



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 08:19 PM EDT

PDB ID : 1EX0  
Title : HUMAN FACTOR XIII, MUTANT W279F ZYMOGEN  
Authors : Garzon, R.J.; Pratt, K.P.; Bishop, P.D.; Le Trong, I.; Stenkamp, R.E.; Teller, D.C.  
Deposited on : unknown  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

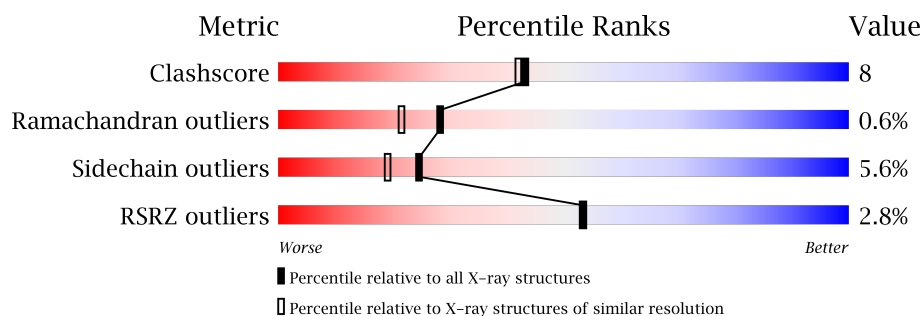
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	731	
1	B	731	

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
4	PGO	A	1340	-	-	-	X
4	PGO	A	1341	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PGO	B	1343	-	-	-	X
4	PGO	B	1344	-	-	-	X
4	PGO	B	1345	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12770 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 COAGULATION FACTOR XIII A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	705	Total	C	N	O	S	0	2	0
			5673	3595	980	1072	26			
1	B	716	Total	C	N	O	S	0	2	0
			5744	3638	993	1086	27			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SAC	SER	MODIFIED RESIDUE	UNP P00488
A	35	ASN	VAL	CONFLICT	UNP P00488
A	36	LEU	PRO	CONFLICT	UNP P00488
A	279	PHE	TRP	ENGINEERED	UNP P00488
A	509	SER	GLU	CONFLICT	UNP P00488
A	510	ARG	GLY	CONFLICT	UNP P00488
B	1	SAC	SER	MODIFIED RESIDUE	UNP P00488
B	35	ASN	VAL	CONFLICT	UNP P00488
B	36	LEU	PRO	CONFLICT	UNP P00488
B	279	PHE	TRP	ENGINEERED	UNP P00488
B	509	SER	GLU	CONFLICT	UNP P00488
B	510	ARG	GLY	CONFLICT	UNP P00488
B	511	SER	VAL	CONFLICT	UNP P00488

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

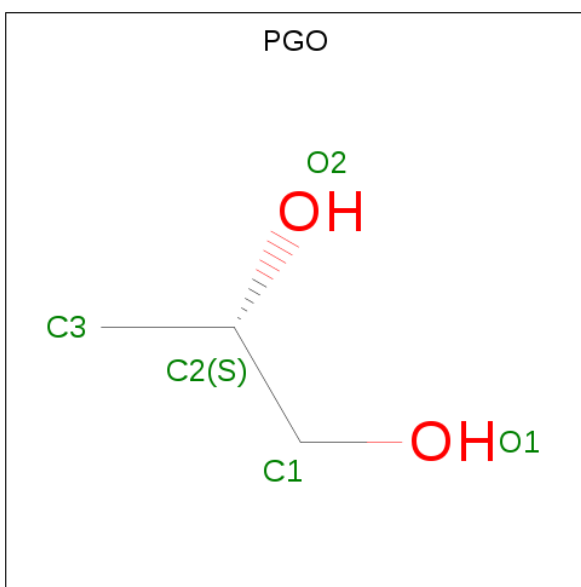
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			5	3	2		
4	B	1	Total	C	O	0	0
			5	3	2		
4	B	1	Total	C	O	0	0
			5	3	2		
4	B	1	Total	C	O	0	0
			5	3	2		

