



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:29 AM UTC

PDB ID : 1EVU / pdb_00001evu
Title : HUMAN FACTOR XIII WITH CALCIUM BOUND IN THE ION SITE
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Deposited on : 2000-04-20
Resolution : 2.01 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

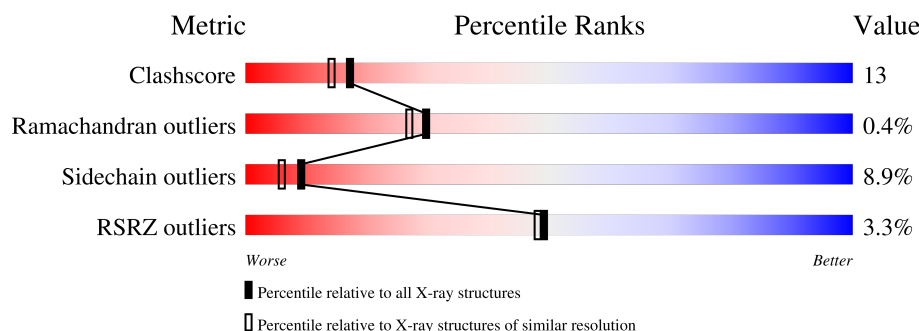
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	4% 60% 28% 6% • •
1	B	731	3% 65% 25% 6% • •

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
1	SAC	A	1	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12593 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	3	0
			5709	3618	981	1084	26			
1	B	708	Total	C	N	O	S	0	4	0
			5718	3623	988	1081	26			

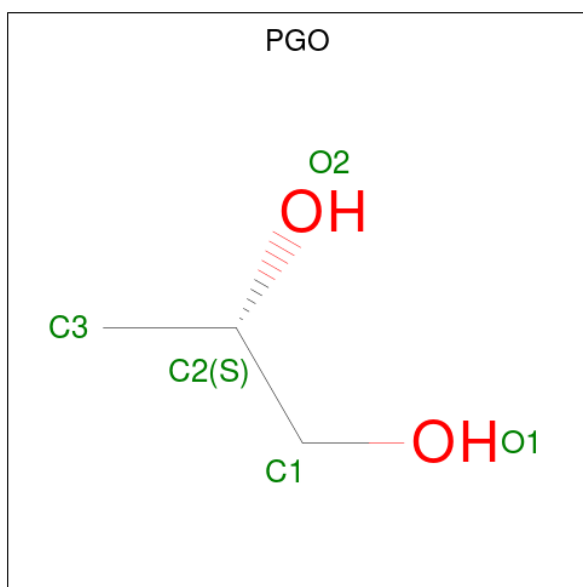
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SAC	SER	modified residue	UNP P00488
B	1	SAC	SER	modified residue	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 S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: C₃H₈O₂).



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

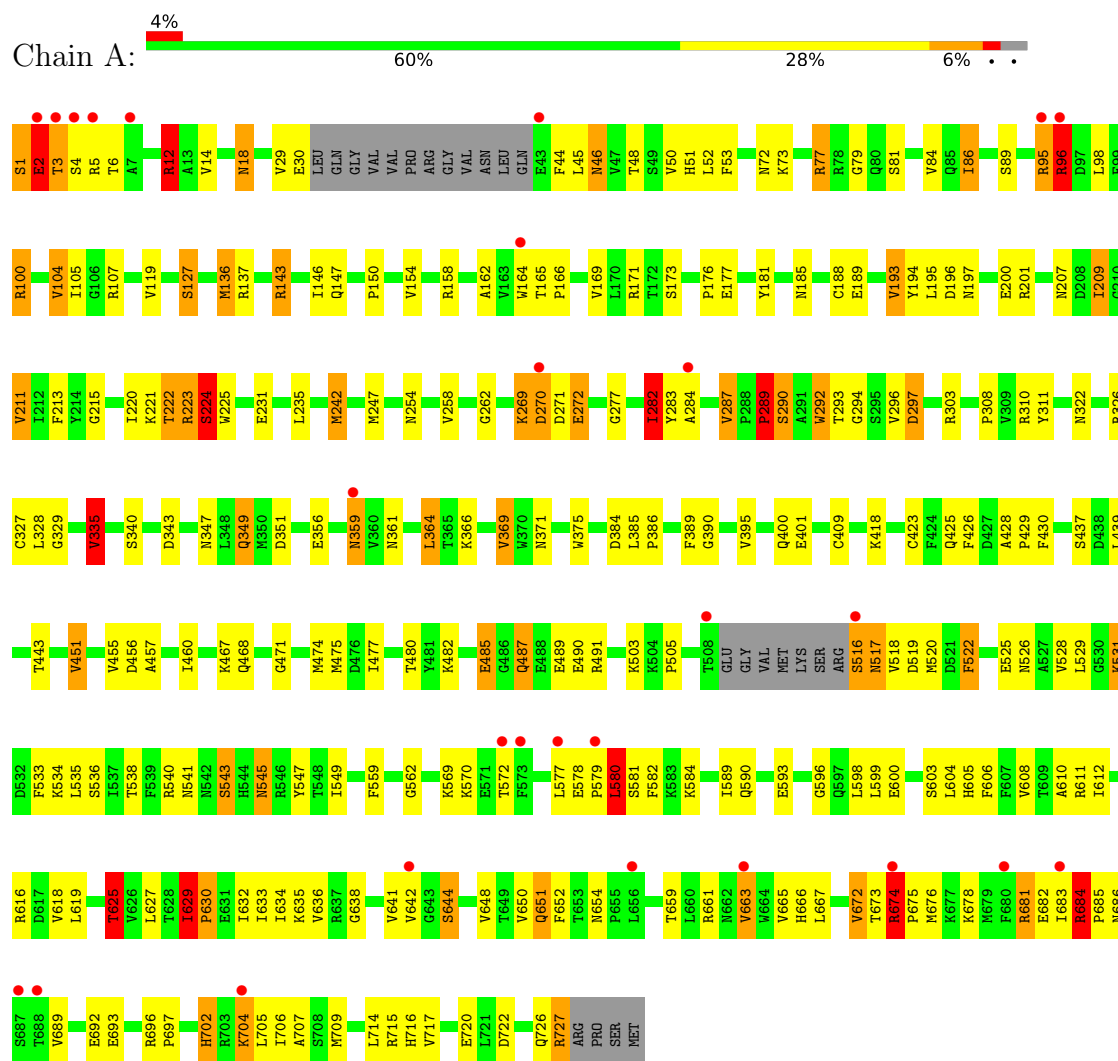
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	542	Total	O	0	0
			542	542		
4	B	617	Total	O	0	0
			617	617		

