



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:42 PM UTC

PDB ID : 1EX0 / pdb_00001ex0
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 : 2000-04-28
Resolution : 2.00 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

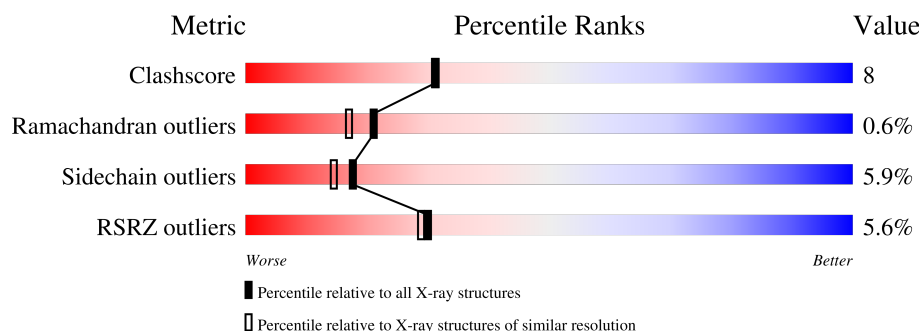
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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	1341	-	-	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			

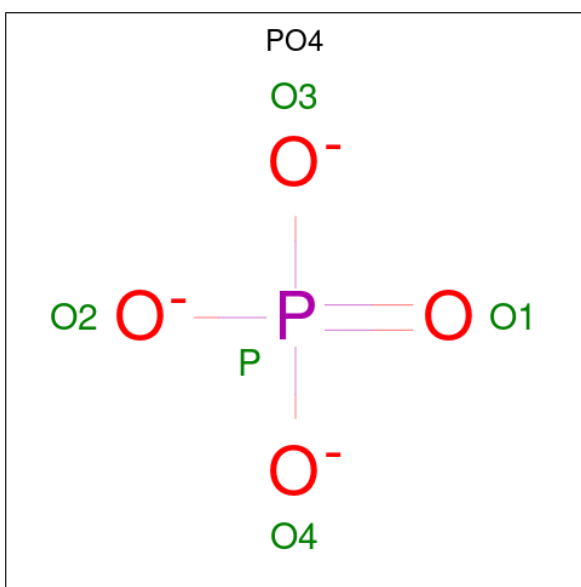
There are 13 discrepancies between the modelled and reference sequences:

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 mutation	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 mutation	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 (CCD ID: CA) (formula: Ca).

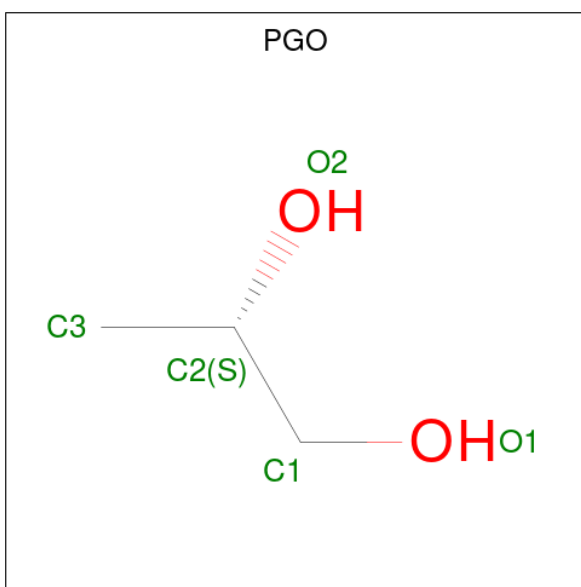
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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 (CCD ID: PGO) (formula: C₃H₈O₂).