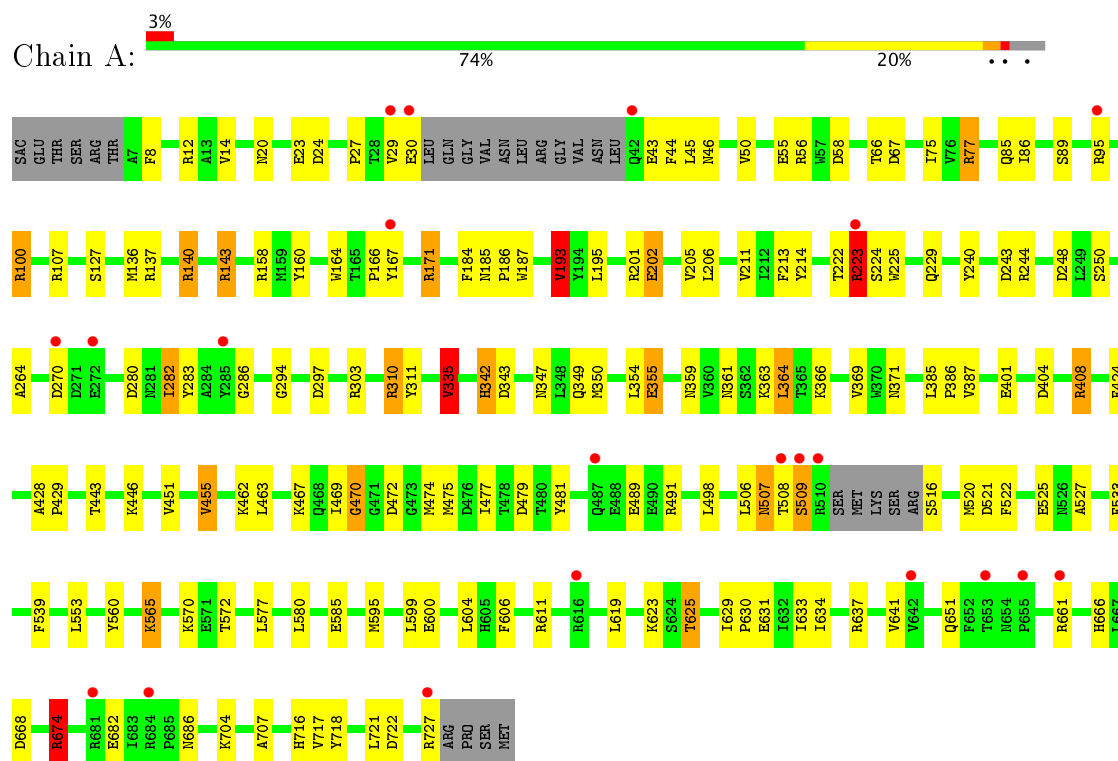
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	554	Total	O	0	0
			554	554		
5	B	752	Total	O	0	0
			752	752		

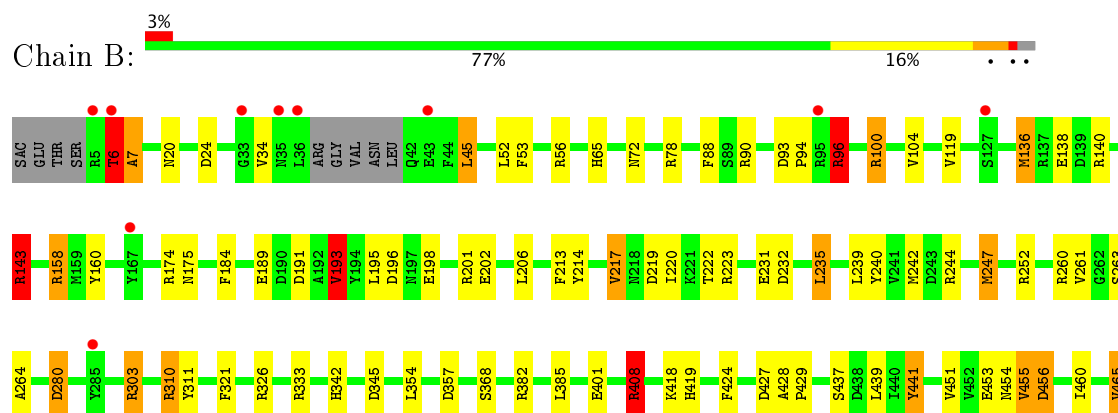
### 3 Residue-property plots

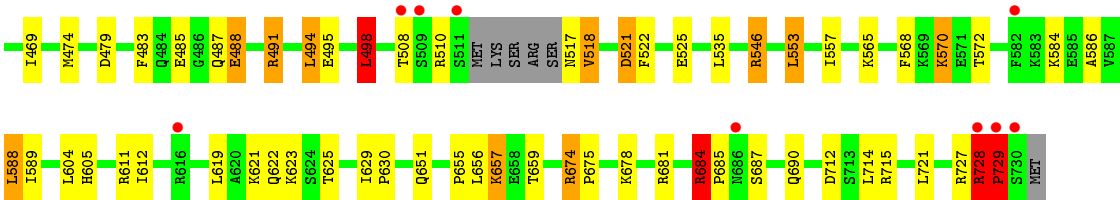
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: COAGULATION FACTOR XIII A CHAIN



#### • Molecule 1: COAGULATION FACTOR XIII A CHAIN







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.54Å 70.64Å 133.38Å 90.00° 106.08° 90.00°	Depositor
Resolution (Å)	19.94 – 2.00 28.51 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.94-2.00) 94.5 (28.51-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 1.79Å)	Xtriage
Refinement program	REFMAC V 3.5	Depositor
R, $R_{free}$	0.187 , 0.234 0.186 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12770	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: PGO, CA, PO4