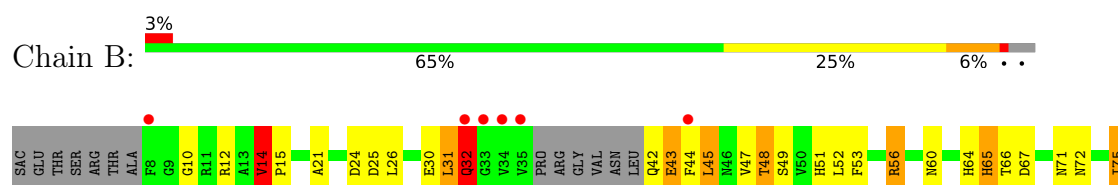
3 Residue-property plots

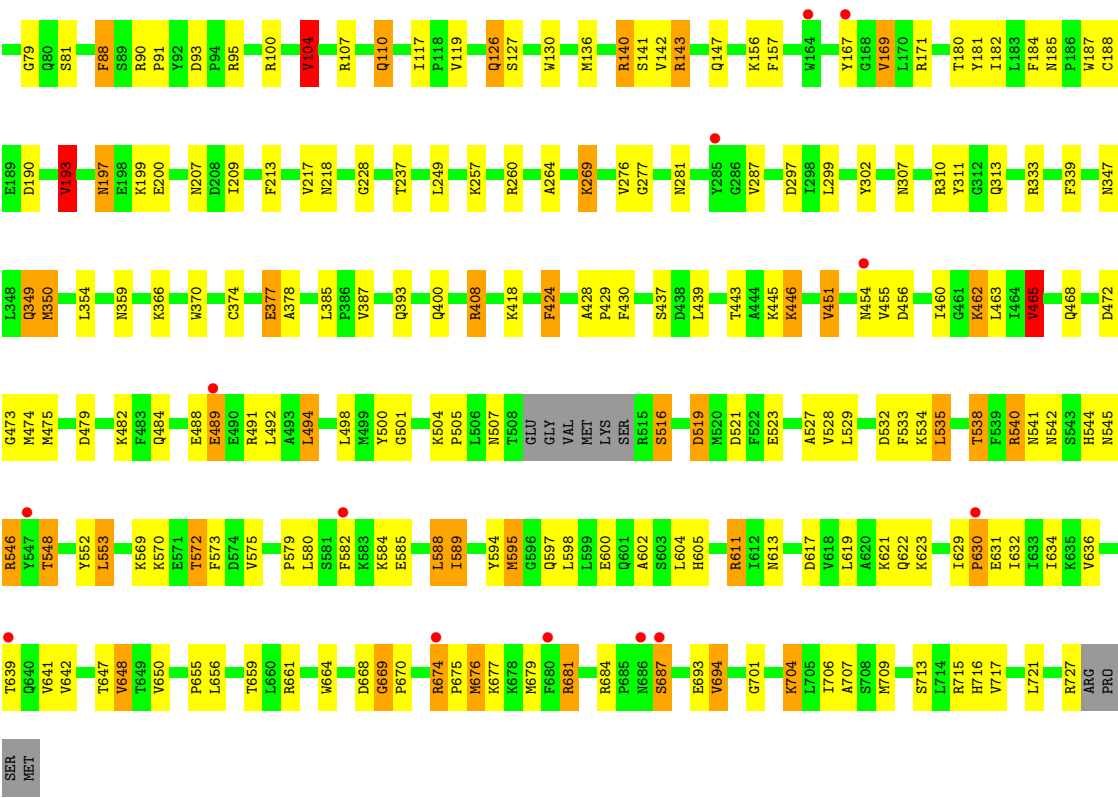
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: COAGULATION FACTOR XIII





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.17Å 70.76Å 133.82Å 90.00° 106.11° 90.00°	Depositor
Resolution (Å)	20.66 – 2.01 20.66 – 2.01	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.66-2.01) 91.9 (20.66-2.01)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.266 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12593	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PGO, SAC

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	0.87	0/5834	1.77	97/7916 (1.2%)
1	B	0.92	0/5851	1.84	113/7938 (1.4%)
All	All	0.90	0/11685	1.81	210/15854 (1.3%)

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	5
1	B	0	3
All	All	0	8

There are no bond length outliers.

