



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2021 – 02:18 PM JST

PDB ID : 7V1V  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

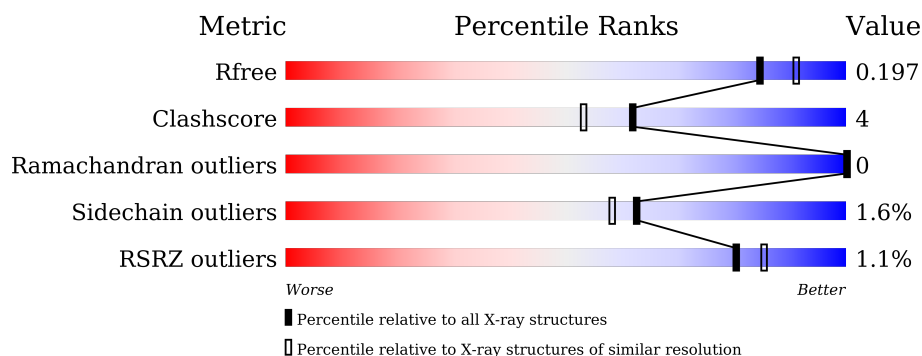
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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  $\geq 3$ , 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	<div> <div>87%</div> <div>10% ..</div> </div>
1	B	460	<div> <div>%</div> <div>85%</div> <div>10% ..</div> </div>
1	C	460	<div> <div>%</div> <div>86%</div> <div>10% .</div> </div>
1	D	460	<div> <div>%</div> <div>86%</div> <div>11% .</div> </div>
1	E	460	<div> <div>2%</div> <div>85%</div> <div>11% ..</div> </div>
1	F	460	<div> <div>2%</div> <div>86%</div> <div>10% ..</div> </div>

## 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 (three-letter code: CA) (formula: Ca).

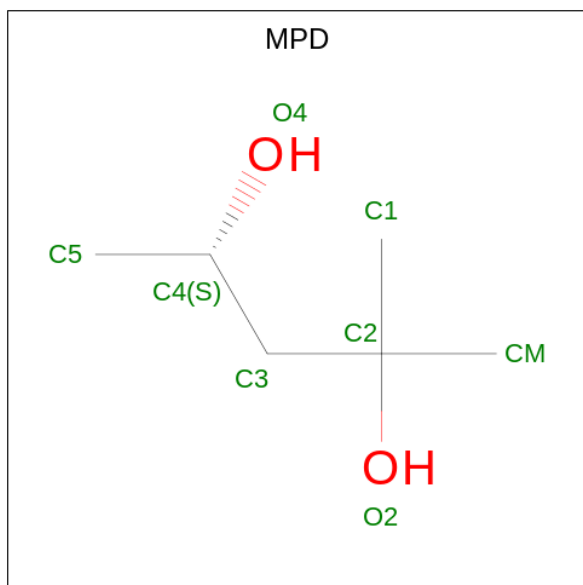
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	2	Total Ca 2 2	0	0
2	D	1	Total Ca 1 1	0	0

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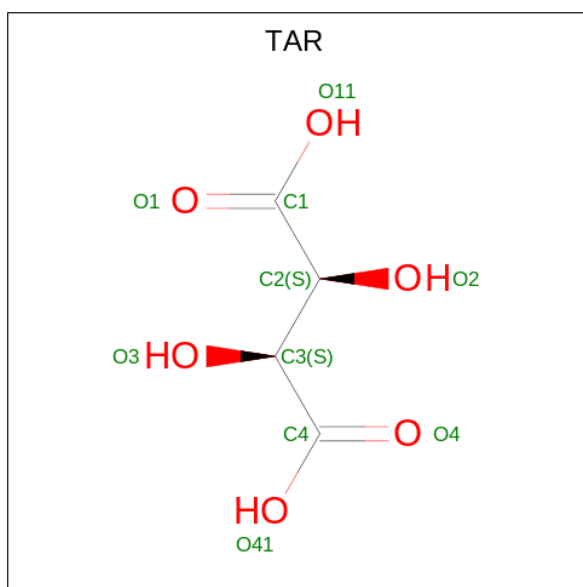
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Ca	0	0
			1	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: 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 (three-letter code: 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		

