



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 10:45 AM JST

PDB ID : 5WXU  
Title : 11S globulin from *Wrightia tinctoria* reveals auxin binding site  
Authors : Kumar, P.; Kesari, P.; Dhindwal, S.; Kumar, P.  
Deposited on : 2017-01-09  
Resolution : 1.70 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

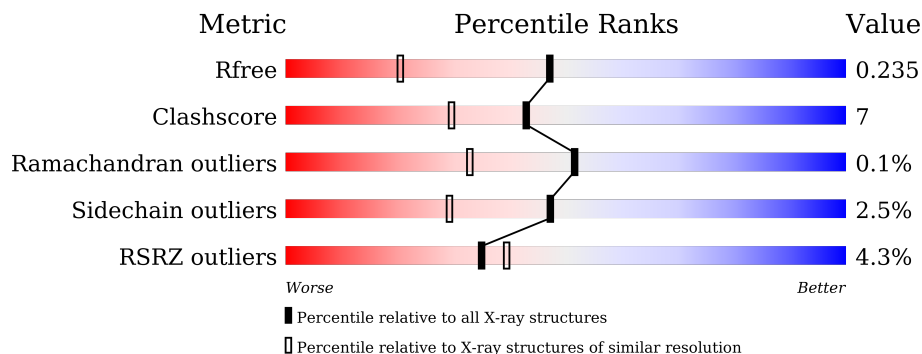
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	479	
1	B	479	
1	C	479	
1	D	479	
1	E	479	
1	F	479	

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	PO4	B	501	-	X	-	-
2	PO4	C	506	-	-	-	X
3	FLC	A	503	-	X	X	-
3	FLC	B	504	-	X	-	-
3	FLC	C	501	-	X	X	-
3	FLC	D	502	-	X	-	-
3	FLC	E	504	-	X	-	-
3	FLC	F	501	-	X	-	-
4	GOL	B	503	-	X	-	-
6	PEG	D	505	-	-	X	-
6	PEG	E	506	-	-	X	-
6	PEG	F	505	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21977 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 11S globulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	399	Total 3360	C 2102	N 620	O 631	S 7	0	20	0
1	B	400	Total 3281	C 2060	N 600	O 614	S 7	0	12	0
1	C	397	Total 3240	C 2035	N 595	O 603	S 7	0	9	0
1	D	396	Total 3192	C 2006	N 584	O 595	S 7	0	4	0
1	E	397	Total 3221	C 2020	N 590	O 604	S 7	0	6	0
1	F	398	Total 3264	C 2047	N 599	O 610	S 8	0	10	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	GLN	ARG	conflict	UNP A0A162EGL7
A	459	ASP	GLY	conflict	UNP A0A162EGL7
B	147	GLN	ARG	conflict	UNP A0A162EGL7
B	459	ASP	GLY	conflict	UNP A0A162EGL7
C	147	GLN	ARG	conflict	UNP A0A162EGL7
C	459	ASP	GLY	conflict	UNP A0A162EGL7
D	147	GLN	ARG	conflict	UNP A0A162EGL7
D	459	ASP	GLY	conflict	UNP A0A162EGL7
E	147	GLN	ARG	conflict	UNP A0A162EGL7
E	459	ASP	GLY	conflict	UNP A0A162EGL7
F	147	GLN	ARG	conflict	UNP A0A162EGL7
F	459	ASP	GLY	conflict	UNP A0A162EGL7

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



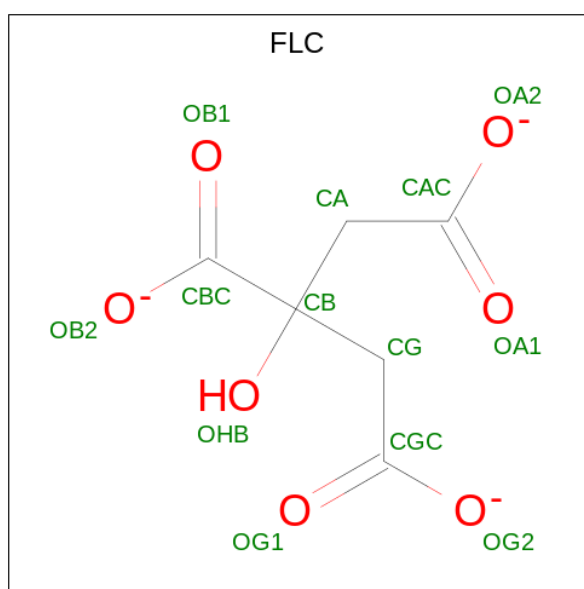
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



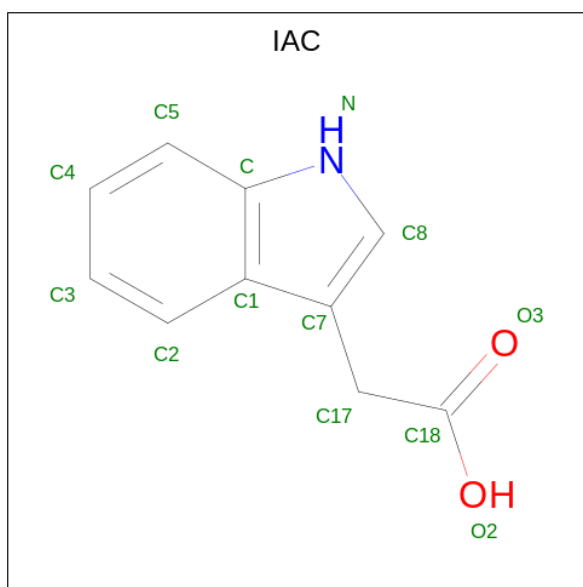
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



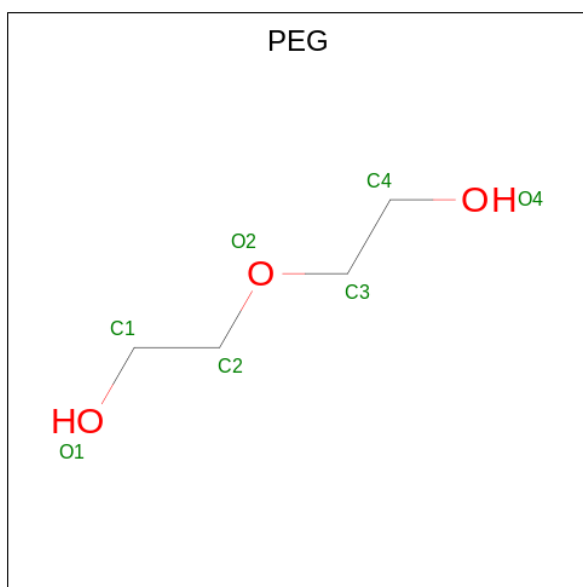
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

- Molecule 5 is 1H-INDOL-3-YLACETIC ACID (three-letter code: IAC) (formula: C<sub>10</sub>H<sub>9</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	26	20	2	4	0	1
5	B	1	26	20	2	4	0	1
5	D	1	26	20	2	4	0	1

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	D	1	7	4	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			7	4	3		
6	F	1	Total	C	O	0	0
			7	4	3		

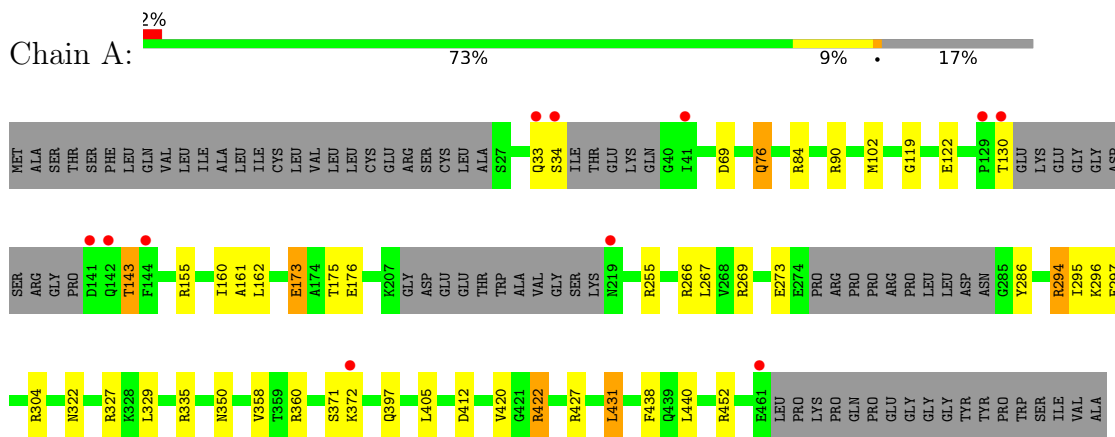
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	388	Total	O	0	0
			388	388		
7	B	346	Total	O	0	0
			346	346		
7	C	327	Total	O	0	0
			327	327		
7	D	339	Total	O	0	0
			339	339		
7	E	352	Total	O	0	0
			352	352		
7	F	346	Total	O	0	0
			346	346		

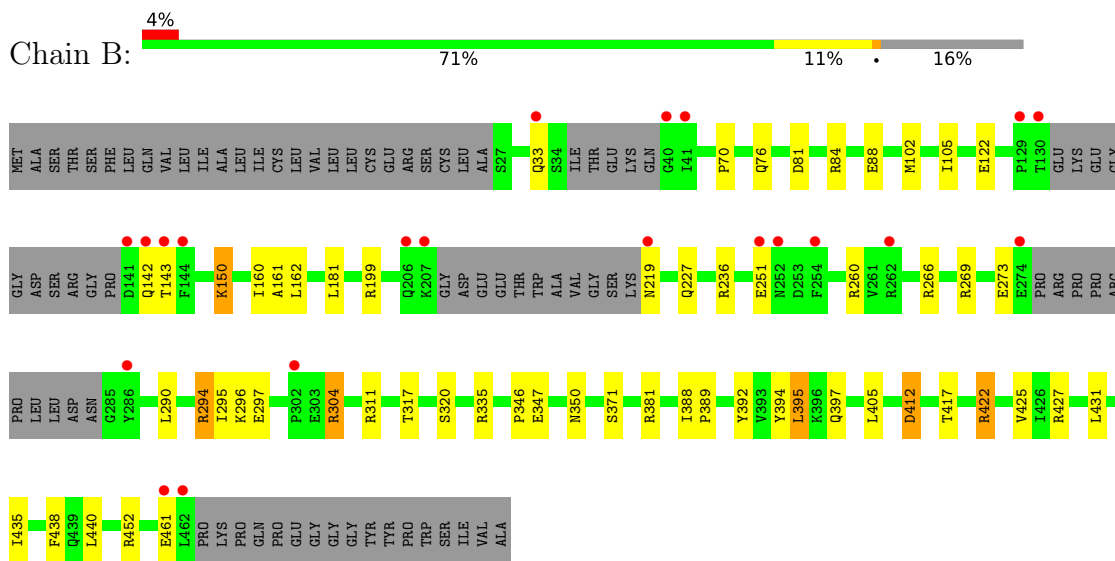
### 3 Residue-property plots [i](#)

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.