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	ARG	NE-CZ-NH2	-13.01	107.49	119.20
1	A	100	ARG	CD-NE-CZ	13.01	142.62	124.40
1	A	282	ILE	N-CA-CB	11.81	121.33	111.64
1	A	147	GLN	OE1-CD-NE2	10.98	133.58	122.60
1	A	371	ASN	OD1-CG-ND2	9.64	132.24	122.60
1	B	197	ASN	OD1-CG-ND2	9.18	131.78	122.60
1	A	605	HIS	CA-CB-CG	-9.04	104.76	113.80
1	B	60	ASN	OD1-CG-ND2	-8.71	113.89	122.60
1	B	359	ASN	OD1-CG-ND2	8.39	130.99	122.60
1	A	215	GLY	CA-C-N	-7.89	109.73	122.36
1	A	215	GLY	C-N-CA	-7.89	109.73	122.36
1	B	218	ASN	CA-CB-CG	-7.88	104.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	ASP	CA-CB-CG	7.83	120.43	112.60
1	B	630	PRO	CA-C-O	-7.72	112.23	121.03
1	A	84	VAL	CA-C-O	-7.67	113.62	121.67
1	B	48	THR	N-CA-C	-7.54	104.60	113.88
1	B	313	GLN	CA-C-O	-7.53	112.44	121.32
1	A	672	VAL	CB-CA-C	-7.47	104.34	111.44
1	A	270	ASP	CB-CA-C	-7.44	108.00	116.63
1	B	193	VAL	CA-CB-CG1	7.37	122.94	110.40
1	B	107	ARG	CD-NE-CZ	7.28	134.60	124.40
1	B	51	HIS	CA-CB-CG	-7.26	106.54	113.80
1	B	56	ARG	NH1-CZ-NH2	7.18	128.64	119.30
1	B	187	TRP	N-CA-C	-7.16	104.15	113.17
1	B	516	SER	CA-C-O	7.08	128.31	119.95
1	B	60	ASN	CA-CB-CG	7.07	119.67	112.60
1	A	322	ASN	CA-CB-CG	-6.89	105.71	112.60
1	B	193	VAL	N-CA-CB	-6.89	100.51	112.08
1	B	281	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	A	213	PHE	CA-CB-CG	-6.83	106.97	113.80
1	A	79	GLY	N-CA-C	-6.73	106.04	115.32
1	A	222	THR	N-CA-CB	6.68	121.35	110.32
1	B	605	HIS	CA-CB-CG	-6.68	107.12	113.80
1	A	262	GLY	O-C-N	6.67	128.66	122.19
1	B	400	GLN	CA-C-O	-6.65	114.19	121.31
1	A	221	LYS	CA-CB-CG	6.64	127.37	114.10
1	B	71	ASN	OD1-CG-ND2	-6.51	116.09	122.60
1	A	270	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	188	CYS	O-C-N	-6.48	115.84	123.22
1	B	171	ARG	CD-NE-CZ	6.47	133.46	124.40
1	B	611	ARG	NE-CZ-NH1	-6.43	115.07	121.50
1	B	287	VAL	N-CA-CB	-6.43	105.55	112.37
1	B	668	ASP	CA-CB-CG	6.43	119.03	112.60
1	B	542	ASN	OD1-CG-ND2	-6.42	116.18	122.60
1	A	389	PHE	CA-C-N	-6.40	115.94	122.27
1	A	389	PHE	C-N-CA	-6.40	115.94	122.27
1	A	50	VAL	O-C-N	-6.38	116.27	123.10
1	B	302	TYR	O-C-N	-6.36	114.50	122.20
1	A	46	ASN	OD1-CG-ND2	6.36	128.96	122.60
1	B	140	ARG	CA-C-O	6.32	126.66	119.27
1	A	104	VAL	CA-CB-CG2	6.28	121.08	110.40
1	A	522	PHE	CA-CB-CG	6.28	120.08	113.80
1	B	140	ARG	O-C-N	-6.24	113.91	122.46
1	B	349	GLN	OE1-CD-NE2	-6.23	116.37	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	588	LEU	CA-C-O	-6.21	113.66	120.43
1	B	32	GLN	CB-CA-C	6.18	120.34	109.89
1	B	79	GLY	N-CA-C	-6.18	106.72	115.30
1	B	648	VAL	O-C-N	6.17	129.47	122.93
1	B	197	ASN	CA-C-O	-6.16	114.24	121.44
1	B	110	GLN	OE1-CD-NE2	6.15	128.75	122.60
1	B	701	GLY	N-CA-C	-6.15	104.09	112.52
1	A	223	ARG	CD-NE-CZ	-6.12	115.83	124.40
1	A	400	GLN	CA-C-O	-6.11	114.91	121.45
1	B	81	SER	N-CA-C	6.11	119.11	110.50
1	B	140	ARG	CA-C-N	6.10	129.53	120.87
1	B	140	ARG	C-N-CA	6.10	129.53	120.87
1	A	201	ARG	CD-NE-CZ	6.08	132.91	124.40
1	A	209	ILE	CA-C-N	-6.08	117.06	122.47
1	A	209	ILE	C-N-CA	-6.08	117.06	122.47