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 5 3 2	0	0
4	A	1	Total C O 5 3 2	0	0
4	B	1	Total C O 5 3 2	0	0
4	B	1	Total C O 5 3 2	0	0
4	B	1	Total C O 5 3 2	0	0

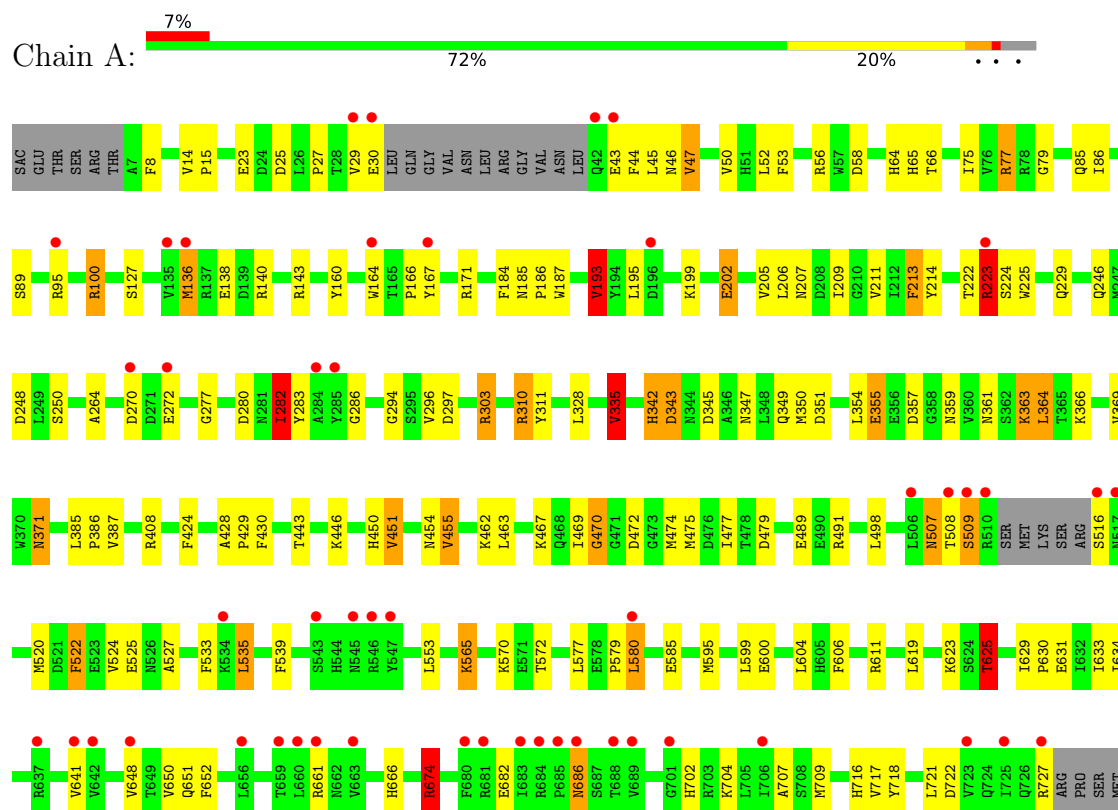
- Molecule 5 is water.