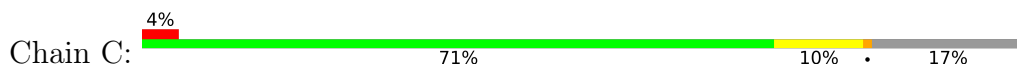
- Molecule 1: 11S globulin

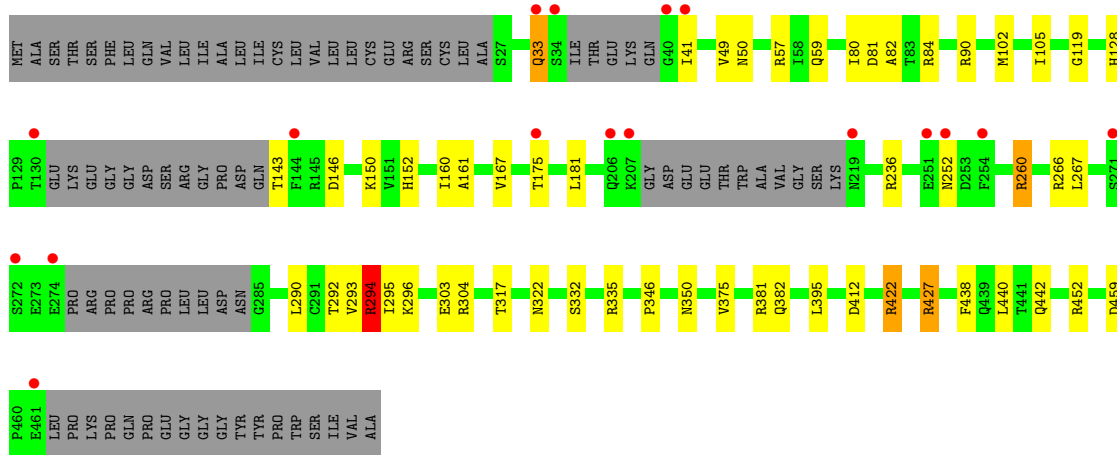


- Molecule 1: 11S globulin

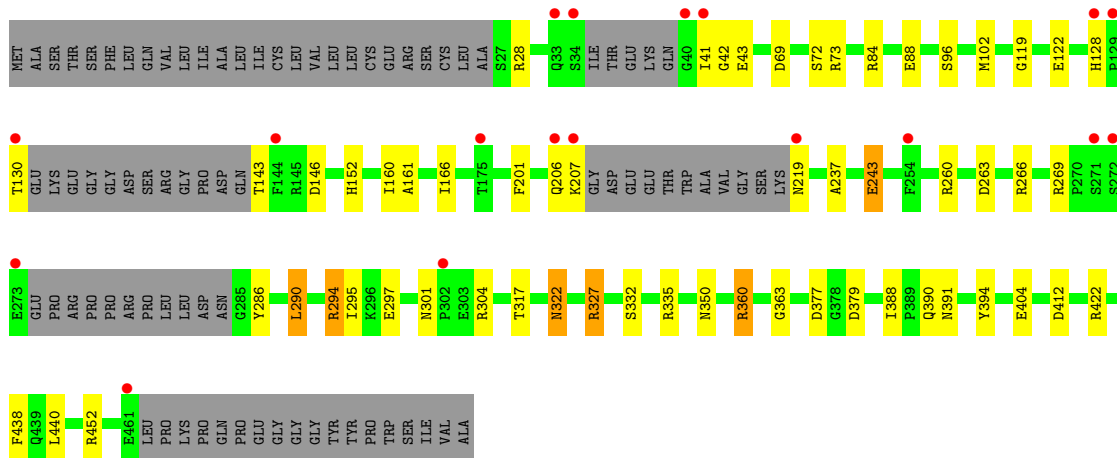


- Molecule 1: 11S globulin





• Molecule 1: 11S globulin

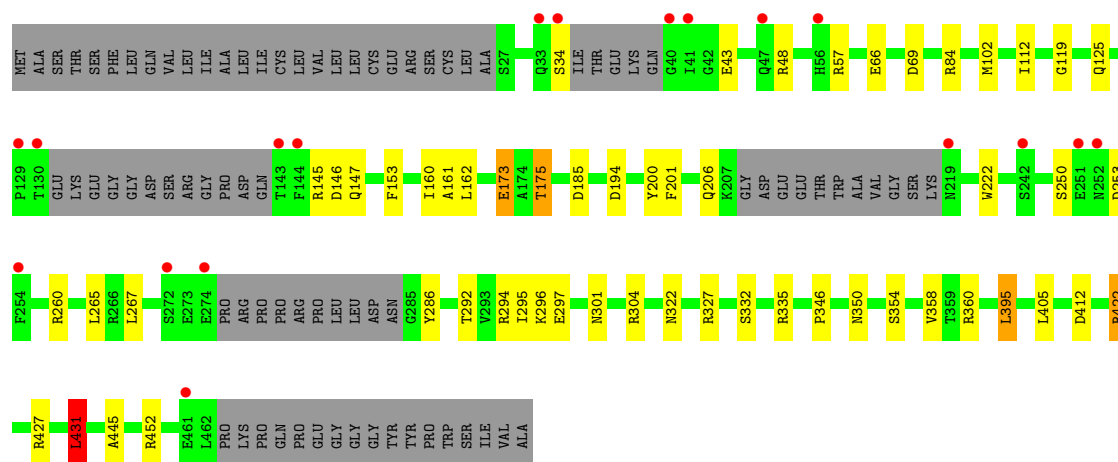


• Molecule 1: 11S globulin



- Molecule 1: 11S globulin

Chain F: 4% 71% 11% 17%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.21Å 114.24Å 202.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.24 – 1.70 31.42 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.2 (101.24-1.70) 94.3 (31.42-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.174 , 0.227 0.185 , 0.235	Depositor DCC
$R_{free}$ test set	13201 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtrriage
Anisotropy	0.445	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.009 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	21977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IAC, FLC, PO4, GOL, PEG

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	1.00	1/3425 (0.0%)	1.08	13/4641 (0.3%)
1	B	1.02	1/3360 (0.0%)	1.11	21/4556 (0.5%)
1	C	1.01	3/3316 (0.1%)	1.12	16/4495 (0.4%)
1	D	1.03	4/3259 (0.1%)	1.09	10/4420 (0.2%)
1	E	1.01	4/3285 (0.1%)	1.12	14/4454 (0.3%)
1	F	1.04	4/3328 (0.1%)	1.08	14/4512 (0.3%)
All	All	1.02	17/19973 (0.1%)	1.10	88/27078 (0.3%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	332	SER	CB-OG	-9.16	1.30	1.42
1	B	122	GLU	CD-OE2	7.75	1.34	1.25
1	D	122	GLU	CD-OE2	6.91	1.33	1.25
1	F	175	THR	CB-CG2	-6.62	1.30	1.52
1	D	332	SER	CB-OG	-6.61	1.33	1.42
1	C	412[A]	ASP	C-O	6.30	1.35	1.23
1	C	412[B]	ASP	C-O	6.30	1.35	1.23
1	E	354	SER	CB-OG	-5.92	1.34	1.42
1	E	332	SER	CB-OG	-5.82	1.34	1.42
1	E	242	SER	CB-OG	-5.70	1.34	1.42
1	D	322	ASN	CG-OD1	5.61	1.36	1.24
1	F	200	TYR	CB-CG	5.55	1.59	1.51
1	C	332	SER	CB-OG	-5.42	1.35	1.42
1	D	43	GLU	CD-OE1	5.40	1.31	1.25
1	A	122	GLU	CD-OE2	5.11	1.31	1.25
1	E	122	GLU	CD-OE2	5.07	1.31	1.25
1	F	43	GLU	CD-OE1	5.06	1.31	1.25