1	A	674	ARG	CD-NE-CZ	6.05	132.88	124.40
1	A	375	TRP	CA-C-O	-6.04	114.92	121.14
1	B	141	SER	N-CA-C	6.02	119.19	110.28
1	A	517	ASN	OD1-CG-ND2	6.00	128.60	122.60
1	A	347	ASN	CA-CB-CG	-5.99	106.61	112.60
1	B	465	VAL	N-CA-CB	-5.97	101.31	112.36
1	B	622	GLN	CA-CB-CG	5.97	126.05	114.10
1	B	545	ASN	OD1-CG-ND2	5.97	128.57	122.60
1	B	378	ALA	N-CA-C	-5.96	99.28	109.24
1	A	423	CYS	O-C-N	-5.96	114.50	122.43
1	B	430	PHE	CA-CB-CG	-5.95	107.85	113.80
1	B	532	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	30	GLU	N-CA-CB	5.94	120.31	111.23
1	B	277	GLY	CA-C-O	-5.93	116.19	121.64
1	A	84	VAL	O-C-N	5.92	129.61	123.04
1	B	21	ALA	O-C-N	-5.91	115.30	122.22
1	A	328	LEU	N-CA-C	-5.91	105.90	113.23
1	B	257	LYS	CA-C-O	-5.90	114.16	120.42
1	B	31	LEU	CA-C-O	5.87	128.65	121.72
1	A	158	ARG	CD-NE-CZ	5.87	132.62	124.40
1	B	107	ARG	N-CA-C	-5.83	106.01	113.23
1	B	228	GLY	CA-C-O	-5.82	113.05	120.03
1	A	143	ARG	CD-NE-CZ	5.78	132.49	124.40
1	B	674	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	A	401	GLU	CG-CD-OE1	5.77	131.66	118.40
1	A	430	PHE	N-CA-C	5.76	117.56	111.28
1	B	347	ASN	OD1-CG-ND2	5.76	128.36	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	684	ARG	CD-NE-CZ	5.75	132.44	124.40
1	B	727	ARG	CD-NE-CZ	5.73	132.43	124.40
1	A	262	GLY	CA-C-O	-5.71	114.60	120.66
1	A	335	VAL	CA-CB-CG1	5.70	120.09	110.40
1	A	86	ILE	CB-CA-C	-5.70	102.34	110.83
1	B	182	ILE	CA-C-O	-5.68	114.23	120.48
1	B	333	ARG	CD-NE-CZ	-5.67	116.47	124.40
1	B	207	ASN	O-C-N	-5.65	115.84	122.96
1	B	500	TYR	CA-C-N	5.64	129.40	123.08
1	B	500	TYR	C-N-CA	5.64	129.40	123.08
1	B	647	THR	CA-C-N	-5.64	114.84	122.91
1	B	647	THR	C-N-CA	-5.64	114.84	122.91
1	A	77	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	A	632	ILE	CB-CA-C	-5.62	103.51	111.21
1	A	612	ILE	N-CA-C	5.62	116.26	108.84
1	B	171	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	B	541	ASN	OD1-CG-ND2	5.59	128.19	122.60
1	A	663	VAL	N-CA-C	5.58	112.19	106.21
1	B	185	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	A	277	GLY	CA-C-O	-5.58	116.51	121.64
1	A	409	CYS	CA-C-O	-5.56	114.69	120.70
1	B	260	ARG	NE-CZ-NH2	-5.56	114.19	119.20
1	B	14	VAL	CA-C-O	5.56	122.96	119.51
1	B	249	LEU	CA-C-O	-5.54	114.55	120.42
1	B	535	LEU	N-CA-CB	-5.53	101.21	110.83
1	B	504	LYS	CA-C-N	5.52	125.18	119.05
1	B	504	LYS	C-N-CA	5.52	125.18	119.05
1	B	197	ASN	O-C-N	5.52	130.33	123.15
1	B	611	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	A	296	VAL	O-C-N	-5.51	116.17	121.90
1	B	600	GLU	CA-C-N	5.51	135.86	125.66
1	B	600	GLU	C-N-CA	5.51	135.86	125.66
1	B	199	LYS	N-CA-CB	5.50	118.20	110.12
1	B	71	ASN	CB-CG-ND2	5.46	124.59	116.40
1	B	185	ASN	CA-C-N	5.45	125.16	119.82
1	B	185	ASN	C-N-CA	5.45	125.16	119.82
1	A	96	ARG	N-CA-C	5.45	121.14	113.02
1	A	430	PHE	CA-CB-CG	-5.44	108.36	113.80
1	B	621	LYS	CA-C-O	-5.43	114.91	120.99
1	B	521	ASP	CA-C-O	-5.43	115.64	121.45
1	B	190	ASP	CA-CB-CG	-5.42	107.18	112.60
1	A	254	ASN	CA-C-N	5.41	125.23	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ASN	C-N-CA	5.41	125.23	119.28
