



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:54 AM UTC

PDB ID : 7V1V / pdb_00007v1v
Title : Difuctose dianhydride I synthase/hydrolase (alphaFFase1) from Bifidobacterium dentium, ligand-free form
Authors : Kashima, T.; Arakawa, T.; Yamada, C.; Fujita, K.; Fushinobu, S.
Deposited on : 2021-08-06
Resolution : 1.96 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

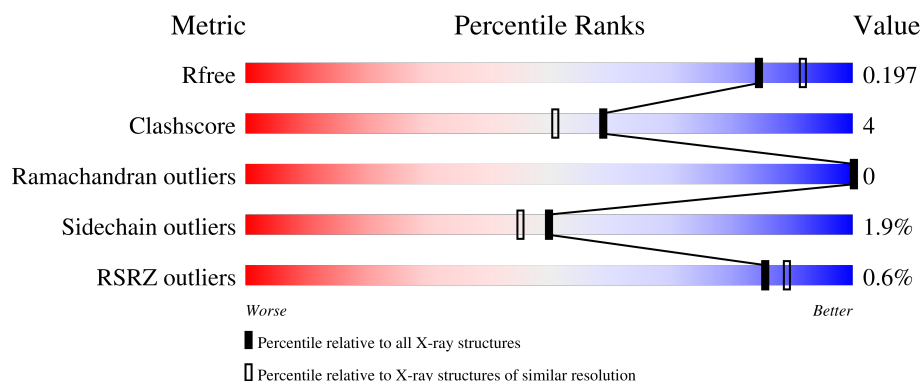
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	460	% 86% 11% .
1	B	460	% 85% 11% ..
1	C	460	85% 12% .
1	D	460	% 86% 10% ..
1	E	460	% 85% 12% ..

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Mol	Chain	Length	Quality of chain
1	F	460	% 85% 11% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24197 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 Difructose dianhydride I synthase/hydrolase (alphaFFase1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3628	2321	611	682	14			
1	B	446	Total	C	N	O	S	0	0	0
			3619	2316	610	679	14			
1	C	446	Total	C	N	O	S	0	0	0
			3619	2316	610	679	14			
1	D	446	Total	C	N	O	S	0	0	0
			3619	2316	610	679	14			
1	E	446	Total	C	N	O	S	0	0	0
			3619	2316	610	679	14			
1	F	447	Total	C	N	O	S	0	0	0
			3628	2321	611	682	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	453	LEU	-	expression tag	UNP A0A6L9SN29
A	454	GLU	-	expression tag	UNP A0A6L9SN29
A	455	HIS	-	expression tag	UNP A0A6L9SN29
A	456	HIS	-	expression tag	UNP A0A6L9SN29
A	457	HIS	-	expression tag	UNP A0A6L9SN29
A	458	HIS	-	expression tag	UNP A0A6L9SN29
A	459	HIS	-	expression tag	UNP A0A6L9SN29
A	460	HIS	-	expression tag	UNP A0A6L9SN29
B	453	LEU	-	expression tag	UNP A0A6L9SN29
B	454	GLU	-	expression tag	UNP A0A6L9SN29
B	455	HIS	-	expression tag	UNP A0A6L9SN29
B	456	HIS	-	expression tag	UNP A0A6L9SN29
B	457	HIS	-	expression tag	UNP A0A6L9SN29
B	458	HIS	-	expression tag	UNP A0A6L9SN29
B	459	HIS	-	expression tag	UNP A0A6L9SN29
B	460	HIS	-	expression tag	UNP A0A6L9SN29
C	453	LEU	-	expression tag	UNP A0A6L9SN29

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Chain	Residue	Modelled	Actual	Comment	Reference
C	454	GLU	-	expression tag	UNP A0A6L9SN29
C	455	HIS	-	expression tag	UNP A0A6L9SN29
C	456	HIS	-	expression tag	UNP A0A6L9SN29
C	457	HIS	-	expression tag	UNP A0A6L9SN29
C	458	HIS	-	expression tag	UNP A0A6L9SN29
C	459	HIS	-	expression tag	UNP A0A6L9SN29
C	460	HIS	-	expression tag	UNP A0A6L9SN29
D	453	LEU	-	expression tag	UNP A0A6L9SN29
D	454	GLU	-	expression tag	UNP A0A6L9SN29
D	455	HIS	-	expression tag	UNP A0A6L9SN29
D	456	HIS	-	expression tag	UNP A0A6L9SN29
D	457	HIS	-	expression tag	UNP A0A6L9SN29
D	458	HIS	-	expression tag	UNP A0A6L9SN29
D	459	HIS	-	expression tag	UNP A0A6L9SN29
D	460	HIS	-	expression tag	UNP A0A6L9SN29
E	453	LEU	-	expression tag	UNP A0A6L9SN29
E	454	GLU	-	expression tag	UNP A0A6L9SN29
E	455	HIS	-	expression tag	UNP A0A6L9SN29
E	456	HIS	-	expression tag	UNP A0A6L9SN29
E	457	HIS	-	expression tag	UNP A0A6L9SN29
E	458	HIS	-	expression tag	UNP A0A6L9SN29
E	459	HIS	-	expression tag	UNP A0A6L9SN29
E	460	HIS	-	expression tag	UNP A0A6L9SN29
F	453	LEU	-	expression tag	UNP A0A6L9SN29
F	454	GLU	-	expression tag	UNP A0A6L9SN29
F	455	HIS	-	expression tag	UNP A0A6L9SN29
F	456	HIS	-	expression tag	UNP A0A6L9SN29
F	457	HIS	-	expression tag	UNP A0A6L9SN29
F	458	HIS	-	expression tag	UNP A0A6L9SN29
F	459	HIS	-	expression tag	UNP A0A6L9SN29
F	460	HIS	-	expression tag	UNP A0A6L9SN29