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

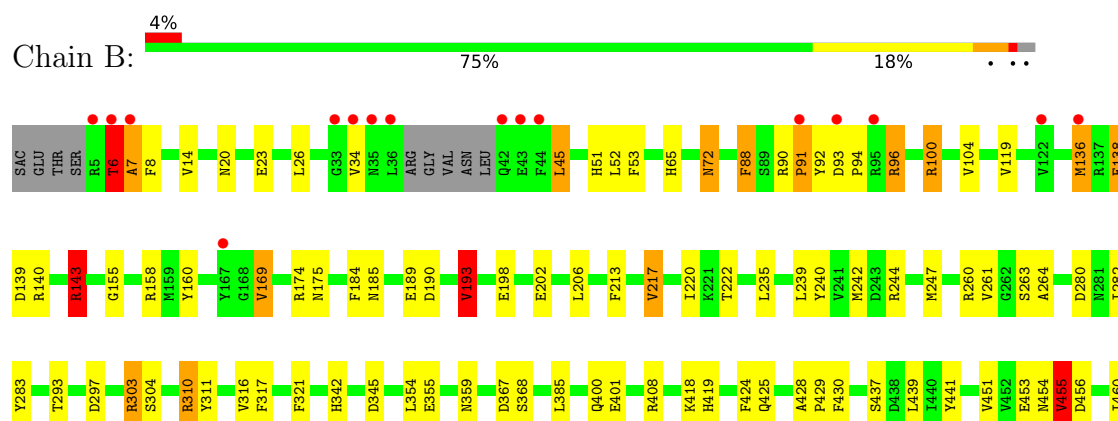
3 Residue-property plots

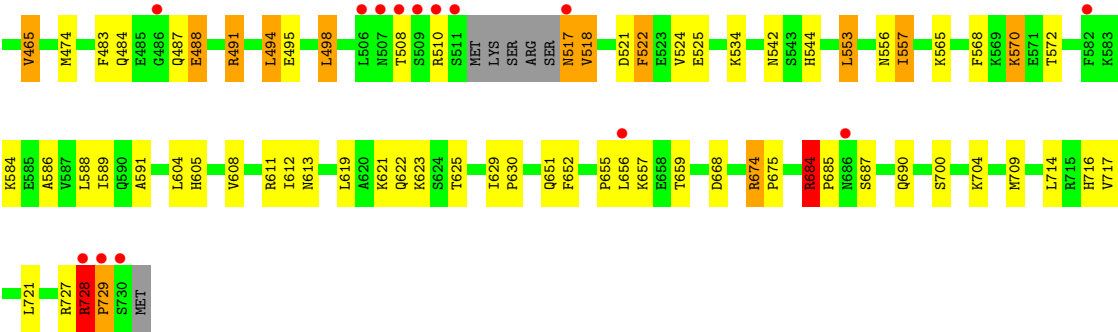
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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, α , β , γ	100.54Å 70.64Å 133.38Å 90.00° 106.08° 90.00°	Depositor
Resolution (Å)	19.94 – 2.00 19.94 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.94-2.00) 96.5 (19.94-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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.	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12770	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PGO, 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	0.76	0/5805	1.60	66/7874 (0.8%)
1	B	0.88	1/5877 (0.0%)	1.69	68/7973 (0.9%)
All	All	0.82	1/11682 (0.0%)	1.65	134/15847 (0.8%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	155	GLY	N-CA	5.62	1.50	1.45