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	0.60	0/5805	1.42	63/7874 (0.8%)
1	B	0.70	0/5877	1.49	77/7973 (1.0%)
All	All	0.65	0/11682	1.46	140/15847 (0.9%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	95	ARG	CD-NE-CZ	21.46	153.65	123.60
1	A	223[A]	ARG	NE-CZ-NH1	17.62	129.11	120.30
1	A	223[B]	ARG	NE-CZ-NH1	17.62	129.11	120.30
1	B	491	ARG	CD-NE-CZ	17.23	147.73	123.60
1	B	303	ARG	CD-NE-CZ	14.82	144.35	123.60
1	B	143	ARG	CD-NE-CZ	13.74	142.84	123.60
1	B	491	ARG	NE-CZ-NH2	-13.70	113.45	120.30
1	B	100	ARG	NE-CZ-NH1	13.38	126.99	120.30
1	A	223[A]	ARG	NE-CZ-NH2	-13.00	113.80	120.30
1	A	223[B]	ARG	NE-CZ-NH2	-13.00	113.80	120.30
1	A	95	ARG	NE-CZ-NH1	12.65	126.63	120.30
1	A	223[A]	ARG	CD-NE-CZ	12.61	141.26	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223[B]	ARG	CD-NE-CZ	12.61	141.26	123.60
1	A	303	ARG	CD-NE-CZ	11.82	140.15	123.60
1	A	56	ARG	NE-CZ-NH2	-11.73	114.44	120.30
1	B	143	ARG	NE-CZ-NH2	-11.57	114.52	120.30
1	A	303	ARG	NE-CZ-NH2	-11.26	114.67	120.30
1	B	143	ARG	NE-CZ-NH1	10.93	125.76	120.30
1	B	252	ARG	NE-CZ-NH2	-10.29	115.15	120.30
1	B	174	ARG	NE-CZ-NH2	10.29	125.45	120.30
1	B	479	ASP	CB-CG-OD1	10.29	127.56	118.30
1	A	143	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	B	684	ARG	CD-NE-CZ	9.42	136.79	123.60
1	A	491	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	B	674	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	B	491	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	A	611	ARG	NE-CZ-NH2	9.29	124.95	120.30
1	B	342	HIS	O-C-N	-9.02	108.27	122.70
1	A	611	ARG	NE-CZ-NH1	-8.90	115.85	120.30
1	B	201	ARG	NE-CZ-NH2	-8.87	115.87	120.30
1	B	441	TYR	CB-CG-CD1	-8.76	115.75	121.00
1	A	158	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	A	479	ASP	CB-CG-OD1	8.70	126.13	118.30
1	A	244	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	B	310	ARG	NE-CZ-NH2	8.40	124.50	120.30
1	B	546	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	A	77	ARG	NE-CZ-NH2	8.35	124.47	120.30
1	B	525	GLU	OE1-CD-OE2	8.31	133.27	123.30
1	B	217	VAL	CB-CA-C	-8.29	95.64	111.40
1	B	232	ASP	CB-CG-OD1	8.26	125.74	118.30
1	B	727	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	521	ASP	CB-CG-OD1	8.13	125.62	118.30
1	A	479	ASP	CB-CG-OD2	-8.05	111.06	118.30
1	B	280	ASP	CB-CG-OD1	8.03	125.53	118.30
1	B	326	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	B	260	ARG	NE-CZ-NH1	-7.95	116.33	120.30
1	A	67	ASP	CB-CG-OD1	7.70	125.23	118.30
1	B	674	ARG	CD-NE-CZ	-7.54	113.04	123.60
1	A	342	HIS	O-C-N	-7.39	110.87	122.70
1	B	244	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	B	100	ARG	CG-CD-NE	7.30	127.13	111.80
1	B	195	LEU	CA-CB-CG	7.29	132.06	115.30
1	B	465	VAL	N-CA-CB	-7.22	95.60	111.50
1	B	90	ARG	CD-NE-CZ	7.18	133.66	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	B	174	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	B	728	ARG	CD-NE-CZ	6.90	133.26	123.60
1	B	345	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	24	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	193	VAL	N-CA-CB	-6.82	96.49	111.50
1	B	24	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	280	ASP	CB-CG-OD2	6.75	124.37	118.30
1	B	333	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	B	456	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	100	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	B	193	VAL	N-CA-CB	-6.65	96.86	111.50
1	A	243	ASP	CB-CG-OD1	6.65	124.28	118.30
1	A	491	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	214	TYR	CB-CG-CD2	6.52	124.91	121.00
1	A	595	MET	CA-C-N	6.49	129.18	116.20
1	B	712	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	B	78	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	B	217	VAL	CG1-CB-CG2	6.44	121.21	110.90
1	A	297	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	244	ARG	CD-NE-CZ	6.38	132.54	123.60
1	A	668	ASP	CB-CG-OD1	6.38	124.04	118.30
1	B	546	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	100	ARG	CG-CD-NE	6.28	124.99	111.80
1	A	342	HIS	CA-C-N	6.22	130.89	117.20
1	B	728	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	B	535	LEU	CA-CB-CG	6.20	129.56	115.30
1	A	491	ARG	CD-NE-CZ	6.20	132.28	123.60
1	B	382	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	B	158	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	158	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	100	ARG	CD-NE-CZ	6.11	132.16	123.60
1	B	217	VAL	CA-CB-CG2	6.10	120.05	110.90
1	B	401	GLU	CG-CD-OE1	6.08	130.46	118.30
1	A	507	ASN	CB-CA-C	6.04	122.47	110.40
1	A	674	ARG	CD-NE-CZ	6.03	132.05	123.60
1	B	357	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	521	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	715	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	90	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	404	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	240	TYR	CB-CG-CD1	5.79	124.48	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	A	560	TYR	CB-CG-CD1	5.77	124.46	121.00
1	A	560	TYR	CB-CG-CD2	-5.76	117.55	121.00
1	A	335	VAL	CA-CB-CG1	5.73	119.50	110.90
1	B	498	LEU	CA-CB-CG	5.72	128.47	115.30
1	B	525	GLU	CG-CD-OE2	-5.72	106.87	118.30
1	B	715	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	240	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	B	427	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	55	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	A	107	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	270	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	95	ARG	NH1-CZ-NH2	-5.61	113.23	119.40
1	B	465	VAL	CG1-CB-CG2	5.60	119.86	110.90
1	B	588	LEU	CA-CB-CG	5.60	128.17	115.30
1	B	455	VAL	CA-CB-CG2	5.58	119.28	110.90
1	A	674	ARG	CG-CD-NE	5.57	123.50	111.80
1	B	342	HIS	CA-C-N	5.54	129.40	117.20
1	B	681	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	12	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	B	408	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	171	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	A	229	GLN	CA-CB-CG	5.45	125.39	113.40
1	B	441	TYR	CB-CG-CD2	5.43	124.26	121.00
1	A	507	ASN	CA-C-O	5.35	131.34	120.10
1	B	469	ILE	C-N-CA	-5.35	111.06	122.30
1	B	196	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	521	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	231	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	B	191	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	219	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	481	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	A	58	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	143	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	419	HIS	CA-CB-CG	-5.09	104.94	113.60
1	A	140	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	600	GLU	C-N-CA	5.08	134.41	121.70
1	B	96	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	B	247	MET	CG-SD-CE	5.05	108.28	100.20
1	A	160	TYR	CB-CG-CD1	-5.04	117.98	121.00
1	A	401	GLU	OE1-CD-OE2	-5.03	117.26	123.30
1	B	235	LEU	CB-CG-CD2	5.03	119.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	727	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	509	SER	Peptide
1	B	729	PRO	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	5673	0	5520	99	0
1	B	5744	0	5579	78	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	1	0
3	B	10	0	0	0	0
4	A	15	0	24	7	0
4	B	15	0	24	1	0
5	A	554	0	0	10	0
5	B	752	0	0	11	0
All	All	12770	0	11147	175	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 8.