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

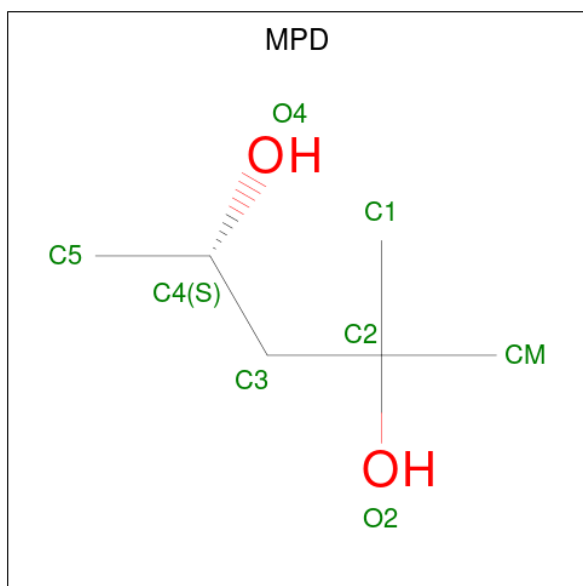
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	2	Total Ca 2 2	0	0
2	D	1	Total Ca 1 1	0	0

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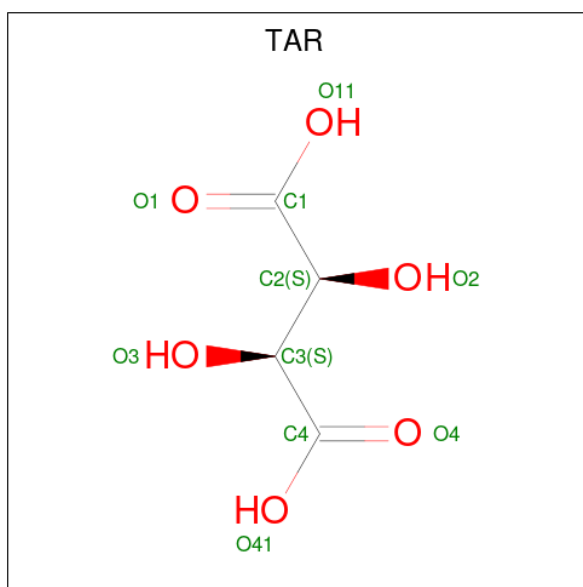
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Ca	0	0
			1	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			10	4	6		
4	E	1	Total	C	O	0	0
			10	4	6		

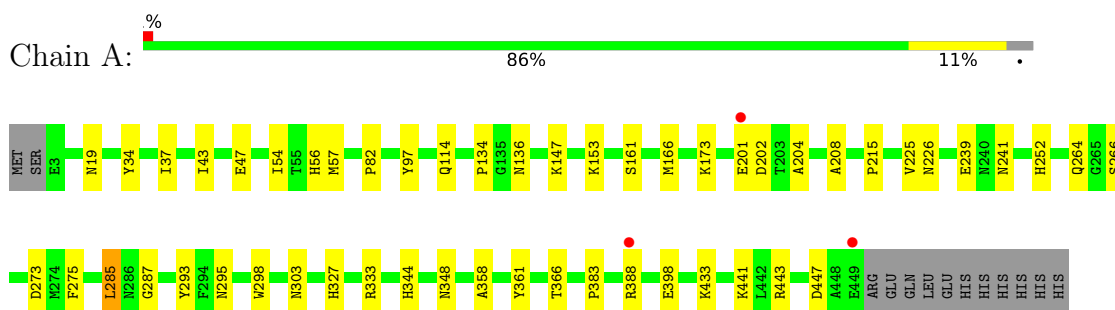
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	410	Total	O	0	0
			410	410		
5	B	408	Total	O	0	0
			408	408		
5	C	402	Total	O	0	0
			402	402		
5	D	461	Total	O	0	0
			461	461		
5	E	372	Total	O	0	0
			372	372		
5	F	370	Total	O	0	0
			370	370		

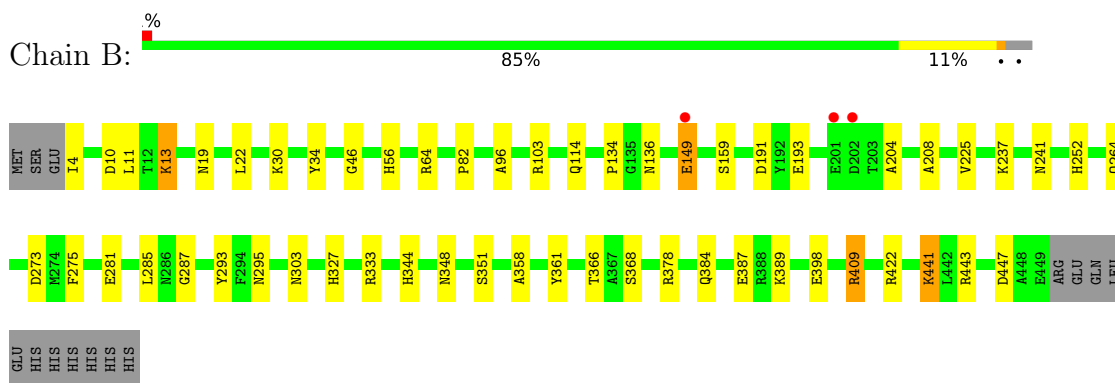
3 Residue-property plots [i](#)

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.

