



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:04 PM UTC

PDB ID : 1L9W / pdb_00001l9w
Title : CRYSTAL STRUCTURE OF 3-DEHYDROQUINASE FROM
SALMONELLA TYPHI COMPLEXED WITH REACTION PRODUCT
Authors : Lee, W.H.; Perles, L.A.; Nagem, R.A.P.; Shrive, A.K.; Hawkins, A.; Sawyer,
L.; Polikarpov, I.
Deposited on : 2002-03-26
Resolution : 2.10 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

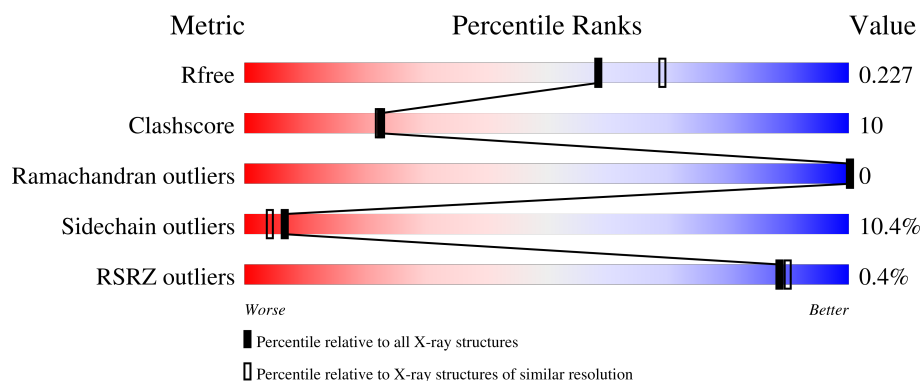
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	252	
1	B	252	
1	C	252	
1	D	252	

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	DHS	A	301	X	X	-	-
2	DHS	B	302	X	X	-	-
2	DHS	C	303	X	X	-	-
2	DHS	D	304	X	-	-	-

2 Entry composition [i](#)

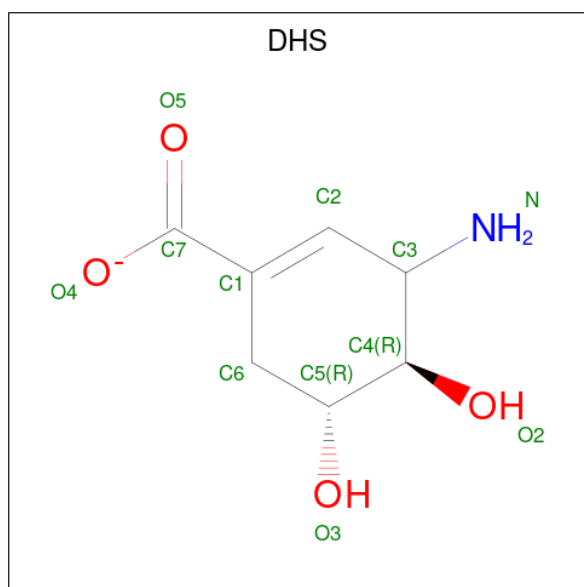
There are 3 unique types of molecules in this entry. The entry contains 7987 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-dehydroquinate dehydratase aroD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1934	1219	335	366	14			
1	B	252	Total	C	N	O	S	0	0	0
			1934	1219	335	366	14			
1	C	252	Total	C	N	O	S	0	0	0
			1934	1219	335	366	14			
1	D	252	Total	C	N	O	S	0	0	0
			1934	1219	335	366	14			

- Molecule 2 is 3-AMINO-4,5-DIHYDROXY-CYCLOHEX-1-ENECARBOXYLATE (CCD ID: DHS) (formula: $C_7H_{10}NO_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	7	4		
2	B	1	Total	C	O	0	0
			11	7	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			11	7	4		
2	D	1	Total	C	O	0	0
			11	7	4		

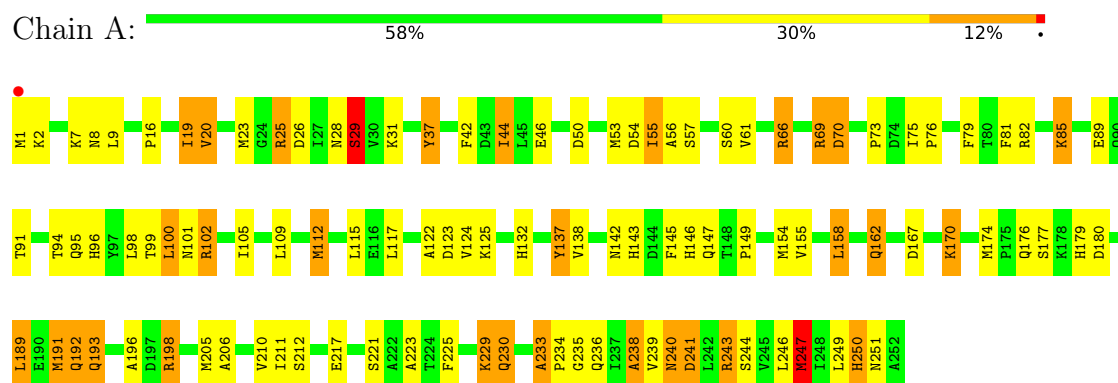
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total	O	0	0
			49	49		
3	B	54	Total	O	1	0
			54	54		
3	C	44	Total	O	2	0
			44	44		
3	D	60	Total	O	5	0
			60	60		

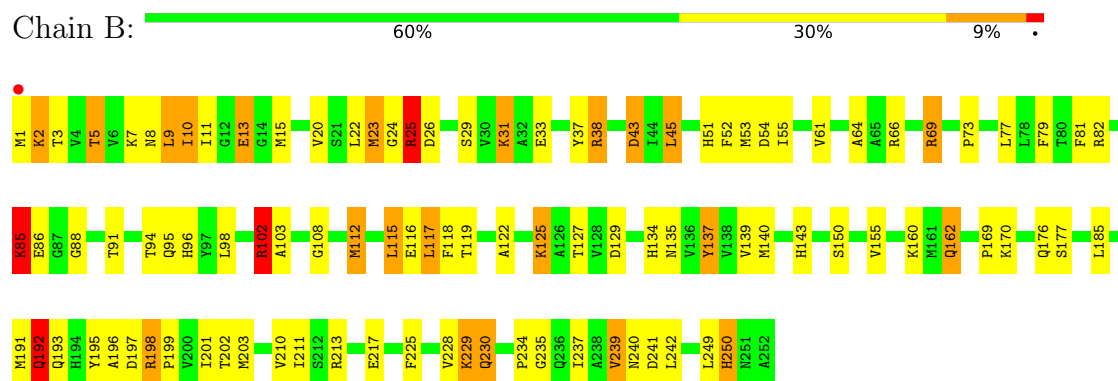
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

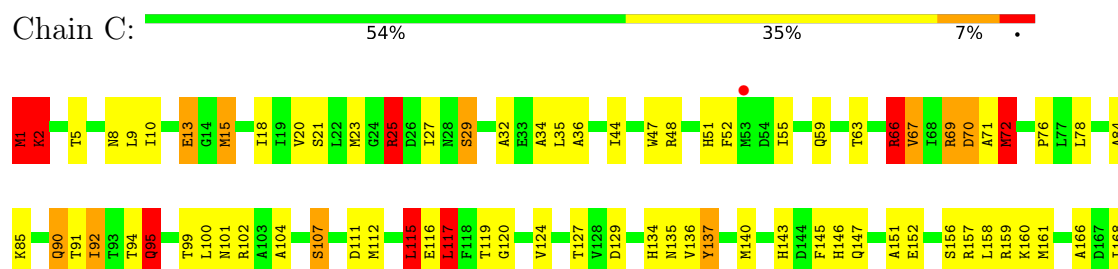
• Molecule 1: 3-dehydroquinate dehydratase aroD