All (175) 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:651:GLN:HE21	1:B:690:GLN:HE21	1.15	0.94
1:B:630:PRO:HG3	1:B:655:PRO:HG3	1.51	0.91
1:A:143:ARG:HB2	4:A:1341:PGO:H12	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136[A]:MET:HG2	1:B:143:ARG:HB2	1.59	0.84
1:B:659:THR:HG22	1:B:685:PRO:HD3	1.64	0.77
1:A:27:PRO:HG2	1:A:30:GLU:HG2	1.66	0.77
1:B:651:GLN:NE2	1:B:690:GLN:HE21	1.86	0.73
1:A:525:GLU:HG2	1:A:533:PHE:HB2	1.69	0.73
1:A:211:VAL:HG22	1:A:467:LYS:HB2	1.70	0.72
1:B:494:LEU:HD22	1:B:498:LEU:HD22	1.73	0.71
1:A:604:LEU:HB2	1:A:625:THR:HG22	1.72	0.70
1:B:684:ARG:HH11	1:B:684:ARG:HG3	1.56	0.70
1:B:674:ARG:HG3	1:B:675:PRO:HD2	1.74	0.69
1:B:136[A]:MET:HG2	1:B:143:ARG:CB	2.22	0.69
1:A:30:GLU:HG3	1:A:171:ARG:HH12	1.58	0.69
1:B:247:MET:HE2	1:B:261:VAL:CG1	2.22	0.69
1:A:187:TRP:CH2	1:A:206:LEU:HD21	2.29	0.68
1:B:656:LEU:HD21	1:B:714:LEU:HD22	1.74	0.68
1:B:565:LYS:HD2	5:B:2030:HOH:O	1.94	0.67
1:B:247:MET:HE2	1:B:261:VAL:HB	1.75	0.67
1:B:136[A]:MET:CG	1:B:143:ARG:HB2	2.25	0.66
1:B:242:MET:HG2	1:B:247:MET:CE	2.25	0.65
1:B:65:HIS:HE1	5:B:1547:HOH:O	1.82	0.63
1:A:363:LYS:HE2	5:A:1557:HOH:O	1.99	0.62
1:B:557:ILE:HD11	1:B:568:PHE:HB3	1.79	0.62
1:A:223[B]:ARG:HG3	1:A:718:TYR:CG	2.34	0.62
1:A:335:VAL:HG22	1:A:477:ILE:HD11	1.81	0.62
1:A:350:MET:HE3	5:A:1444:HOH:O	2.01	0.61
1:B:213:PHE:CE2	1:B:474:MET:HB3	2.35	0.60
1:A:475:MET:HE2	5:A:1750:HOH:O	2.01	0.60
1:A:213:PHE:CE1	1:A:474:MET:HB3	2.37	0.59
1:A:143:ARG:HD3	4:A:1341:PGO:O1	2.03	0.59
1:A:350:MET:HE1	1:A:369:VAL:HG23	1.85	0.59
1:B:247:MET:HE2	1:B:261:VAL:CB	2.32	0.59
1:A:202:GLU:HA	1:A:206:LEU:HD23	1.84	0.58
1:A:661:ARG:NH1	1:A:682:GLU:HB3	2.18	0.58
1:A:443:THR:HB	1:A:451:VAL:HG13	1.85	0.58
1:A:633:ILE:HB	1:A:651:GLN:HB3	1.86	0.58
1:A:282:ILE:HG22	1:B:6:THR:H	1.69	0.58
1:A:704:LYS:HE2	1:A:722:ASP:OD1	2.05	0.57
1:B:522:PHE:O	1:B:623:LYS:HE3	2.04	0.57
1:B:242:MET:HG2	1:B:247:MET:HE1	1.87	0.56
1:B:6:THR:O	1:B:7:ALA:HB3	2.06	0.56
1:A:225:TRP:CE2	1:A:294:GLY:HA2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:ARG:CG	1:B:729:PRO:HD3	2.37	0.55
1:A:187:TRP:HH2	1:A:206:LEU:HD21	1.71	0.55
1:A:347:ASN:ND2	1:A:349:GLN:H	2.05	0.55
1:B:655:PRO:HD2	1:B:656:LEU:HD22	1.88	0.55
1:A:100:ARG:HG2	1:A:164:TRP:CZ3	2.41	0.55
1:B:368:SER:HB2	5:B:1928:HOH:O	2.06	0.55
1:A:385:LEU:HD22	1:A:424:PHE:HB3	1.89	0.54
1:A:282:ILE:HG13	1:A:283:TYR:N	2.20	0.54
1:B:220:ILE:HD13	1:B:474:MET:SD	2.48	0.54
1:A:455:VAL:HG11	1:A:508:THR:HG21	1.90	0.54
1:B:140:ARG:HH11	1:B:140:ARG:HG3	1.73	0.54
1:A:187:TRP:CZ2	1:A:206:LEU:HD21	2.42	0.54
1:B:104:VAL:HG21	1:B:160:TYR:HE1	1.73	0.53
1:B:521:ASP:OD1	1:B:621:LYS:HE2	2.09	0.53
1:A:475:MET:HG3	5:A:1737:HOH:O	2.08	0.53