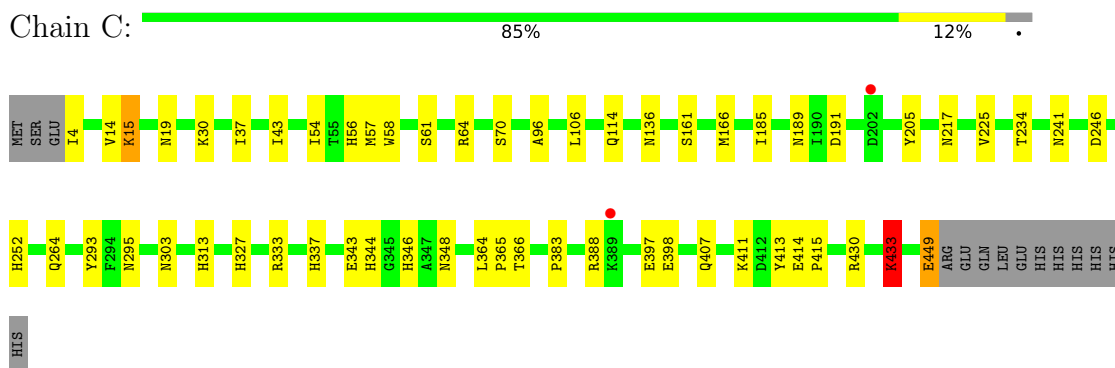
- Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)



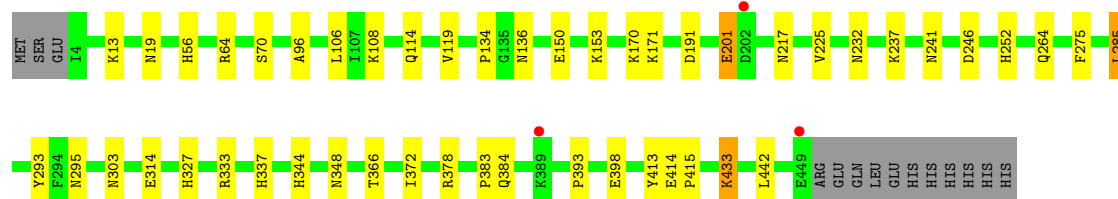
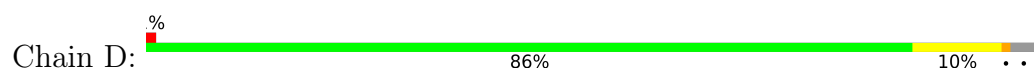
- Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)



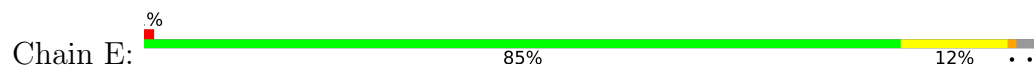
- Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)



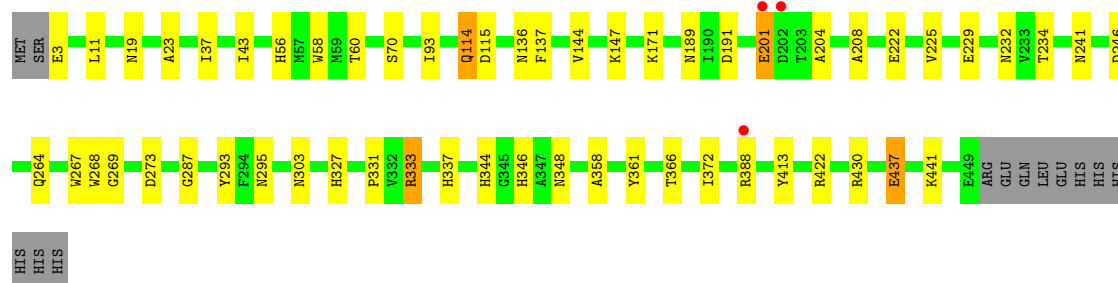
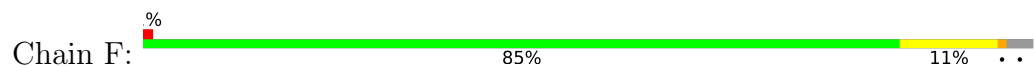
- Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)



- Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)



- Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.55Å 156.97Å 100.91Å 90.00° 109.93° 90.00°	Depositor
Resolution (Å)	49.69 – 1.96 49.69 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.69-1.96) 99.9 (49.69-1.96)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.153 , 0.191 0.162 , 0.197	Depositor DCC
R_{free} test set	10456 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.105 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24197	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: MPD, CA, TAR

