



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:08 PM UTC

PDB ID : 3PRL / pdb_00003prl
Title : Crystal structure of NADP-dependent glyceraldehyde-3-phosphate dehydrogenase from *Bacillus halodurans* C-125
Authors : Malashkevich, V.N.; Toro, R.; Seidel, R.; Garrett, S.; Foti, R.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2010-11-29
Resolution : 2.00 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

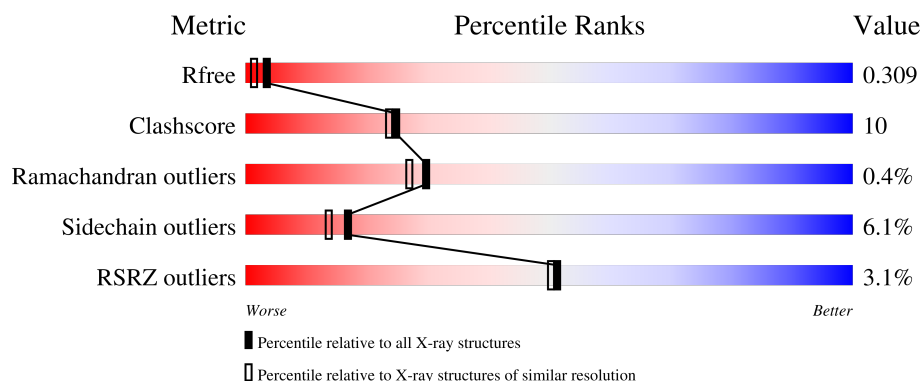
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

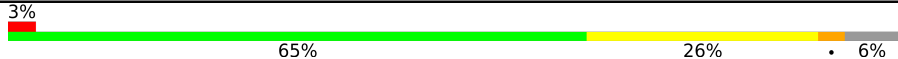
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	505	
1	B	505	
1	C	505	
1	D	505	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	506	-	-	-	X
2	SO4	B	506	-	-	-	X
2	SO4	C	506	-	-	-	X
2	SO4	C	507	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14939 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 NADP-dependent glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3573	2251	621	694	7			
1	B	476	Total	C	N	O	S	0	0	0
			3578	2254	622	695	7			
1	C	475	Total	C	N	O	S	0	1	0
			3579	2255	621	696	7			
1	D	480	Total	C	N	O	S	0	3	0
			3636	2294	628	707	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9KAQ0
A	2	VAL	-	expression tag	UNP Q9KAQ0
A	484	ALA	-	expression tag	UNP Q9KAQ0
A	485	GLU	-	expression tag	UNP Q9KAQ0
A	486	ASN	-	expression tag	UNP Q9KAQ0
A	487	LEU	-	expression tag	UNP Q9KAQ0
A	488	TYR	-	expression tag	UNP Q9KAQ0
A	489	PHE	-	expression tag	UNP Q9KAQ0
A	490	GLN	-	expression tag	UNP Q9KAQ0
A	491	SER	-	expression tag	UNP Q9KAQ0
A	492	HIS	-	expression tag	UNP Q9KAQ0
A	493	HIS	-	expression tag	UNP Q9KAQ0
A	494	HIS	-	expression tag	UNP Q9KAQ0
A	495	HIS	-	expression tag	UNP Q9KAQ0
A	496	HIS	-	expression tag	UNP Q9KAQ0
A	497	HIS	-	expression tag	UNP Q9KAQ0
A	498	TRP	-	expression tag	UNP Q9KAQ0
A	499	SER	-	expression tag	UNP Q9KAQ0
A	500	HIS	-	expression tag	UNP Q9KAQ0
A	501	PRO	-	expression tag	UNP Q9KAQ0
A	502	GLN	-	expression tag	UNP Q9KAQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	503	PHE	-	expression tag	UNP Q9KAQ0
A	504	GLU	-	expression tag	UNP Q9KAQ0
A	505	LYS	-	expression tag	UNP Q9KAQ0
B	1	MET	-	expression tag	UNP Q9KAQ0
B	2	VAL	-	expression tag	UNP Q9KAQ0
B	484	ALA	-	expression tag	UNP Q9KAQ0
B	485	GLU	-	expression tag	UNP Q9KAQ0
B	486	ASN	-	expression tag	UNP Q9KAQ0
B	487	LEU	-	expression tag	UNP Q9KAQ0
B	488	TYR	-	expression tag	UNP Q9KAQ0
B	489	PHE	-	expression tag	UNP Q9KAQ0
B	490	GLN	-	expression tag	UNP Q9KAQ0
B	491	SER	-	expression tag	UNP Q9KAQ0
B	492	HIS	-	expression tag	UNP Q9KAQ0
B	493	HIS	-	expression tag	UNP Q9KAQ0
B	494	HIS	-	expression tag	UNP Q9KAQ0
B	495	HIS	-	expression tag	UNP Q9KAQ0
B	496	HIS	-	expression tag	UNP Q9KAQ0
B	497	HIS	-	expression tag	UNP Q9KAQ0
B	498	TRP	-	expression tag	UNP Q9KAQ0
B	499	SER	-	expression tag	UNP Q9KAQ0
B	500	HIS	-	expression tag	UNP Q9KAQ0
B	501	PRO	-	expression tag	UNP Q9KAQ0
B	502	GLN	-	expression tag	UNP Q9KAQ0
B	503	PHE	-	expression tag	UNP Q9KAQ0
B	504	GLU	-	expression tag	UNP Q9KAQ0
B	505	LYS	-	expression tag	UNP Q9KAQ0
C	1	MET	-	expression tag	UNP Q9KAQ0
C	2	VAL	-	expression tag	UNP Q9KAQ0
C	484	ALA	-	expression tag	UNP Q9KAQ0
C	485	GLU	-	expression tag	UNP Q9KAQ0
C	486	ASN	-	expression tag	UNP Q9KAQ0
C	487	LEU	-	expression tag	UNP Q9KAQ0
C	488	TYR	-	expression tag	UNP Q9KAQ0
C	489	PHE	-	expression tag	UNP Q9KAQ0
C	490	GLN	-	expression tag	UNP Q9KAQ0
C	491	SER	-	expression tag	UNP Q9KAQ0
C	492	HIS	-	expression tag	UNP Q9KAQ0
C	493	HIS	-	expression tag	UNP Q9KAQ0
C	494	HIS	-	expression tag	UNP Q9KAQ0
C	495	HIS	-	expression tag	UNP Q9KAQ0
C	496	HIS	-	expression tag	UNP Q9KAQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	497	HIS	-	expression tag	UNP Q9KAQ0
C	498	TRP	-	expression tag	UNP Q9KAQ0
C	499	SER	-	expression tag	UNP Q9KAQ0
C	500	HIS	-	expression tag	UNP Q9KAQ0
C	501	PRO	-	expression tag	UNP Q9KAQ0
C	502	GLN	-	expression tag	UNP Q9KAQ0
C	503	PHE	-	expression tag	UNP Q9KAQ0
C	504	GLU	-	expression tag	UNP Q9KAQ0
C	505	LYS	-	expression tag	UNP Q9KAQ0
D	1	MET	-	expression tag	UNP Q9KAQ0
D	2	VAL	-	expression tag	UNP Q9KAQ0
D	484	ALA	-	expression tag	UNP Q9KAQ0
D	485	GLU	-	expression tag	UNP Q9KAQ0
D	486	ASN	-	expression tag	UNP Q9KAQ0
D	487	LEU	-	expression tag	UNP Q9KAQ0
D	488	TYR	-	expression tag	UNP Q9KAQ0
D	489	PHE	-	expression tag	UNP Q9KAQ0
D	490	GLN	-	expression tag	UNP Q9KAQ0
D	491	SER	-	expression tag	UNP Q9KAQ0
D	492	HIS	-	expression tag	UNP Q9KAQ0
D	493	HIS	-	expression tag	UNP Q9KAQ0
D	494	HIS	-	expression tag	UNP Q9KAQ0
D	495	HIS	-	expression tag	UNP Q9KAQ0
D	496	HIS	-	expression tag	UNP Q9KAQ0
D	497	HIS	-	expression tag	UNP Q9KAQ0
D	498	TRP	-	expression tag	UNP Q9KAQ0
D	499	SER	-	expression tag	UNP Q9KAQ0
D	500	HIS	-	expression tag	UNP Q9KAQ0
D	501	PRO	-	expression tag	UNP Q9KAQ0
D	502	GLN	-	expression tag	UNP Q9KAQ0
D	503	PHE	-	expression tag	UNP Q9KAQ0
D	504	GLU	-	expression tag	UNP Q9KAQ0
D	505	LYS	-	expression tag	UNP Q9KAQ0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