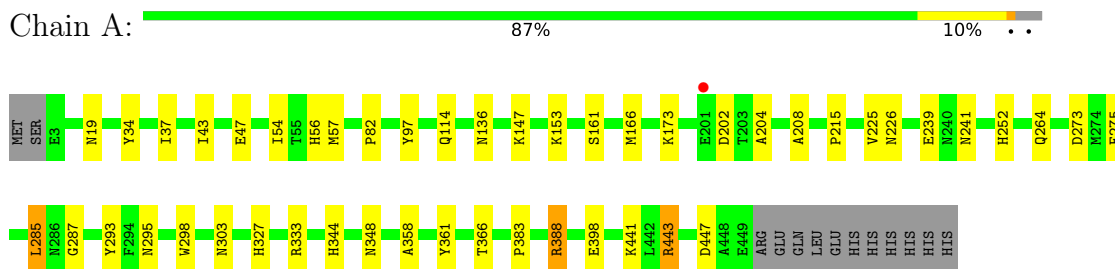
- Molecule 5 is water.

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		

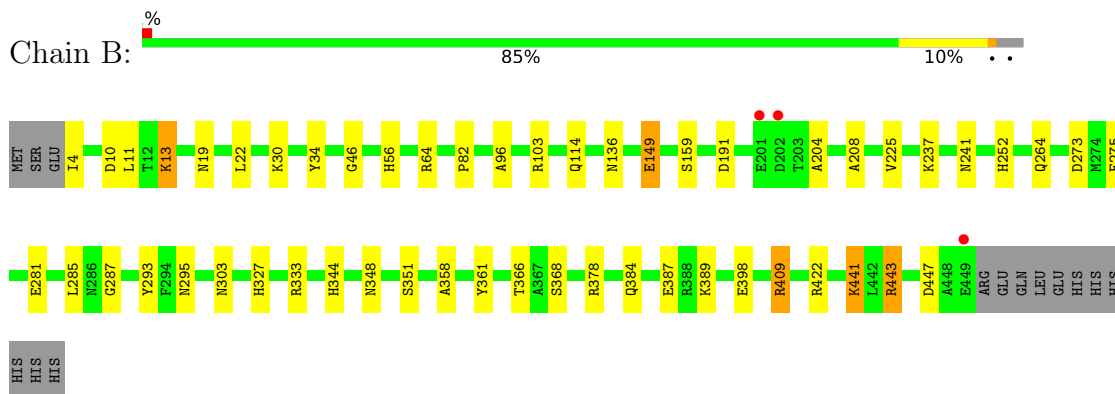
### 3 Residue-property plots

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.

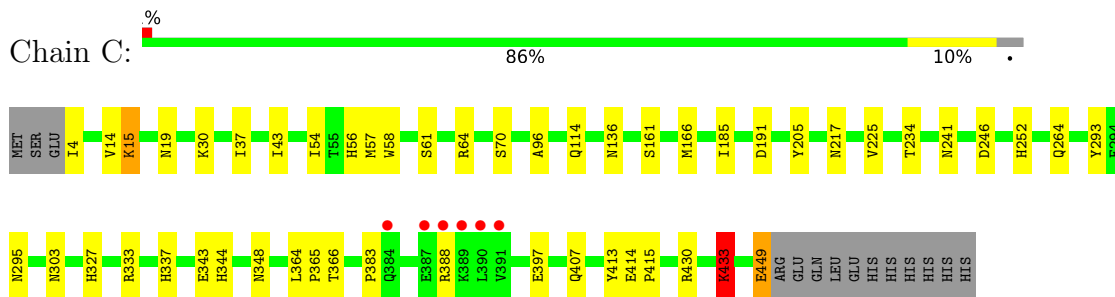
- Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)



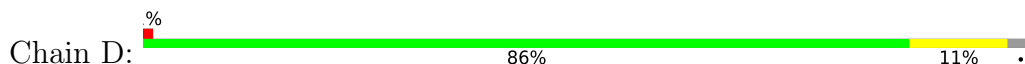
- Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)

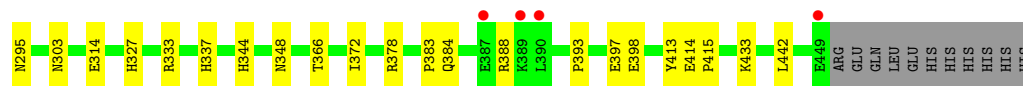


- Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)