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	1.04	0/3744	1.27	3/5098 (0.1%)
1	B	1.04	0/3735	1.25	3/5086 (0.1%)
1	C	1.05	3/3735 (0.1%)	1.25	3/5086 (0.1%)
1	D	1.03	0/3735	1.25	3/5086 (0.1%)
1	E	1.04	0/3735	1.24	3/5086 (0.1%)
1	F	1.05	4/3744 (0.1%)	1.28	8/5098 (0.2%)
All	All	1.04	7/22428 (0.0%)	1.26	23/30540 (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	F	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	144	VAL	C-O	5.96	1.30	1.24
1	C	313	HIS	CE1-NE2	5.67	1.38	1.32
1	F	333	ARG	C-O	5.51	1.30	1.23
1	C	106	LEU	C-O	5.24	1.30	1.23
1	F	137	PHE	C-O	5.20	1.30	1.23
1	F	23	ALA	C-O	5.19	1.30	1.23
1	C	346	HIS	CE1-NE2	5.10	1.37	1.32

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	134	PRO	CA-C-N	7.53	126.77	121.65
1	D	134	PRO	C-N-CA	7.53	126.77	121.65
1	B	134	PRO	CA-C-N	7.42	126.70	121.65
1	B	134	PRO	C-N-CA	7.42	126.70	121.65
1	F	189	ASN	CA-CB-CG	6.87	119.47	112.60
1	E	346	HIS	CA-CB-CG	-6.42	107.38	113.80
1	C	398	GLU	CB-CA-C	-5.73	101.88	110.88
1	F	437	GLU	CB-CG-CD	5.50	121.96	112.60
1	E	189	ASN	CA-CB-CG	5.46	118.06	112.60
1	B	409	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	A	266	SER	O-C-N	5.39	124.82	120.83
1	F	430	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	D	433	LYS	N-CA-CB	5.30	118.01	110.16
1	C	433	LYS	CB-CA-C	5.25	120.75	110.67
1	E	126	PHE	CA-CB-CG	-5.19	108.61	113.80
1	C	189	ASN	CA-CB-CG	5.18	117.78	112.60
1	F	60	THR	CA-CB-OG1	-5.12	101.93	109.60
1	A	134	PRO	CA-C-N	5.09	125.11	121.65
1	A	134	PRO	C-N-CA	5.09	125.11	121.65
1	F	114	GLN	CA-C-N	5.07	127.59	120.28
1	F	114	GLN	C-N-CA	5.07	127.59	120.28
1	F	346	HIS	CA-CB-CG	-5.05	108.75	113.80
1	F	430	ARG	NE-CZ-NH1	-5.00	116.50	121.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	268	TRP	Peptide

5.2 Too-close contacts [i](#)

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	3628	0	3422	39	0
1	B	3619	0	3416	39	0
1	C	3619	0	3416	39	0
1	D	3619	0	3416	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3619	0	3416	35	0
1	F	3628	0	3422	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	B	8	0	14	3	0
3	F	8	0	14	2	0
4	C	10	0	4	0	0
4	E	10	0	4	0	0
5	A	410	0	0	6	0
5	B	408	0	0	3	0
5	C	402	0	0	5	0
5	D	461	0	0	3	0
5	E	372	0	0	3	0
5	F	370	0	0	2	0
All	All	24197	0	20544	187	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 4.