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	452	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	E	335	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	C	452	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	F	260	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	E	294[A]	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	E	294[B]	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	E	84	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	D	84	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	E	294[A]	ARG	NE-CZ-NH2	8.29	124.44	120.30
1	E	294[B]	ARG	NE-CZ-NH2	8.29	124.44	120.30
1	C	427[A]	ARG	NE-CZ-NH2	8.25	124.43	120.30
1	C	427[B]	ARG	NE-CZ-NH2	8.25	124.43	120.30
1	A	294[A]	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	A	294[B]	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	B	452	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	F	452	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	E	335	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	C	335	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	155	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	C	84	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	C	294[A]	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	C	294[B]	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	B	84	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	B	335	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	D	335	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	B	294[A]	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	294[B]	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	E	452	ARG	CG-CD-NE	7.01	126.52	111.80
1	E	199	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	69	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	A	335	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	C	146	ASP	CB-CG-OD1	6.67	124.31	118.30
1	B	412[A]	ASP	CB-CG-OD1	-6.67	112.30	118.30
1	B	412[B]	ASP	CB-CG-OD1	-6.67	112.30	118.30
1	F	422	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	F	422	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	E	422	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	F	146	ASP	CB-CG-OD1	6.40	124.06	118.30
1	F	84	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	D	335	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	377	ASP	CB-CG-OD1	6.23	123.91	118.30
1	D	260	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	294[A]	ARG	NE-CZ-NH2	-6.10	117.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	294[B]	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	255	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	199	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	84[A]	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	84[B]	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	422	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	F	395	LEU	CA-CB-CG	5.80	128.63	115.30
1	F	431	LEU	CA-CB-CG	5.74	128.50	115.30
1	C	335	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	422	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	C	422	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	431	LEU	CA-CB-CG	5.69	128.39	115.30
1	F	395	LEU	CB-CA-C	-5.68	99.41	110.20
1	B	395	LEU	CB-CA-C	-5.66	99.45	110.20
1	C	84	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	F	335	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	E	255	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	69	ASP	CB-CG-OD1	5.53	123.28	118.30
1	E	304	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	459	ASP	CB-CG-OD2	-5.50	113.36	118.30
1	F	69	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	D	377	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	B	431	LEU	CB-CG-CD2	5.48	120.31	111.00
1	B	381	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	E	343	MET	CG-SD-CE	5.45	108.92	100.20
1	E	48	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	D	146	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	69	ASP	CB-CG-OD1	5.34	123.11	118.30
1	F	145	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	260	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	431	LEU	CA-CB-CG	5.28	127.45	115.30
1	F	292	THR	CA-CB-CG2	-5.25	105.05	112.40
1	B	405	LEU	CA-CB-CG	5.24	127.34	115.30
1	B	422	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	294	ARG	CG-CD-NE	-5.16	100.97	111.80
1	B	122	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	B	335	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	304	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	335	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	F	185	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	B	84	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	422[A]	ARG	NE-CZ-NH1	-5.02	117.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422[B]	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	B	150[A]	LYS	CD-CE-NZ	5.02	123.24	111.70
1	B	150[B]	LYS	CD-CE-NZ	5.02	123.24	111.70

There are no chirality outliers.

There are no planarity outliers.

## 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	3360	0	3297	40	0
1	B	3281	0	3247	39	0
1	C	3240	0	3207	54	0
1	D	3192	0	3155	43	0
1	E	3221	0	3168	47	0
1	F	3264	0	3218	47	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
2	E	20	0	0	0	0
2	F	15	0	0	0	0
3	A	13	0	5	4	0
3	B	13	0	5	2	0
3	C	13	0	5	5	0
3	D	13	0	5	3	0
3	E	13	0	5	2	0
3	F	13	0	5	3	0
4	A	18	0	24	2	0
4	B	12	0	16	0	0
4	C	12	0	16	0	0
4	E	6	0	8	0	0
4	F	6	0	8	0	0
5	A	26	0	16	8	0
5	B	26	0	16	8	0
5	D	26	0	16	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	7	0	10	10	0
6	E	7	0	10	7	0
6	F	7	0	10	12	0
7	A	388	0	0	8	3
7	B	346	0	0	7	0
7	C	327	0	0	14	0
7	D	339	0	0	15	3
7	E	352	0	0	12	3
7	F	346	0	0	10	1
All	All	21977	0	19472	266	5

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 7.