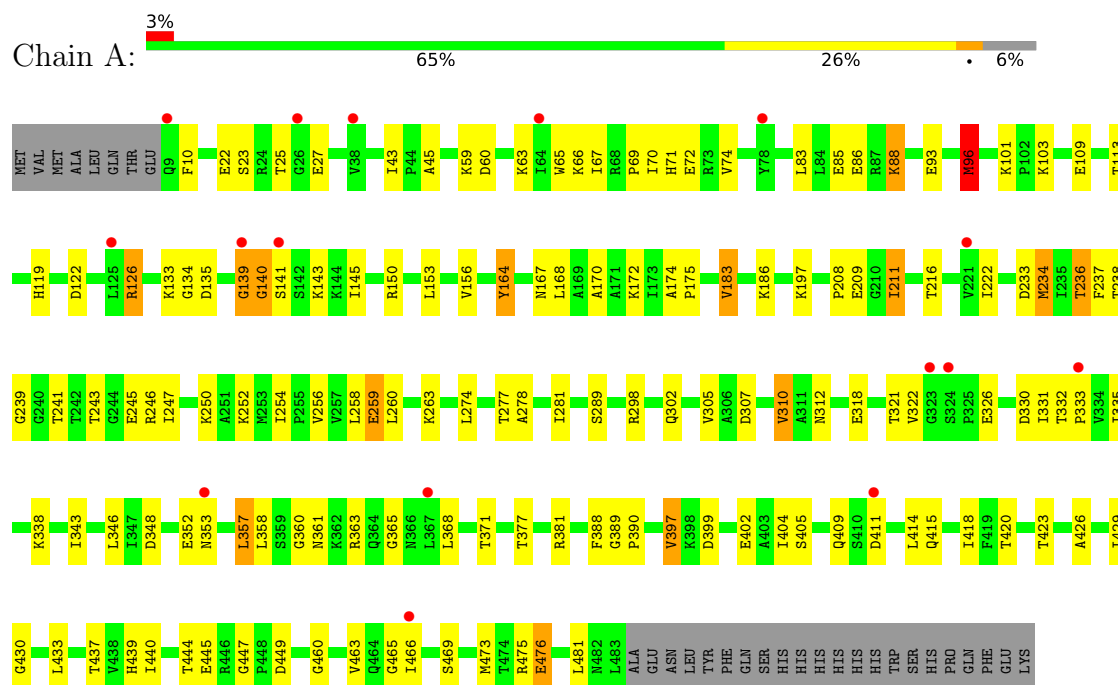
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	148	Total	O	0	0
			148	148		
3	B	184	Total	O	0	0
			184	184		
3	C	116	Total	O	0	0
			116	116		
3	D	105	Total	O	0	0
			105	105		

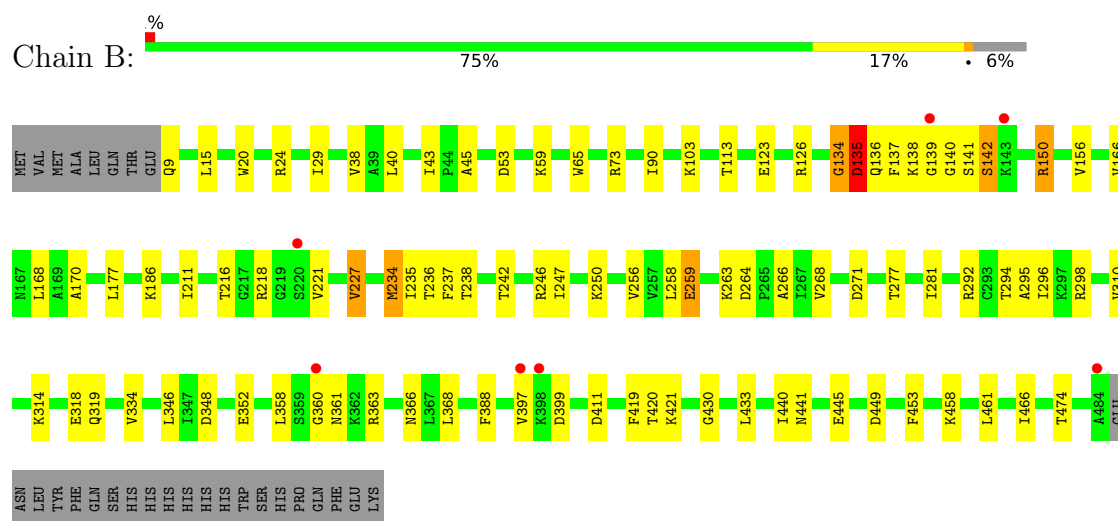
3 Residue-property plots [i](#)

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.