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ARG	CD-NE-CZ	20.89	153.65	124.40
1	B	491	ARG	CD-NE-CZ	16.66	147.73	124.40
1	B	303	ARG	CD-NE-CZ	14.25	144.35	124.40
1	B	143	ARG	CD-NE-CZ	13.17	142.84	124.40
1	B	217	VAL	CB-CA-C	-12.52	95.64	112.04
1	B	342	HIS	O-C-N	-12.31	108.27	122.68
1	A	303	ARG	CD-NE-CZ	11.25	140.15	124.40
1	B	430	PHE	CA-CB-CG	-10.56	103.24	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	VAL	N-CA-CB	-10.40	96.86	112.15
1	A	342	HIS	O-C-N	-10.09	110.87	122.68
1	A	507	ASN	CA-C-O	9.55	131.34	120.54
1	A	507	ASN	CA-CB-CG	9.12	121.72	112.60
1	B	465	VAL	N-CA-CB	-9.06	95.60	112.36
1	A	193	VAL	N-CA-CB	-8.94	96.49	111.23
1	B	419	HIS	CA-CB-CG	-8.86	104.94	113.80
1	B	684	ARG	CD-NE-CZ	8.85	136.79	124.40
1	A	282	ILE	N-CA-CB	8.54	118.65	111.64
1	B	674	ARG	CD-NE-CZ	-8.11	113.04	124.40
1	A	280	ASP	CA-CB-CG	8.06	120.67	112.60
1	A	371	ASN	OD1-CG-ND2	7.91	130.51	122.60
1	B	51	HIS	CA-CB-CG	-7.87	105.94	113.80
1	A	479	ASP	CA-CB-CG	7.83	120.43	112.60
1	B	556	ASN	CA-CB-CG	7.77	120.37	112.60
1	A	507	ASN	CB-CA-C	7.73	122.47	109.80
1	A	522	PHE	CA-CB-CG	7.72	121.52	113.80
1	B	345	ASP	CA-CB-CG	7.61	120.21	112.60
1	A	207	ASN	OD1-CG-ND2	7.40	130.00	122.60
1	B	668	ASP	CA-CB-CG	7.25	119.85	112.60
1	B	14	VAL	CA-C-O	-7.25	115.02	119.51
1	A	535	LEU	CA-C-O	-7.24	112.28	120.32
1	B	88	PHE	CA-CB-CG	7.10	120.90	113.80
1	B	174	ARG	NE-CZ-NH2	6.94	125.45	119.20
1	B	175	ASN	CA-CB-CG	6.88	119.48	112.60
1	B	217	VAL	N-CA-CB	6.88	119.07	110.47
1	B	100	ARG	CG-CD-NE	6.88	127.13	112.00
1	B	522	PHE	CA-CB-CG	6.88	120.68	113.80
1	A	595	MET	CA-C-O	-6.75	112.64	120.20
1	B	613	ASN	OD1-CG-ND2	6.66	129.26	122.60
1	A	209	ILE	CA-C-N	-6.65	115.36	122.67
1	A	209	ILE	C-N-CA	-6.65	115.36	122.67
1	B	90	ARG	CD-NE-CZ	6.61	133.66	124.40
1	B	517	ASN	CA-CB-CG	-6.59	106.01	112.60
1	A	430	PHE	CA-CB-CG	-6.52	107.28	113.80
1	B	652	PHE	CA-CB-CG	-6.51	107.28	113.80
1	B	297	ASP	CA-CB-CG	6.51	119.11	112.60
1	B	8	PHE	CA-CB-CG	6.47	120.27	113.80
1	B	674	ARG	NE-CZ-NH2	6.44	125.00	119.20
1	B	491	ARG	NE-CZ-NH2	-6.39	113.45	119.20
1	A	611	ARG	NE-CZ-NH2	6.38	124.95	119.20
1	A	213	PHE	CA-CB-CG	-6.38	107.42	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	728	ARG	CD-NE-CZ	6.33	133.26	124.40
1	A	160	TYR	CA-C-N	-6.33	114.33	123.06
1	A	160	TYR	C-N-CA	-6.33	114.33	123.06
1	A	454	ASN	OD1-CG-ND2	6.26	128.86	122.60
1	B	525	GLU	CA-C-O	-6.24	114.33	121.19
1	A	600	GLU	O-C-N	-6.23	115.37	122.97
1	B	517	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	B	716	HIS	CA-C-N	6.18	131.15	123.12
1	B	716	HIS	C-N-CA	6.18	131.15	123.12
1	A	296	VAL	N-CA-C	6.17	116.33	110.53
1	B	91	PRO	CA-C-O	6.00	127.99	120.97
1	B	727	ARG	CA-C-O	-5.94	115.77	122.01
1	A	357	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	557	ILE	N-CA-C	-5.93	101.06	108.89
1	A	100	ARG	CG-CD-NE	5.90	124.99	112.00
1	A	328	LEU	N-CA-C	-5.90	106.08	113.28
1	B	310	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	A	77	ARG	NE-CZ-NH2	5.86	124.47	119.20