All (187) 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:149:GLU:HG2	5:B:906:HOH:O	1.32	1.26
1:D:201:GLU:HB2	5:D:1278:HOH:O	1.60	0.99
1:B:443:ARG:HD2	1:B:447:ASP:OD2	1.66	0.94
1:C:430:ARG:O	1:C:433:LYS:HD2	1.74	0.87
1:C:449:GLU:O	1:C:449:GLU:HG2	1.78	0.83
1:B:409:ARG:HD3	1:F:229:GLU:OE2	1.80	0.82
1:E:114:GLN:HE22	1:E:366:THR:H	1.31	0.79
1:D:114:GLN:HE22	1:D:366:THR:H	1.30	0.76
1:E:443:ARG:HD2	1:E:447:ASP:OD2	1.86	0.76
1:C:114:GLN:HE22	1:C:366:THR:H	1.34	0.74
1:A:275:PHE:HB2	1:A:285:LEU:HB2	1.68	0.74
1:A:443:ARG:HD2	1:A:447:ASP:OD2	1.87	0.74
1:C:388:ARG:NH1	5:C:601:HOH:O	2.18	0.72
1:B:4:ILE:N	3:B:502:MPD:H4	2.04	0.72
1:A:295:ASN:OD1	1:F:56:HIS:HE1	1.78	0.67
1:F:114:GLN:HE22	1:F:366:THR:H	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:HIS:HE1	1:C:295:ASN:OD1	1.77	0.66
1:A:114:GLN:HE22	1:A:366:THR:H	1.42	0.65
1:E:275:PHE:HB2	1:E:285:LEU:HB2	1.77	0.65
1:C:344:HIS:H	1:C:348:ASN:HD22	1.45	0.64
1:B:136:ASN:HD21	1:D:303:ASN:HD21	1.45	0.64
1:C:234:THR:HG23	1:D:398:GLU:OE2	1.97	0.63
1:D:275:PHE:HB2	1:D:285:LEU:HB2	1.79	0.63
1:E:318:ASP:C	5:E:776:HOH:O	2.41	0.63
1:C:56:HIS:HD2	1:C:191:ASP:OD2	1.82	0.62
1:F:37:ILE:HD12	1:F:43:ILE:HG21	1.80	0.62
1:A:37:ILE:HD12	1:A:43:ILE:HG21	1.82	0.62
1:D:201:GLU:CB	5:D:1278:HOH:O	2.34	0.61
1:F:241:ASN:HA	1:F:348:ASN:HD21	1.66	0.61
1:B:295:ASN:OD1	1:E:56:HIS:HE1	1.84	0.60
1:B:19:ASN:ND2	1:D:333:ARG:H	2.00	0.60
1:D:56:HIS:HE1	1:E:295:ASN:OD1	1.85	0.59
1:B:56:HIS:HE1	1:D:295:ASN:OD1	1.84	0.59
1:E:344:HIS:H	1:E:348:ASN:HD22	1.49	0.59
1:C:293:TYR:OH	1:C:327:HIS:HE1	1.86	0.58
1:A:333:ARG:H	1:F:19:ASN:ND2	2.01	0.58
1:F:201:GLU:H	1:F:201:GLU:CD	2.09	0.58
1:C:225:VAL:H	1:C:264:GLN:HE22	1.50	0.58
1:A:147:LYS:HD3	5:C:755:HOH:O	2.03	0.57
1:D:19:ASN:HD21	1:E:333:ARG:H	1.52	0.57
1:A:344:HIS:H	1:A:348:ASN:HD22	1.52	0.57
1:A:241:ASN:HA	1:A:348:ASN:HD21	1.70	0.56
1:B:11:LEU:O	1:D:252:HIS:HE1	1.89	0.56
1:A:293:TYR:OH	1:A:327:HIS:HE1	1.89	0.56
1:D:19:ASN:ND2	1:E:333:ARG:H	2.05	0.55
1:C:136:ASN:HD21	1:F:303:ASN:HD21	1.53	0.55
1:B:56:HIS:HD2	1:B:191:ASP:OD2	1.90	0.55
1:A:239:GLU:HG3	5:A:923:HOH:O	2.06	0.55
1:C:14:VAL:O	1:C:15:LYS:HD3	2.07	0.55
1:F:293:TYR:OH	1:F:327:HIS:HE1	1.90	0.54
1:A:252:HIS:HD2	5:F:938:HOH:O	1.89	0.54
1:A:19:ASN:ND2	1:C:333:ARG:H	2.06	0.54
1:B:293:TYR:OH	1:B:327:HIS:HE1	1.90	0.54
1:C:241:ASN:HA	1:C:348:ASN:HD21	1.72	0.54
1:B:344:HIS:H	1:B:348:ASN:HD22	1.54	0.53
1:E:293:TYR:OH	1:E:327:HIS:HE1	1.90	0.53
1:B:351:SER:O	1:F:388:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLU:CD	5:A:601:HOH:O	2.50	0.53
1:C:37:ILE:HD12	1:C:43:ILE:HG21	1.90	0.53
1:F:222:GLU:O	3:F:601:MPD:H12	2.08	0.53
1:B:114:GLN:HE22	1:B:366:THR:H	1.57	0.52
1:C:56:HIS:HE1	1:F:295:ASN:OD1	1.92	0.52
1:E:241:ASN:HA	1:E:348:ASN:HD21	1.75	0.52
1:A:97:TYR:CE2	1:A:153:LYS:HE3	2.44	0.52
1:B:22:LEU:HD13	1:B:46:GLY:HA3	1.91	0.52
1:D:241:ASN:HA	1:D:348:ASN:HD21	1.74	0.51
1:E:387:GLU:OE1	1:E:387:GLU:HA	2.10	0.51
1:A:303:ASN:HD21	1:F:136:ASN:HD21	1.58	0.51
1:F:344:HIS:H	1:F:348:ASN:HD22	1.58	0.51
1:F:204:ALA:HB1	1:F:361:TYR:HB3	1.93	0.51
1:B:19:ASN:HD21	1:D:333:ARG:H	1.59	0.50
1:B:443:ARG:O	1:B:443:ARG:HD3	2.11	0.50
1:D:293:TYR:OH	1:D:327:HIS:HE1	1.94	0.50
1:E:56:HIS:HD2	1:E:191:ASP:OD2	1.94	0.50
1:D:136:ASN:HD21	1:E:303:ASN:HD21	1.60	0.50
1:D:246:ASP:OD1	1:D:337:HIS:CE1	2.65	0.50
1:B:241:ASN:HA	1:B:348:ASN:HD21	1.77	0.49
5:A:910:HOH:O	1:C:252:HIS:HD2	1.96	0.49
5:C:773:HOH:O	1:D:217:ASN:HB2	2.11	0.49
1:E:343:GLU:HA	1:E:348:ASN:HD21	1.78	0.49
1:A:57:MET:O	1:A:161:SER:HA	2.12	0.49
1:B:398:GLU:OE1	1:F:234:THR:HG23	2.13	0.49
1:C:19:ASN:ND2	1:F:333:ARG:H	2.11	0.48
1:A:19:ASN:HD21	1:C:333:ARG:H	1.60	0.48
1:D:56:HIS:HD2	1:D:191:ASP:OD2	1.96	0.48
1:B:10:ASP:OD1	1:B:13:LYS:HE2	2.14	0.48
1:B:443:ARG:CD	1:B:447:ASP:OD2	2.52	0.48
1:B:208:ALA:HA	1:B:358:ALA:O	2.13	0.48
3:B:502:MPD:O4	3:B:502:MPD:HM1	2.13	0.48
1:A:398:GLU:OE2	5:A:601:HOH:O	2.20	0.47
5:D:1207:HOH:O	1:E:252:HIS:HD2	1.97	0.47
1:B:303:ASN:HD21	1:E:136:ASN:HD21	1.61	0.47
1:D:225:VAL:H	1:D:264:GLN:HE22	1.62	0.47
1:B:409:ARG:CD	1:F:229:GLU:OE2	2.57	0.47
1:C:205:TYR:CE2	1:C:364:LEU:HD11	2.50	0.47
1:D:70:SER:HB3	1:D:413:TYR:CZ	2.50	0.47
1:F:246:ASP:OD1	1:F:337:HIS:HE1	1.97	0.47
1:A:225:VAL:H	1:A:264:GLN:HE22	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ILE:N	5:C:619:HOH:O	2.48	0.46
1:A:383:PRO:HB2	1:E:383:PRO:HB2	1.97	0.46
1:C:19:ASN:HD21	1:F:333:ARG:H	1.63	0.46