All (266) 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:C:57[A]:ARG:HH21	1:C:59[A]:GLN:NE2	1.01	1.48
1:C:57[A]:ARG:NH2	1:C:59[A]:GLN:HE22	1.08	1.47
1:B:294[A]:ARG:NH2	1:B:297:GLU:OE1	1.75	1.20
1:E:84:ARG:HD2	7:E:747:HOH:O	1.53	1.04
1:C:57[A]:ARG:NH2	1:C:59[A]:GLN:NE2	1.79	1.01
1:C:292:THR:OG1	7:C:601:HOH:O	1.71	1.00
1:D:102:MET:CE	7:D:717:HOH:O	2.11	0.96
1:A:102:MET:HE3	1:A:162:LEU:HD12	1.51	0.93
1:D:42:GLY:N	7:D:603:HOH:O	2.00	0.93
1:B:295[B]:ILE:HG22	1:B:295[B]:ILE:O	1.71	0.91
1:C:102:MET:CE	7:C:644:HOH:O	2.19	0.91
1:F:102[B]:MET:SD	7:F:834:HOH:O	2.28	0.91
1:B:427[B]:ARG:NH2	7:B:601:HOH:O	1.83	0.88
1:E:422:ARG:HE	6:E:506:PEG:H21	1.39	0.88
1:F:422:ARG:HE	6:F:505:PEG:H12	1.36	0.88
1:D:102:MET:HE2	7:D:717:HOH:O	1.70	0.87
1:D:243:GLU:OE2	7:D:602:HOH:O	1.92	0.86
1:D:422:ARG:HE	6:D:505:PEG:H32	1.42	0.85
1:C:152:HIS:ND1	3:C:501:FLC:HG2	1.91	0.85
3:C:501:FLC:OB2	1:E:304:ARG:HA	1.78	0.84
1:C:102:MET:HE2	7:C:644:HOH:O	1.78	0.83
1:A:294[A]:ARG:NH2	1:F:294[A]:ARG:NH1	2.27	0.82
5:A:507[A]:IAC:H171	6:F:505:PEG:H21	1.60	0.81
1:F:173:GLU:HG3	7:F:732:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57[A]:ARG:CZ	1:C:59[A]:GLN:NE2	2.44	0.81
1:F:102[B]:MET:HE3	1:F:162:LEU:HD12	1.62	0.81
1:D:294:ARG:NH2	1:D:297:GLU:OE1	2.14	0.79
3:B:504:FLC:OB2	1:D:304:ARG:HA	1.82	0.79
1:F:422:ARG:HE	6:F:505:PEG:C1	1.95	0.79
1:B:102:MET:HE2	1:B:162:LEU:HB2	1.64	0.78
1:E:102:MET:CE	7:E:609:HOH:O	2.32	0.78
1:E:297:GLU:OE2	1:E:322[B]:ASN:ND2	2.16	0.78
1:F:297:GLU:OE1	1:F:322[B]:ASN:OD1	2.02	0.77
5:B:506[B]:IAC:O3	6:D:505:PEG:H42	1.85	0.77
1:D:327:ARG:NH1	1:D:412:ASP:OD2	2.17	0.76
1:D:422:ARG:NE	6:D:505:PEG:H32	2.01	0.76
1:B:88:GLU:OE1	1:B:260:ARG:NH2	2.18	0.75
1:A:102:MET:CE	1:A:162:LEU:HD12	2.16	0.75
1:E:304:ARG:HH21	1:E:322[B]:ASN:ND2	1.84	0.74
3:D:502:FLC:OHB	3:D:502:FLC:OG2	2.05	0.74
1:A:350[A]:ASN:O	7:A:601:HOH:O	2.06	0.73
1:E:304:ARG:HH21	1:E:322[B]:ASN:HD21	1.36	0.72
5:B:506[B]:IAC:C18	6:D:505:PEG:H42	2.19	0.72
1:A:294[A]:ARG:HH21	1:F:294[A]:ARG:NH1	1.87	0.72
5:A:507[A]:IAC:O3	6:F:505:PEG:H22	1.88	0.72
1:F:147:GLN:OE1	7:F:601:HOH:O	2.08	0.72
1:E:207:LYS:NZ	7:E:601:HOH:O	2.23	0.71
1:F:327:ARG:NH1	1:F:412:ASP:OD1	2.21	0.70
1:E:102:MET:HE3	7:E:609:HOH:O	1.90	0.69
6:F:505:PEG:O4	7:F:602:HOH:O	2.10	0.69
1:A:322[B]:ASN:ND2	7:A:605:HOH:O	2.25	0.68
1:B:161:ALA:O	1:B:295[B]:ILE:CG2	2.41	0.68
1:A:327:ARG:NH1	1:A:412:ASP:OD2	2.25	0.68
1:B:427[B]:ARG:NE	7:B:601:HOH:O	2.25	0.67
1:F:194:ASP:HB2	7:F:696:HOH:O	1.94	0.67
1:B:160:ILE:HG23	1:B:295[A]:ILE:HG22	1.77	0.67
1:E:304:ARG:NH2	1:E:322[B]:ASN:ND2	2.42	0.67
1:D:422:ARG:HE	6:D:505:PEG:C3	2.07	0.66
1:C:161:ALA:O	1:C:295[A]:ILE:HG23	1.96	0.66
1:C:33:GLN:HA	7:C:812:HOH:O	1.95	0.66
1:C:57[A]:ARG:HE	1:C:59[A]:GLN:NE2	1.94	0.66
1:C:350[B]:ASN:O	7:C:602:HOH:O	2.09	0.66
1:D:152:HIS:ND1	3:D:502:FLC:OG2	2.27	0.66
1:C:350[B]:ASN:CG	7:C:620:HOH:O	2.33	0.65
1:F:301[B]:ASN:OD1	1:F:301[B]:ASN:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ARG:HA	3:D:502:FLC:OB2	1.97	0.65
1:E:297:GLU:OE1	1:E:322[B]:ASN:OD1	2.15	0.65
1:B:317:THR:HB	7:B:630:HOH:O	1.95	0.65
5:D:506[B]:IAC:O2	6:E:506:PEG:H11	1.97	0.65
3:A:503:FLC:OB1	1:F:304:ARG:HA	1.98	0.64
1:E:422:ARG:NE	6:E:506:PEG:H21	2.11	0.63
1:C:57[A]:ARG:NE	1:C:59[A]:GLN:NE2	2.45	0.63
1:D:301:ASN:O	7:D:604:HOH:O	2.15	0.63
1:F:301[B]:ASN:ND2	7:F:606:HOH:O	2.30	0.63
1:B:435:ILE:CD1	1:C:143:THR:HG21	2.28	0.62
1:F:102[B]:MET:CE	1:F:162:LEU:HD12	2.29	0.62
1:C:150:LYS:HE2	7:C:746:HOH:O	1.98	0.62
1:D:161:ALA:O	1:D:295:ILE:HG23	2.00	0.62
1:E:422:ARG:HE	6:E:506:PEG:C2	2.12	0.61
1:C:82:ALA:N	7:C:612:HOH:O	2.34	0.61
1:A:297:GLU:OE1	1:A:322[B]:ASN:OD1	2.19	0.61
1:C:317:THR:OG1	7:C:603:HOH:O	2.16	0.61
1:D:119:GLY:O	5:D:506[B]:IAC:H5	2.01	0.61
1:F:350:ASN:O	7:F:603:HOH:O	2.16	0.61
1:D:143:THR:O	1:D:143:THR:OG1	2.18	0.61
1:C:57[A]:ARG:HE	1:C:59[A]:GLN:HE21	1.47	0.60
1:C:160:ILE:HG23	1:C:295[B]:ILE:HG23	1.84	0.60
1:E:295:ILE:O	1:E:295:ILE:HG22	2.00	0.59
1:A:422[A]:ARG:O	5:B:506[A]:IAC:H3	2.03	0.59
1:B:296:LYS:HE3	3:B:504:FLC:HG2	1.83	0.59
1:C:252:ASN:N	7:C:605:HOH:O	2.22	0.59
1:C:152:HIS:ND1	3:C:501:FLC:CG	2.66	0.59
1:B:161:ALA:O	1:B:295[B]:ILE:HG23	2.02	0.59
1:A:296:LYS:HG2	3:A:503:FLC:OG1	2.03	0.58
1:E:161:ALA:O	1:E:295:ILE:HG23	2.02	0.58
1:C:160:ILE:HG23	1:C:295[B]:ILE:CG2	2.33	0.58
1:F:102[B]:MET:HE3	1:F:162:LEU:CD1	2.34	0.58
1:D:237:ALA:O	1:E:452:ARG:HD3	2.04	0.58
1:C:296:LYS:HE3	3:C:501:FLC:HG1	1.86	0.58
1:C:422:ARG:HD2	6:F:505:PEG:H41	1.86	0.57
5:A:507[A]:IAC:H171	6:F:505:PEG:C2	2.32	0.57
1:F:160:ILE:HG23	1:F:295[B]:ILE:CG2	2.34	0.57
1:C:290:LEU:O	1:C:293[B]:VAL:HG23	2.04	0.57
1:A:161:ALA:O	1:A:295[A]:ILE:HG23	2.05	0.56
1:C:41:ILE:O	1:C:41:ILE:HG23	2.03	0.56
1:E:354:SER:HB3	7:E:700:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:ALA:O	1:F:295[A]:ILE:HG23	2.05	0.56
5:B:506[B]:IAC:C18	6:D:505:PEG:C4	2.83	0.56
1:C:57[A]:ARG:NE	1:C:59[A]:GLN:HE21	2.01	0.56
1:D:304:ARG:NH2	1:D:317:THR:O	2.35	0.56
5:A:507[A]:IAC:C18	1:C:422:ARG:O	2.53	0.55
1:F:346:PRO:HB3	1:F:395:LEU:HG	1.88	0.55
1:D:42:GLY:CA	7:D:603:HOH:O	2.47	0.55
1:E:296:LYS:HG2	3:E:504:FLC:OG2	2.06	0.55
1:F:422:ARG:NE	6:F:505:PEG:C1	2.68	0.55
1:E:327:ARG:NH1	1:E:412:ASP:OD1	2.38	0.54
1:A:427[B]:ARG:NH2	7:A:602:HOH:O	2.11	0.54
1:E:322[B]:ASN:OD1	1:E:322[B]:ASN:O	2.25	0.54
1:C:382:GLN:NE2	7:C:614:HOH:O	2.40	0.54
1:C:322:ASN:O	1:E:294[A]:ARG:HD3	2.08	0.53
1:E:427[B]:ARG:NH2	7:E:602:HOH:O	2.23	0.53
1:A:90[B]:ARG:NH2	7:A:609:HOH:O	2.42	0.53
1:B:150[B]:LYS:HE2	7:B:798:HOH:O	2.08	0.53
1:F:296:LYS:HE3	3:F:501:FLC:HG2	1.91	0.53
1:B:143:THR:HG21	1:B:266:ARG:CZ	2.40	0.52
1:B:347:GLU:HB2	1:B:417:THR:O	2.09	0.52
1:C:304:ARG:HA	3:E:504:FLC:OB1	2.10	0.52
1:D:206:GLN:N	7:D:612:HOH:O	2.40	0.51
1:A:175[A]:THR:HG22	4:A:506:GOL:H2	1.92	0.51
1:B:105:ILE:HD12	1:B:181:LEU:HD23	1.91	0.51
1:D:350:ASN:O	7:D:605:HOH:O	2.19	0.51
1:F:173:GLU:HB3	7:F:656:HOH:O	2.11	0.51
1:A:286[A]:TYR:CE1	1:E:290:LEU:HD21	2.46	0.51
1:A:427[B]:ARG:NE	7:A:602:HOH:O	2.40	0.51
1:A:173:GLU:HG3	7:A:620:HOH:O	2.11	0.51
1:E:422:ARG:HH21	6:E:506:PEG:H12	1.75	0.51
1:E:349:ASN:ND2	7:E:604:HOH:O	2.27	0.51
5:A:507[B]:IAC:C18	7:F:602:HOH:O	2.59	0.50
1:C:438:PHE:HB2	1:C:440:LEU:HG	1.93	0.50
1:B:304:ARG:NH2	1:B:317:THR:O	2.44	0.50
1:B:102:MET:HE2	1:B:162:LEU:CB	2.39	0.50
1:D:286:TYR:HB3	1:D:290:LEU:HD23	1.94	0.50
1:A:304:ARG:NH2	1:A:322[B]:ASN:ND2	2.60	0.50
1:C:119:GLY:O	5:D:506[A]:IAC:H5	2.11	0.50
1:C:293[A]:VAL:HG13	1:C:293[A]:VAL:O	2.11	0.50
1:C:160:ILE:HG23	1:C:295[A]:ILE:HG22	1.94	0.49
1:F:57[B]:ARG:HG2	1:F:57[B]:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ARG:O	5:D:506[B]:IAC:C18	2.61	0.49
6:D:505:PEG:O1	7:D:606:HOH:O	2.19	0.49
1:D:438:PHE:HB2	1:D:440:LEU:HG	1.94	0.49
1:B:143:THR:HG21	1:B:266:ARG:NE	2.27	0.49
1:D:295:ILE:HG22	1:D:295:ILE:O	2.12	0.49
1:F:358:VAL:HG22	1:F:405:LEU:CD2	2.43	0.48
1:B:311:ARG:HD2	1:D:128:HIS:CE1	2.48	0.48
1:F:296:LYS:HG2	3:F:501:FLC:OA1	2.13	0.48
1:F:422:ARG:NE	6:F:505:PEG:H11	2.27	0.48
1:A:143:THR:HG22	1:C:442:GLN:NE2	2.29	0.48
1:C:294[A]:ARG:NH1	3:C:501:FLC:OG1	2.47	0.48
1:E:86:VAL:HG22	1:E:179:VAL:HG22	1.95	0.48
1:C:143:THR:O	1:C:143:THR:OG1	2.24	0.48
1:D:160:ILE:HG23	1:D:295:ILE:HG22	1.96	0.48
1:E:422:ARG:NH2	6:E:506:PEG:H12	2.29	0.48
1:F:102[B]:MET:HE3	1:F:162:LEU:HB2	1.95	0.48
5:A:507[A]:IAC:C18	6:F:505:PEG:H22	2.44	0.47
1:A:294[A]:ARG:HG3	3:A:503:FLC:CGC	2.44	0.47
1:A:176:GLU:HG2	4:A:506:GOL:O1	2.14	0.47
1:A:422[A]:ARG:NH1	1:F:125:GLN:OE1	2.48	0.47
1:A:372:LYS:HG3	1:B:227:GLN:HB3	1.97	0.47
5:B:506[B]:IAC:H5	1:F:119:GLY:O	2.14	0.47
1:F:327:ARG:HD2	1:F:412:ASP:OD1	2.14	0.47
5:A:507[B]:IAC:H2	6:F:505:PEG:H21	1.96	0.47
1:C:350[B]:ASN:ND2	7:C:620:HOH:O	2.48	0.47
7:C:603:HOH:O	1:E:292:THR:HB	2.14	0.46
5:D:506[A]:IAC:C18	7:E:617:HOH:O	2.62	0.46
1:B:160:ILE:HG23	1:B:295[A]:ILE:CG2	2.44	0.46
1:B:294[A]:ARG:NH1	1:D:322:ASN:O	2.49	0.46
5:B:506[A]:IAC:H171	6:D:505:PEG:H31	1.97	0.46
1:E:431:LEU:HD22	1:E:445:ALA:HB1	1.98	0.46
1:A:397:GLN:OE1	1:B:236:ARG:NH2	2.49	0.46
3:A:503:FLC:CAC	7:A:738:HOH:O	2.64	0.46
1:F:57[A]:ARG:NH2	1:F:66:GLU:OE2	2.49	0.46
1:C:90[A]:ARG:HB2	1:C:90[A]:ARG:NH1	2.31	0.45
1:C:105:ILE:HD12	1:C:181:LEU:HD23	1.99	0.45
1:E:422:ARG:HH21	6:E:506:PEG:C1	2.29	0.45
1:A:143:THR:HG23	1:A:266:ARG:NH1	2.32	0.45
1:C:304:ARG:NH2	1:C:317:THR:O	2.41	0.45
1:A:295[A]:ILE:O	1:A:295[A]:ILE:HG22	2.17	0.45
5:B:506[A]:IAC:O3	6:D:505:PEG:H11	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:LEU:N	1:E:202:LEU:HD12	2.32	0.45
1:E:322[B]:ASN:OD1	1:E:322[B]:ASN:C	2.54	0.45
1:E:160:ILE:HG23	1:E:295:ILE:HG22	1.98	0.45
1:B:320:SER:OG	1:B:412[B]:ASP:OD1	2.30	0.44
1:B:388:ILE:HD13	1:B:394:TYR:CD2	2.51	0.44
1:B:425:VAL:HG21	1:C:167:VAL:HG21	1.98	0.44
1:D:96:SER:HB3	1:D:201:PHE:CD2	2.52	0.44
1:E:207:LYS:NZ	7:E:618:HOH:O	2.48	0.44
1:E:92:LEU:O	1:E:258:MET:HA	2.17	0.44
1:C:128:HIS:CD2	1:E:311:ARG:HD2	2.52	0.44
1:F:295[B]:ILE:CG2	1:F:295[B]:ILE:O	2.64	0.44
1:A:119:GLY:O	5:A:507[B]:IAC:H5	2.18	0.44
1:D:102:MET:HE1	7:D:717:HOH:O	2.01	0.44
1:D:263:ASP:N	7:D:601:HOH:O	1.76	0.44
1:E:70:PRO:HB3	1:E:81[A]:ASP:OD1	2.17	0.44
1:E:304:ARG:NH2	1:E:322[B]:ASN:HD22	2.15	0.44
1:D:143:THR:HG23	1:D:266:ARG:CZ	2.48	0.44
1:B:397:GLN:OE1	1:C:236:ARG:NH1	2.51	0.44
1:C:422:ARG:CD	6:F:505:PEG:H41	2.48	0.44
1:D:388:ILE:HD13	1:D:394:TYR:CD2	2.53	0.44
1:E:427[B]:ARG:NE	7:E:602:HOH:O	2.44	0.44
1:D:390:GLN:O	1:D:391:ASN:HB2	2.18	0.43
1:A:360:ARG:NH1	7:A:624:HOH:O	2.52	0.43
1:D:143:THR:HG23	1:D:266:ARG:NH2	2.32	0.43
1:F:427[C]:ARG:NH2	7:F:630:HOH:O	2.51	0.43
1:C:143:THR:HG23	1:C:266:ARG:NH2	2.33	0.43
1:C:143:THR:HG23	1:C:266:ARG:CZ	2.47	0.43
1:C:49:VAL:HG22	1:C:375:VAL:HG12	2.01	0.43
1:E:84:ARG:CD	7:E:747:HOH:O	2.35	0.43
1:E:200:TYR:HB3	1:E:225:VAL:CG1	2.48	0.43
5:B:506[A]:IAC:C18	7:D:606:HOH:O	2.67	0.43
1:F:201:PHE:CE1	1:F:222:TRP:NE1	2.87	0.43
1:A:294[A]:ARG:NH2	1:F:294[A]:ARG:HH11	2.12	0.42
1:F:112:ILE:CD1	1:F:153:PHE:CE2	3.02	0.42
1:E:96:SER:HB3	1:E:201:PHE:CD2	2.54	0.42
1:F:265:LEU:CD2	1:F:267:LEU:HD21	2.49	0.42
1:F:431:LEU:HD22	1:F:445:ALA:HB1	2.02	0.42
1:E:231:PRO:HA	1:E:245:ILE:HG21	2.01	0.42
1:F:304:ARG:NH2	1:F:322[B]:ASN:ND2	2.67	0.42
1:D:166:ILE:N	7:D:615:HOH:O	2.52	0.42
1:A:420:VAL:CG1	1:A:452:ARG:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294[A]:ARG:HH21	1:F:294[A]:ARG:HH11	1.62	0.42
1:A:438:PHE:HB2	1:A:440:LEU:HG	2.01	0.42
1:B:294[A]:ARG:NH1	1:D:294:ARG:NH2	2.68	0.42
1:B:294[A]:ARG:HH12	1:D:294:ARG:HE	1.66	0.42
1:D:422:ARG:HH21	6:D:505:PEG:C4	2.33	0.42
1:A:273:GLU:O	1:F:360:ARG:NH2	2.53	0.42
1:A:358:VAL:HG22	1:A:405:LEU:CD2	2.49	0.42
1:D:360:ARG:HB2	1:D:404:GLU:HB3	2.02	0.42
1:E:295:ILE:O	1:E:295:ILE:CG2	2.67	0.42
1:B:219:ASN:N	7:B:619:HOH:O	2.53	0.41
1:A:160:ILE:HG23	1:A:295[B]:ILE:HG23	2.03	0.41
1:B:273:GLU:O	1:D:360:ARG:NH2	2.52	0.41
1:B:70:PRO:HB3	1:B:81:ASP:OD1	2.21	0.41
1:C:346:PRO:HB3	1:C:395:LEU:HG	2.03	0.41
1:B:346:PRO:HB3	1:B:395:LEU:HG	2.03	0.41
1:B:389:PRO:HB2	1:B:392:TYR:CD1	2.56	0.41
1:B:438:PHE:HB2	1:B:440:LEU:HG	2.03	0.41
1:D:363:GLY:O	1:D:379:ASP:HA	2.21	0.41
1:F:250:SER:OG	1:F:253:ASP:HB3	2.20	0.41
1:A:143:THR:HG22	1:C:442:GLN:CD	2.41	0.41
1:A:267:LEU:C	1:A:267:LEU:HD12	2.41	0.41
1:D:28:ARG:HD2	7:E:631:HOH:O	2.20	0.41
1:D:219:ASN:N	7:D:635:HOH:O	2.54	0.41
1:F:160:ILE:HG23	1:F:295[A]:ILE:HG22	2.03	0.41
1:E:33:GLN:HA	1:E:33:GLN:OE1	2.20	0.41
1:A:161:ALA:HB1	1:A:329:LEU:HD12	2.02	0.40
1:A:294[A]:ARG:NH2	1:F:294[A]:ARG:CZ	2.83	0.40
1:B:290[B]:LEU:HD12	1:F:286:TYR:CZ	2.56	0.40
7:C:603:HOH:O	1:E:292:THR:CB	2.68	0.40
1:F:295[B]:ILE:O	1:F:295[B]:ILE:HG23	2.22	0.40
1:A:33:GLN:HB3	1:A:76:GLN:HE22	1.86	0.40
1:C:303:GLU:HB3	1:E:153:PHE:CD1	2.56	0.40
3:F:501:FLC:OG1	3:F:501:FLC:OHB	2.39	0.40
1:D:41:ILE:HG13	7:D:603:HOH:O	2.21	0.40