1	A	270	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	591	ALA	CA-C-O	5.82	126.92	120.63
1	B	244	ARG	CD-NE-CZ	5.81	132.54	124.40
1	A	79	GLY	N-CA-C	-5.81	107.30	115.32
1	A	345	ASP	CA-CB-CG	-5.79	106.81	112.60
1	A	58	ASP	CA-C-N	5.72	128.26	120.54
1	A	58	ASP	C-N-CA	5.72	128.26	120.54
1	B	217	VAL	CA-CB-CG2	5.67	120.05	110.40
1	A	25	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	611	ARG	NE-CZ-NH1	-5.65	115.85	121.50
1	A	229	GLN	CA-CB-CG	5.64	125.39	114.10
1	A	491	ARG	CD-NE-CZ	5.62	132.28	124.40
1	A	625	THR	N-CA-CB	-5.62	101.08	111.53
1	B	293	THR	CA-CB-OG1	-5.58	101.23	109.60
1	B	26	LEU	N-CA-CB	5.55	118.53	110.32
1	A	100	ARG	CD-NE-CZ	5.54	132.16	124.40
1	B	317	PHE	CA-CB-CG	5.53	119.33	113.80
1	B	282	ILE	O-C-N	-5.51	117.74	121.98
1	B	100	ARG	NE-CZ-NH1	5.49	126.99	121.50
1	A	277	GLY	CA-C-O	-5.49	116.59	121.64
1	B	400	GLN	OE1-CD-NE2	5.48	128.08	122.60
1	B	23	GLU	CA-C-O	-5.47	114.72	121.06
1	A	674	ARG	CD-NE-CZ	5.46	132.05	124.40
1	B	700	SER	CA-C-O	-5.46	114.95	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	GLN	O-C-N	-5.45	116.11	122.81
1	B	608	VAL	N-CA-CB	5.45	119.07	112.10
1	A	595	MET	N-CA-C	5.42	118.69	111.75
1	A	343	ASP	N-CA-C	5.41	119.17	112.24
1	A	246	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	B	359	ASN	OD1-CG-ND2	5.41	128.01	122.60
1	B	524	VAL	CA-C-O	-5.38	114.74	120.39
1	B	169	VAL	N-CA-C	5.37	117.06	108.89
1	A	138	GLU	N-CA-CB	5.36	119.18	110.77
1	A	335	VAL	CA-CB-CG1	5.35	119.50	110.40
1	A	450	HIS	CA-C-O	-5.32	114.55	120.66
1	A	56	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	A	65	HIS	CA-CB-CG	5.25	119.05	113.80
1	B	401	GLU	CG-CD-OE1	5.24	130.46	118.40
1	A	674	ARG	CG-CD-NE	5.23	123.50	112.00
1	B	455	VAL	CA-CB-CG2	5.22	119.28	110.40
1	B	143	ARG	NE-CZ-NH2	-5.21	114.52	119.20
1	B	260	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	B	542	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	A	95	ARG	NE-CZ-NH1	5.13	126.63	121.50
1	A	207	ASN	CB-CG-ND2	-5.12	108.72	116.40
1	A	648	VAL	CA-C-N	-5.11	115.94	123.00
1	A	648	VAL	C-N-CA	-5.11	115.94	123.00
1	A	223[A]	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	A	223[B]	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	A	272	GLU	CA-C-O	-5.09	113.45	119.05
1	A	47	VAL	N-CA-CB	5.08	116.25	110.72
1	A	524	VAL	CA-C-O	-5.08	115.06	120.39
1	B	544	HIS	CA-CB-CG	-5.07	108.73	113.80
1	A	64	HIS	N-CA-C	-5.07	107.09	113.28
1	A	351	ASP	CA-C-N	-5.07	116.36	123.10
1	A	351	ASP	C-N-CA	-5.07	116.36	123.10
1	B	185	ASN	CA-CB-CG	-5.06	107.54	112.60
1	A	15	PRO	O-C-N	5.06	123.64	121.31
1	B	367	ASP	CA-CB-CG	-5.04	107.56	112.60
1	A	303	ARG	NE-CZ-NH2	-5.03	114.67	119.20
1	A	335	VAL	N-CA-CB	-5.03	101.90	111.21
1	B	283	TYR	CA-CB-CG	-5.03	104.85	113.90
1	B	316	VAL	CB-CA-C	-5.02	105.46	112.04
1	B	304	SER	CA-CB-OG	-5.02	101.07	111.10
1	B	190	ASP	CA-CB-CG	-5.01	107.58	112.60
1	B	525	GLU	CG-CD-OE2	-5.01	106.87	118.40