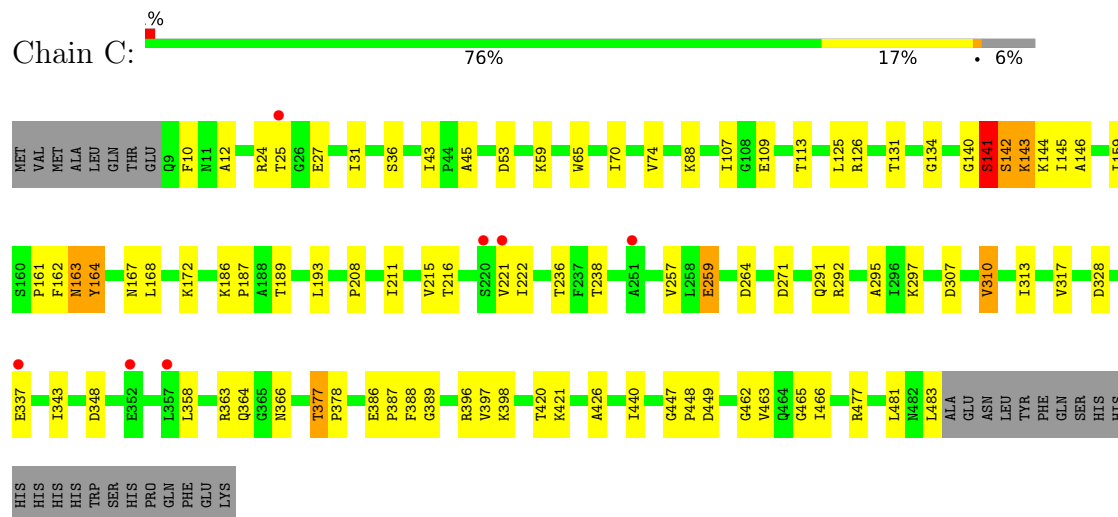
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



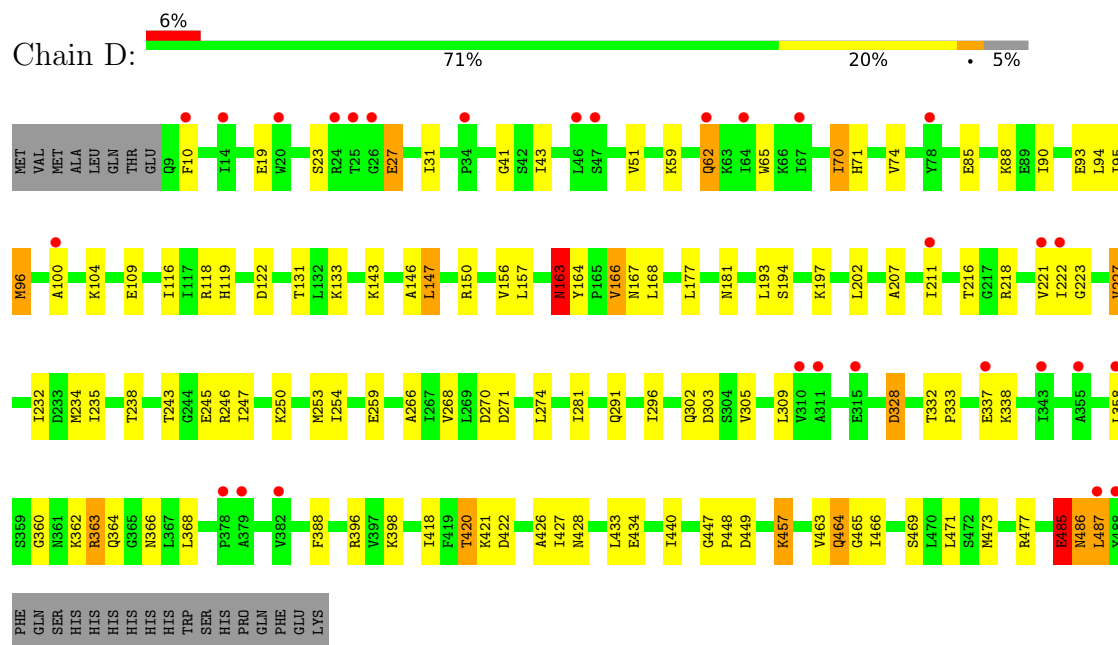
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



• Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



• Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.30Å 131.43Å 83.89Å 90.00° 102.95° 90.00°	Depositor
Resolution (Å)	19.98 – 2.00 19.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.98-2.00) 99.3 (19.98-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.248 , 0.306 0.251 , 0.309	Depositor DCC
R_{free} test set	6163 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14939	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.52% 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.70	0/3627	1.03	13/4919 (0.3%)
1	B	0.76	2/3632 (0.1%)	1.01	2/4926 (0.0%)
1	C	0.70	0/3636	1.01	8/4932 (0.2%)
1	D	0.68	0/3701	1.00	6/5020 (0.1%)
All	All	0.71	2/14596 (0.0%)	1.01	29/19797 (0.1%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	GLY	C-O	-6.32	1.17	1.23
1	B	135	ASP	C-O	-5.03	1.17	1.24

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	460	GLY	N-CA-C	7.87	122.53	110.88
1	C	164	TYR	CA-C-N	7.74	127.45	119.56
1	C	164	TYR	C-N-CA	7.74	127.45	119.56
1	D	486	ASN	N-CA-C	7.66	127.11	110.80
1	C	141	SER	N-CA-C	7.50	126.78	110.80
1	D	485	GLU	N-CA-C	7.34	122.51	112.90
1	A	335	ILE	N-CA-C	7.04	117.75	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ILE	N-CA-C	6.99	114.92	109.19
1	B	136	GLN	N-CA-C	-6.90	104.97	113.19
1	D	166	VAL	N-CA-C	-6.87	105.65	111.56
1	D	465	GLY	N-CA-C	-6.78	102.78	112.81
1	A	183	VAL	N-CA-C	6.30	117.19	108.12
1	A	465	GLY	N-CA-C	-6.01	105.56	112.29
1	A	222	ILE	N-CA-C	5.79	119.20	113.53
1	C	162	PHE	CA-C-N	5.69	130.23	121.19
1	C	162	PHE	C-N-CA	5.69	130.23	121.19
1	C	465	GLY	N-CA-C	-5.65	105.96	112.29
1	A	164	TYR	CA-C-N	5.55	125.16	119.56
1	A	164	TYR	C-N-CA	5.55	125.16	119.56
1	A	103	LYS	N-CA-C	5.51	118.00	111.33
1	A	139	GLY	N-CA-C	-5.44	104.82	111.35
1	D	362	LYS	N-CA-C	5.39	117.89	110.35
1	A	96	MET	N-CA-CB	5.36	117.99	110.12
1	D	457	LYS	CB-CA-C	-5.31	110.47	116.63
1	C	377	THR	CA-C-N	5.14	124.93	119.28
1	C	377	THR	C-N-CA	5.14	124.93	119.28
1	A	377	THR	CA-C-N	5.04	126.14	119.84
1	A	377	THR	C-N-CA	5.04	126.14	119.84
1	B	103	LYS	N-CA-C	5.01	117.12	111.11