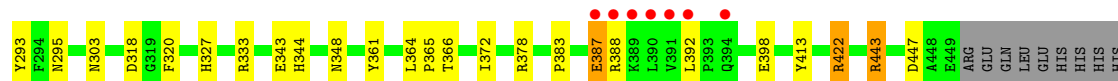
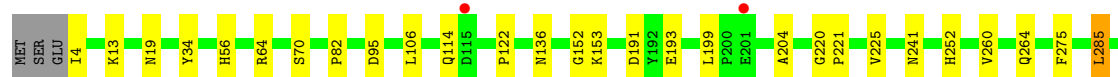
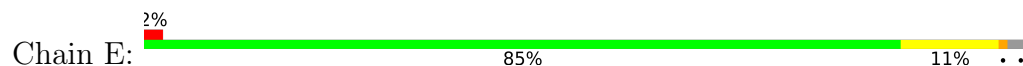


- Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)

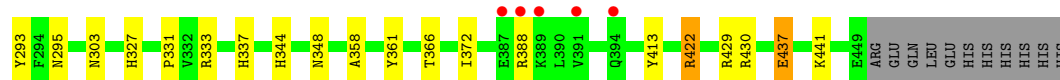
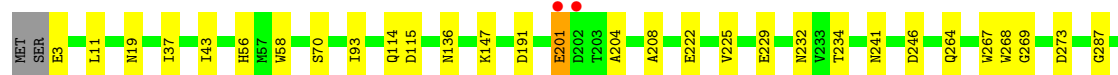
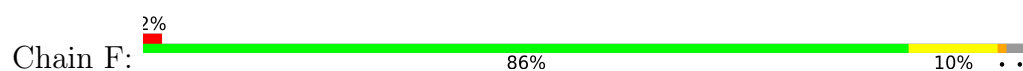




- Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)



- 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, $\alpha$ , $\beta$ , $\gamma$	98.55Å 156.97Å 100.91Å 90.00° 109.93° 90.00°	Depositor
Resolution (Å)	49.69 – 1.96 49.64 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.69-1.96) 99.9 (49.64-1.96)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	17.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TAR, MPD, CA

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	0.72	0/3744	0.88	3/5098 (0.1%)
1	B	0.72	0/3735	0.91	5/5086 (0.1%)
1	C	0.73	0/3735	0.85	1/5086 (0.0%)
1	D	0.72	2/3735 (0.1%)	0.85	0/5086
1	E	0.72	0/3735	0.85	2/5086 (0.0%)
1	F	0.74	1/3744 (0.0%)	0.89	5/5098 (0.1%)
All	All	0.72	3/22428 (0.0%)	0.87	16/30540 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	437	GLU	CD-OE2	5.60	1.31	1.25
1	D	213	GLU	CD-OE2	5.58	1.31	1.25
1	D	397	GLU	CD-OE2	5.41	1.31	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	409	ARG	NE-CZ-NH2	-11.93	114.33	120.30
1	B	409	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	B	443	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	B	443	ARG	NE-CZ-NH1	9.32	124.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	443	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	F	430	ARG	NE-CZ-NH1	-7.61	116.50	120.30
1	F	430	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	388	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	E	443	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	F	422	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	F	429	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	F	429	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	433	LYS	CB-CA-C	5.17	120.75	110.40
1	B	409	ARG	CD-NE-CZ	5.12	130.78	123.60
1	E	193	GLU	CB-CA-C	5.02	120.44	110.40

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 ⓘ

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	38	0
1	C	3619	0	3416	39	0
1	D	3619	0	3416	36	0
1	E	3619	0	3416	35	0
1	F	3628	0	3422	36	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	185	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 (185) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:318:ASP:C	5:E:776:HOH:O	2.41	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: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:F:201:GLU:H	1:F:201:GLU:CD	2.09	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:398:GLU:CD	5:A:601:HOH:O	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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%)	385 (99%)	3 (1%)	81	80
1	B	387/401 (96%)	378 (98%)	9 (2%)	50	42
1	C	387/401 (96%)	382 (99%)	5 (1%)	69	65
1	D	387/401 (96%)	379 (98%)	8 (2%)	53	46
1	E	387/401 (96%)	380 (98%)	7 (2%)	59	53
1	F	388/401 (97%)	382 (98%)	6 (2%)	65	60
All	All	2324/2406 (97%)	2286 (98%)	38 (2%)	62	58