1	A	188	CYS	O-C-N	-5.39	116.93	123.13
1	A	171	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	B	104	VAL	CA-CB-CG2	5.38	119.55	110.40
1	A	629	ILE	CA-C-N	5.36	125.28	119.76
1	A	629	ILE	C-N-CA	5.36	125.28	119.76
1	A	48	THR	N-CA-C	-5.35	107.30	113.88
1	A	154	VAL	N-CA-CB	-5.35	104.89	110.72
1	B	408	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	A	193	VAL	N-CA-CB	-5.34	102.42	111.23
1	A	137	ARG	NE-CZ-NH2	-5.34	114.40	119.20
1	B	64	HIS	CE1-NE2-CD2	5.34	114.34	109.00
1	B	377	GLU	CA-C-O	-5.34	114.52	120.66
1	B	424	PHE	CA-CB-CG	-5.34	108.46	113.80
1	A	326	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	B	209	ILE	CA-C-N	-5.33	116.32	122.77
1	B	209	ILE	C-N-CA	-5.33	116.32	122.77
1	B	260	ARG	NH1-CZ-NH2	5.33	126.22	119.30
1	B	157	PHE	CA-C-N	-5.32	114.72	122.65
1	B	157	PHE	C-N-CA	-5.32	114.72	122.65
1	A	104	VAL	CB-CA-C	5.32	119.91	110.71
1	B	143	ARG	NE-CZ-NH1	-5.29	116.20	121.50
1	A	526	ASN	CA-C-O	-5.28	115.03	121.05
1	A	351	ASP	CA-C-N	-5.27	116.27	123.12
1	A	351	ASP	C-N-CA	-5.27	116.27	123.12
1	B	297	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	489	GLU	CA-CB-CG	5.26	124.62	114.10
1	A	3	THR	N-CA-C	5.25	118.38	109.76
1	A	343	ASP	CA-CB-CG	-5.25	107.35	112.60
1	B	88	PHE	N-CA-C	5.25	117.63	110.55
1	B	631	GLU	O-C-N	-5.24	116.67	122.86
1	A	390	GLY	N-CA-C	-5.21	104.59	112.41
1	B	276	VAL	CB-CA-C	-5.21	104.38	111.15
1	A	451	VAL	CA-C-O	5.20	125.88	120.36
1	A	630	PRO	CB-CA-C	-5.20	104.75	111.46
1	B	14	VAL	N-CA-C	5.20	113.79	107.61
1	A	638	GLY	N-CA-C	-5.19	104.00	112.83
1	A	395	VAL	CA-C-N	-5.18	115.50	123.07
1	A	395	VAL	C-N-CA	-5.18	115.50	123.07
1	A	651	GLN	N-CA-C	5.17	116.84	108.41
1	B	619	LEU	CA-C-O	-5.16	115.24	120.71
1	B	65	HIS	CA-CB-CG	-5.16	108.64	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	THR	CA-CB-OG1	-5.14	101.88	109.60
1	A	329	GLY	CA-C-N	-5.14	118.31	123.04
1	A	329	GLY	C-N-CA	-5.14	118.31	123.04
1	B	374	CYS	O-C-N	5.14	129.01	123.10
1	A	289	PRO	O-C-N	-5.13	115.60	122.22
1	A	625	THR	N-CA-CB	-5.13	101.98	111.52
1	B	169	VAL	N-CA-C	5.13	117.15	109.20
1	A	272	GLU	CA-C-N	-5.13	116.63	122.83
1	A	272	GLU	C-N-CA	-5.13	116.63	122.83
1	A	224	SER	CA-C-O	-5.12	115.37	121.16
1	A	457	ALA	CA-C-O	-5.12	113.36	119.35
1	B	171	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	A	207	ASN	N-CA-C	5.09	117.08	109.59
1	B	307	ASN	OD1-CG-ND2	-5.09	117.50	122.60
1	A	535	LEU	CA-C-O	-5.09	114.02	120.28
1	A	46	ASN	N-CA-CB	-5.07	102.05	111.13
1	B	387	VAL	CA-CB-CG1	5.07	119.02	110.40
1	A	12[A]	ARG	CA-C-O	-5.06	115.33	120.89
1	A	12[B]	ARG	CA-C-O	-5.06	115.33	120.89
1	A	349	GLN	CB-CG-CD	5.05	121.19	112.60
1	A	351	ASP	N-CA-CB	5.04	118.65	110.43
1	A	242	MET	N-CA-C	5.04	116.77	111.28
1	A	343	ASP	O-C-N	-5.03	115.81	122.40
1	B	545	ASN	CA-CB-CG	-5.03	107.57	112.60
1	A	150	PRO	N-CA-C	-5.02	108.07	114.35
1	A	359	ASN	OD1-CG-ND2	5.02	127.62	122.60
1	B	716	HIS	CA-CB-CG	-5.01	108.78	113.80
1	B	501	GLY	N-CA-C	5.01	120.44	114.48
1	B	681	ARG	N-CA-C	5.01	117.39	111.33
1	A	127	SER	CA-C-O	-5.00	115.68	121.19