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	135	ASP	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	3573	0	3656	96	0
1	B	3578	0	3661	65	0
1	C	3579	0	3662	60	0
1	D	3636	0	3716	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
3	A	148	0	0	4	0
3	B	184	0	0	8	0
3	C	116	0	0	6	0
3	D	105	0	0	7	0
All	All	14939	0	14695	285	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 10.

All (285) 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:227:VAL:HG21	1:B:247:ILE:HD12	1.40	1.01
1:A:156:VAL:HG13	1:A:234:MET:CE	1.90	1.01
1:A:156:VAL:HG13	1:A:234:MET:HE1	1.41	0.98
1:B:156:VAL:HG13	1:B:234:MET:CE	1.93	0.98
1:B:156:VAL:HG13	1:B:234:MET:HE1	1.49	0.94
1:D:164:TYR:HB2	1:D:168:LEU:HG	1.50	0.92
1:C:74:VAL:HG21	1:C:125:LEU:HD13	1.55	0.89
1:B:363:ARG:HG2	1:B:368:LEU:HG	1.53	0.89
1:B:271:ASP:O	1:B:421:LYS:HG2	1.74	0.88
1:B:266:ALA:HB2	1:B:296:ILE:HD12	1.59	0.83
1:D:268:VAL:HG12	3:D:533:HOH:O	1.78	0.83
1:B:134:GLY:O	1:B:135:ASP:HB3	1.77	0.83
1:D:177:LEU:HD22	1:D:211:ILE:HG22	1.61	0.82
1:A:426:ALA:HB1	1:A:440:ILE:HD12	1.62	0.81
1:D:227:VAL:HG21	1:D:247:ILE:HG12	1.62	0.81
1:A:96:MET:HE1	1:A:326:GLU:HG3	1.62	0.81
1:D:271:ASP:O	1:D:421:LYS:HG2	1.83	0.79
1:C:348:ASP:HB2	3:C:518:HOH:O	1.81	0.78
1:A:96:MET:HB3	1:A:101:LYS:O	1.82	0.78
1:D:157:LEU:HD23	1:D:235:ILE:HD12	1.66	0.78
1:D:486:ASN:O	1:D:487:LEU:HB2	1.83	0.77
1:B:156:VAL:HG13	1:B:234:MET:HE2	1.69	0.75
1:B:134:GLY:O	1:B:135:ASP:CB	2.33	0.75
1:A:25:THR:CG2	1:A:27:GLU:HG2	2.16	0.74
1:D:90:ILE:O	1:D:93:GLU:HG3	1.87	0.74
1:B:65:TRP:CZ2	1:B:73:ARG:HG2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:THR:HG23	1:C:259:GLU:OE2	1.86	0.74
1:A:256:VAL:HG11	3:A:528:HOH:O	1.88	0.74
1:A:25:THR:HG23	1:A:27:GLU:H	1.53	0.73
1:D:232:ILE:HG21	1:D:235:ILE:HD11	1.71	0.72
1:A:25:THR:HG23	1:A:27:GLU:HG2	1.71	0.72
1:D:104:LYS:HG3	1:D:328:ASP:OD2	1.90	0.72
1:A:234:MET:C	1:A:234:MET:HE3	2.15	0.71
1:A:430:GLY:O	1:D:477:ARG:NH2	2.23	0.71
1:D:486:ASN:O	1:D:487:LEU:CB	2.39	0.71
1:C:27:GLU:HG3	1:C:45:ALA:HB3	1.73	0.70
1:B:135:ASP:HA	1:B:137:PHE:O	1.92	0.69
1:A:156:VAL:HG13	1:A:234:MET:HE2	1.73	0.69
1:D:418:ILE:HD11	1:D:433:LEU:HD11	1.74	0.69
1:A:43:ILE:HD12	1:A:216:THR:HB	1.74	0.68
1:A:175:PRO:HG2	1:A:473:MET:HE3	1.74	0.68
1:B:238:THR:HG23	1:B:259:GLU:HG3	1.75	0.67
1:A:415:GLN:HG2	1:A:437:THR:HB	1.78	0.66
1:A:85:GLU:O	1:A:88:LYS:HG3	1.96	0.66
1:A:208:PRO:HB2	1:A:211:ILE:HG12	1.77	0.66
1:B:142:SER:N	3:B:604:HOH:O	2.23	0.66
1:D:332:THR:HB	1:D:333:PRO:CD	2.25	0.66
1:D:469:SER:O	1:D:473:MET:HG2	1.96	0.65
1:A:343:ILE:HD13	1:A:389:GLY:HA3	1.79	0.64
1:A:469:SER:O	1:A:473:MET:HG2	1.97	0.64
1:A:139:GLY:O	1:A:141:SER:N	2.31	0.63
1:B:314:LYS:O	1:B:318:GLU:HG3	1.98	0.63
1:C:43:ILE:HD12	1:C:216:THR:HB	1.80	0.63
1:A:245:GLU:OE1	1:D:253:MET:HG3	1.98	0.63
1:A:134:GLY:O	1:A:140:GLY:HA3	1.98	0.63
1:A:357:LEU:HD11	1:A:361:ASN:HB2	1.81	0.63
1:B:238:THR:HG23	1:B:259:GLU:CG	2.28	0.63
1:A:133:LYS:HD2	1:A:145:ILE:HG22	1.81	0.63
1:D:157:LEU:HB3	1:D:235:ILE:HD13	1.80	0.62
1:C:126:ARG:NH2	1:D:122:ASP:HB2	2.14	0.62
1:C:25:THR:HG23	1:C:27:GLU:H	1.65	0.62
1:A:357:LEU:CD1	1:A:361:ASN:HB2	2.29	0.62
1:C:271:ASP:O	1:C:421:LYS:HG2	1.99	0.62
1:C:88:LYS:HG2	1:C:107:ILE:HG23	1.80	0.61
1:B:411:ASP:HB3	1:B:458:LYS:HG3	1.82	0.61
1:B:24:ARG:NH2	1:B:53:ASP:OD2	2.21	0.61