• Molecule 1: 3-dehydroquinate dehydratase aroD



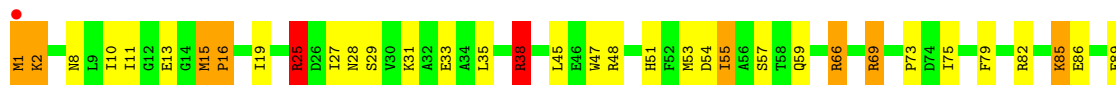
• Molecule 1: 3-dehydroquinate dehydratase aroD





• Molecule 1: 3-dehydroquinate dehydratase aroD

Chain D: 58% 34% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.61Å 158.56Å 85.89Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 10.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.10) 75.1 (10.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.09Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.177 , 0.245 0.165 , 0.227	Depositor DCC
R_{free} test set	2479 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7987	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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: DHS

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	1.22	4/1965 (0.2%)	2.23	97/2661 (3.6%)
1	B	1.29	4/1965 (0.2%)	2.33	94/2661 (3.5%)
1	C	1.19	0/1965	2.27	96/2661 (3.6%)
1	D	1.17	1/1965 (0.1%)	2.33	93/2661 (3.5%)
All	All	1.22	9/7860 (0.1%)	2.29	380/10644 (3.6%)

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
1	C	0	3
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	HIS	CG-ND1	6.28	1.45	1.38
1	D	94	THR	C-O	-5.90	1.17	1.24
1	B	225	PHE	C-N	-5.27	1.28	1.33
1	B	112	MET	CA-CB	5.27	1.63	1.53
1	A	138	VAL	C-O	-5.22	1.18	1.24
1	B	239	VAL	CA-CB	5.07	1.60	1.54
1	A	244	SER	N-CA	5.06	1.52	1.46
1	A	79	PHE	CA-CB	5.04	1.60	1.53
1	B	69	ARG	CD-NE	-5.02	1.39	1.46