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

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	105	0
1	B	5744	0	5579	82	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	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 8.

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: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
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:B:247:MET:HE2	1:B:261:VAL:CG1	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:242:MET:HG2	1:B:247:MET:HE3	1.73	0.70
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: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:A:350:MET:HE3	5:A:1444:HOH:O	1.96	0.66
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:B:213:PHE:CE2	1:B:474:MET:HB3	2.35	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: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:282:ILE:HG22	1:B:6:THR:H	1.69	0.58
1:A:633:ILE:HB	1:A:651:GLN:HB3	1.86	0.58
1:B:247:MET:HE2	1:B:261:VAL:HB	1.86	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: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
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:247:MET:HE2	1:B:261:VAL:CB	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:VAL:HG11	1:A:508:THR:HG21	1.90	0.54
1:B:140:ARG:HG3	1:B:140:ARG:HH11	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:350:MET:HE1	1:A:369:VAL:HG23	1.91	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:247:MET:HE2	1:B:261:VAL:HG11	1.91	0.53
1:A:350:MET:CE	1:A:369:VAL:HG23	2.39	0.52
1:A:29:VAL:O	1:A:30:GLU:C	2.51	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:HH11	1:A:674:ARG:HG2	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:A:475:MET:HE2	5:A:1750:HOH:O	2.10	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:A:462:LYS:NZ	3:A:1330:PO4:O3	2.46	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:709:MET:HE3	1:A:717:VAL:HB	1.96	0.48
1:A:186:PRO:HG2	1:A:205:VAL:HG21	1.96	0.48
1:A:282:ILE:CG2	1:B:6:THR:H	2.26	0.47
1:A:469:ILE:O	1:A:470:GLY:C	2.57	0.47
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:A:350:MET:HE2	5:A:1452:HOH:O	2.14	0.47
1:A:652:PHE:CZ	1:A:709:MET:HE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:85:GLN:OE1	4:A:1341:PGO:H11	2.15	0.46
1:A:184:PHE:HB3	1:A:193:VAL:HG11	1.97	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:B:52:LEU:O	1:B:53:PHE:C	2.58	0.46
1:A:8:PHE:O	1:B:280:ASP:HA	2.16	0.46
1:A:46:ASN:OD1	1:A:89:SER:HB3	2.15	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:709:MET:HE3	1:B:717:VAL:HB	1.97	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:684:ARG:HB2	1:B:687:SER:HG	1.81	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:B:91:PRO:O	1:B:92:TYR:C	2.60	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:66:THR:HG21	1:A:75:ILE:HG22	1.99	0.44
1:A:223[B]:ARG:HD2	1:A:224:SER:O	2.17	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: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:72:ASN:C	1:B:72:ASN:HD22	2.27	0.43
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:52:LEU:O	1:A:53:PHE:C	2.62	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:HG3	1:B:684:ARG:NH1	2.29	0.42
1:B:589:ILE:HD12	1:B:589:ILE:N	2.34	0.42
1:A:310[A]:ARG:HA	1:A:311:TYR:HA	1.66	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:O	1:A:508:THR:HG22	2.20	0.41
1:A:535:LEU:C	1:A:535:LEU:HD23	2.45	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:44:PHE:CZ	1:A:166:PRO:HD2	2.55	0.41
1:A:211:VAL:HG22	1:A:467:LYS:CG	2.50	0.41
1:B:657:LYS:HD2	5:B:1739:HOH:O	2.20	0.41
1:B:93:ASP:HA	1:B:94:PRO:HD2	1.81	0.41
1:B:20:ASN:HD22	1:B:20:ASN:C	2.29	0.41
1:B:263:SER:HB3	1:B:321:PHE:CZ	2.56	0.41
1:A:446:LYS:HA	1:A:446:LYS:HD3	1.93	0.41
1:A:579:PRO:O	1:A:580:LEU:C	2.64	0.41
1:A:702:HIS:ND1	1:A:702:HIS:C	2.77	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:136[A]:MET:O	1:B:136[A]:MET:HG3	2.21	0.41
1:B:138:GLU:O	1:B:139:ASP:C	2.64	0.41
1:B:213:PHE:CD2	1:B:222:THR:HG22	2.56	0.41
1:B:418:LYS:HE2	1:B:483:PHE:CE1	2.55	0.41
1:A:385:LEU:HB3	1:A:386:PRO:CD	2.51	0.41

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

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	701/731 (96%)	677 (97%)	22 (3%)	2 (0%)	36	35
1	B	712/731 (97%)	682 (96%)	24 (3%)	6 (1%)	16	11
All	All	1413/1462 (97%)	1359 (96%)	46 (3%)	8 (1%)	21	17