1:A:136:MET:HG2	4:A:1341:PGO:H2	1.90	0.53
1:A:342:HIS:O	1:A:343:ASP:HB2	2.09	0.53
1:B:242:MET:HG2	1:B:247:MET:HE3	1.91	0.53
1:A:350:MET:CE	1:A:369:VAL:HG23	2.39	0.52
1:A:520:MET:HB2	1:A:619:LEU:HD13	1.90	0.52
1:B:189:GLU:HG2	5:B:1573:HOH:O	2.08	0.52
1:B:488:GLU:OE2	1:B:491:ARG:NH1	2.37	0.52
1:B:605:HIS:CE1	1:B:622:GLN:HE21	2.27	0.52
1:A:387:VAL:HG23	5:A:1546:HOH:O	2.08	0.52
1:A:248:ASP:OD2	1:A:250:SER:HB2	2.10	0.51
1:A:674:ARG:HG2	1:A:674:ARG:HH11	1.75	0.51
1:B:100:ARG:HB2	1:B:119:VAL:O	2.10	0.51
1:A:50:VAL:HG22	1:A:86:ILE:HD12	1.93	0.51
1:B:437:SER:HB2	1:B:460:ILE:HD13	1.93	0.51
1:B:65:HIS:HD2	5:B:1351:HOH:O	1.94	0.50
1:A:211:VAL:HG22	1:A:467:LYS:CB	2.41	0.49
1:A:363:LYS:O	1:A:366:LYS:HE3	2.12	0.49
1:A:143:ARG:HB2	4:A:1341:PGO:C1	2.36	0.49
1:A:641:VAL:HG13	1:A:727:ARG:HB2	1.92	0.49
1:B:385:LEU:HD22	1:B:424:PHE:HB3	1.94	0.49
4:B:1345:PGO:H32	5:B:1732:HOH:O	2.13	0.48
1:A:286:GLY:HA3	1:A:310[A]:ARG:HG3	1.95	0.48
1:A:186:PRO:HG2	1:A:205:VAL:HG21	1.96	0.48
1:A:29:VAL:O	1:A:30:GLU:C	2.51	0.48
1:A:282:ILE:CG2	1:B:6:THR:H	2.26	0.47
1:A:350:MET:HE2	5:A:1452:HOH:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:THR:HG21	5:A:1506:HOH:O	2.14	0.47
1:A:443:THR:HB	1:A:451:VAL:CG1	2.45	0.47
1:A:213:PHE:CD1	1:A:222:THR:HG22	2.50	0.47
1:B:140:ARG:HG3	1:B:140:ARG:NH1	2.30	0.47
1:A:223[B]:ARG:HG3	1:A:718:TYR:CB	2.45	0.47
1:A:184:PHE:HB3	1:A:193:VAL:HG11	1.97	0.46
1:A:85:GLN:OE1	4:A:1341:PGO:H11	2.15	0.46
1:A:77:ARG:HB3	1:A:185:ASN:HB2	1.96	0.46
1:A:666:HIS:O	1:A:707:ALA:HA	2.16	0.46
1:B:184:PHE:HB3	1:B:193:VAL:HG11	1.96	0.46
1:A:310[B]:ARG:HA	1:A:311:TYR:HA	1.68	0.46
1:A:343:ASP:HA	5:A:1711:HOH:O	2.15	0.46
1:A:522:PHE:O	1:A:623:LYS:HE3	2.16	0.46
1:A:46:ASN:OD1	1:A:89:SER:HB3	2.15	0.46
1:A:8:PHE:O	1:B:280:ASP:HA	2.16	0.46
1:B:354:LEU:HD21	1:B:441:TYR:HB3	1.97	0.46
1:B:198:GLU:O	1:B:202:GLU:HG3	2.16	0.45
1:B:487:GLN:HB2	5:B:1813:HOH:O	2.16	0.45
1:B:104:VAL:CG2	1:B:158:ARG:HB2	2.47	0.45
1:B:104:VAL:CG2	1:B:160:TYR:HE1	2.30	0.45
1:B:553:LEU:O	1:B:570:LYS:HE2	2.16	0.45
1:A:223[A]:ARG:HH22	1:A:716:HIS:CE1	2.35	0.44
1:B:136[A]:MET:CG	1:B:143:ARG:CB	2.90	0.44
1:B:611:ARG:HG3	5:B:2031:HOH:O	2.17	0.44
1:A:539:PHE:HB3	1:A:577:LEU:HD11	1.99	0.44
1:A:223[A]:ARG:NH2	1:A:716:HIS:CE1	2.86	0.44
1:A:355:GLU:HG3	1:A:359:ASN:HB3	1.98	0.44
1:A:472:ASP:OD2	1:A:704:LYS:NZ	2.45	0.44
1:B:6:THR:O	1:B:7:ALA:CB	2.66	0.44
1:A:223[B]:ARG:HD2	1:A:224:SER:O	2.17	0.44
1:A:66:THR:HG21	1:A:75:ILE:HG22	1.99	0.44
1:B:684:ARG:HB2	1:B:687:SER:OG	2.18	0.44
1:A:264:ALA:HA	1:A:408:ARG:HG2	2.00	0.44
1:B:518:VAL:HG22	1:B:619:LEU:HD11	2.00	0.44
1:A:206:LEU:N	1:A:206:LEU:HD22	2.33	0.43
1:B:240:TYR:CD2	1:B:303:ARG:HD2	2.52	0.43