1:C:57:MET:O	1:C:161:SER:HA	2.16	0.46
1:A:333:ARG:H	1:F:19:ASN:HD21	1.62	0.46
1:E:443:ARG:CD	1:E:447:ASP:OD2	2.60	0.46
1:A:398:GLU:CG	5:A:601:HOH:O	2.63	0.46
1:A:208:ALA:HA	1:A:358:ALA:O	2.16	0.46
1:A:136:ASN:HD21	1:C:303:ASN:HD21	1.64	0.46
1:D:344:HIS:H	1:D:348:ASN:HD22	1.63	0.46
1:E:364:LEU:HB3	1:E:365:PRO:HA	1.97	0.45
1:F:56:HIS:HD2	1:F:191:ASP:OD2	1.99	0.45
1:A:273:ASP:OD1	1:A:287:GLY:HA3	2.17	0.45
5:C:773:HOH:O	1:D:217:ASN:CB	2.65	0.45
1:D:106:LEU:HD22	1:D:372:ILE:HD13	1.99	0.45
1:B:204:ALA:HB1	1:B:361:TYR:HB3	1.98	0.45
1:D:150:GLU:OE1	1:D:153:LYS:NZ	2.43	0.45
1:B:443:ARG:HD3	1:B:443:ARG:C	2.43	0.44
1:C:246:ASP:OD1	1:C:337:HIS:HE1	2.00	0.44
1:E:152:GLY:O	1:E:153:LYS:HD3	2.16	0.44
1:E:64:ARG:HB3	1:E:95:ASP:HB3	1.99	0.44
1:A:252:HIS:HE1	1:F:11:LEU:O	2.01	0.44
5:B:877:HOH:O	1:D:252:HIS:HD2	1.99	0.44
1:C:344:HIS:H	1:C:348:ASN:ND2	2.12	0.44
1:B:11:LEU:O	1:D:252:HIS:CE1	2.71	0.43
1:B:225:VAL:H	1:B:264:GLN:HE22	1.67	0.43
1:C:414:GLU:N	1:C:415:PRO:CD	2.82	0.43
1:F:70:SER:HB3	1:F:413:TYR:CZ	2.53	0.43
1:F:201:GLU:CD	1:F:201:GLU:N	2.76	0.43
1:E:220:GLY:N	1:E:221:PRO:CD	2.81	0.43
1:C:430:ARG:HA	1:C:433:LYS:HE3	2.00	0.43
1:B:333:ARG:H	1:E:19:ASN:ND2	2.16	0.43
1:C:30:LYS:HE2	1:F:232:ASN:O	2.19	0.43
1:E:422:ARG:HA	1:E:422:ARG:HD3	1.83	0.43
1:B:30:LYS:HD3	1:D:232:ASN:HD22	1.84	0.42
1:C:64:ARG:HA	1:C:96:ALA:O	2.19	0.42
1:C:70:SER:HB3	1:C:413:TYR:CZ	2.54	0.42
1:B:252:HIS:HD2	5:E:954:HOH:O	2.01	0.42
1:D:246:ASP:OD1	1:D:337:HIS:HE1	2.00	0.42
1:B:333:ARG:H	1:E:19:ASN:HD21	1.68	0.42
1:F:225:VAL:H	1:F:264:GLN:HE22	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:ILE:N	5:E:720:HOH:O	2.52	0.42
1:E:70:SER:HB3	1:E:413:TYR:CZ	2.54	0.42
1:E:106:LEU:HD21	1:E:378:ARG:CZ	2.50	0.42
1:F:208:ALA:HA	1:F:358:ALA:O	2.19	0.42
3:B:502:MPD:H51	5:B:644:HOH:O	2.19	0.42
1:C:54:ILE:HB	1:C:166:MET:HB2	2.01	0.42
1:C:364:LEU:HB3	1:C:365:PRO:HA	2.02	0.42
1:D:442:LEU:HD12	1:D:442:LEU:HA	1.90	0.42
1:E:204:ALA:HB1	1:E:361:TYR:HB3	2.02	0.42
1:B:34:TYR:CE2	1:B:82:PRO:HB3	2.55	0.42
1:F:273:ASP:OD1	1:F:287:GLY:HA3	2.20	0.42
1:A:34:TYR:CE1	1:A:82:PRO:HB3	2.54	0.42
1:A:226:ASN:HD22	1:A:226:ASN:HA	1.74	0.42
1:A:344:HIS:H	1:A:348:ASN:ND2	2.17	0.42
1:E:225:VAL:H	1:E:264:GLN:HE22	1.67	0.42
1:B:103:ARG:HD2	1:B:378:ARG:O	2.20	0.42
1:D:64:ARG:HA	1:D:96:ALA:O	2.19	0.41
1:A:295:ASN:HA	1:F:58:TRP:CD1	2.55	0.41
1:C:61:SER:HA	1:C:185:ILE:O	2.20	0.41
1:A:47:GLU:HG2	1:A:173:LYS:HG3	2.01	0.41
1:B:273:ASP:OD1	1:B:287:GLY:HA3	2.20	0.41
1:E:34:TYR:CE2	1:E:82:PRO:HB3	2.55	0.41
1:A:202:ASP:OD1	1:A:202:ASP:N	2.53	0.41
1:C:58:TRP:CD1	1:F:295:ASN:HA	2.55	0.41
1:B:237:LYS:HE3	1:B:281:GLU:HG3	2.03	0.41
1:C:383:PRO:HB2	1:D:383:PRO:HB2	2.02	0.41
1:D:106:LEU:HD21	1:D:378:ARG:CZ	2.50	0.41
1:F:327:HIS:HB3	1:F:331:PRO:HA	2.02	0.41
1:A:54:ILE:HB	1:A:166:MET:HB2	2.03	0.41
1:A:204:ALA:HB1	1:A:361:TYR:HB3	2.01	0.41
1:A:215:PRO:HB3	1:E:388:ARG:NH2	2.36	0.41
1:A:241:ASN:HA	1:A:348:ASN:ND2	2.35	0.41
1:A:298:TRP:O	1:F:147:LYS:HE2	2.20	0.41
1:B:64:ARG:HA	1:B:96:ALA:O	2.20	0.41
1:C:217:ASN:ND2	1:D:393:PRO:HB3	2.36	0.41
1:E:122:PRO:HD3	1:E:372:ILE:HD11	2.03	0.41
1:E:260:VAL:O	1:E:320:PHE:HA	2.21	0.41
1:F:70:SER:HB2	1:F:93:ILE:HG13	2.03	0.41
3:F:601:MPD:H12	5:F:811:HOH:O	2.20	0.41
1:D:108:LYS:HA	1:D:119:VAL:O	2.21	0.41
5:A:896:HOH:O	1:F:3:GLU:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:PHE:HB2	1:B:285:LEU:HB2	2.03	0.40
1:B:441:LYS:N	1:B:441:LYS:HE3	2.35	0.40
1:D:414:GLU:HB3	1:D:415:PRO:HD3	2.03	0.40
1:F:267:TRP:CZ2	1:F:269:GLY:HA3	2.56	0.40
1:C:114:GLN:NE2	1:C:366:THR:H	2.11	0.40
1:C:343:GLU:HA	1:C:348:ASN:HD21	1.87	0.40
1:F:114:GLN:NE2	1:F:366:THR:H	2.15	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	445/460 (97%)	432 (97%)	13 (3%)	0	100	100
1	B	444/460 (96%)	430 (97%)	14 (3%)	0	100	100
1	C	444/460 (96%)	431 (97%)	13 (3%)	0	100	100
1	D	444/460 (96%)	431 (97%)	13 (3%)	0	100	100
1	E	444/460 (96%)	426 (96%)	18 (4%)	0	100	100
1	F	445/460 (97%)	429 (96%)	16 (4%)	0	100	100
All	All	2666/2760 (97%)	2579 (97%)	87 (3%)	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	388/401 (97%)	383 (99%)	5 (1%)	61	58
1	B	387/401 (96%)	377 (97%)	10 (3%)	40	33
1	C	387/401 (96%)	381 (98%)	6 (2%)	55	52
1	D	387/401 (96%)	378 (98%)	9 (2%)	44	38
1	E	387/401 (96%)	379 (98%)	8 (2%)	47	41
1	F	388/401 (97%)	381 (98%)	7 (2%)	51	47
All	All	2324/2406 (97%)	2279 (98%)	45 (2%)	50	45