1:D:202:LEU:CD2	1:D:207:ALA:HB2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:ALA:HB1	1:C:440:ILE:HD12	1.83	0.60
1:B:271:ASP:O	1:B:421:LYS:CG	2.47	0.60
1:D:164:TYR:CB	1:D:168:LEU:HG	2.29	0.60
1:D:62:GLN:HE22	1:D:181:ASN:HA	1.67	0.60
1:D:164:TYR:HB2	1:D:168:LEU:CG	2.30	0.60
1:D:232:ILE:HG21	1:D:235:ILE:CD1	2.31	0.59
1:D:485:GLU:O	1:D:486:ASN:CG	2.45	0.59
1:C:291:GLN:O	1:C:292:ARG:HG3	2.02	0.59
1:B:430:GLY:O	1:C:477:ARG:NH2	2.35	0.59
1:A:65:TRP:HB2	1:A:211:ILE:HD11	1.85	0.58
1:A:426:ALA:CB	1:A:440:ILE:HD12	2.31	0.58
1:A:238:THR:HG23	1:A:259:GLU:HG3	1.84	0.58
1:D:131:THR:HG22	1:D:147:LEU:HD12	1.85	0.58
1:C:271:ASP:O	1:C:421:LYS:CG	2.52	0.58
1:C:141:SER:O	1:C:142:SER:CB	2.51	0.57
1:D:246:ARG:O	1:D:250:LYS:HG3	2.04	0.57
1:A:259:GLU:HG3	1:A:259:GLU:O	2.03	0.57
1:A:289:SER:HB3	1:A:390:PRO:HG3	1.86	0.57
1:C:24:ARG:NH2	1:C:53:ASP:OD2	2.36	0.57
1:A:25:THR:HG21	1:A:27:GLU:HG2	1.86	0.57
1:D:332:THR:HB	1:D:333:PRO:HD2	1.86	0.56
1:B:113:THR:HG23	1:B:170:ALA:HB3	1.86	0.56
1:D:485:GLU:HG2	3:D:633:HOH:O	2.03	0.56
1:A:274:LEU:HD11	1:A:305:VAL:HB	1.87	0.56
1:A:343:ILE:CD1	1:A:389:GLY:HA3	2.36	0.56
1:C:337:GLU:HA	1:C:366:ASN:HD21	1.71	0.56
1:D:305:VAL:HG21	3:D:533:HOH:O	2.06	0.55
1:B:259:GLU:HG3	1:B:259:GLU:O	2.07	0.55
1:B:419:PHE:HA	1:B:441:ASN:OD1	2.07	0.55
1:A:119:HIS:HD2	1:A:466:ILE:HG21	1.73	0.54
1:D:51:VAL:HG21	1:D:222:ILE:HG22	1.90	0.54
1:B:43:ILE:HD12	1:B:216:THR:HB	1.88	0.53
1:B:348:ASP:O	1:B:352:GLU:HB2	2.08	0.53
1:B:334:VAL:HG22	1:B:366:ASN:O	2.07	0.53
1:A:310:VAL:HG13	1:A:358:LEU:CD1	2.38	0.53
1:D:363:ARG:HB2	1:D:368:LEU:HG	1.90	0.53
1:C:10:PHE:CE1	1:C:12:ALA:HB2	2.43	0.53
1:A:246:ARG:HG3	3:A:619:HOH:O	2.08	0.53
1:C:59:LYS:NZ	3:C:629:HOH:O	2.42	0.53
1:A:69:PRO:HG2	1:A:72:GLU:HG3	1.91	0.53
1:C:186:LYS:NZ	1:C:187:PRO:O	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:GLU:HG3	1:D:167:ASN:HB2	1.90	0.52
1:D:163:ASN:ND2	1:D:291:GLN:O	2.42	0.52
1:B:168:LEU:HD13	1:B:238:THR:HG21	1.90	0.52
1:A:397:VAL:HG13	1:A:402:GLU:HB3	1.91	0.52
1:C:396:ARG:HD3	3:C:520:HOH:O	2.10	0.52
1:D:157:LEU:HB3	1:D:235:ILE:CD1	2.39	0.52
1:C:313:ILE:O	1:C:317:VAL:HG23	2.09	0.52
1:C:257:VAL:HG22	1:C:462:GLY:HA3	1.91	0.52
1:D:157:LEU:CD2	1:D:235:ILE:HD12	2.39	0.51
1:B:186:LYS:HD2	3:B:512:HOH:O	2.11	0.51
1:D:43:ILE:HD12	1:D:216:THR:HB	1.92	0.51
1:B:440:ILE:HG13	1:C:481:LEU:HD23	1.91	0.51
1:A:241:THR:O	1:A:245:GLU:HG2	2.09	0.51
1:A:243:THR:O	1:A:247:ILE:HG12	2.10	0.51
1:A:246:ARG:O	1:A:250:LYS:HG3	2.11	0.51
1:C:186:LYS:HB2	1:C:215:VAL:HG23	1.92	0.51
1:A:122:ASP:HB2	1:B:126:ARG:NH2	2.26	0.51
1:D:65:TRP:HB2	1:D:211:ILE:CD1	2.41	0.51
1:B:294:THR:HG21	1:B:453:PHE:CE1	2.45	0.50
1:C:164:TYR:HB3	1:C:167:ASN:HB3	1.94	0.50
1:A:263:LYS:HG3	1:A:298:ARG:HG3	1.94	0.50
1:B:399:ASP:HB2	3:B:550:HOH:O	2.12	0.50
1:D:94:LEU:HD23	1:D:194:SER:HA	1.92	0.50
1:D:303:ASP:OD2	1:D:398:LYS:HA	2.12	0.50
1:A:172:LYS:HE3	1:A:236:THR:HG22	1.92	0.50
1:D:202:LEU:HD23	1:D:207:ALA:HB2	1.93	0.50
1:D:10:PHE:CZ	1:D:197:LYS:HE2	2.46	0.49
1:B:15:LEU:HD13	1:B:20:TRP:CE2	2.47	0.49
1:A:153:LEU:O	3:A:618:HOH:O	2.20	0.49
1:C:43:ILE:HD11	1:C:189:THR:HG23	1.95	0.49
1:D:197:LYS:HE3	3:D:537:HOH:O	2.13	0.49
1:A:277:THR:O	1:A:281:ILE:HG12	2.13	0.48
1:B:135:ASP:C	1:B:137:PHE:H	2.22	0.48
1:A:332:THR:HB	1:A:333:PRO:CD	2.43	0.48