All (380) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	ARG	CD-NE-CZ	24.77	159.07	124.40
1	B	25	ARG	CD-NE-CZ	22.13	155.38	124.40
1	D	38	ARG	NE-CZ-NH2	16.78	134.30	119.20
1	B	69	ARG	CD-NE-CZ	16.43	147.40	124.40
1	A	25	ARG	CD-NE-CZ	15.89	146.64	124.40
1	D	38	ARG	CD-NE-CZ	14.64	144.90	124.40
1	C	240	ASN	CA-CB-CG	-14.36	98.24	112.60
1	D	38	ARG	NE-CZ-NH1	-13.63	107.87	121.50
1	B	95	GLN	OE1-CD-NE2	-13.55	109.05	122.60
1	D	95	GLN	OE1-CD-NE2	-12.35	110.25	122.60
1	B	8	ASN	CA-CB-CG	-11.88	100.72	112.60
1	A	146	HIS	CA-CB-CG	-11.06	102.74	113.80
1	B	191	MET	CA-C-O	10.99	132.02	120.70
1	A	179	HIS	CA-CB-CG	-10.79	103.01	113.80
1	C	59	GLN	OE1-CD-NE2	-10.56	112.04	122.60
1	B	38	ARG	NE-CZ-NH1	-10.54	110.96	121.50
1	D	135	ASN	OD1-CG-ND2	-10.22	112.38	122.60
1	D	124	VAL	CA-C-O	-9.79	110.77	120.95
1	C	179	HIS	CA-CB-CG	-9.76	104.04	113.80
1	C	111	ASP	CA-CB-CG	-9.37	103.23	112.60
1	A	124	VAL	N-CA-CB	9.36	122.55	110.57
1	C	228	VAL	N-CA-C	-9.06	102.50	110.74
1	D	124	VAL	N-CA-CB	9.05	122.85	110.54
1	C	240	ASN	OD1-CG-ND2	8.93	131.53	122.60
1	B	45	LEU	CD1-CG-CD2	-8.79	91.45	110.80
1	C	99	THR	CA-C-O	-8.72	111.67	120.82
1	B	230	GLN	CB-CG-CD	8.68	127.36	112.60
1	A	210	VAL	O-C-N	-8.65	113.16	121.90
1	A	198	ARG	NE-CZ-NH2	-8.65	111.42	119.20
1	B	135	ASN	OD1-CG-ND2	-8.62	113.98	122.60
1	C	32	ALA	CA-C-O	8.59	129.84	120.82
1	A	247	MET	O-C-N	8.53	130.86	122.07
1	C	92	ILE	CA-C-O	-8.52	112.93	121.45
1	C	70	ASP	CA-C-O	-8.48	111.56	120.55
1	C	95	GLN	CB-CG-CD	8.45	126.97	112.60
1	C	107	SER	O-C-N	-8.26	113.36	122.12
1	A	238	ALA	CA-C-O	-8.26	111.51	120.92
1	D	135	ASN	CB-CG-ND2	8.25	128.78	116.40
1	D	193	GLN	OE1-CD-NE2	8.25	130.85	122.60
1	B	79	PHE	O-C-N	-8.25	113.81	123.22
1	A	95	GLN	CB-CG-CD	8.16	126.48	112.60
1	B	192	GLN	OE1-CD-NE2	8.15	130.75	122.60
1	B	198	ARG	NE-CZ-NH2	-8.09	111.92	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	MET	CA-CB-CG	7.99	130.07	114.10
1	C	115	LEU	CA-C-O	-7.97	112.09	120.70
1	B	38	ARG	NE-CZ-NH2	7.97	126.37	119.20
1	C	69	ARG	CD-NE-CZ	7.84	135.37	124.40
1	C	13	GLU	CA-CB-CG	7.82	129.73	114.10
1	B	213	ARG	CD-NE-CZ	7.81	135.33	124.40
1	A	192	GLN	OE1-CD-NE2	7.78	130.38	122.60
1	B	134	HIS	CA-CB-CG	-7.59	106.21	113.80
1	B	250	HIS	O-C-N	-7.59	113.49	122.15
1	C	238	ALA	CA-C-O	7.56	129.50	121.19
1	B	102	ARG	CD-NE-CZ	7.55	134.97	124.40
1	D	28	ASN	CA-C-N	7.54	130.25	120.44
1	D	28	ASN	C-N-CA	7.54	130.25	120.44
1	A	198	ARG	NE-CZ-NH1	7.51	129.01	121.50
1	C	102	ARG	CD-NE-CZ	7.49	134.88	124.40
1	A	42	PHE	CA-CB-CG	7.45	121.25	113.80
1	D	66	ARG	CD-NE-CZ	7.44	134.82	124.40
1	B	85	LYS	CB-CG-CD	7.43	128.40	111.30
1	D	25	ARG	CD-NE-CZ	7.41	134.77	124.40
1	C	243	ARG	CD-NE-CZ	7.41	134.77	124.40
1	A	210	VAL	CA-C-O	7.30	128.60	120.64
1	B	23	MET	O-C-N	-7.26	114.77	123.27
1	D	16	PRO	N-CA-CB	7.25	109.63	103.25
1	C	59	GLN	CB-CG-CD	7.19	124.82	112.60
1	D	69	ARG	NH1-CZ-NH2	-7.17	109.98	119.30
1	C	194	HIS	CA-C-O	-7.16	111.32	119.41
1	D	223	ALA	CA-C-O	-7.15	113.80	121.45
1	D	204	SER	CA-C-O	-7.13	112.61	120.38
1	B	15	MET	CA-C-N	7.12	127.17	119.90
1	B	15	MET	C-N-CA	7.12	127.17	119.90
1	D	45	LEU	O-C-N	-7.11	115.23	123.27
1	D	243	ARG	CA-C-N	-7.11	110.20	120.29
1	D	243	ARG	C-N-CA	-7.11	110.20	120.29
1	D	69	ARG	NE-CZ-NH1	7.09	128.59	121.50
1	A	233	ALA	CA-C-O	-7.06	114.06	120.13
1	C	47	TRP	O-C-N	-7.06	114.65	123.05
1	D	92	ILE	CA-C-O	-7.05	114.73	121.64
1	B	69	ARG	NE-CZ-NH1	7.02	128.52	121.50
1	D	215	ALA	CB-CA-C	-6.99	99.88	111.13
1	A	54	ASP	CB-CG-OD2	-6.97	102.38	118.40
1	B	5	THR	CA-CB-OG1	-6.95	99.18	109.60
1	A	102	ARG	NE-CZ-NH1	6.94	128.44	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ASN	CA-CB-CG	-6.93	105.67	112.60
1	D	95	GLN	CG-CD-NE2	6.91	126.77	116.40
1	D	82	ARG	CD-NE-CZ	6.91	134.07	124.40
1	C	151	ALA	CA-C-N	6.88	129.38	120.44
1	C	151	ALA	C-N-CA	6.88	129.38	120.44
1	C	161	MET	CA-C-O	6.85	127.68	120.42
1	B	234	PRO	CA-C-O	-6.85	113.85	121.32
1	C	134	HIS	CA-CB-CG	-6.80	107.00	113.80
1	D	190	GLU	CA-C-O	6.78	127.94	120.82
1	A	60	SER	N-CA-CB	6.74	120.14	110.16
1	B	191	MET	O-C-N	-6.73	114.82	122.09
1	A	247	MET	CA-C-O	-6.72	113.76	120.82
1	B	118	PHE	CA-C-N	6.70	129.81	120.29
1	B	118	PHE	C-N-CA	6.70	129.81	120.29
1	C	25	ARG	NE-CZ-NH2	6.68	125.21	119.20
1	D	127	THR	CA-C-O	6.68	127.65	119.97
1	D	19	ILE	CA-C-O	-6.67	113.40	120.48
1	A	7	LYS	CA-C-N	-6.67	111.99	122.73
1	A	7	LYS	C-N-CA	-6.67	111.99	122.73
1	B	241	ASP	CA-CB-CG	-6.64	105.96	112.60
1	A	28	ASN	CB-CG-ND2	-6.61	106.49	116.40
1	B	235	GLY	CA-C-O	6.57	125.28	119.56
1	C	204	SER	CA-C-O	-6.57	113.27	120.43
1	D	157	ARG	O-C-N	6.55	129.06	122.12
1	D	94	THR	N-CA-C	-6.54	104.07	111.07
1	A	167	ASP	CA-CB-CG	-6.53	106.07	112.60
1	B	160	LYS	CA-C-N	6.52	130.22	120.31
1	B	160	LYS	C-N-CA	6.52	130.22	120.31
1	B	210	VAL	O-C-N	-6.52	115.50	121.89
1	D	137	TYR	CA-C-O	6.51	128.41	120.92
1	C	137	TYR	CA-CB-CG	-6.50	102.20	113.90
1	A	112	MET	CA-C-O	-6.49	113.53	121.06
1	D	241	ASP	O-C-N	-6.49	115.24	122.12
1	D	15	MET	CA-C-N	6.49	126.52	119.90
1	D	15	MET	C-N-CA	6.49	126.52	119.90
1	C	66	ARG	CB-CA-C	-6.48	100.03	110.79
1	D	250	HIS	CA-CB-CG	-6.47	107.33	113.80
1	D	146	HIS	CA-CB-CG	-6.47	107.33	113.80
1	A	9	LEU	O-C-N	-6.43	116.00	123.27
1	A	191	MET	O-C-N	-6.42	115.45	122.07
1	B	150	SER	N-CA-CB	-6.39	101.60	110.29