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

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Mol	Chain	Res	Type
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%)	578 (93%)	43 (7%)	14	11
1	B	627/644 (97%)	594 (95%)	33 (5%)	20	18
All	All	1248/1288 (97%)	1172 (94%)	76 (6%)	18	14

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	23	GLU
1	A	43	GLU
1	A	45	LEU
1	A	47	VAL
1	A	127	SER
1	A	136	MET
1	A	140	ARG
1	A	167	TYR
1	A	193	VAL
1	A	195	LEU
1	A	199	LYS
1	A	202	GLU
1	A	223[A]	ARG
1	A	223[B]	ARG
1	A	282	ILE
1	A	297	ASP
1	A	303	ARG
1	A	310[A]	ARG
1	A	310[B]	ARG
1	A	335	VAL

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Mol	Chain	Res	Type
1	A	354	LEU
1	A	355	GLU
1	A	363	LYS
1	A	364	LEU
1	A	451	VAL
1	A	455	VAL
1	A	463	LEU
1	A	489	GLU
1	A	498	LEU
1	A	507	ASN
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	650	VAL
1	A	674	ARG
1	A	686	ASN
1	B	6	THR
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	169	VAL
1	B	193	VAL
1	B	206	LEU
1	B	217	VAL
1	B	235	LEU
1	B	239	LEU
1	B	355	GLU
1	B	451	VAL
1	B	455	VAL
1	B	465	VAL
1	B	484	GLN
1	B	488	GLU

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Mol	Chain	Res	Type
1	B	494	LEU
1	B	498	LEU
1	B	518	VAL
1	B	534	LYS
1	B	553	LEU
1	B	570	LYS
1	B	572	THR
1	B	588	LEU
1	B	604	LEU
1	B	684	ARG
1	B	704	LYS
1	B	721	LEU
1	B	728	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	218	ASN
1	A	313	GLN
1	A	347	ASN
1	A	359	ASN
1	A	371	ASN
1	A	415	GLN
1	A	526	ASN
1	A	662	ASN
1	A	686	ASN
1	B	32	GLN
1	B	51	HIS
1	B	65	HIS
1	B	72	ASN
1	B	175	ASN
1	B	371	ASN
1	B	415	GLN
1	B	421	HIS
1	B	425	GLN
1	B	601	GLN
1	B	622	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 oligosaccharides 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	$\# Z > 2$
4	PGO	A	1342	-	4,4,4	0.86	0	4,4,4	1.01	0
4	PGO	B	1345	-	4,4,4	0.94	0	4,4,4	0.94	0
3	PO4	A	1330	-	4,4,4	0.86	0	6,6,6	0.93	0
4	PGO	A	1341	-	4,4,4	0.96	0	4,4,4	1.14	0
4	PGO	B	1343	-	4,4,4	1.06	0	4,4,4	1.73	1 (25%)
3	PO4	B	1332	-	4,4,4	1.42	1 (25%)	6,6,6	1.04	0
4	PGO	B	1344	-	4,4,4	0.96	0	4,4,4	1.41	1 (25%)
3	PO4	B	1331	-	4,4,4	0.75	0	6,6,6	0.71	0
4	PGO	A	1340	-	4,4,4	1.03	0	4,4,4	1.36	1 (25%)