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ILE	Mainchain
1	A	12[B]	ARG	Mainchain
1	A	2	GLU	Peptide
1	A	3	THR	Peptide
1	A	596	GLY	Peptide
1	B	32	GLN	Peptide
1	B	632	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	B	75	ILE	Mainchain

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	5709	0	5546	174	0
1	B	5718	0	5564	118	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	5	0	8	0	0
4	A	542	0	0	11	0
4	B	617	0	0	15	0
All	All	12593	0	11118	284	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 13.

All (284) 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:A:629:ILE:HD11	1:A:717:VAL:HG22	1.27	1.08
1:B:548:THR:HG22	1:B:613:ASN:HD22	1.15	1.07
1:B:44:PHE:O	1:B:45:LEU:HB2	1.53	1.06
1:A:676:MET:HE1	1:A:693:GLU:HG2	1.41	1.02
1:A:528:VAL:HB	1:A:531:LYS:HD3	1.43	1.00
1:B:630:PRO:HG3	1:B:655:PRO:HG3	1.51	0.93
1:B:443:THR:HB	1:B:451:VAL:HG13	1.49	0.92
1:B:595:MET:HE2	1:B:595:MET:HA	1.49	0.91
1:A:290:SER:HG	1:A:716:HIS:HD1	0.90	0.90
1:A:242:MET:CE	1:A:258:VAL:HG22	2.09	0.82
1:A:211:VAL:HG22	1:A:467:LYS:HB2	1.61	0.81
1:A:681:ARG:HH11	1:A:681:ARG:HB3	1.45	0.80
1:A:528:VAL:HB	1:A:531:LYS:CD	2.11	0.80
1:A:242:MET:HE3	1:A:258:VAL:HG13	1.64	0.79
1:A:95:ARG:NH1	1:A:96:ARG:NH1	2.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559[A]:PHE:CE1	1:A:599:LEU:HD13	2.20	0.76
1:A:641:VAL:HB	1:A:644:SER:HB2	1.66	0.75
1:B:519:ASP:HB3	1:B:540:ARG:HD3	1.69	0.75
1:B:629:ILE:HG23	1:B:630:PRO:HD2	1.68	0.75
1:A:681:ARG:HD2	1:A:682:GLU:HG2	1.69	0.74
1:A:709:MET:HE3	1:A:717:VAL:HG21	1.70	0.73
1:A:684:ARG:H	1:A:684:ARG:HD2	1.53	0.73
1:A:242:MET:HE1	1:A:258:VAL:HG22	1.70	0.73
1:A:633:ILE:HB	1:A:651:GLN:HB3	1.71	0.72
1:A:335:VAL:HG22	1:A:477:ILE:HD11	1.70	0.72
1:A:290:SER:OG	1:A:716:HIS:ND1	2.09	0.71
1:B:529:LEU:HD21	1:B:656:LEU:HD21	1.75	0.69
1:A:559[A]:PHE:CD1	1:A:599:LEU:HD13	2.28	0.68
1:A:5:ARG:O	1:A:6:THR:HB	1.93	0.68
1:A:100:ARG:HG2	1:A:164:TRP:CZ3	2.28	0.68
1:B:595:MET:HA	1:B:595:MET:CE	2.21	0.68
1:B:540:ARG:HG3	1:B:582:PHE:CE2	2.30	0.67
1:B:548:THR:HG22	1:B:613:ASN:ND2	2.00	0.67
1:B:197:ASN:ND2	1:B:200:GLU:OE1	2.25	0.66
1:A:418:LYS:HD2	1:A:480:THR:O	1.96	0.66
1:B:569:LYS:CD	1:B:589:ILE:HD13	2.26	0.65
1:A:18:ASN:C	1:A:18:ASN:HD22	2.05	0.65
1:A:272:GLU:O	4:A:1507:HOH:O	2.14	0.64
1:A:642:VAL:HG23	1:A:726:GLN:O	1.97	0.64
1:A:650:VAL:HG11	1:A:665:VAL:HG11	1.80	0.64
1:A:727:ARG:HA	1:A:727:ARG:HH11	1.62	0.64
1:A:1:SAC:H2A1	1:A:1:SAC:C	2.25	0.63
1:B:594:TYR:CE1	1:B:595:MET:HE3	2.34	0.63
1:B:349:GLN:OE1	1:B:505:PRO:HD2	1.99	0.63
1:B:676:MET:HE3	1:B:693:GLU:HG3	1.80	0.63
1:B:156:LYS:HD2	1:B:181:TYR:CZ	2.33	0.62
1:A:726:GLN:O	1:A:727:ARG:HB2	1.99	0.62
1:A:1:SAC:HB2	1:B:713:SER:O	1.99	0.62
1:A:46:ASN:HD22	1:A:89:SER:HB3	1.64	0.62
1:B:472:ASP:OD2	1:B:704:LYS:NZ	2.33	0.61
1:B:674:ARG:HD2	1:B:675:PRO:HD2	1.82	0.61
1:A:2:GLU:OE1	1:B:598:LEU:HD12	1.99	0.61
1:A:579:PRO:O	1:A:580:LEU:C	2.44	0.61
1:A:682:GLU:CD	1:A:684:ARG:HE	2.09	0.61
1:A:100:ARG:HB2	1:A:119:VAL:O	2.02	0.60
1:A:559[B]:PHE:HD1	1:A:599:LEU:HD13	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:LYS:HD2	1:A:570:LYS:N	2.17	0.60