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	GLU
1	A	285	LEU
1	A	388	ARG
1	A	433	LYS
1	A	441	LYS
1	B	13	LYS
1	B	149	GLU
1	B	159	SER
1	B	193	GLU
1	B	368	SER
1	B	384	GLN
1	B	387	GLU
1	B	389	LYS
1	B	422	ARG
1	B	441	LYS
1	C	15	LYS
1	C	397	GLU
1	C	407	GLN
1	C	411	LYS
1	C	433	LYS
1	C	449	GLU
1	D	13	LYS
1	D	170	LYS
1	D	171	LYS
1	D	201	GLU
1	D	237	LYS
1	D	285	LEU
1	D	314	GLU

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Mol	Chain	Res	Type
1	D	384	GLN
1	D	433	LYS
1	E	13	LYS
1	E	199	LEU
1	E	239	GLU
1	E	285	LEU
1	E	387	GLU
1	E	392	LEU
1	E	398	GLU
1	E	422	ARG
1	F	115	ASP
1	F	171	LYS
1	F	201	GLU
1	F	372	ILE
1	F	422	ARG
1	F	437	GLU
1	F	441	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	56	HIS
1	A	114	GLN
1	A	143	ASN
1	A	226	ASN
1	A	232	ASN
1	A	252	HIS
1	A	264	GLN
1	A	303	ASN
1	A	327	HIS
1	A	337	HIS
1	A	348	ASN
1	A	400	GLN
1	B	19	ASN
1	B	32	GLN
1	B	56	HIS
1	B	114	GLN
1	B	232	ASN
1	B	252	HIS
1	B	264	GLN
1	B	303	ASN