1:A:214:TYR:CD1	1:A:223[A]:ARG:HD2	2.53	0.43
1:A:44:PHE:CE1	1:A:166:PRO:HD2	2.53	0.43
1:A:455:VAL:HG11	1:A:508:THR:CG2	2.49	0.43
1:A:469:ILE:O	1:A:470:GLY:C	2.57	0.43
1:A:527:ALA:HB2	1:A:533:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:VAL:HG11	1:B:508:THR:HG21	2.00	0.43
1:B:629:ILE:CG2	1:B:630:PRO:HD2	2.49	0.43
1:A:136:MET:HB3	1:A:143:ARG:HB3	2.01	0.42
1:A:286:GLY:CA	1:A:310[A]:ARG:HG3	2.49	0.42
1:A:721:LEU:HD13	1:A:722:ASP:O	2.18	0.42
1:B:684:ARG:NH1	1:B:684:ARG:HG3	2.29	0.42
1:B:728:ARG:HG3	1:B:729:PRO:HD3	2.01	0.42
1:B:589:ILE:N	1:B:589:ILE:HD12	2.34	0.42
1:A:310[A]:ARG:HA	1:A:311:TYR:HA	1.66	0.42
1:A:462:LYS:NZ	3:A:1330:PO4:O3	2.46	0.42
1:A:136:MET:HG2	4:A:1341:PGO:C2	2.50	0.42
1:A:565:LYS:HB2	1:A:599:LEU:HD11	2.02	0.42
1:B:453:GLU:O	1:B:454[A]:ASN:HB2	2.20	0.42
1:A:136:MET:HG2	4:A:1341:PGO:C3	2.50	0.42
1:A:385:LEU:HB3	1:A:386:PRO:HD2	2.01	0.42
1:A:428:ALA:N	1:A:429:PRO:CD	2.83	0.42
1:A:508:THR:HG22	1:A:508:THR:O	2.20	0.41
1:A:634:ILE:HB	1:A:721:LEU:HB2	2.02	0.41
1:B:439:LEU:HB2	1:B:456:ASP:HB3	2.02	0.41
1:B:491:ARG:NH2	1:B:495:GLU:OE1	2.53	0.41
1:A:629:ILE:CG2	1:A:630:PRO:HD2	2.50	0.41
1:B:310:ARG:HA	1:B:311:TYR:HA	1.82	0.41
1:B:517:ASN:N	5:B:1709:HOH:O	2.53	0.41
1:B:625:THR:HG21	5:B:1487:HOH:O	2.19	0.41
1:A:211:VAL:HG22	1:A:467:LYS:CG	2.50	0.41
1:A:44:PHE:CZ	1:A:166:PRO:HD2	2.55	0.41
1:B:657:LYS:HD2	5:B:1739:HOH:O	2.20	0.41
1:B:52:LEU:O	1:B:53:PHE:C	2.58	0.41
1:B:93:ASP:HA	1:B:94:PRO:HD2	1.81	0.41
1:B:263:SER:HB3	1:B:321:PHE:CZ	2.56	0.41
1:A:446:LYS:HD3	1:A:446:LYS:HA	1.93	0.41
1:B:136[A]:MET:O	1:B:136[A]:MET:HG3	2.21	0.41
1:B:418:LYS:HE2	1:B:483:PHE:CE1	2.55	0.41
1:A:361:ASN:ND2	1:A:364:LEU:HD22	2.36	0.41
1:A:371:ASN:ND2	5:A:1399:HOH:O	2.52	0.41
1:B:213:PHE:CD2	1:B:222:THR:HG22	2.56	0.41
1:A:385:LEU:HB3	1:A:386:PRO:CD	2.51	0.41
1:A:686:ASN:HD22	1:A:686:ASN:N	2.19	0.41
1:B:45:LEU:HG	1:B:88:PHE:CD1	2.56	0.41
1:A:100:ARG:HD2	5:A:1647:HOH:O	2.20	0.40
1:B:428:ALA:N	1:B:429:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ARG:HB3	1:A:185:ASN:CB	2.51	0.40
1:B:518:VAL:HG13	1:B:612:ILE:CD1	2.51	0.40
1:B:264:ALA:HA	1:B:408:ARG:HG2	2.03	0.40
1:B:96:ARG:H	1:B:96:ARG:HD3	1.87	0.40
1:A:211:VAL:HG23	1:A:213:PHE:CE2	2.56	0.40
1:A:606:PHE:HE2	1:A:625:THR:HB	1.86	0.40
1:A:629:ILE:CG2	1:A:717:VAL:HG22	2.51	0.40
1:B:584:LYS:NZ	1:B:586:ALA:HB2	2.36	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	701/731 (96%)	677 (97%)	22 (3%)	2 (0%)	44	40
1	B	712/731 (97%)	682 (96%)	24 (3%)	6 (1%)	22	15
All	All	1413/1462 (97%)	1359 (96%)	46 (3%)	8 (1%)	28	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	SER
1	B	7	ALA
1	B	34	VAL
1	B	6	THR
1	B	510	ARG
1	B	729	PRO
1	A	470	GLY
1	B	728	ARG