All (5) 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)
7:D:746:HOH:O	7:E:883:HOH:O[4_556]	1.46	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:868:HOH:O	7:F:750:HOH:O[3_545]	1.58	0.62
7:D:858:HOH:O	7:E:883:HOH:O[4_556]	1.94	0.26
7:A:898:HOH:O	7:E:651:HOH:O[2_454]	2.08	0.12
7:A:898:HOH:O	7:D:601:HOH:O[2_454]	2.17	0.03

## 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	409/479 (85%)	393 (96%)	16 (4%)	0	100	100
1	B	402/479 (84%)	385 (96%)	16 (4%)	1 (0%)	47	30
1	C	396/479 (83%)	384 (97%)	12 (3%)	0	100	100
1	D	390/479 (81%)	378 (97%)	12 (3%)	0	100	100
1	E	393/479 (82%)	378 (96%)	13 (3%)	2 (0%)	29	13
1	F	398/479 (83%)	382 (96%)	16 (4%)	0	100	100
All	All	2388/2874 (83%)	2300 (96%)	85 (4%)	3 (0%)	51	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	41	ILE
1	B	33	GLN
1	E	193	LEU

### 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	369/416 (89%)	360 (98%)	9 (2%)	49	31
1	B	362/416 (87%)	354 (98%)	8 (2%)	52	34
1	C	356/416 (86%)	344 (97%)	12 (3%)	37	18
1	D	350/416 (84%)	340 (97%)	10 (3%)	42	23
1	E	353/416 (85%)	343 (97%)	10 (3%)	43	25
1	F	358/416 (86%)	351 (98%)	7 (2%)	55	38
All	All	2148/2496 (86%)	2092 (97%)	56 (3%)	47	28

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	76	GLN
1	A	130	THR
1	A	143	THR
1	A	173	GLU
1	A	269	ARG
1	A	371[A]	SER
1	A	371[B]	SER
1	A	431	LEU
1	B	76	GLN
1	B	142	GLN
1	B	251	GLU
1	B	269	ARG
1	B	350[A]	ASN
1	B	350[B]	ASN
1	B	371	SER
1	B	461	GLU
1	C	33	GLN
1	C	50	ASN
1	C	80	ILE
1	C	81	ASP
1	C	175	THR
1	C	260	ARG
1	C	267	LEU
1	C	294[A]	ARG
1	C	294[B]	ARG
1	C	381	ARG
1	C	427[A]	ARG

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Mol	Chain	Res	Type
1	C	427[B]	ARG
1	D	72	SER
1	D	73	ARG
1	D	88	GLU
1	D	130	THR
1	D	207	LYS
1	D	243	GLU
1	D	269	ARG
1	D	290	LEU
1	D	327	ARG
1	D	360	ARG
1	E	33	GLN
1	E	34	SER
1	E	48	ARG
1	E	175	THR
1	E	262	ARG
1	E	269	ARG
1	E	354	SER
1	E	360	ARG
1	E	371	SER
1	E	452	ARG
1	F	34	SER
1	F	48	ARG
1	F	173	GLU
1	F	175	THR
1	F	206	GLN
1	F	354	SER
1	F	431	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	GLN
1	B	76	GLN
1	B	142	GLN
1	C	382	GLN
1	D	128	HIS
1	D	223	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