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Mol	Chain	Res	Type
1	B	327	HIS
1	B	348	ASN
1	B	384	GLN
1	C	19	ASN
1	C	27	GLN
1	C	56	HIS
1	C	114	GLN
1	C	143	ASN
1	C	226	ASN
1	C	252	HIS
1	C	264	GLN
1	C	286	ASN
1	C	303	ASN
1	C	327	HIS
1	C	337	HIS
1	C	348	ASN
1	C	400	GLN
1	D	19	ASN
1	D	56	HIS
1	D	114	GLN
1	D	143	ASN
1	D	224	GLN
1	D	226	ASN
1	D	232	ASN
1	D	252	HIS
1	D	264	GLN
1	D	286	ASN
1	D	303	ASN
1	D	327	HIS
1	D	337	HIS
1	D	348	ASN
1	E	19	ASN
1	E	27	GLN
1	E	56	HIS
1	E	114	GLN
1	E	226	ASN
1	E	252	HIS
1	E	264	GLN
1	E	286	ASN
1	E	303	ASN
1	E	327	HIS
1	E	348	ASN

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Mol	Chain	Res	Type
1	F	19	ASN
1	F	32	GLN
1	F	56	HIS
1	F	114	GLN
1	F	189	ASN
1	F	217	ASN
1	F	226	ASN
1	F	232	ASN
1	F	252	HIS
1	F	264	GLN
1	F	303	ASN
1	F	327	HIS
1	F	337	HIS
1	F	348	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](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MPD	F	601	-	7,7,7	0.24	0	9,10,10	0.42	0
4	TAR	E	601	-	9,9,9	0.90	0	12,12,12	1.13	0
4	TAR	C	501	-	9,9,9	1.06	0	12,12,12	1.39	2 (16%)
3	MPD	B	502	-	7,7,7	0.21	0	9,10,10	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	F	601	-	-	0/5/5/5	-
4	TAR	E	601	-	-	8/12/12/12	-
4	TAR	C	501	-	-	8/12/12/12	-
3	MPD	B	502	-	-	1/5/5/5	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	TAR	C3-C2-C1	2.85	116.15	109.82
4	C	501	TAR	O4-C4-C3	-2.29	115.51	121.62

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	MPD	C2-C3-C4-C5
4	C	501	TAR	O11-C1-C2-O2
4	E	601	TAR	O3-C3-C4-O4
4	E	601	TAR	O3-C3-C4-O41
4	C	501	TAR	O1-C1-C2-O2
4	E	601	TAR	C2-C3-C4-O4
4	E	601	TAR	C2-C3-C4-O41
4	C	501	TAR	O3-C3-C4-O4
4	C	501	TAR	O3-C3-C4-O41
4	C	501	TAR	C1-C2-C3-C4
4	C	501	TAR	C2-C3-C4-O4
4	C	501	TAR	O2-C2-C3-O3
4	E	601	TAR	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	E	601	TAR	O1-C1-C2-C3
4	E	601	TAR	O11-C1-C2-C3
4	E	601	TAR	O11-C1-C2-O2
4	C	501	TAR	C2-C3-C4-O41

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	601	MPD	2	0
3	B	502	MPD	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	447/460 (97%)	-0.37	3 (0%) 84 88	11, 16, 29, 70	0
1	B	446/460 (96%)	-0.39	3 (0%) 84 88	10, 16, 29, 71	0
1	C	446/460 (96%)	-0.36	2 (0%) 88 91	11, 16, 32, 64	0
1	D	446/460 (96%)	-0.42	3 (0%) 84 88	10, 15, 29, 67	0
1	E	446/460 (96%)	-0.34	3 (0%) 84 88	11, 17, 34, 64	0
1	F	447/460 (97%)	-0.29	3 (0%) 84 88	11, 18, 34, 71	0
All	All	2678/2760 (97%)	-0.36	17 (0%) 85 89	10, 16, 32, 71	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	389	LYS	3.2
1	B	201	GLU	3.0
1	B	202	ASP	3.0
1	A	201	GLU	3.0
1	F	201	GLU	2.9
1	D	202	ASP	2.8
1	F	202	ASP	2.5
1	A	449	GLU	2.3
1	D	389	LYS	2.3
1	D	449	GLU	2.2
1	A	388	ARG	2.2
1	E	388	ARG	2.1
1	E	202	ASP	2.1
1	B	149	GLU	2.1
1	E	389	LYS	2.1
1	C	202	ASP	2.1
1	F	388	ARG	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
3	MPD	B	502	8/8	0.54	0.25	43,52,53,55	0
4	TAR	E	601	10/10	0.85	0.13	38,51,54,59	0
4	TAR	C	501	10/10	0.86	0.12	39,44,45,50	0
3	MPD	F	601	8/8	0.89	0.12	28,29,33,35	0
2	CA	A	501	1/1	0.99	0.02	16,16,16,16	0
2	CA	B	501	1/1	0.99	0.02	14,14,14,14	0
2	CA	C	502	1/1	1.00	0.01	12,12,12,12	0
2	CA	C	503	1/1	1.00	0.02	13,13,13,13	0
2	CA	D	801	1/1	1.00	0.01	11,11,11,11	0
2	CA	E	602	1/1	1.00	0.02	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.