### 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	621/644 (96%)	583 (94%)	38 (6%)	22	16
1	B	627/644 (97%)	592 (94%)	35 (6%)	25	19
All	All	1248/1288 (97%)	1175 (94%)	73 (6%)	25	18

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	20	ASN
1	A	23	GLU
1	A	43	GLU
1	A	45	LEU
1	A	127	SER
1	A	140	ARG
1	A	167	TYR
1	A	193	VAL
1	A	195	LEU
1	A	202	GLU
1	A	223[A]	ARG
1	A	223[B]	ARG
1	A	282	ILE
1	A	310[A]	ARG
1	A	310[B]	ARG
1	A	335	VAL
1	A	354	LEU
1	A	355	GLU
1	A	364	LEU
1	A	408	ARG
1	A	455	VAL
1	A	463	LEU
1	A	489	GLU
1	A	498	LEU
1	A	506	LEU
1	A	507	ASN

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Mol	Chain	Res	Type
1	A	516	SER
1	A	553	LEU
1	A	565	LYS
1	A	570	LYS
1	A	572	THR
1	A	580	LEU
1	A	585	GLU
1	A	625	THR
1	A	631	GLU
1	A	637	ARG
1	A	674	ARG
1	B	6	THR
1	B	20	ASN
1	B	45	LEU
1	B	72	ASN
1	B	96	ARG
1	B	136[A]	MET
1	B	136[B]	MET
1	B	138	GLU
1	B	143	ARG
1	B	175	ASN
1	B	193	VAL
1	B	206	LEU
1	B	217	VAL
1	B	223	ARG
1	B	235	LEU
1	B	239	LEU
1	B	408	ARG
1	B	451	VAL
1	B	465	VAL
1	B	485	GLU
1	B	488	GLU
1	B	494	LEU
1	B	498	LEU
1	B	518	VAL
1	B	546	ARG
1	B	553	LEU
1	B	570	LYS
1	B	572	THR
1	B	588	LEU
1	B	604	LEU
1	B	657	LYS