1:A:629:ILE:HD12	1:A:630:PRO:HD2	1.82	0.60
4:A:1583:HOH:O	1:B:366:LYS:HE3	2.00	0.60
1:A:629:ILE:CD1	1:A:717:VAL:HG22	2.18	0.60
1:B:694:VAL:HG12	4:B:1525:HOH:O	2.01	0.60
1:A:667:LEU:HD23	1:A:676:MET:HE3	1.84	0.59
1:B:544:HIS:CE1	1:B:580:LEU:HD11	2.37	0.59
1:A:439:LEU:HB2	1:A:456:ASP:HB3	1.85	0.59
1:A:269:LYS:O	1:A:270:ASP:HB2	2.03	0.59
1:A:468:GLN:HG3	1:A:471:GLY:H	1.67	0.59
1:A:51:HIS:HB3	4:A:1391:HOH:O	2.02	0.59
1:B:269:LYS:HD2	4:B:1257:HOH:O	2.01	0.59
1:A:242:MET:HE2	1:A:247:MET:SD	2.43	0.59
1:A:672:VAL:O	4:A:1332:HOH:O	2.17	0.59
1:B:569:LYS:HD3	1:B:589:ILE:HD13	1.84	0.58
1:B:629:ILE:CG2	1:B:630:PRO:HD2	2.33	0.58
1:A:629:ILE:HD12	1:A:630:PRO:CD	2.34	0.58
1:B:538:THR:HG21	1:B:584:LYS:NZ	2.18	0.58
1:A:629:ILE:HD11	1:A:717:VAL:CG2	2.18	0.58
1:A:224:SER:HB2	1:A:720:GLU:OE1	2.03	0.58
1:A:516:SER:O	1:A:517:ASN:HB2	2.03	0.57
1:A:225:TRP:CE2	1:A:294:GLY:HA2	2.39	0.57
1:B:385:LEU:HD22	1:B:424:PHE:HB3	1.86	0.57
1:A:538:THR:HG21	1:A:582:PHE:CZ	2.40	0.56
1:A:704:LYS:HE2	1:A:722:ASP:OD1	2.05	0.56
1:B:217:VAL:HG21	1:B:462:LYS:HD2	1.85	0.56
1:B:636:VAL:HG12	1:B:648:VAL:HG22	1.88	0.56
1:B:213:PHE:CE1	1:B:474:MET:HB3	2.40	0.56
1:B:446:LYS:HB2	1:B:446:LYS:NZ	2.21	0.55
1:A:578:GLU:O	1:A:581:SER:OG	2.22	0.55
1:B:488:GLU:OE1	1:B:491:ARG:NH1	2.40	0.55
1:A:1:SAC:O	1:A:2:GLU:HB3	2.06	0.55
1:A:443:THR:HB	1:A:451:VAL:HG13	1.88	0.55
1:B:26:LEU:HD11	1:B:104:VAL:HG11	1.88	0.55
1:A:611:ARG:HD2	1:A:616:ARG:CZ	2.35	0.55
1:B:93:ASP:OD1	1:B:95:ARG:HB2	2.07	0.55
1:A:520:MET:HE3	1:A:619:LEU:HB2	1.88	0.54
1:B:437:SER:HB2	1:B:460:ILE:HD13	1.90	0.54
1:B:552:TYR:CD1	1:B:572:THR:HB	2.42	0.54
1:A:369:VAL:HG13	4:A:1380:HOH:O	2.07	0.54
1:A:543:SER:OG	1:A:545:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:THR:HG23	4:B:1763:HOH:O	2.08	0.53
1:B:674:ARG:NH1	4:B:1516:HOH:O	2.41	0.53
1:A:545:ASN:ND2	1:A:547:TYR:CZ	2.76	0.53
1:A:559[A]:PHE:CD2	1:B:10:GLY:HA2	2.43	0.53
1:B:44:PHE:O	1:B:45:LEU:CB	2.38	0.53
1:A:562:GLY:HA2	4:A:1297:HOH:O	2.07	0.53
1:A:189:GLU:HA	1:A:194:TYR:CG	2.43	0.53
1:A:443:THR:HB	1:A:451:VAL:CG1	2.38	0.53
1:A:666:HIS:O	1:A:707:ALA:HA	2.08	0.53
1:B:679:MET:HE1	1:B:681:ARG:HD3	1.90	0.53
1:A:520:MET:SD	1:A:608:VAL:HG12	2.49	0.53
1:B:538:THR:HB	1:B:584:LYS:HG2	1.91	0.52
1:A:659:THR:HG22	1:A:685:PRO:CD	2.39	0.52
1:A:702:HIS:ND1	1:A:702:HIS:C	2.68	0.52
1:B:66:THR:HG21	1:B:75:ILE:HG22	1.92	0.52
1:A:520:MET:HB2	1:A:619:LEU:HD13	1.92	0.52
1:A:522:PHE:HZ	1:A:606:PHE:HB2	1.75	0.52
1:A:661:ARG:NH1	1:A:681:ARG:HG2	2.25	0.52
1:B:110:GLN:HG2	4:B:1678:HOH:O	2.08	0.52
1:A:136:MET:HB3	1:A:143:ARG:HB3	1.91	0.51
1:A:518:VAL:CG1	1:A:619:LEU:HD11	2.41	0.51
1:A:648:VAL:HG11	1:A:705:LEU:HD13	1.91	0.51
1:A:611:ARG:HD2	1:A:616:ARG:NH2	2.26	0.51
1:A:673:THR:OG1	1:A:676:MET:HE2	2.11	0.51
1:A:676:MET:CE	1:A:693:GLU:HG2	2.29	0.51
1:A:654:ASN:O	1:A:686:ASN:HA	2.10	0.51
1:B:31:LEU:HD22	1:B:167:TYR:HB2	1.92	0.51
1:B:136:MET:HB2	1:B:143:ARG:HB3	1.91	0.51
1:A:162:ALA:HB3	1:A:164:TRP:CZ3	2.45	0.51
1:A:659:THR:HG22	1:A:685:PRO:HD2	1.93	0.51
1:A:282:ILE:HG13	1:A:283:TYR:N	2.25	0.50