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	LEU
1	A	388	ARG
1	A	441	LYS
1	B	13	LYS
1	B	149	GLU
1	B	159	SER
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	433	LYS
1	C	449	GLU
1	D	13	LYS
1	D	170	LYS
1	D	171	LYS
1	D	285	LEU
1	D	314	GLU
1	D	384	GLN
1	D	388	ARG
1	D	433	LYS
1	E	13	LYS
1	E	199	LEU
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	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 (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	27	GLN
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	384	GLN
1	A	400	GLN
1	B	19	ASN
1	B	56	HIS
1	B	114	GLN
1	B	232	ASN
1	B	252	HIS
1	B	264	GLN
1	B	303	ASN
1	B	327	HIS
1	B	348	ASN
1	C	19	ASN
1	C	27	GLN
1	C	56	HIS
1	C	114	GLN
1	C	143	ASN
1	C	189	ASN
1	C	226	ASN
1	C	252	HIS
1	C	264	GLN
1	C	303	ASN
1	C	327	HIS
1	C	337	HIS
1	C	348	ASN
1	D	19	ASN
1	D	56	HIS
1	D	77	ASN
1	D	114	GLN
1	D	143	ASN
1	D	226	ASN

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Mol	Chain	Res	Type
1	D	232	ASN
1	D	252	HIS
1	D	264	GLN
1	D	295	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	189	ASN
1	E	226	ASN
1	E	252	HIS
1	E	264	GLN
1	E	303	ASN
1	E	327	HIS
1	E	348	ASN
1	F	19	ASN
1	F	27	GLN
1	F	56	HIS
1	F	114	GLN
1	F	143	ASN
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	295	ASN
1	F	303	ASN
1	F	327	HIS
1	F	337	HIS
1	F	348	ASN

### 5.3.3 RNA ⓘ

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 monosaccharides 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	B	502	-	7,7,7	0.23	0	9,10,10	0.88	0
3	MPD	F	601	-	7,7,7	0.24	0	9,10,10	0.41	0
4	TAR	C	501	-	3,9,9	0.52	0	6,12,12	1.01	0
4	TAR	E	601	-	3,9,9	0.48	0	6,12,12	1.21	1 (16%)

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	B	502	-	-	0/5/5/5	-
3	MPD	F	601	-	-	0/5/5/5	-
4	TAR	C	501	-	-	1/4/12/12	-
4	TAR	E	601	-	-	1/4/12/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	601	TAR	C1-C2-C3	-2.42	107.90	113.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	MPD	3	0
3	F	601	MPD	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	447/460 (97%)	-0.39	1 (0%) 95 97	11, 16, 29, 70	0
1	B	446/460 (96%)	-0.41	3 (0%) 87 92	10, 16, 29, 71	0
1	C	446/460 (96%)	-0.42	6 (1%) 77 83	11, 16, 32, 64	0
1	D	446/460 (96%)	-0.43	4 (0%) 84 89	10, 15, 29, 67	0
1	E	446/460 (96%)	-0.37	9 (2%) 65 73	11, 17, 34, 64	0
1	F	447/460 (97%)	-0.33	7 (1%) 72 79	11, 18, 34, 71	0
All	All	2678/2760 (97%)	-0.39	30 (1%) 80 85	10, 16, 32, 71	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	389	LYS	6.2
1	D	389	LYS	4.5
1	F	387	GLU	4.4
1	A	201	GLU	4.2
1	B	201	GLU	4.0
1	F	201	GLU	4.0
1	F	389	LYS	3.9
1	E	389	LYS	3.6
1	E	387	GLU	3.6
1	C	387	GLU	3.4
1	C	391	VAL	3.4
1	E	201	GLU	3.0
1	D	449	GLU	3.0
1	D	387	GLU	2.9
1	C	390	LEU	2.9
1	D	390	LEU	2.8
1	E	391	VAL	2.8
1	F	391	VAL	2.7
1	E	115	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	202	ASP	2.5
1	B	449	GLU	2.5
1	C	384	GLN	2.4
1	E	394	GLN	2.4
1	F	388	ARG	2.4
1	B	202	ASP	2.4
1	E	388	ARG	2.3
1	E	392	LEU	2.3
1	C	388	ARG	2.1
1	E	390	LEU	2.1
1	F	394	GLN	2.1

## 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 monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MPD	B	502	8/8	0.63	0.27	43,52,53,55	0
4	TAR	C	501	10/10	0.86	0.24	39,44,45,50	0
4	TAR	E	601	10/10	0.86	0.22	38,51,54,59	0
3	MPD	F	601	8/8	0.92	0.14	28,29,33,35	0
2	CA	B	501	1/1	0.99	0.07	14,14,14,14	0
2	CA	E	602	1/1	1.00	0.05	12,12,12,12	0
2	CA	A	501	1/1	1.00	0.06	16,16,16,16	0
2	CA	C	502	1/1	1.00	0.08	12,12,12,12	0
2	CA	C	503	1/1	1.00	0.04	13,13,13,13	0
2	CA	D	801	1/1	1.00	0.08	11,11,11,11	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.