1	D	57	SER	O-C-N	-6.38	115.94	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	SER	CB-CA-C	-6.38	100.86	110.88
1	D	66	ARG	NE-CZ-NH1	6.37	127.86	121.50
1	A	250	HIS	CA-CB-CG	-6.36	107.44	113.80
1	C	156	SER	O-C-N	-6.34	115.54	122.07
1	A	94	THR	CA-CB-OG1	-6.33	100.10	109.60
1	C	156	SER	CA-C-N	6.33	128.67	120.44
1	C	156	SER	C-N-CA	6.33	128.67	120.44
1	D	91	THR	N-CA-CB	6.32	120.50	110.57
1	C	146	HIS	CA-CB-CG	-6.30	107.50	113.80
1	B	13	GLU	CA-CB-CG	6.30	126.70	114.10
1	D	101	ASN	CB-CG-ND2	6.30	125.84	116.40
1	D	59	GLN	CA-C-O	-6.29	112.73	119.97
1	B	11	ILE	CA-C-O	-6.29	113.84	120.57
1	C	224	THR	CA-C-O	-6.26	113.97	120.99
1	D	15	MET	N-CA-CB	-6.25	100.17	109.98
1	B	235	GLY	O-C-N	-6.23	116.92	122.77
1	C	95	GLN	OE1-CD-NE2	-6.21	116.39	122.60
1	B	26	ASP	CB-CG-OD2	6.20	132.66	118.40
1	C	231	ALA	CA-C-O	-6.20	114.34	121.47
1	C	101	ASN	CA-CB-CG	-6.19	106.41	112.60
1	B	122	ALA	CA-C-O	-6.18	113.86	120.42
1	D	27	ILE	CA-C-O	-6.17	114.85	121.27
1	C	242	LEU	O-C-N	-6.17	115.71	122.07
1	C	92	ILE	CA-CB-CG1	6.17	120.88	110.40
1	A	193	GLN	OE1-CD-NE2	6.16	128.76	122.60
1	D	243	ARG	CA-C-O	-6.14	114.04	120.55
1	D	106	ASP	CA-C-O	6.14	127.03	119.97
1	A	8	ASN	CA-CB-CG	6.12	118.72	112.60
1	C	52	PHE	CA-CB-CG	6.12	119.92	113.80
1	B	125	LYS	O-C-N	-6.12	115.64	122.12
1	C	159	ARG	CD-NE-CZ	6.11	132.95	124.40
1	C	94	THR	CA-C-O	6.09	127.22	120.82
1	A	155	VAL	CA-C-O	6.08	127.28	120.95
1	D	106	ASP	CA-CB-CG	-6.08	106.53	112.60
1	D	220	GLY	N-CA-C	6.06	124.48	115.64
1	B	38	ARG	CD-NE-CZ	-6.05	115.93	124.40
1	C	116	GLU	CA-C-N	6.04	128.70	120.54
1	C	116	GLU	C-N-CA	6.04	128.70	120.54
1	C	1	MET	CA-C-O	6.04	131.07	120.80
1	B	64	ALA	O-C-N	-6.03	115.73	122.12
1	B	98	LEU	CA-C-N	6.02	128.84	120.29
1	B	98	LEU	C-N-CA	6.02	128.84	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	SER	O-C-N	-6.01	115.19	122.22
1	C	71	ALA	CA-C-O	-6.00	111.86	119.31
1	B	96	HIS	CA-CB-CG	-6.00	107.80	113.80
1	C	242	LEU	CA-C-O	6.00	127.12	120.82
1	A	147	GLN	OE1-CD-NE2	5.97	128.57	122.60
1	A	46	GLU	CA-C-O	-5.97	113.97	120.36
1	C	168	ILE	CA-C-N	5.95	125.88	119.76
1	C	168	ILE	C-N-CA	5.95	125.88	119.76
1	A	66	ARG	CA-C-N	5.92	128.58	120.46
1	A	66	ARG	C-N-CA	5.92	128.58	120.46
1	A	9	LEU	N-CA-C	5.89	118.84	109.24
1	C	67	VAL	CB-CA-C	-5.89	104.19	112.14
1	C	119	THR	CA-C-O	-5.89	113.20	119.97
1	C	145	PHE	CA-CB-CG	-5.89	107.91	113.80
1	C	157	ARG	NE-CZ-NH1	5.88	127.38	121.50
1	B	5	THR	O-C-N	5.88	130.87	123.23
1	B	195	TYR	N-CA-C	5.88	120.84	113.43
1	B	91	THR	O-C-N	-5.86	116.38	123.29
1	D	33	GLU	CA-C-N	5.86	128.13	120.28
1	D	33	GLU	C-N-CA	5.86	128.13	120.28
1	A	177	SER	CA-C-O	-5.86	115.15	121.36
1	A	69	ARG	NE-CZ-NH2	-5.85	113.93	119.20
1	C	48	ARG	CA-C-O	5.85	127.29	120.98
1	C	100	LEU	N-CA-CB	5.84	118.71	110.12
1	B	198	ARG	CD-NE-CZ	5.84	132.58	124.40
1	A	239	VAL	O-C-N	-5.83	115.98	121.87
1	B	31	LYS	CA-C-O	-5.83	114.70	120.82
1	C	190	GLU	CA-C-O	5.81	126.71	120.55
1	C	215	ALA	CB-CA-C	-5.81	101.36	110.94
1	B	24	GLY	O-C-N	-5.80	118.20	123.36
1	D	183	THR	OG1-CB-CG2	-5.80	97.71	109.30
1	D	163	ALA	O-C-N	-5.79	115.14	122.27
1	A	91	THR	CB-CA-C	-5.78	99.77	109.48
1	A	189	LEU	CA-C-O	-5.78	114.30	120.42
1	B	137	TYR	CA-C-N	5.78	130.63	123.12
1	B	137	TYR	C-N-CA	5.78	130.63	123.12
1	C	72	MET	O-C-N	-5.76	116.56	121.23
1	C	185	LEU	N-CA-CB	5.76	118.58	110.12
1	D	245	VAL	CA-C-O	-5.75	114.97	120.95
1	B	11	ILE	O-C-N	5.75	129.41	123.03
1	D	198	ARG	NE-CZ-NH1	5.74	127.24	121.50
1	A	50	ASP	CA-CB-CG	-5.74	106.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	LEU	O-C-N	5.73	128.20	122.12
1	D	242	LEU	CA-C-O	5.72	127.03	120.90
1	A	25	ARG	CA-CB-CG	-5.70	102.69	114.10
1	B	10	ILE	CB-CA-C	5.70	118.87	110.77
1	A	16	PRO	CB-CA-C	5.70	118.53	111.23
1	A	57	SER	O-C-N	-5.70	116.72	123.22
1	B	9	LEU	CA-C-N	-5.70	115.53	123.10
1	B	9	LEU	C-N-CA	-5.70	115.53	123.10
1	A	20	VAL	CA-C-O	5.69	127.33	120.67
1	A	137	TYR	CA-CB-CG	-5.69	103.67	113.90
1	D	218	VAL	CB-CA-C	-5.69	105.09	111.80
1	D	143	HIS	CA-CB-CG	-5.66	108.14	113.80
1	B	54	ASP	CA-CB-CG	-5.65	106.95	112.60
1	C	10	ILE	N-CA-CB	5.64	118.47	111.41
1	D	11	ILE	CA-C-O	-5.64	114.54	120.57
1	C	119	THR	N-CA-C	-5.64	105.28	111.82
1	B	64	ALA	CA-C-N	5.60	127.79	120.28
1	B	64	ALA	C-N-CA	5.60	127.79	120.28
1	B	103	ALA	N-CA-CB	5.60	118.36	110.12
1	D	205	MET	N-CA-C	5.59	118.07	110.35
1	A	42	PHE	CA-C-O	-5.59	115.45	121.38
1	D	89	GLU	N-CA-C	5.59	119.27	112.23
1	D	96	HIS	CA-CB-CG	-5.58	108.22	113.80
1	B	177	SER	CA-C-O	-5.57	115.47	121.38
1	B	185	LEU	N-CA-CB	5.57	118.80	110.22
1	B	143	HIS	CE1-NE2-CD2	5.56	114.56	109.00
1	A	180	ASP	CA-C-O	-5.56	114.66	120.55
1	C	52	PHE	O-C-N	5.55	129.53	123.04
1	D	101	ASN	CA-CB-CG	-5.54	107.06	112.60
1	C	2	LYS	CA-CB-CG	5.53	125.16	114.10
1	A	235	GLY	N-CA-C	5.52	122.39	115.21
1	C	176	GLN	N-CA-C	-5.52	107.19	114.31
1	C	90	GLN	CA-C-O	5.51	127.62	121.40
1	D	176	GLN	N-CA-C	-5.51	106.73	113.50
1	D	10	ILE	CB-CG1-CD1	5.50	125.36	113.80
1	D	219	PHE	N-CA-C	5.49	119.67	112.92
1	D	47	TRP	CA-C-O	-5.49	114.48	120.36
1	D	35	LEU	CA-C-O	-5.48	114.61	120.42
1	D	229	LYS	N-CA-C	-5.47	104.79	112.12
1	C	78	LEU	CB-CA-C	5.47	119.16	110.19
1	D	157	ARG	CA-C-O	-5.47	114.76	120.55
1	D	48	ARG	O-C-N	-5.46	115.96	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	SER	O-C-N	-5.46	117.00	123.22
1	A	81	PHE	CA-CB-CG	-5.46	108.34	113.80
1	D	194	HIS	CA-CB-CG	5.45	119.25	113.80