1:D:418:ILE:HD11	1:D:433:LEU:CD1	2.43	0.48
1:A:302:GLN:HE21	1:A:399:ASP:HA	1.79	0.48
1:A:83:LEU:O	1:A:86:GLU:HG2	2.14	0.48
1:C:131:THR:HA	1:C:146:ALA:O	2.14	0.48
1:A:96:MET:CB	1:A:101:LYS:O	2.58	0.48
1:B:449:ASP:O	1:B:466:ILE:HG12	2.14	0.48
1:C:159:ILE:O	1:C:172:LYS:HE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ILE:HD11	3:D:585:HOH:O	2.13	0.47
1:A:71:HIS:O	1:A:74:VAL:HG22	2.14	0.47
1:A:418:ILE:HD11	1:A:433:LEU:HD11	1.95	0.47
1:D:150:ARG:HG3	3:D:577:HOH:O	2.14	0.47
1:A:174:ALA:N	1:A:175:PRO:HD2	2.29	0.47
1:B:135:ASP:O	1:D:70:ILE:HG23	2.13	0.47
1:D:281:ILE:HD12	1:D:296:ILE:HG21	1.96	0.47
1:C:386:GLU:HA	1:C:387:PRO:HD3	1.74	0.47
1:D:10:PHE:O	1:D:41:GLY:HA3	2.14	0.47
1:D:177:LEU:HD22	1:D:211:ILE:CG2	2.39	0.47
1:D:266:ALA:HB1	1:D:281:ILE:HD11	1.97	0.47
1:A:23:SER:OG	1:A:25:THR:HG22	2.13	0.47
1:C:113:THR:OG1	1:C:167:ASN:HA	2.15	0.47
1:C:31:ILE:HD12	1:C:193:LEU:HG	1.97	0.47
1:A:321:THR:N	1:A:330:ASP:OD2	2.40	0.47
1:A:60:ASP:HA	1:A:63:LYS:HE2	1.96	0.47
1:A:234:MET:HE3	1:A:234:MET:O	2.13	0.47
1:D:333:PRO:HB3	1:D:366:ASN:HB3	1.96	0.47
1:B:135:ASP:HB2	1:B:140:GLY:O	2.15	0.46
1:D:464[A]:GLN:CD	1:D:469:SER:OG	2.57	0.46
1:A:238:THR:HG23	1:A:259:GLU:CG	2.45	0.46
1:A:126:ARG:HD2	1:B:126:ARG:CD	2.46	0.46
1:C:109:GLU:HG3	1:C:167:ASN:HB2	1.97	0.46
1:D:27:GLU:H	1:D:27:GLU:HG2	1.63	0.46
1:A:332:THR:HB	1:A:333:PRO:HD2	1.97	0.46
1:A:439:HIS:CD2	1:A:444:THR:HA	2.50	0.46
1:D:449:ASP:O	1:D:466:ILE:HG12	2.16	0.46
1:B:264:ASP:HB2	1:B:295:ALA:O	2.15	0.46
1:C:164:TYR:HB2	1:C:168:LEU:HG	1.96	0.46
1:D:238:THR:OG1	1:D:259[A]:GLU:OE2	2.30	0.46
1:B:234:MET:HE3	1:B:235:ILE:CA	2.46	0.46
1:A:69:PRO:HD2	1:A:72:GLU:OE1	2.15	0.46
1:A:418:ILE:HD11	1:A:433:LEU:CD1	2.46	0.46
1:B:292:ARG:HD3	3:B:576:HOH:O	2.15	0.46
1:B:263:LYS:HE3	1:B:298:ARG:HG3	1.97	0.45
1:A:363:ARG:NE	1:A:365:GLY:O	2.49	0.45
1:D:235:ILE:HG12	1:D:254:ILE:HD11	1.98	0.45
1:D:131:THR:HA	1:D:146:ALA:O	2.17	0.45
1:A:27:GLU:HG3	1:A:45:ALA:HB3	1.97	0.45
1:B:256:VAL:HG11	3:B:607:HOH:O	2.15	0.45
1:B:314:LYS:HE2	1:B:358:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:THR:HG22	1:D:422:ASP:H	1.82	0.45
1:B:135:ASP:HB2	1:D:71:HIS:HD2	1.82	0.45
1:B:141:SER:O	1:B:142:SER:CB	2.65	0.45
1:B:256:VAL:HG13	1:B:461:LEU:HD23	1.98	0.45
1:C:343:ILE:CD1	1:C:389:GLY:HA3	2.46	0.45
1:D:426:ALA:HB1	1:D:440:ILE:HD12	1.99	0.44
1:B:246:ARG:HG3	1:B:250:LYS:HE2	1.98	0.44
1:C:65:TRP:HB2	1:C:211:ILE:HD11	1.99	0.44
1:C:363:ARG:NH2	3:C:535:HOH:O	2.51	0.44
1:B:135:ASP:C	1:B:137:PHE:N	2.72	0.44
1:B:445:GLU:OE2	1:C:144:LYS:NZ	2.49	0.44
1:A:113:THR:HG23	1:A:170:ALA:HB3	2.00	0.44
1:A:164:TYR:HB2	1:A:168:LEU:HG	1.99	0.44
1:A:475:ARG:HD2	1:A:476:GLU:O	2.17	0.44
1:C:297:LYS:NZ	1:C:386:GLU:OE2	2.48	0.44
1:A:135:ASP:O	1:C:70:ILE:HG23	2.18	0.44
1:B:268:VAL:CG1	1:B:277:THR:HG21	2.48	0.44
1:A:168:LEU:HD13	1:A:238:THR:HG21	1.99	0.44
1:C:238:THR:HG23	1:C:259:GLU:CD	2.43	0.44
1:C:420:THR:CG2	1:C:426:ALA:HB2	2.48	0.44
1:D:119:HIS:NE2	3:D:553:HOH:O	2.36	0.44
1:A:22:GLU:HG2	1:A:23:SER:H	1.82	0.43
1:A:346:LEU:HD12	1:A:381:ARG:NH2	2.33	0.43
1:B:150:ARG:HD3	1:B:474:THR:OG1	2.18	0.43
1:C:141:SER:O	1:C:142:SER:OG	2.30	0.43
1:D:164:TYR:HB3	1:D:167:ASN:HB3	2.01	0.43
1:D:168:LEU:HD13	1:D:238:THR:HG21	2.01	0.43
1:A:331:ILE:HD12	1:A:390:PRO:HB3	2.00	0.43