42 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	PO4	C	505	-	4,4,4	1.28	0	6,6,6	2.03	3 (50%)
2	PO4	E	502	-	4,4,4	1.29	0	6,6,6	1.07	1 (16%)
6	PEG	E	506	-	6,6,6	0.85	0	5,5,5	1.18	0
3	FLC	F	501	-	12,12,12	1.84	3 (25%)	17,17,17	5.92	11 (64%)
2	PO4	D	501	-	4,4,4	0.76	0	6,6,6	1.70	2 (33%)
2	PO4	E	507	-	4,4,4	0.78	0	6,6,6	0.59	0
3	FLC	E	504	-	12,12,12	1.40	2 (16%)	17,17,17	4.92	13 (76%)
5	IAC	B	506[B]	-	13,14,14	1.46	2 (15%)	14,19,19	1.06	0
6	PEG	D	505	-	6,6,6	0.96	0	5,5,5	1.92	3 (60%)
2	PO4	B	501	-	4,4,4	2.32	1 (25%)	6,6,6	2.46	3 (50%)
2	PO4	B	502	-	4,4,4	0.91	0	6,6,6	1.69	1 (16%)
5	IAC	B	506[A]	-	13,14,14	1.34	1 (7%)	14,19,19	1.53	3 (21%)
3	FLC	A	503	-	12,12,12	1.67	3 (25%)	17,17,17	4.81	12 (70%)
3	FLC	D	502	-	12,12,12	1.59	2 (16%)	17,17,17	4.41	9 (52%)
2	PO4	D	504	-	4,4,4	0.72	0	6,6,6	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	B	507	-	5,5,5	0.88	0	5,5,5	0.66	0
2	PO4	A	501	-	4,4,4	1.32	1 (25%)	6,6,6	1.30	0
2	PO4	F	504	-	4,4,4	1.10	0	6,6,6	1.57	1 (16%)
5	IAC	A	507[B]	-	13,14,14	1.49	1 (7%)	14,19,19	1.06	1 (7%)
2	PO4	A	502	-	4,4,4	0.41	0	6,6,6	1.30	1 (16%)
4	GOL	A	506	-	5,5,5	0.50	0	5,5,5	0.36	0
2	PO4	F	502	-	4,4,4	1.03	0	6,6,6	1.33	0
2	PO4	E	505	-	4,4,4	0.71	0	6,6,6	1.10	1 (16%)
4	GOL	B	503	-	5,5,5	1.63	2 (40%)	5,5,5	1.72	2 (40%)
5	IAC	A	507[A]	-	13,14,14	1.60	2 (15%)	14,19,19	1.31	2 (14%)
5	IAC	D	506[B]	-	13,14,14	1.43	2 (15%)	14,19,19	1.12	1 (7%)
4	GOL	E	503	-	5,5,5	0.54	0	5,5,5	0.63	0
2	PO4	F	503	-	4,4,4	0.91	0	6,6,6	1.90	2 (33%)
4	GOL	A	504	-	5,5,5	0.38	0	5,5,5	0.46	0
5	IAC	D	506[A]	-	13,14,14	1.49	2 (15%)	14,19,19	1.20	2 (14%)
4	GOL	F	506	-	5,5,5	0.85	0	5,5,5	0.78	0
2	PO4	E	501	-	4,4,4	1.22	1 (25%)	6,6,6	1.59	1 (16%)
2	PO4	D	503	-	4,4,4	0.86	0	6,6,6	0.39	0
3	FLC	B	504	-	12,12,12	1.96	5 (41%)	17,17,17	5.42	10 (58%)
3	FLC	C	501	-	12,12,12	1.75	1 (8%)	17,17,17	4.66	12 (70%)
4	GOL	A	505	-	5,5,5	0.66	0	5,5,5	0.54	0
4	GOL	C	502	-	5,5,5	0.63	0	5,5,5	0.75	0
4	GOL	C	503	-	5,5,5	0.59	0	5,5,5	0.82	0
2	PO4	B	505	-	4,4,4	0.96	0	6,6,6	2.02	2 (33%)
2	PO4	C	504	-	4,4,4	0.91	0	6,6,6	1.14	0
2	PO4	C	506	-	4,4,4	0.85	0	6,6,6	0.34	0
6	PEG	F	505	-	6,6,6	1.08	1 (16%)	5,5,5	2.15	2 (40%)

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
6	PEG	E	506	-	-	3/4/4/4	-
3	FLC	F	501	-	-	11/16/16/16	-
5	IAC	B	506[B]	-	-	2/4/4/4	0/2/2/2
3	FLC	E	504	-	-	9/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	D	505	-	-	2/4/4/4	-
5	IAC	B	506[A]	-	-	2/4/4/4	0/2/2/2
3	FLC	D	502	-	-	10/16/16/16	-
3	FLC	A	503	-	-	14/16/16/16	-
4	GOL	B	507	-	-	2/4/4/4	-
5	IAC	A	507[B]	-	-	0/4/4/4	0/2/2/2
4	GOL	A	506	-	-	2/4/4/4	-
4	GOL	B	503	-	-	4/4/4/4	-
5	IAC	A	507[A]	-	-	2/4/4/4	0/2/2/2
5	IAC	D	506[B]	-	-	0/4/4/4	0/2/2/2
4	GOL	E	503	-	-	3/4/4/4	-
4	GOL	A	504	-	-	1/4/4/4	-
5	IAC	D	506[A]	-	-	0/4/4/4	0/2/2/2
4	GOL	F	506	-	-	2/4/4/4	-
3	FLC	B	504	-	-	9/16/16/16	-
3	FLC	C	501	-	-	9/16/16/16	-
4	GOL	A	505	-	-	4/4/4/4	-
4	GOL	C	502	-	-	2/4/4/4	-
4	GOL	C	503	-	-	4/4/4/4	-
6	PEG	F	505	-	-	1/4/4/4	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PO4	P-O1	4.57	1.61	1.50
3	C	501	FLC	OHB-CB	4.24	1.51	1.43
3	D	502	FLC	OHB-CB	3.92	1.50	1.43
3	F	501	FLC	CG-CB	3.55	1.58	1.53
3	A	503	FLC	CG-CB	-3.26	1.49	1.53
3	B	504	FLC	OHB-CB	3.24	1.49	1.43
3	B	504	FLC	CB-CBC	3.16	1.56	1.53
5	D	506[A]	IAC	C5-C	-3.10	1.36	1.41
5	D	506[B]	IAC	C5-C	-2.94	1.36	1.41
5	B	506[A]	IAC	C5-C	-2.72	1.37	1.41
3	F	501	FLC	CB-CBC	-2.70	1.50	1.53
5	A	507[A]	IAC	O2-C18	-2.67	1.21	1.30
3	E	504	FLC	OHB-CB	2.65	1.48	1.43
3	B	504	FLC	OG1-CGC	2.61	1.30	1.22
5	A	507[B]	IAC	C5-C	-2.57	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	506[B]	IAC	C2-C1	-2.54	1.37	1.42
3	B	504	FLC	CG-CB	2.53	1.57	1.53
5	A	507[A]	IAC	C5-C	-2.49	1.37	1.41
3	A	503	FLC	CB-CBC	-2.44	1.50	1.53
3	A	503	FLC	CG-CGC	2.35	1.57	1.50
5	B	506[B]	IAC	C5-C	-2.35	1.37	1.41
3	B	504	FLC	OA1-CAC	2.30	1.29	1.22
3	F	501	FLC	OG1-CGC	2.25	1.29	1.22
4	B	503	GOL	C1-C2	2.22	1.60	1.51
6	F	505	PEG	O1-C1	2.19	1.53	1.42
5	D	506[B]	IAC	C2-C1	-2.12	1.37	1.42
3	D	502	FLC	OB1-CBC	2.12	1.29	1.22
5	D	506[A]	IAC	C1-C	2.04	1.48	1.42
2	E	501	PO4	P-O1	2.04	1.55	1.50
2	A	501	PO4	P-O1	2.03	1.55	1.50
4	B	503	GOL	O1-C1	2.03	1.51	1.42
3	E	504	FLC	CB-CBC	-2.03	1.51	1.53