1	B	155	VAL	O-C-N	-5.45	116.59	121.87
1	B	211	ILE	CA-C-O	5.44	126.71	121.05
1	A	210	VAL	N-CA-C	5.43	118.67	111.17
1	B	242	LEU	O-C-N	-5.43	116.48	122.07
1	C	129	ASP	CA-CB-CG	-5.43	107.17	112.60
1	D	28	ASN	CA-CB-CG	-5.42	107.17	112.60
1	A	223	ALA	CA-C-O	-5.42	115.47	121.33
1	A	143	HIS	CA-CB-CG	-5.42	108.38	113.80
1	B	66	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	B	139	VAL	CA-C-O	-5.40	114.33	120.65
1	C	182	LEU	CA-C-O	5.40	126.28	120.55
1	A	246	LEU	N-CA-CB	5.40	118.54	110.22
1	C	70	ASP	CA-CB-CG	-5.40	107.20	112.60
1	C	210	VAL	N-CA-C	5.40	116.77	110.62
1	D	238	ALA	O-C-N	-5.39	117.07	123.11
1	B	108	GLY	N-CA-C	-5.38	108.20	115.36
1	C	44	ILE	CA-C-O	-5.38	114.84	120.76
1	C	100	LEU	CB-CA-C	-5.38	101.85	110.79
1	B	119	THR	N-CA-C	-5.38	105.49	111.36
1	C	159	ARG	O-C-N	5.38	127.83	122.12
1	C	210	VAL	O-C-N	-5.37	116.63	121.89
1	A	191	MET	CA-C-O	5.36	126.45	120.82
1	C	193	GLN	OE1-CD-NE2	5.36	127.96	122.60
1	B	61	VAL	CA-C-O	-5.36	115.49	121.17
1	D	11	ILE	O-C-N	5.35	128.97	123.03
1	A	122	ALA	CA-C-O	-5.35	115.20	120.82
1	D	108	GLY	N-CA-C	-5.35	108.24	115.36
1	A	37	TYR	CA-C-O	5.35	125.96	119.38
1	A	81	PHE	N-CA-C	-5.34	99.06	108.20
1	C	72	MET	CA-C-O	5.34	127.16	121.28
1	A	225	PHE	CA-C-N	5.34	126.31	121.82
1	A	225	PHE	C-N-CA	5.34	126.31	121.82
1	A	69	ARG	CD-NE-CZ	5.33	131.87	124.40
1	C	66	ARG	CD-NE-CZ	-5.33	116.94	124.40
1	B	143	HIS	CB-CG-ND1	-5.33	114.70	122.70
1	A	198	ARG	N-CA-CB	-5.31	105.82	111.29
1	A	211	ILE	CB-CG1-CD1	-5.30	102.67	113.80
1	B	162	GLN	OE1-CD-NE2	5.29	127.89	122.60
1	D	248	ILE	O-C-N	-5.29	116.74	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	GLN	CA-CB-CG	5.29	124.68	114.10
1	B	116	GLU	CA-CB-CG	-5.28	103.54	114.10
1	A	212	SER	CA-C-N	5.28	129.53	120.72
1	A	212	SER	C-N-CA	5.28	129.53	120.72
1	C	220	GLY	CA-C-O	-5.28	113.81	118.77
1	B	129	ASP	O-C-N	-5.27	115.78	122.27
1	D	73	PRO	CA-C-N	-5.27	114.29	122.67
1	D	73	PRO	C-N-CA	-5.27	114.29	122.67
1	B	10	ILE	CB-CG1-CD1	5.26	124.84	113.80
1	D	54	ASP	CA-CB-CG	-5.26	107.34	112.60
1	D	8	ASN	CA-CB-CG	-5.25	107.34	112.60
1	D	92	ILE	O-C-N	5.25	128.78	122.95
1	A	123	ASP	O-C-N	5.25	127.69	122.12
1	C	36	ALA	CA-C-O	5.25	126.11	120.55
1	B	94	THR	CA-C-O	5.25	126.00	119.97
1	B	52	PHE	CA-CB-CG	5.25	119.05	113.80
1	B	31	LYS	CB-CA-C	5.24	119.11	110.88
1	D	224	THR	CA-C-O	-5.24	115.12	120.89
1	A	70	ASP	CA-C-O	-5.24	115.00	120.55
1	C	2	LYS	N-CA-C	-5.23	100.57	108.52
1	C	136	VAL	CA-C-O	-5.23	114.94	120.48
1	A	82	ARG	CD-NE-CZ	5.23	131.72	124.40
1	D	137	TYR	CA-CB-CG	-5.23	104.49	113.90
1	B	43	ASP	CA-CB-CG	-5.22	107.38	112.60
1	A	56	ALA	N-CA-C	-5.22	105.77	111.82
1	B	102	ARG	CB-CA-C	-5.21	102.13	110.79
1	C	143	HIS	CA-CB-CG	-5.21	108.59	113.80
1	C	59	GLN	CG-CD-OE1	5.20	131.21	120.80
1	D	79	PHE	N-CA-CB	-5.20	101.43	110.17
1	A	44	ILE	CA-C-N	-5.20	115.55	122.72
1	A	44	ILE	C-N-CA	-5.20	115.55	122.72
1	A	170	LYS	CA-C-N	-5.19	115.23	122.71
1	A	170	LYS	C-N-CA	-5.19	115.23	122.71
1	B	240	ASN	CA-C-N	5.19	127.19	120.44
1	B	240	ASN	C-N-CA	5.19	127.19	120.44
1	B	37	TYR	CA-C-N	5.19	127.75	120.28
1	B	37	TYR	C-N-CA	5.19	127.75	120.28
1	A	247	MET	CB-CA-C	-5.19	102.74	110.88
1	C	243	ARG	CA-C-O	-5.18	115.06	120.55
1	B	213	ARG	CG-CD-NE	5.18	123.40	112.00
1	B	230	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	C	15	MET	N-CA-CB	-5.17	103.06	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	75	ILE	CA-CB-CG2	5.17	119.29	110.50
1	D	31	LYS	CA-C-O	-5.16	115.40	120.82
1	A	158	LEU	N-CA-C	5.16	116.90	111.28
1	B	81	PHE	CA-CB-CG	-5.15	108.65	113.80
1	C	104	ALA	CB-CA-C	-5.15	102.79	110.88
1	A	95	GLN	CG-CD-OE1	5.14	131.07	120.80
1	A	101	ASN	CA-CB-CG	-5.14	107.46	112.60
1	A	89	GLU	N-CA-C	5.13	119.25	112.89
1	A	241	ASP	CA-C-O	5.12	126.19	120.82
1	A	19	ILE	CA-C-N	5.11	130.12	123.06
1	A	19	ILE	C-N-CA	5.11	130.12	123.06
1	A	105	ILE	N-CA-CB	-5.11	103.60	110.54
1	C	29	SER	CA-CB-OG	-5.10	100.90	111.10
1	B	117	LEU	CB-CA-C	-5.10	102.66	110.81
1	B	135	ASN	CA-CB-CG	5.10	117.70	112.60
1	B	55	ILE	CA-C-O	-5.09	112.86	119.53
1	A	95	GLN	CG-CD-NE2	-5.09	108.77	116.40
1	D	218	VAL	CA-C-O	-5.09	115.35	120.69
1	A	28	ASN	CA-C-N	-5.09	112.03	120.68
1	A	28	ASN	C-N-CA	-5.09	112.03	120.68
1	B	160	LYS	O-C-N	-5.09	116.73	122.12
1	C	76	PRO	O-C-N	-5.09	115.78	122.64
1	D	157	ARG	CD-NE-CZ	5.08	131.51	124.40
1	C	101	ASN	OD1-CG-ND2	5.08	127.68	122.60
1	C	127	THR	CA-C-N	5.07	126.95	120.56
1	C	127	THR	C-N-CA	5.07	126.95	120.56
1	D	243	ARG	O-C-N	5.07	127.49	122.12
1	B	3	THR	O-C-N	-5.06	116.33	123.11
1	D	249	LEU	CA-C-O	5.06	125.78	120.42
1	A	132	HIS	CA-C-O	-5.05	115.07	120.42
1	A	243	ARG	NE-CZ-NH1	5.05	126.55	121.50
1	D	198	ARG	CD-NE-CZ	5.04	131.46	124.40
1	D	91	THR	CA-C-N	-5.04	116.18	123.03
1	D	91	THR	C-N-CA	-5.04	116.18	123.03
1	C	36	ALA	CB-CA-C	-5.04	102.43	110.79
1	C	21	SER	CA-CB-OG	-5.03	101.04	111.10
1	A	29	SER	CA-CB-OG	-5.03	101.05	111.10
1	A	112	MET	O-C-N	5.03	129.10	123.27
1	C	117	LEU	CA-CB-CG	5.03	133.90	116.30
1	C	20	VAL	CA-C-O	-5.02	115.05	120.67
1	A	142	ASN	CA-CB-CG	-5.02	107.58	112.60
1	A	73	PRO	CB-CA-C	-5.01	103.87	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ASP	CA-CB-CG	-5.01	107.59	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	43	ASP	Mainchain
1	C	107	SER	Mainchain
1	C	115	LEU	Mainchain
1	C	84	ALA	Mainchain