1:B:141:SER:O	1:B:142:SER:HB2	2.19	0.43
1:B:236:THR:HG21	3:B:602:HOH:O	2.18	0.43
1:C:134:GLY:HA3	3:C:534:HOH:O	2.19	0.43
1:B:218:ARG:HB2	1:B:221:VAL:HG23	2.00	0.43
1:C:221:VAL:HG12	1:C:222:ILE:HG23	2.00	0.43
1:D:116:ILE:HG23	1:D:466:ILE:HD11	2.00	0.43
1:D:270:ASP:HB2	1:D:302:GLN:NE2	2.33	0.43
1:A:109:GLU:HG3	1:A:167:ASN:HB2	2.01	0.43
1:B:9:GLN:HB2	1:B:40:LEU:O	2.18	0.43
1:D:270:ASP:OD1	1:D:270:ASP:C	2.61	0.43
1:A:405:SER:O	1:A:409:GLN:HG3	2.19	0.42
1:C:449:ASP:O	1:C:466:ILE:HG12	2.19	0.42
1:C:208:PRO:HB2	1:C:211:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:THR:HB	1:C:378:PRO:CD	2.49	0.42
1:D:96:MET:O	1:D:100:ALA:HA	2.19	0.42
1:D:157:LEU:HB2	1:D:232:ILE:HD12	2.01	0.42
1:D:243:THR:HA	1:D:246:ARG:HH11	1.83	0.42
1:D:274:LEU:HD22	1:D:309:LEU:HB2	1.99	0.42
1:A:63:LYS:HA	1:A:66:LYS:HE2	2.02	0.42
1:A:245:GLU:OE2	1:D:253:MET:SD	2.77	0.42
1:A:481:LEU:HD21	1:D:427:ILE:HD11	2.01	0.42
1:A:445:GLU:HG3	1:A:447:GLY:O	2.18	0.42
1:A:239:GLY:O	1:A:260:LEU:HA	2.20	0.42
1:D:65:TRP:HB2	1:D:211:ILE:HD11	2.02	0.42
1:A:70:ILE:HG22	3:C:611:HOH:O	2.20	0.42
1:B:138:LYS:HA	1:B:139:GLY:HA2	1.89	0.42
1:C:131:THR:HB	1:C:145:ILE:HD11	2.02	0.42
1:D:202:LEU:HD22	1:D:207:ALA:HB2	2.00	0.42
1:B:113:THR:HG21	1:B:166:VAL:HG12	2.02	0.42
1:A:449:ASP:O	1:A:466:ILE:HG12	2.20	0.42
1:B:237:PHE:HB3	1:B:258:LEU:HD23	2.01	0.42
1:B:433:LEU:O	1:C:477:ARG:NH2	2.52	0.42
1:C:447:GLY:HA2	1:C:448:PRO:C	2.44	0.42
1:A:10:PHE:CZ	1:A:197:LYS:HE2	2.55	0.41
1:A:404:ILE:HD11	1:A:429:ILE:HG23	2.02	0.41
1:C:143:LYS:O	1:C:483:LEU:N	2.45	0.41
1:D:447:GLY:HA2	1:D:448:PRO:C	2.45	0.41
1:C:377:THR:HB	1:C:378:PRO:HD2	2.02	0.41
1:A:145:ILE:O	1:A:145:ILE:HG13	2.19	0.41
1:A:241:THR:HA	1:A:260:LEU:HB3	2.03	0.41
1:B:186:LYS:NZ	3:B:669:HOH:O	2.20	0.41
1:C:310:VAL:HG13	1:C:358:LEU:CD1	2.50	0.41
1:D:31:ILE:HD12	1:D:193:LEU:HG	2.03	0.41
1:C:264:ASP:HB2	1:C:295:ALA:O	2.21	0.41
1:A:156:VAL:HB	1:A:183:VAL:HG22	2.02	0.41
1:B:29:ILE:HG13	1:B:45:ALA:HB2	2.03	0.41
1:C:161:PRO:HG3	1:C:238:THR:CG2	2.51	0.41
1:C:291:GLN:C	1:C:292:ARG:HG3	2.45	0.41
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.97	0.41
1:A:278:ALA:CB	1:A:312:ASN:HB3	2.50	0.41
1:B:177:LEU:HD22	1:B:211:ILE:HD12	2.03	0.41
1:C:134:GLY:O	1:C:140:GLY:HA3	2.20	0.41
1:A:234:MET:HE2	1:A:234:MET:HB3	1.91	0.41
1:A:360:GLY:O	1:A:371:THR:OG1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ARG:NH2	3:B:561:HOH:O	2.42	0.41
1:D:95:ILE:HD11	1:D:166:VAL:HG21	2.02	0.41
1:A:237:PHE:HB3	1:A:258:LEU:HD23	2.03	0.40
1:C:88:LYS:HB3	1:C:88:LYS:HE2	1.88	0.40
1:C:163:ASN:HD22	1:C:163:ASN:HA	1.67	0.40
1:A:126:ARG:HD3	1:B:123:GLU:OE2	2.21	0.40
1:A:357:LEU:HD13	1:A:361:ASN:HB2	2.02	0.40
1:B:363:ARG:CG	1:B:368:LEU:HG	2.37	0.40
1:C:271:ASP:O	1:C:421:LYS:HG3	2.21	0.40
1:D:85:GLU:OE2	1:D:118:ARG:NH2	2.53	0.40
1:D:434:GLU:OE1	1:D:457:LYS:HE2	2.21	0.40
1:A:233:ASP:OD1	3:A:530:HOH:O	2.22	0.40
1:D:156:VAL:HG22	1:D:234:MET:HB3	2.04	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	473/505 (94%)	452 (96%)	20 (4%)	1 (0%)	43	42
1	B	474/505 (94%)	451 (95%)	22 (5%)	1 (0%)	43	42
1	C	474/505 (94%)	454 (96%)	18 (4%)	2 (0%)	30	27
1	D	481/505 (95%)	451 (94%)	27 (6%)	3 (1%)	21	17
All	All	1902/2020 (94%)	1808 (95%)	87 (5%)	7 (0%)	30	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	GLY
1	C	141	SER