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Mol	Chain	Res	Type
1	B	678	LYS
1	B	684	ARG
1	B	721	LEU
1	B	728	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	GLN
1	A	347	ASN
1	A	371	ASN
1	A	400	GLN
1	A	415	GLN
1	A	450	HIS
1	A	526	ASN
1	A	686	ASN
1	B	32	GLN
1	B	65	HIS
1	B	72	ASN
1	B	175	ASN
1	B	371	ASN
1	B	415	GLN
1	B	597	GLN
1	B	601	GLN
1	B	622	GLN
1	B	640	GLN
1	B	651	GLN
1	B	702	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	PO4	A	1330	-	4,4,4	0.67	0	6,6,6	0.77	0
4	PGO	A	1340	-	4,4,4	1.21	1 (25%)	2,4,4	2.31	1 (50%)
4	PGO	A	1341	-	4,4,4	1.07	1 (25%)	2,4,4	1.22	0
4	PGO	A	1342	-	4,4,4	0.88	0	2,4,4	2.08	1 (50%)
3	PO4	B	1331	-	4,4,4	0.57	0	6,6,6	0.60	0
3	PO4	B	1332	-	4,4,4	1.19	0	6,6,6	0.88	0
4	PGO	B	1343	-	4,4,4	1.26	1 (25%)	2,4,4	3.45	1 (50%)
4	PGO	B	1344	-	4,4,4	1.08	1 (25%)	2,4,4	2.50	1 (50%)
4	PGO	B	1345	-	4,4,4	1.04	0	2,4,4	1.18	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	PO4	A	1330	-	-	0/0/0/0	0/0/0/0
4	PGO	A	1340	-	-	0/2/2/2	0/0/0/0
4	PGO	A	1341	-	-	0/2/2/2	0/0/0/0
4	PGO	A	1342	-	-	0/2/2/2	0/0/0/0
3	PO4	B	1331	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1332	-	-	0/0/0/0	0/0/0/0
4	PGO	B	1343	-	-	0/2/2/2	0/0/0/0
4	PGO	B	1344	-	-	0/2/2/2	0/0/0/0
4	PGO	B	1345	-	-	0/2/2/2	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1341	PGO	C1-C2	2.03	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1344	PGO	C1-C2	2.08	1.55	1.50
4	A	1340	PGO	C1-C2	2.32	1.56	1.50
4	B	1343	PGO	C1-C2	2.41	1.56	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1343	PGO	O1-C1-C2	-4.87	99.82	110.83
4	B	1344	PGO	O1-C1-C2	-3.41	103.11	110.83
4	A	1340	PGO	O1-C1-C2	-3.12	103.77	110.83
4	A	1342	PGO	O1-C1-C2	-2.94	104.17	110.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1330	PO4	1	0
4	A	1341	PGO	7	0
4	B	1345	PGO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 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	705/731 (96%)	-0.30	21 (2%) 51 51	18, 30, 65, 88	2 (0%)
1	B	716/731 (97%)	-0.58	19 (2%) 55 54	14, 23, 52, 107	2 (0%)
All	All	1421/1462 (97%)	-0.44	40 (2%) 53 53	14, 27, 60, 107	4 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	LEU	9.5
1	B	511	SER	9.1
1	B	6	THR	8.0
1	B	729	PRO	5.8
1	B	35	ASN	5.5
1	A	167	TYR	5.5
1	B	5	ARG	5.2
1	B	730	SER	4.6
1	A	42	GLN	4.5
1	A	270	ASP	4.3
1	B	167	TYR	4.2
1	A	285	TYR	3.4
1	A	223[A]	ARG	3.4
1	B	95	ARG	3.3
1	B	728	ARG	3.2
1	A	510	ARG	3.2
1	B	127	SER	3.0
1	A	727	ARG	3.0
1	A	95	ARG	2.9
1	A	30	GLU	2.8
1	A	509	SER	2.7
1	B	33	GLY	2.7
1	A	616	ARG	2.6
1	B	509	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	508	THR	2.5
1	A	29	VAL	2.5
1	A	655	PRO	2.4
1	A	272	GLU	2.4
1	B	508	THR	2.4
1	A	653	THR	2.4
1	A	661	ARG	2.4
1	B	582	PHE	2.3
1	A	684	ARG	2.3
1	B	43	GLU	2.3
1	A	681	ARG	2.2
1	B	686	ASN	2.2
1	A	487	GLN	2.2
1	A	642	VAL	2.2
1	B	616	ARG	2.2
1	B	285	TYR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	PGO	B	1344	5/5	0.59	0.20	6.45	62,62,63,65	0
4	PGO	A	1340	5/5	0.93	0.17	6.38	45,46,47,48	0
4	PGO	B	1345	5/5	0.82	0.15	5.19	50,53,53,54	0
4	PGO	B	1343	5/5	0.84	0.15	2.86	46,49,50,51	0
4	PGO	A	1341	5/5	0.87	0.15	2.47	58,59,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PGO	A	1342	5/5	0.97	0.08	1.51	48,48,49,49	0
3	PO4	B	1332	5/5	0.93	0.13	0.45	64,64,65,65	0
2	CA	A	1320	1/1	0.98	0.08	0.19	30,30,30,30	0
3	PO4	A	1330	5/5	0.96	0.09	0.10	36,36,40,40	0
3	PO4	B	1331	5/5	0.99	0.06	-1.13	25,26,29,29	0
2	CA	B	1321	1/1	0.98	0.03	-3.34	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.