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	1934	0	1963	38	0
1	B	1934	0	1963	43	0
1	C	1934	0	1963	49	0
1	D	1934	0	1963	39	0
2	A	11	0	7	2	0
2	B	11	0	7	1	0
2	C	11	0	6	2	0
2	D	11	0	6	0	0
3	A	49	0	0	1	0
3	B	54	0	0	3	1
3	C	44	0	0	2	1
3	D	60	0	0	10	0
All	All	7987	0	7878	163	1

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 (163) 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:25:ARG:HH21	1:B:51:HIS:HB3	1.23	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:GLN:NE2	3:D:305:HOH:O	1.98	0.91
1:C:211:ILE:HD11	1:D:211:ILE:HD11	1.55	0.88
1:D:140:MET:HE3	1:D:166:ALA:HB2	1.55	0.86
1:B:25:ARG:NH2	1:B:51:HIS:HB3	1.96	0.79
1:D:85:LYS:HE2	1:D:86:GLU:HG3	1.64	0.78
1:C:227:ALA:O	1:C:239:VAL:HG22	1.85	0.77
1:D:112:MET:HG2	1:D:137:TYR:HB2	1.67	0.76
1:A:53:MET:HE3	1:A:53:MET:HA	1.70	0.74
1:B:102:ARG:HH11	1:B:102:ARG:HG2	1.54	0.71
1:A:240:ASN:N	1:A:240:ASN:HD22	1.89	0.70
1:C:176:GLN:OE1	3:C:341:HOH:O	2.09	0.70
1:B:162:GLN:HE22	1:B:196:ALA:HA	1.56	0.70
1:A:217:GLU:OE2	1:A:250:HIS:HD2	1.76	0.68
1:C:208:GLU:HG3	3:C:345:HOH:O	1.91	0.68
1:D:25:ARG:HG3	1:D:53:MET:HG3	1.75	0.68
1:B:230:GLN:HG2	3:B:346:HOH:O	1.94	0.67
1:C:95:GLN:H	1:C:95:GLN:CD	2.02	0.67
1:D:66:ARG:NE	3:D:324:HOH:O	2.21	0.67
1:D:86:GLU:OE2	3:D:311:HOH:O	2.12	0.67
1:A:174:MET:HE2	1:A:205:MET:HE3	1.76	0.66
1:D:85:LYS:HE2	1:D:86:GLU:CG	2.28	0.64
1:D:120:GLY:O	1:D:124:VAL:HG13	1.98	0.64
1:B:217:GLU:OE2	1:B:250:HIS:HD2	1.82	0.62
1:A:243:ARG:O	1:A:247:MET:HG2	1.99	0.62
1:D:121:ASP:OD2	1:D:160:LYS:NZ	2.32	0.62
1:D:1:MET:HE2	1:D:198:ARG:O	1.99	0.62
1:B:85:LYS:HE2	1:B:86:GLU:HG3	1.83	0.61
1:D:149:PRO:HD2	1:D:173:VAL:HG11	1.83	0.61
1:C:63:THR:O	1:C:67:VAL:HG23	2.00	0.60
1:C:217:GLU:OE2	1:C:250:HIS:HD2	1.85	0.59
1:C:66:ARG:NH1	1:C:70:ASP:OD1	2.32	0.59
1:A:96:HIS:HE1	3:A:329:HOH:O	1.85	0.59
1:C:55:ILE:HD12	1:C:92:ILE:HG21	1.85	0.58
1:A:217:GLU:OE2	1:A:250:HIS:CD2	2.56	0.58
1:D:55:ILE:HD11	1:D:90:GLN:NE2	2.19	0.58
1:C:120:GLY:O	1:C:124:VAL:HG22	2.03	0.57
1:C:25:ARG:NH2	1:C:51:HIS:ND1	2.52	0.57
1:A:240:ASN:HD22	1:A:240:ASN:H	1.52	0.56
1:C:229:LYS:HB3	1:C:229:LYS:NZ	2.19	0.56
1:B:162:GLN:HE21	1:B:198:ARG:HG2	1.70	0.56
1:D:198:ARG:HB2	1:D:199:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:LYS:HG3	1:C:230:GLN:H	1.70	0.56
1:D:66:ARG:NH2	3:D:326:HOH:O	2.23	0.55
1:C:229:LYS:HG3	1:C:230:GLN:HG2	1.87	0.55
1:D:15:MET:HE3	1:D:246:LEU:CB	2.37	0.55
1:B:170:LYS:HZ3	2:B:302:DHS:C3	2.19	0.55
1:B:228:VAL:HG12	1:B:229:LYS:HG3	1.89	0.55
1:A:112:MET:HG2	1:A:137:TYR:HB2	1.88	0.55
1:B:192:GLN:HG3	1:B:193:GLN:N	2.23	0.54
1:C:112:MET:HG2	1:C:137:TYR:HB2	1.89	0.54
1:D:229:LYS:HG3	3:D:356:HOH:O	2.06	0.54
1:D:170:LYS:HA	1:D:201:ILE:O	2.08	0.53
1:A:75:ILE:HD12	1:A:75:ILE:N	2.23	0.53
1:D:155:VAL:O	1:D:159:ARG:HG3	2.08	0.53
1:A:145:PHE:HA	1:A:205:MET:HE1	1.91	0.53
1:B:45:LEU:C	1:B:45:LEU:HD23	2.34	0.53
1:B:23:MET:CE	1:B:230:GLN:HG3	2.38	0.52
1:B:82:ARG:O	1:B:88:GLY:HA3	2.09	0.52
1:B:38:ARG:NH1	1:C:135:ASN:OD1	2.34	0.52
1:A:240:ASN:N	1:A:240:ASN:ND2	2.56	0.52
1:A:158:LEU:HD13	1:A:191:MET:HG2	1.92	0.52
1:A:240:ASN:H	1:A:240:ASN:ND2	2.07	0.52
1:D:38:ARG:HD3	3:D:321:HOH:O	2.10	0.52
1:B:5:THR:HG23	1:B:9:LEU:O	2.09	0.52
1:B:115:LEU:HD21	1:B:127:THR:HB	1.92	0.52
1:D:38:ARG:NE	3:D:342:HOH:O	2.13	0.51
1:B:85:LYS:HE2	1:B:86:GLU:CG	2.41	0.51
1:B:2:LYS:HB3	1:B:197:ASP:O	2.11	0.51
1:B:102:ARG:HG2	1:B:102:ARG:NH1	2.24	0.51
1:C:55:ILE:HG12	1:C:90:GLN:HE22	1.76	0.51
1:C:18:ILE:HD11	1:C:246:LEU:HD12	1.93	0.50
1:C:15:MET:HE3	1:C:246:LEU:HB2	1.93	0.50
1:A:170:LYS:HZ1	2:A:301:DHS:H2	1.76	0.50
1:B:20:VAL:CG1	1:B:239:VAL:HG11	2.42	0.49
1:C:140:MET:HE3	1:C:166:ALA:HB2	1.94	0.49
1:B:23:MET:HE1	1:B:230:GLN:HG3	1.93	0.49
1:D:25:ARG:HH21	1:D:51:HIS:HB3	1.78	0.49
1:A:162:GLN:HE22	1:A:196:ALA:HA	1.78	0.48
1:D:16:PRO:HD3	1:D:217:GLU:HB2	1.95	0.48
1:D:113:ILE:HD12	1:D:115:LEU:HD13	1.95	0.48
1:A:37:TYR:HE1	1:A:229:LYS:HE2	1.79	0.48
1:B:45:LEU:HD22	1:B:77:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD13	1:A:189:LEU:O	2.14	0.48
1:C:178:LYS:HD3	1:D:218:VAL:O	2.13	0.48
1:A:85:LYS:H	1:A:85:LYS:HD3	1.78	0.47
1:B:33:GLU:OE2	1:B:229:LYS:HE2	2.14	0.47
1:B:7:LYS:HE3	1:B:73:PRO:O	2.15	0.47
1:D:15:MET:HE3	1:D:246:LEU:HB3	1.96	0.47
1:B:140:MET:HE3	1:B:140:MET:HB2	1.81	0.47
1:C:55:ILE:HD11	1:C:90:GLN:NE2	2.30	0.47
1:C:242:LEU:O	1:C:246:LEU:HG	2.15	0.47
1:D:184:LEU:C	1:D:184:LEU:HD13	2.40	0.46
1:A:23:MET:HE1	1:A:230:GLN:HE21	1.80	0.46
1:B:22:LEU:C	1:B:22:LEU:HD23	2.40	0.46
1:A:98:LEU:O	1:A:102:ARG:HG3	2.15	0.46
1:C:23:MET:HE1	1:C:230:GLN:HG3	1.97	0.46
1:D:15:MET:HE3	1:D:246:LEU:HB2	1.96	0.45
1:A:66:ARG:NH1	1:A:70:ASP:OD1	2.42	0.45
1:C:1:MET:HE3	1:C:196:ALA:HB1	1.98	0.45
1:D:1:MET:HE1	3:D:337:HOH:O	2.16	0.45
1:A:162:GLN:HG3	1:A:198:ARG:NE	2.32	0.45
1:C:158:LEU:HD13	1:C:191:MET:HG2	1.98	0.45
1:D:200:VAL:HG12	1:D:201:ILE:N	2.31	0.45
1:C:72:MET:HE3	1:C:72:MET:HB2	1.66	0.45
1:A:162:GLN:HG3	1:A:198:ARG:CZ	2.47	0.45
1:B:198:ARG:HB2	1:B:199:PRO:CD	2.46	0.45
1:D:95:GLN:CG	3:D:305:HOH:O	2.65	0.45
1:C:66:ARG:HD2	1:C:70:ASP:OD1	2.17	0.45
1:B:162:GLN:NE2	1:B:197:ASP:H	2.15	0.44
1:C:8:ASN:OD1	1:C:8:ASN:N	2.50	0.44
1:C:1:MET:HB3	1:C:2:LYS:H	1.36	0.44
1:A:19:ILE:HG12	1:A:44:ILE:HB	2.00	0.44
1:C:203:MET:HE2	2:C:303:DHS:O5	2.17	0.44
1:D:25:ARG:NH2	1:D:51:HIS:ND1	2.66	0.44
1:A:233:ALA:HB1	1:A:234:PRO:HD2	2.00	0.43
1:A:240:ASN:ND2	1:A:241:ASP:H	2.15	0.43
1:A:26:ASP:OD2	1:A:29:SER:OG	2.35	0.43
1:A:61:VAL:HG11	1:A:100:LEU:HD21	2.01	0.43
1:C:27:ILE:H	1:C:27:ILE:HG13	1.58	0.43
1:B:162:GLN:HG2	1:B:198:ARG:CZ	2.48	0.43
1:C:55:ILE:CG1	1:C:90:GLN:HE22	2.31	0.43
1:C:117:LEU:HD21	1:C:160:LYS:HG2	1.99	0.43
1:A:205:MET:O	1:A:206:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:MET:HE3	1:B:230:GLN:CD	2.44	0.43
1:A:236:GLN:NE2	2:A:301:DHS:O5	2.47	0.43
1:B:2:LYS:HB3	1:B:2:LYS:HE3	1.85	0.43
1:B:162:GLN:HE22	1:B:197:ASP:H	1.65	0.43
1:C:198:ARG:HB2	1:C:199:PRO:HD2	2.00	0.43
1:B:202:THR:O	3:B:339:HOH:O	2.21	0.43
1:A:69:ARG:HD2	1:A:109:LEU:O	2.19	0.42
1:A:230:GLN:HE21	1:A:230:GLN:HB3	1.65	0.42
1:B:170:LYS:HA	1:B:201:ILE:O	2.18	0.42
1:C:23:MET:CE	1:C:230:GLN:HG3	2.49	0.42
1:D:2:LYS:HB3	1:D:2:LYS:HE3	1.94	0.42
1:A:55:ILE:H	1:A:55:ILE:HG13	1.46	0.42
1:C:207:LYS:NZ	1:D:252:ALA:O	2.47	0.42
1:C:92:ILE:HG21	1:C:92:ILE:HD13	1.90	0.42
1:B:112:MET:HG2	1:B:137:TYR:HB2	2.02	0.42
1:C:34:ALA:HB1	1:C:72:MET:CE	2.50	0.42
1:C:247:MET:O	1:C:248:ILE:C	2.62	0.42
1:A:75:ILE:HG22	1:A:76:PRO:O	2.20	0.41
1:B:20:VAL:HG11	1:B:239:VAL:HG11	2.01	0.41
1:C:55:ILE:CD1	1:C:92:ILE:HG21	2.49	0.41
1:B:203:MET:HE3	3:B:339:HOH:O	2.20	0.41
1:C:5:THR:HA	1:C:9:LEU:O	2.19	0.41
1:B:162:GLN:HG2	1:B:198:ARG:NE	2.36	0.41
1:B:198:ARG:HB2	1:B:199:PRO:HD2	2.02	0.41
1:A:189:LEU:HD11	1:A:193:GLN:OE1	2.20	0.41
1:A:238:ALA:HB1	1:A:240:ASN:HD21	1.84	0.41
1:B:38:ARG:NH1	1:C:135:ASN:HA	2.36	0.41
1:C:66:ARG:HD2	1:C:66:ARG:HH11	1.64	0.41
1:C:69:ARG:O	1:C:69:ARG:HG3	2.21	0.41
1:C:178:LYS:HZ2	1:C:178:LYS:HG2	1.51	0.41
1:A:149:PRO:O	1:A:154:MET:HE2	2.21	0.41
1:C:95:GLN:CD	1:C:95:GLN:N	2.75	0.41
1:B:169:PRO:HD2	1:B:199:PRO:O	2.22	0.40
1:B:102:ARG:HH11	1:B:102:ARG:CG	2.27	0.40
1:D:25:ARG:NH2	1:D:51:HIS:HB3	2.36	0.40
1:C:182:LEU:HD11	1:D:186:THR:HA	2.03	0.40
1:D:192:GLN:HG3	1:D:193:GLN:N	2.37	0.40
1:D:38:ARG:NH1	3:D:342:HOH:O	2.53	0.40
1:C:170:LYS:HZ1	2:C:303:DHS:H2	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:352:HOH:O	3:C:324:HOH:O[1_655]	2.18	0.02