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Mol	Chain	Res	Type
1	B	360	GLY
1	C	142	SER
1	D	163	ASN
1	D	360	GLY
1	D	223	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/414 (93%)	354 (92%)	32 (8%)	10	7
1	B	386/414 (93%)	368 (95%)	18 (5%)	23	22
1	C	387/414 (94%)	374 (97%)	13 (3%)	32	33
1	D	393/414 (95%)	360 (92%)	33 (8%)	10	7
All	All	1552/1656 (94%)	1456 (94%)	96 (6%)	17	13

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	88	LYS
1	A	93	GLU
1	A	96	MET
1	A	126	ARG
1	A	143	LYS
1	A	150	ARG
1	A	186	LYS
1	A	209	GLU
1	A	211	ILE
1	A	234	MET
1	A	236	THR
1	A	252	LYS
1	A	259	GLU
1	A	307	ASP
1	A	310	VAL

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Mol	Chain	Res	Type
1	A	318	GLU
1	A	322	VAL
1	A	338	LYS
1	A	348	ASP
1	A	352	GLU
1	A	353	ASN
1	A	357	LEU
1	A	368	LEU
1	A	388	PHE
1	A	397	VAL
1	A	411	ASP
1	A	414	LEU
1	A	420	THR
1	A	423	THR
1	A	463	VAL
1	A	476	GLU
1	B	38	VAL
1	B	59	LYS
1	B	90	ILE
1	B	135	ASP
1	B	142	SER
1	B	150	ARG
1	B	227	VAL
1	B	234	MET
1	B	242	THR
1	B	259	GLU
1	B	281	ILE
1	B	310	VAL
1	B	319	GLN
1	B	346	LEU
1	B	361	ASN
1	B	388	PHE
1	B	397	VAL
1	B	420	THR
1	C	36	SER
1	C	143	LYS
1	C	163	ASN
1	C	236	THR
1	C	259	GLU
1	C	307	ASP
1	C	310	VAL
1	C	328	ASP

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Mol	Chain	Res	Type
1	C	364	GLN
1	C	388	PHE
1	C	397	VAL
1	C	398	LYS
1	C	463	VAL
1	D	19	GLU
1	D	23	SER
1	D	27	GLU
1	D	59	LYS
1	D	62	GLN
1	D	70	ILE
1	D	74	VAL
1	D	88	LYS
1	D	96	MET
1	D	133	LYS
1	D	143	LYS
1	D	147	LEU
1	D	163	ASN
1	D	218	ARG
1	D	221	VAL
1	D	227	VAL
1	D	245	GLU
1	D	328	ASP
1	D	337	GLU
1	D	338	LYS
1	D	358	LEU
1	D	363	ARG
1	D	364	GLN
1	D	388	PHE
1	D	396	ARG
1	D	420	THR
1	D	428	ASN
1	D	463	VAL
1	D	464[A]	GLN
1	D	464[B]	GLN
1	D	471	LEU
1	D	485	GLU
1	D	487	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	119	HIS
1	A	302	GLN
1	A	344	GLN
1	A	361	ASN
1	A	401	ASN
1	B	11	ASN
1	B	366	ASN
1	B	409	GLN
1	B	428	ASN
1	B	464	GLN
1	C	9	GLN
1	C	97	HIS
1	C	163	ASN
1	C	319	GLN
1	C	364	GLN
1	C	366	ASN
1	D	62	GLN
1	D	97	HIS
1	D	163	ASN
1	D	302	GLN
1	D	344	GLN
1	D	353	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 [i](#)

4 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	SO4	C	507	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	C	506	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	506	-	4,4,4	0.22	0	6,6,6	0.09	0
2	SO4	B	506	-	4,4,4	0.22	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	475/505 (94%)	0.46	16 (3%) 48 47	15, 26, 40, 52	0
1	B	476/505 (94%)	0.27	7 (1%) 72 71	13, 23, 36, 44	0
1	C	475/505 (94%)	0.41	7 (1%) 72 71	15, 27, 40, 47	1 (0%)
1	D	480/505 (95%)	0.79	29 (6%) 27 26	16, 32, 48, 59	3 (0%)
All	All	1906/2020 (94%)	0.48	59 (3%) 51 50	13, 26, 42, 59	4 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	355	ALA	4.0
1	D	488	TYR	3.8
1	B	139	GLY	3.7
1	D	487	LEU	3.3
1	D	47	SER	3.2
1	A	78	TYR	3.1
1	C	220	SER	3.1
1	D	311	ALA	3.1
1	C	221	VAL	3.0
1	D	337	GLU	3.0
1	B	360	GLY	3.0
1	B	484	ALA	2.9
1	D	379	ALA	2.9
1	A	367	LEU	2.7
1	D	64	ILE	2.7
1	D	343	ILE	2.7
1	B	398	LYS	2.6
1	D	382	VAL	2.6
1	D	67	ILE	2.5
1	D	222	ILE	2.5
1	D	310	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	315	GLU	2.5
1	D	62	GLN	2.4
1	A	221	VAL	2.4
1	A	353	ASN	2.4
1	C	352	GLU	2.3
1	D	358	LEU	2.3
1	A	411	ASP	2.3
1	D	25	THR	2.3
1	C	357	LEU	2.3
1	D	221	VAL	2.3
1	A	141	SER	2.3
1	A	139	GLY	2.3
1	D	14	ILE	2.2
1	D	100	ALA	2.2
1	D	46	LEU	2.2
1	A	26	GLY	2.2
1	C	337	GLU	2.2
1	D	24	ARG	2.2
1	D	378	PRO	2.1
1	A	64	ILE	2.1
1	A	466	ILE	2.1
1	A	323	GLY	2.1
1	D	34	PRO	2.1
1	A	38	VAL	2.1
1	D	26	GLY	2.1
1	B	220	SER	2.1
1	D	10	PHE	2.1
1	A	125	LEU	2.1
1	A	9	GLN	2.1
1	A	333	PRO	2.1
1	D	78[A]	TYR	2.1
1	B	143	LYS	2.1
1	C	251	ALA	2.1
1	C	25	THR	2.0
1	D	211	ILE	2.0
1	B	397	VAL	2.0
1	A	324	SER	2.0
1	D	20	TRP	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 [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	SO4	C	506	5/5	0.66	0.64	118,119,120,120	5
2	SO4	A	506	5/5	0.71	0.69	107,109,109,109	5
2	SO4	B	506	5/5	0.78	0.65	113,115,115,115	5
2	SO4	C	507	5/5	0.79	0.75	99,102,102,102	5

6.5 Other polymers [i](#)

There are no such residues in this entry.