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	501	FLC	OHB-CB-CBC	-16.00	86.40	108.86
3	B	504	FLC	OHB-CB-CBC	-12.71	91.02	108.86
3	E	504	FLC	OHB-CB-CBC	-12.62	91.15	108.86
3	B	504	FLC	OHB-CB-CG	-12.41	80.36	109.40
3	A	503	FLC	CG-CB-CA	10.50	136.57	109.16
3	A	503	FLC	OHB-CB-CA	-10.14	85.67	109.40
3	D	502	FLC	OHB-CB-CA	-9.36	87.49	109.40
3	D	502	FLC	OHB-CB-CBC	-9.20	95.95	108.86
3	C	501	FLC	OHB-CB-CA	-8.86	88.67	109.40
3	F	501	FLC	OHB-CB-CA	-8.62	89.22	109.40
3	C	501	FLC	OHB-CB-CG	-8.51	89.49	109.40
3	C	501	FLC	CG-CB-CA	8.37	131.00	109.16
3	F	501	FLC	OHB-CB-CG	-8.34	89.88	109.40
3	B	504	FLC	CG-CB-CBC	8.11	127.53	110.11
3	E	504	FLC	OHB-CB-CA	-7.95	90.81	109.40
3	F	501	FLC	OB1-CBC-CB	-7.86	111.12	122.25
3	E	504	FLC	OHB-CB-CG	-7.58	91.67	109.40
3	F	501	FLC	CG-CB-CBC	7.39	125.98	110.11
3	D	502	FLC	OHB-CB-CG	-6.73	93.65	109.40
3	A	503	FLC	OG2-CGC-CG	6.29	134.55	114.35
3	B	504	FLC	OHB-CB-CA	-6.17	94.97	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	FLC	CG-CB-CA	6.11	125.11	109.16
3	C	501	FLC	OB2-CBC-CB	5.77	123.07	113.05
3	A	503	FLC	OB2-CBC-CB	5.48	122.57	113.05
3	E	504	FLC	CA-CB-CBC	5.38	121.66	110.11
3	D	502	FLC	CA-CB-CBC	5.30	121.49	110.11
3	C	501	FLC	OHB-CB-CBC	-5.21	101.55	108.86
3	B	504	FLC	OB2-CBC-CB	5.09	121.89	113.05
3	E	504	FLC	CB-CG-CGC	4.94	125.78	113.81
3	A	503	FLC	OG1-CGC-CG	-4.67	109.31	122.94
3	F	501	FLC	CG-CB-CA	4.58	121.10	109.16
3	C	501	FLC	CB-CA-CAC	4.53	124.77	113.81
3	F	501	FLC	CB-CA-CAC	-4.39	103.19	113.81
3	E	504	FLC	CG-CB-CBC	4.35	119.46	110.11
3	A	503	FLC	OHB-CB-CG	-4.25	99.47	109.40
3	C	501	FLC	CA-CB-CBC	4.21	119.15	110.11
2	B	501	PO4	O3-P-O2	-3.86	95.57	107.97
3	D	502	FLC	OB2-CBC-CB	3.80	119.65	113.05
3	E	504	FLC	CG-CB-CA	3.68	118.75	109.16
6	F	505	PEG	O2-C2-C1	3.66	126.13	110.07
3	B	504	FLC	OG2-CGC-OG1	3.63	132.34	123.30
3	A	503	FLC	CA-CB-CBC	3.55	117.74	110.11
3	A	503	FLC	OB1-CBC-CB	-3.54	117.25	122.25
5	B	506[A]	IAC	C2-C1-C	3.50	122.81	118.17
3	E	504	FLC	OB2-CBC-CB	3.44	119.02	113.05
3	B	504	FLC	CA-CB-CBC	3.43	117.48	110.11
3	D	502	FLC	OA1-CAC-CA	-3.41	112.99	122.94
3	C	501	FLC	OG1-CGC-CG	-3.40	113.00	122.94
3	A	503	FLC	CG-CB-CBC	-3.38	102.84	110.11
3	F	501	FLC	CB-CG-CGC	3.34	121.91	113.81
3	A	503	FLC	OHB-CB-CBC	-3.33	104.19	108.86
2	F	503	PO4	O2-P-O1	-3.33	98.73	110.89
3	C	501	FLC	OG2-CGC-CG	3.29	124.90	114.35
3	C	501	FLC	OB1-CBC-CB	-3.26	117.64	122.25
3	D	502	FLC	OB1-CBC-CB	-3.12	117.83	122.25
2	B	505	PO4	O3-P-O2	-3.09	98.05	107.97
2	B	505	PO4	O4-P-O3	3.05	117.76	107.97
2	B	502	PO4	O3-P-O1	-3.04	99.75	110.89
5	A	507[A]	IAC	C17-C7-C1	3.02	132.41	126.50
6	F	505	PEG	O1-C1-C2	2.94	128.85	111.81
2	C	505	PO4	O3-P-O1	2.93	121.61	110.89
3	F	501	FLC	OB2-CBC-CB	2.91	118.09	113.05
2	F	504	PO4	O4-P-O3	2.89	117.26	107.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	PO4	O2-P-O1	2.89	121.47	110.89
3	A	503	FLC	OG2-CGC-OG1	-2.89	116.10	123.30
3	B	504	FLC	OB2-CBC-OB1	-2.84	114.79	123.82
2	B	501	PO4	O4-P-O3	-2.83	98.89	107.97
3	E	504	FLC	OA1-CAC-CA	-2.83	114.68	122.94
5	D	506[B]	IAC	C17-C7-C1	2.66	131.72	126.50
2	C	505	PO4	O2-P-O1	-2.66	101.17	110.89
3	E	504	FLC	OG2-CGC-OG1	-2.62	116.77	123.30
2	C	505	PO4	O4-P-O2	-2.59	99.65	107.97
3	C	501	FLC	OA2-CAC-CA	2.59	122.66	114.35
5	D	506[A]	IAC	O2-C18-O3	-2.52	117.01	123.30
2	D	501	PO4	O4-P-O1	-2.50	101.75	110.89
2	E	501	PO4	O4-P-O2	-2.48	100.02	107.97
5	A	507[B]	IAC	C17-C7-C1	2.48	131.35	126.50
5	A	507[A]	IAC	O2-C18-O3	-2.47	117.15	123.30
3	B	504	FLC	OG1-CGC-CG	-2.45	115.77	122.94
6	D	505	PEG	O1-C1-C2	2.44	125.99	111.81
3	C	501	FLC	OA1-CAC-CA	-2.41	115.91	122.94
3	E	504	FLC	OB1-CBC-CB	-2.33	118.95	122.25
5	B	506[A]	IAC	C3-C2-C1	-2.33	117.66	120.89
4	B	503	GOL	C3-C2-C1	2.31	120.70	111.70
6	D	505	PEG	O2-C2-C1	2.31	120.23	110.07
3	D	502	FLC	OA2-CAC-OA1	2.26	128.94	123.30
6	D	505	PEG	O2-C3-C4	2.26	120.00	110.07
3	F	501	FLC	OA2-CAC-CA	2.26	121.60	114.35
2	D	501	PO4	O4-P-O2	2.24	115.17	107.97
3	A	503	FLC	OA2-CAC-CA	2.22	121.47	114.35
5	B	506[A]	IAC	C5-C-C1	-2.21	116.72	120.76
3	E	504	FLC	CB-CA-CAC	2.20	119.14	113.81
3	F	501	FLC	OB2-CBC-OB1	2.19	130.78	123.82
3	E	504	FLC	OG1-CGC-CG	2.17	129.29	122.94
3	B	504	FLC	CG-CB-CA	2.17	114.81	109.16
2	E	505	PO4	O3-P-O2	2.12	114.78	107.97
2	E	502	PO4	O4-P-O2	2.11	114.73	107.97
5	D	506[A]	IAC	O2-C18-C17	2.10	122.00	114.02
2	A	502	PO4	O4-P-O2	2.08	114.65	107.97
2	F	503	PO4	O4-P-O3	2.04	114.52	107.97
4	B	503	GOL	O1-C1-C2	2.02	119.91	110.20

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	FLC	CA-CB-CBC-OB1
3	A	503	FLC	CA-CB-CBC-OB2
3	A	503	FLC	OHB-CB-CBC-OB1
3	A	503	FLC	OHB-CB-CBC-OB2
3	A	503	FLC	CA-CB-CG-CGC
3	B	504	FLC	CA-CB-CBC-OB1
3	B	504	FLC	CA-CB-CBC-OB2
3	B	504	FLC	CG-CB-CBC-OB1
3	B	504	FLC	CG-CB-CBC-OB2
3	B	504	FLC	OHB-CB-CBC-OB1
3	B	504	FLC	OHB-CB-CBC-OB2
3	C	501	FLC	OHB-CB-CBC-OB1
3	C	501	FLC	OHB-CB-CBC-OB2
3	D	502	FLC	CA-CB-CBC-OB2
3	D	502	FLC	CG-CB-CBC-OB1
3	D	502	FLC	CG-CB-CBC-OB2
3	D	502	FLC	OHB-CB-CBC-OB1
3	D	502	FLC	OHB-CB-CBC-OB2
3	D	502	FLC	CA-CB-CG-CGC
3	E	504	FLC	CA-CB-CBC-OB1
3	E	504	FLC	CA-CB-CBC-OB2
3	E	504	FLC	CG-CB-CBC-OB1
3	E	504	FLC	CG-CB-CBC-OB2
3	E	504	FLC	OHB-CB-CBC-OB1
3	E	504	FLC	OHB-CB-CBC-OB2
3	E	504	FLC	CA-CB-CG-CGC
3	F	501	FLC	CAC-CA-CB-CBC
3	F	501	FLC	CA-CB-CBC-OB1
3	F	501	FLC	CA-CB-CBC-OB2
3	F	501	FLC	CG-CB-CBC-OB1
3	F	501	FLC	CG-CB-CBC-OB2
3	F	501	FLC	OHB-CB-CBC-OB1
3	F	501	FLC	OHB-CB-CBC-OB2
3	F	501	FLC	CA-CB-CG-CGC
4	A	505	GOL	O1-C1-C2-O2
4	A	505	GOL	O1-C1-C2-C3
4	A	505	GOL	C1-C2-C3-O3
4	B	503	GOL	O1-C1-C2-C3
4	B	503	GOL	C1-C2-C3-O3
4	B	507	GOL	C1-C2-C3-O3
4	C	502	GOL	C1-C2-C3-O3
4	C	503	GOL	O1-C1-C2-C3
4	F	506	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	504	FLC	CAC-CA-CB-CG
3	B	504	FLC	CBC-CB-CG-CGC
3	B	504	FLC	OHB-CB-CG-CGC
4	A	506	GOL	O1-C1-C2-O2
6	D	505	PEG	O2-C3-C4-O4
6	E	506	PEG	O1-C1-C2-O2
6	F	505	PEG	O2-C3-C4-O4
3	A	503	FLC	OHB-CB-CG-CGC
3	C	501	FLC	CA-CB-CG-CGC
3	F	501	FLC	OHB-CB-CG-CGC
4	A	504	GOL	C1-C2-C3-O3
4	A	506	GOL	O1-C1-C2-C3
4	C	503	GOL	C1-C2-C3-O3
4	E	503	GOL	C1-C2-C3-O3
3	A	503	FLC	CG-CB-CBC-OB2
4	B	507	GOL	O2-C2-C3-O3
4	C	502	GOL	O2-C2-C3-O3
4	C	503	GOL	O1-C1-C2-O2
3	C	501	FLC	CAC-CA-CB-CG
3	E	504	FLC	CAC-CA-CB-CBC
4	B	503	GOL	O1-C1-C2-O2
4	B	503	GOL	O2-C2-C3-O3
4	F	506	GOL	O1-C1-C2-O2
3	A	503	FLC	CAC-CA-CB-CG
3	D	502	FLC	OHB-CB-CG-CGC
3	D	502	FLC	CA-CB-CBC-OB1
6	D	505	PEG	O1-C1-C2-O2
4	A	505	GOL	O2-C2-C3-O3
6	E	506	PEG	O2-C3-C4-O4
4	C	503	GOL	O2-C2-C3-O3
4	E	503	GOL	O1-C1-C2-O2
4	E	503	GOL	O2-C2-C3-O3
3	A	503	FLC	CAC-CA-CB-OHB
3	C	501	FLC	OHB-CB-CG-CGC
5	B	506[A]	IAC	C7-C17-C18-O3
5	B	506[A]	IAC	C7-C17-C18-O2
5	B	506[B]	IAC	C7-C17-C18-O2
6	E	506	PEG	C1-C2-O2-C3
3	A	503	FLC	CBC-CB-CG-CGC
3	D	502	FLC	CAC-CA-CB-CG
3	F	501	FLC	CAC-CA-CB-OHB
5	A	507[A]	IAC	C7-C17-C18-O2

