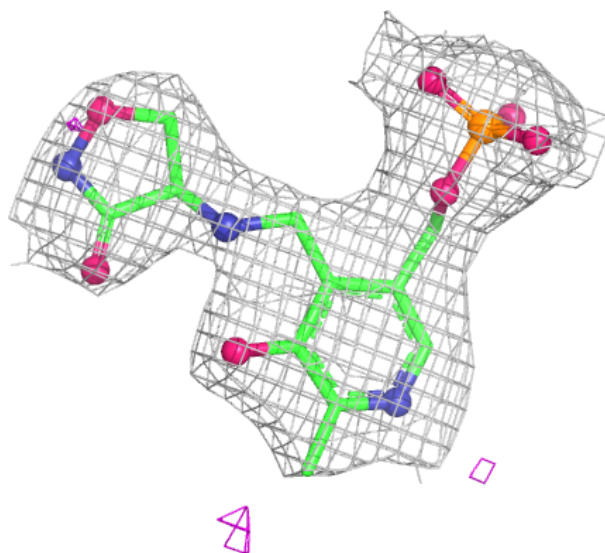
Electron density around DCS A 501:

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



Electron density around DCS B 502:

$2mF_o-DF_c$ (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.