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	250/252 (99%)	246 (98%)	4 (2%)	0	100	100
1	B	250/252 (99%)	242 (97%)	8 (3%)	0	100	100
1	C	250/252 (99%)	245 (98%)	5 (2%)	0	100	100
1	D	250/252 (99%)	243 (97%)	7 (3%)	0	100	100
All	All	1000/1008 (99%)	976 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	209/209 (100%)	189 (90%)	20 (10%)	8	5
1	B	209/209 (100%)	191 (91%)	18 (9%)	10	7
1	C	209/209 (100%)	185 (88%)	24 (12%)	5	3
1	D	209/209 (100%)	184 (88%)	25 (12%)	5	3
All	All	836/836 (100%)	749 (90%)	87 (10%)	7	4

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	20	VAL
1	A	25	ARG
1	A	29	SER
1	A	31	LYS
1	A	55	ILE
1	A	85	LYS
1	A	99	THR
1	A	100	LEU
1	A	115	LEU
1	A	117	LEU
1	A	125	LYS
1	A	176	GLN
1	A	192	GLN
1	A	229	LYS
1	A	230	GLN
1	A	240	ASN
1	A	247	MET
1	A	249	LEU
1	B	1	MET
1	B	2	LYS
1	B	10	ILE
1	B	13	GLU
1	B	25	ARG
1	B	29	SER
1	B	31	LYS
1	B	69	ARG
1	B	85	LYS
1	B	102	ARG
1	B	115	LEU
1	B	117	LEU
1	B	125	LYS
1	B	176	GLN
1	B	192	GLN
1	B	229	LYS
1	B	237	ILE
1	B	249	LEU
1	C	1	MET
1	C	2	LYS
1	C	13	GLU
1	C	25	ARG
1	C	29	SER

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Mol	Chain	Res	Type
1	C	35	LEU
1	C	66	ARG
1	C	72	MET
1	C	85	LYS
1	C	91	THR
1	C	95	GLN
1	C	115	LEU
1	C	117	LEU
1	C	147	GLN
1	C	152	GLU
1	C	178	LYS
1	C	182	LEU
1	C	192	GLN
1	C	203	MET
1	C	208	GLU
1	C	229	LYS
1	C	239	VAL
1	C	248	ILE
1	C	249	LEU
1	D	1	MET
1	D	2	LYS
1	D	13	GLU
1	D	25	ARG
1	D	29	SER
1	D	38	ARG
1	D	55	ILE
1	D	69	ARG
1	D	85	LYS
1	D	91	THR
1	D	115	LEU
1	D	117	LEU
1	D	124	VAL
1	D	125	LYS
1	D	147	GLN
1	D	156	SER
1	D	160	LYS
1	D	182	LEU
1	D	192	GLN
1	D	207	LYS
1	D	208	GLU
1	D	229	LYS
1	D	239	VAL