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
4	PGO	A	1342	-	-	2/2/2/2	-
4	PGO	B	1345	-	-	2/2/2/2	-
4	PGO	A	1341	-	-	0/2/2/2	-
4	PGO	B	1343	-	-	0/2/2/2	-
4	PGO	B	1344	-	-	0/2/2/2	-
4	PGO	A	1340	-	-	0/2/2/2	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1332	PO4	P-O3	-2.09	1.48	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1343	PGO	O1-C1-C2	-2.78	99.82	114.54
4	B	1344	PGO	O1-C1-C2	-2.16	103.11	114.54
4	A	1340	PGO	O1-C1-C2	-2.03	103.77	114.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1345	PGO	O1-C1-C2-C3
4	B	1345	PGO	O1-C1-C2-O2
4	A	1342	PGO	O1-C1-C2-C3
4	A	1342	PGO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1345	PGO	1	0
3	A	1330	PO4	1	0
4	A	1341	PGO	7	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	705/731 (96%)	0.23	49 (6%)	22 21	18, 30, 63, 88	4 (0%)
1	B	716/731 (97%)	-0.23	30 (4%)	40 39	14, 23, 51, 107	4 (0%)
All	All	1421/1462 (97%)	-0.00	79 (5%)	30 29	14, 27, 59, 107	8 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	511	SER	11.3
1	A	510	ARG	9.7
1	B	729	PRO	8.5
1	B	36	LEU	8.1
1	B	6	THR	7.8
1	B	728	ARG	7.6
1	A	509	SER	7.2
1	A	29	VAL	4.8
1	A	683	ILE	4.6
1	A	223[A]	ARG	4.1
1	B	510	ARG	4.1
1	B	730	SER	4.1
1	B	33	GLY	4.0
1	A	30	GLU	4.0
1	A	660	LEU	3.9
1	A	727	ARG	3.8
1	A	167	TYR	3.7
1	A	725	ILE	3.7
1	A	270	ASP	3.7
1	A	661	ARG	3.5
1	B	35	ASN	3.5
1	B	508	THR	3.4
1	A	42	GLN	3.4
1	A	506	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	7	ALA	3.3
1	B	509	SER	3.1
1	B	582	PHE	3.1
1	A	272	GLU	3.0
1	B	34	VAL	3.0
1	B	517	ASN	2.9
1	A	543	SER	2.9
1	B	507	ASN	2.8
1	A	43	GLU	2.7
1	B	486	GLY	2.7
1	A	95	ARG	2.7
1	B	95	ARG	2.7
1	B	5	ARG	2.7
1	A	508	THR	2.7
1	A	516	SER	2.7
1	B	686	ASN	2.6
1	A	648	VAL	2.6
1	B	43	GLU	2.6
1	A	706	ILE	2.6
1	B	136[A]	MET	2.5
1	A	659	THR	2.5
1	A	681	ARG	2.5
1	B	93	ASP	2.5
1	A	701	GLY	2.5
1	A	686	ASN	2.5
1	A	688	THR	2.5
1	A	284	ALA	2.4
1	A	663	VAL	2.4
1	A	680	PHE	2.4
1	B	42	GLN	2.4
1	A	689	VAL	2.4
1	A	285	TYR	2.4
1	B	506	LEU	2.4
1	B	167	TYR	2.3
1	A	517	ASN	2.3
1	A	135	VAL	2.3
1	A	545	ASN	2.3
1	A	637	ARG	2.3
1	A	642	VAL	2.2
1	B	44	PHE	2.2
1	A	656	LEU	2.2
1	B	656	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	136	MET	2.2
1	A	547	TYR	2.1
1	A	685	PRO	2.1
1	A	164	TRP	2.1
1	A	641	VAL	2.1
1	A	546	ARG	2.1
1	A	580	LEU	2.0
1	B	91	PRO	2.0
1	A	534	LYS	2.0
1	A	723	VAL	2.0
1	B	122	VAL	2.0
1	A	196	ASP	2.0
1	A	684	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PGO	B	1344	5/5	0.64	0.19	62,62,63,65	0
4	PGO	B	1343	5/5	0.76	0.17	46,49,50,51	0
3	PO4	B	1332	5/5	0.80	0.17	64,64,65,65	0
4	PGO	B	1345	5/5	0.83	0.14	50,53,53,54	0
4	PGO	A	1340	5/5	0.89	0.11	45,46,47,48	0
4	PGO	A	1341	5/5	0.91	0.12	58,59,59,60	0
4	PGO	A	1342	5/5	0.92	0.09	48,48,49,49	0
3	PO4	A	1330	5/5	0.95	0.08	36,36,40,40	0
2	CA	A	1320	1/1	0.97	0.11	30,30,30,30	0
2	CA	B	1321	1/1	0.98	0.07	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	B	1331	5/5	0.99	0.05	25,26,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.