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Mol	Chain	Res	Type	Atoms
5	B	506[B]	IAC	C7-C17-C18-O3
3	D	502	FLC	CAC-CA-CB-CBC
5	A	507[A]	IAC	C7-C17-C18-O3
3	F	501	FLC	CAC-CA-CB-CG
3	A	503	FLC	CB-CA-CAC-OA1
3	C	501	FLC	CG-CB-CBC-OB1
3	C	501	FLC	CG-CB-CBC-OB2
3	A	503	FLC	CB-CA-CAC-OA2
3	A	503	FLC	CB-CG-CGC-OG1
3	C	501	FLC	CB-CA-CAC-OA1
3	A	503	FLC	CB-CG-CGC-OG2
3	C	501	FLC	CB-CA-CAC-OA2
3	E	504	FLC	CAC-CA-CB-CG

There are no ring outliers.

16 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	506	PEG	7	0
3	F	501	FLC	3	0
3	E	504	FLC	2	0
5	B	506[B]	IAC	4	0
6	D	505	PEG	10	0
5	B	506[A]	IAC	4	0
3	A	503	FLC	4	0
3	D	502	FLC	3	0
5	A	507[B]	IAC	3	0
4	A	506	GOL	2	0
5	A	507[A]	IAC	5	0
5	D	506[B]	IAC	3	0
5	D	506[A]	IAC	2	0
3	B	504	FLC	2	0
3	C	501	FLC	5	0
6	F	505	PEG	12	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	399/479 (83%)	-0.08	11 (2%) 53 57	14, 21, 42, 69	0
1	B	400/479 (83%)	0.00	21 (5%) 26 29	15, 23, 50, 85	0
1	C	397/479 (82%)	0.01	17 (4%) 35 39	15, 24, 47, 75	0
1	D	396/479 (82%)	0.01	18 (4%) 33 37	15, 23, 42, 98	0
1	E	397/479 (82%)	-0.04	17 (4%) 35 39	15, 23, 49, 75	0
1	F	398/479 (83%)	-0.05	18 (4%) 33 37	15, 22, 47, 77	0
All	All	2387/2874 (83%)	-0.02	102 (4%) 35 39	14, 23, 46, 98	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	40	GLY	10.2
1	D	130	THR	7.9
1	B	130	THR	7.4
1	A	41	ILE	6.8
1	D	144	PHE	6.7
1	C	41	ILE	6.7
1	D	272	SER	6.5
1	B	142	GLN	6.4
1	F	41	ILE	6.1
1	F	130	THR	5.7
1	B	141	ASP	5.5
1	E	130	THR	5.4
1	C	130	THR	5.3
1	B	41	ILE	5.2
1	E	41	ILE	5.2
1	A	130	THR	5.2
1	D	41	ILE	5.0
1	F	34	SER	5.0
1	B	40	GLY	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	34	SER	5.0
1	C	144	PHE	4.8
1	C	219	ASN	4.8
1	C	272	SER	4.6
1	A	141	ASP	4.6
1	D	129	PRO	4.2
1	A	33	GLN	4.1
1	A	219	ASN	3.9
1	E	219	ASN	3.9
1	B	274	GLU	3.9
1	D	33	GLN	3.8
1	C	34	SER	3.7
1	E	262	ARG	3.7
1	B	462	LEU	3.7
1	B	144	PHE	3.7
1	E	144	PHE	3.7
1	F	143	THR	3.7
1	D	207	LYS	3.7
1	D	271	SER	3.7
1	B	33	GLN	3.6
1	F	33	GLN	3.6
1	F	274	GLU	3.6
1	E	34	SER	3.6
1	C	40	GLY	3.4
1	D	206	GLN	3.3
1	D	461	GLU	3.3
1	D	40	GLY	3.3
1	A	34	SER	3.3
1	A	144	PHE	3.3
1	C	274	GLU	3.3
1	A	142	GLN	3.2
1	D	273	GLU	3.1
1	B	461	GLU	3.1
1	C	252	ASN	3.1
1	D	128	HIS	3.0
1	F	56	HIS	3.0
1	F	219	ASN	3.0
1	B	129	PRO	3.0
1	B	219	ASN	2.9
1	E	143	THR	2.9
1	F	144	PHE	2.8
1	E	263	ASP	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	461	GLU	2.8
1	D	219	ASN	2.7
1	A	461	GLU	2.7
1	D	254	PHE	2.7
1	E	207	LYS	2.7
1	B	302	PRO	2.7
1	F	252	ASN	2.6
1	C	461	GLU	2.6
1	E	274	GLU	2.6
1	B	252	ASN	2.6
1	F	272	SER	2.6
1	B	207	LYS	2.5
1	F	461	GLU	2.5
1	B	206	GLN	2.5
1	B	262	ARG	2.5
1	C	271	SER	2.5
1	B	254	PHE	2.5
1	E	272	SER	2.4
1	E	129	PRO	2.4
1	B	251	GLU	2.4
1	B	143	THR	2.4
1	E	47	GLN	2.4
1	F	251	GLU	2.3
1	E	206	GLN	2.3
1	F	242	SER	2.3
1	C	175	THR	2.3
1	D	302	PRO	2.3
1	C	251	GLU	2.3
1	C	33	GLN	2.2
1	F	40	GLY	2.2
1	C	207	LYS	2.2
1	A	129	PRO	2.2
1	B	286	TYR	2.1
1	F	47	GLN	2.1
1	F	129	PRO	2.1
1	C	254	PHE	2.1
1	F	254	PHE	2.1
1	C	206	GLN	2.1
1	D	175	THR	2.1
1	E	33	GLN	2.1
1	A	372	LYS	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 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
2	PO4	E	507	5/5	0.42	0.31	76,78,99,101	0
4	GOL	A	506	6/6	0.49	0.27	49,61,63,67	0
4	GOL	B	503	6/6	0.55	0.24	40,55,58,58	0
2	PO4	D	503	5/5	0.56	0.39	100,101,114,121	0
3	FLC	F	501	13/13	0.64	0.32	37,55,63,78	0
2	PO4	C	506	5/5	0.65	0.53	101,107,122,124	0
3	FLC	C	501	13/13	0.70	0.28	33,51,67,67	0
3	FLC	B	504	13/13	0.70	0.34	36,57,68,79	0
3	FLC	D	502	13/13	0.72	0.27	31,51,68,74	0
4	GOL	C	502	6/6	0.73	0.25	37,56,59,67	0
2	PO4	D	504	5/5	0.75	0.21	89,98,102,102	0
3	FLC	E	504	13/13	0.76	0.32	44,66,83,95	0
6	PEG	E	506	7/7	0.76	0.17	28,38,44,46	0
4	GOL	F	506	6/6	0.77	0.24	39,52,54,55	0
3	FLC	A	503	13/13	0.77	0.29	33,59,82,87	0
4	GOL	B	507	6/6	0.79	0.27	34,49,51,51	0
2	PO4	E	505	5/5	0.79	0.25	68,86,92,93	0
4	GOL	A	505	6/6	0.80	0.17	45,51,60,62	0
4	GOL	E	503	6/6	0.84	0.14	47,50,53,54	0
4	GOL	C	503	6/6	0.85	0.23	43,54,66,73	0
6	PEG	D	505	7/7	0.85	0.17	35,36,44,44	0
4	GOL	A	504	6/6	0.85	0.13	35,47,50,52	0
6	PEG	F	505	7/7	0.86	0.14	28,34,41,42	0
2	PO4	B	501	5/5	0.92	0.11	26,35,45,48	0
2	PO4	C	505	5/5	0.94	0.13	33,42,48,50	0
2	PO4	E	501	5/5	0.95	0.08	32,39,45,51	0
5	IAC	B	506[A]	13/13	0.95	0.12	21,23,25,26	13

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	IAC	B	506[B]	13/13	0.95	0.12	21,21,22,22	13
5	IAC	A	507[B]	13/13	0.96	0.12	23,24,29,32	13
2	PO4	F	504	5/5	0.96	0.20	45,46,54,55	0
2	PO4	D	501	5/5	0.96	0.08	34,35,46,46	0
2	PO4	A	501	5/5	0.96	0.08	30,33,37,37	0
2	PO4	F	503	5/5	0.96	0.08	34,42,44,45	0
5	IAC	A	507[A]	13/13	0.96	0.12	20,21,24,29	13
5	IAC	D	506[B]	13/13	0.97	0.10	19,20,23,23	13
2	PO4	B	505	5/5	0.97	0.17	37,38,45,52	0
2	PO4	B	502	5/5	0.97	0.20	30,32,40,43	0
5	IAC	D	506[A]	13/13	0.97	0.10	20,20,22,26	13
2	PO4	F	502	5/5	0.98	0.18	35,37,47,47	0
2	PO4	A	502	5/5	0.98	0.14	34,34,41,43	0
2	PO4	C	504	5/5	0.98	0.15	35,36,47,48	0
2	PO4	E	502	5/5	0.99	0.17	35,39,44,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.