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Mol	Chain	Res	Type
1	D	244	SER
1	D	249	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	162	GLN
1	A	230	GLN
1	A	240	ASN
1	A	250	HIS
1	B	95	GLN
1	B	162	GLN
1	B	250	HIS
1	C	90	GLN
1	C	162	GLN
1	C	250	HIS
1	D	90	GLN
1	D	101	ASN
1	D	162	GLN
1	D	230	GLN
1	D	250	HIS

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 ⓘ

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	DHS	A	301	1	11,11,12	3.04	5 (45%)	13,15,17	5.39	9 (69%)
2	DHS	D	304	1	11,11,12	2.93	4 (36%)	13,15,17	4.56	9 (69%)
2	DHS	C	303	1	11,11,12	2.76	5 (45%)	13,15,17	6.61	10 (76%)
2	DHS	B	302	1	11,11,12	2.54	3 (27%)	13,15,17	4.26	12 (92%)

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	DHS	A	301	1	2/2/4/6	4/4/17/20	0/1/1/1
2	DHS	D	304	1	1/1/4/6	4/4/17/20	0/1/1/1
2	DHS	C	303	1	2/2/4/6	4/4/17/20	0/1/1/1
2	DHS	B	302	1	2/2/4/6	4/4/17/20	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	304	DHS	C3-C4	7.11	1.60	1.52
2	B	302	DHS	C3-C4	6.74	1.60	1.52
2	A	301	DHS	C3-C4	6.58	1.59	1.52
2	C	303	DHS	C6-C1	5.07	1.59	1.51
2	C	303	DHS	C3-C2	5.06	1.60	1.50
2	D	304	DHS	C3-C2	4.03	1.58	1.50
2	A	301	DHS	C3-C2	3.69	1.57	1.50
2	A	301	DHS	C5-C4	3.66	1.57	1.52
2	A	301	DHS	C7-C1	3.34	1.56	1.49
2	B	302	DHS	C3-C2	3.28	1.56	1.50
2	D	304	DHS	C5-C4	3.07	1.56	1.52
2	A	301	DHS	C6-C1	2.99	1.56	1.51
2	C	303	DHS	C5-C4	2.88	1.56	1.52
2	D	304	DHS	C6-C5	-2.53	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	303	DHS	C3-C4	2.34	1.55	1.52
2	C	303	DHS	C6-C5	-2.30	1.49	1.52
2	B	302	DHS	C6-C5	2.13	1.56	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	303	DHS	C3-C2-C1	-10.93	100.93	123.04
2	C	303	DHS	O3-C5-C6	10.71	133.16	109.38
2	A	301	DHS	O2-C4-C5	-10.21	87.80	110.20
2	C	303	DHS	O2-C4-C5	-10.10	88.04	110.20
2	C	303	DHS	C6-C1-C2	-8.74	101.84	119.76
2	A	301	DHS	O3-C5-C6	8.70	128.71	109.38
2	B	302	DHS	C3-C2-C1	-8.48	105.88	123.04
2	D	304	DHS	C3-C2-C1	-8.43	105.99	123.04
2	A	301	DHS	C6-C1-C2	-7.98	103.40	119.76
2	A	301	DHS	C3-C2-C1	-7.82	107.22	123.04
2	D	304	DHS	O3-C5-C6	7.56	126.17	109.38
2	D	304	DHS	O2-C4-C5	-7.41	93.94	110.20
2	C	303	DHS	O2-C4-C3	6.92	121.38	109.53
2	B	302	DHS	O4-C7-O5	-6.29	108.92	123.90
2	C	303	DHS	O4-C7-C1	6.05	128.21	115.43
2	A	301	DHS	O4-C7-O5	-5.84	110.01	123.90
2	C	303	DHS	O5-C7-C1	-5.27	112.40	121.64
2	B	302	DHS	C2-C1-C7	5.23	129.25	119.66
2	D	304	DHS	C5-C6-C1	5.15	121.68	111.77
2	C	303	DHS	C6-C1-C7	-4.21	109.26	116.99
2	C	303	DHS	O3-C5-C4	-4.06	101.30	110.20
2	D	304	DHS	C2-C1-C7	3.94	126.88	119.66
2	B	302	DHS	O2-C4-C3	3.93	116.25	109.53
2	B	302	DHS	O3-C5-C4	3.86	118.68	110.20
2	B	302	DHS	O3-C5-C6	3.76	117.73	109.38
2	D	304	DHS	O4-C7-O5	-3.58	115.36	123.90
2	A	301	DHS	O5-C7-C1	-3.57	115.39	121.64
2	B	302	DHS	C6-C1-C2	-3.49	112.61	119.76
2	D	304	DHS	O2-C4-C3	3.47	115.48	109.53
2	D	304	DHS	O4-C7-C1	3.27	122.34	115.43
2	B	302	DHS	O4-C7-C1	3.21	122.20	115.43
2	B	302	DHS	C5-C6-C1	-3.17	105.68	111.77
2	A	301	DHS	C6-C1-C7	-2.99	111.51	116.99
2	B	302	DHS	O2-C4-C5	-2.76	104.14	110.20
2	A	301	DHS	O4-C7-C1	2.72	121.19	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	DHS	O5-C7-C1	-2.64	117.00	121.64
2	A	301	DHS	O2-C4-C3	2.63	114.03	109.53
2	B	302	DHS	C3-C4-C5	-2.30	107.77	110.69
2	C	303	DHS	O4-C7-O5	-2.29	118.45	123.90
2	D	304	DHS	C6-C1-C2	-2.23	115.19	119.76

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	DHS	C4
2	A	301	DHS	C5
2	B	302	DHS	C4
2	B	302	DHS	C5
2	C	303	DHS	C4
2	C	303	DHS	C5
2	D	304	DHS	C4

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	DHS	C6-C1-C7-O4
2	A	301	DHS	C6-C1-C7-O5
2	A	301	DHS	C2-C1-C7-O4
2	A	301	DHS	C2-C1-C7-O5
2	B	302	DHS	C6-C1-C7-O4
2	B	302	DHS	C6-C1-C7-O5
2	B	302	DHS	C2-C1-C7-O4
2	C	303	DHS	C6-C1-C7-O4
2	C	303	DHS	C6-C1-C7-O5
2	C	303	DHS	C2-C1-C7-O4
2	C	303	DHS	C2-C1-C7-O5
2	D	304	DHS	C6-C1-C7-O4
2	D	304	DHS	C6-C1-C7-O5
2	D	304	DHS	C2-C1-C7-O4
2	D	304	DHS	C2-C1-C7-O5
2	B	302	DHS	C2-C1-C7-O5

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	DHS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	303	DHS	2	0
2	B	302	DHS	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	252/252 (100%)	-0.62	1 (0%) 88 90	15, 27, 43, 76	0
1	B	252/252 (100%)	-0.59	1 (0%) 88 90	15, 27, 43, 77	0
1	C	252/252 (100%)	-0.50	1 (0%) 88 90	18, 29, 44, 66	0
1	D	252/252 (100%)	-0.55	1 (0%) 88 90	18, 29, 44, 73	0
All	All	1008/1008 (100%)	-0.56	4 (0%) 88 90	15, 28, 44, 77	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	3.2
1	A	1	MET	3.0
1	B	1	MET	2.4
1	C	53	MET	2.3

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	DHS	D	304	11/12	0.78	0.12	21,32,37,38	0
2	DHS	A	301	11/12	0.81	0.10	24,28,29,30	0
2	DHS	C	303	11/12	0.82	0.12	27,31,33,33	0
2	DHS	B	302	11/12	0.88	0.10	21,29,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.