1:A:223:ARG:HD3	1:A:224:SER:N	2.26	0.50
1:A:211:VAL:HG13	1:A:467:LYS:HD2	1.93	0.50
1:A:52:LEU:O	1:A:53:PHE:C	2.55	0.50
1:A:516:SER:O	1:A:517:ASN:CB	2.60	0.50
1:A:604:LEU:HB2	1:A:625:THR:HG22	1.93	0.50
1:A:289:PRO:HD3	1:A:311:TYR:HB2	1.94	0.50
1:B:519:ASP:HB3	1:B:540:ARG:CD	2.41	0.50
1:A:437:SER:HB2	1:A:460:ILE:HD13	1.94	0.49
1:B:706:ILE:HG23	4:B:1534:HOH:O	2.12	0.49
1:A:642:VAL:HG23	1:A:727:ARG:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LEU:HA	1:A:327:CYS:SG	2.51	0.49
1:A:242:MET:CE	1:A:258:VAL:HG13	2.39	0.49
1:B:14:VAL:HG23	1:B:15:PRO:HD2	1.94	0.49
1:A:73:LYS:HE3	1:A:176:PRO:O	2.13	0.49
1:A:475:MET:HE2	4:A:1654:HOH:O	2.12	0.49
1:B:65:HIS:HD2	4:B:1278:HOH:O	1.94	0.49
1:B:468:GLN:HG2	1:B:473:GLY:O	2.13	0.49
1:A:652:PHE:CE2	1:A:709:MET:HE2	2.48	0.49
1:B:65:HIS:HE1	4:B:1462:HOH:O	1.94	0.49
1:A:529:LEU:HD11	1:A:598:LEU:CD1	2.42	0.49
1:A:72:ASN:OD1	1:A:72:ASN:C	2.55	0.49
1:A:297:ASP:N	1:A:297:ASP:OD1	2.44	0.49
1:B:679:MET:HE3	1:B:681:ARG:HA	1.95	0.48
1:A:636:VAL:HG12	1:A:648:VAL:HG22	1.94	0.48
1:A:12[B]:ARG:NH2	4:A:1366:HOH:O	2.44	0.48
1:A:635:LYS:HD2	4:A:1455:HOH:O	2.13	0.48
1:A:681:ARG:HH11	1:A:681:ARG:CB	2.22	0.48
1:B:546:ARG:NH1	1:B:546:ARG:HG3	2.29	0.48
1:B:579:PRO:O	1:B:580:LEU:C	2.53	0.48
1:A:425:GLN:HG2	4:B:1316:HOH:O	2.14	0.48
1:A:1:SAC:C2A	1:B:602:ALA:HB2	2.44	0.47
1:A:95:ARG:NH1	1:A:96:ARG:HH11	2.07	0.47
1:A:356:GLU:O	1:A:611:ARG:NE	2.46	0.47
1:B:594:TYR:CD1	1:B:595:MET:HE3	2.48	0.47
1:A:385:LEU:HB3	1:A:386:PRO:HD2	1.96	0.47
1:A:271:ASP:HA	1:A:308:PRO:HG2	1.97	0.47
1:B:126:GLN:O	1:B:147:GLN:NE2	2.45	0.47
1:A:98:LEU:HD23	1:A:164:TRP:HB2	1.96	0.47
1:A:223:ARG:NH2	1:A:292:TRP:O	2.47	0.47
1:B:140:ARG:N	1:B:140:ARG:HD2	2.30	0.47
1:B:684:ARG:O	1:B:687:SER:HB3	2.15	0.47
1:A:209:ILE:HD13	1:A:704:LYS:HB2	1.96	0.47
1:A:223:ARG:HD3	1:A:224:SER:O	2.14	0.47
1:A:287:VAL:HG13	1:A:310:ARG:O	2.15	0.47
1:A:487:GLN:NE2	1:A:489:GLU:OE1	2.47	0.47
1:B:548:THR:CG2	1:B:613:ASN:HD22	2.06	0.47
1:A:1:SAC:CB	1:B:713:SER:O	2.63	0.47
1:B:529:LEU:HD11	1:B:595:MET:HE1	1.97	0.47
1:B:639:THR:HB	1:B:641:VAL:HG23	1.96	0.47
1:A:570:LYS:HD2	1:A:570:LYS:H	1.80	0.46
1:B:90:ARG:HB2	1:B:91:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:VAL:O	1:B:642:VAL:C	2.55	0.46
1:A:349:GLN:OE1	1:A:505:PRO:HD2	2.15	0.46
1:B:465:VAL:HG21	1:B:474:MET:SD	2.56	0.46
1:B:674:ARG:CD	1:B:675:PRO:HD2	2.45	0.46
1:A:165:THR:HB	1:A:166:PRO:HD2	1.98	0.46
1:A:197:ASN:HB3	1:A:200:GLU:HB2	1.98	0.46
1:A:522:PHE:CZ	1:A:606:PHE:HB2	2.50	0.46
1:B:494:LEU:HD22	1:B:494:LEU:O	2.16	0.46
1:A:209:ILE:HG21	1:A:704:LYS:HD3	1.97	0.46
1:A:538:THR:CG2	1:A:582:PHE:CZ	2.99	0.46
1:A:282:ILE:HG13	1:A:283:TYR:H	1.80	0.45
1:A:630:PRO:O	1:A:717:VAL:HG13	2.16	0.45
1:A:648:VAL:CG1	1:A:705:LEU:HD13	2.47	0.45
1:B:527:ALA:HB2	1:B:533:PHE:HB3	1.98	0.45
1:A:1:SAC:H	1:B:715:ARG:H	1.65	0.45
1:B:24:ASP:HA	4:B:1519:HOH:O	2.16	0.45
1:A:489:GLU:CD	1:A:489:GLU:H	2.24	0.45
1:A:519:ASP:HB2	1:A:540:ARG:HB3	1.98	0.45
1:A:536:SER:CB	1:A:584:LYS:HE2	2.46	0.45
1:A:600:GLU:OE1	1:A:715:ARG:NH1	2.49	0.45
1:B:594:TYR:HE1	1:B:595:MET:HE3	1.80	0.45
1:A:4:SER:OG	1:B:597:GLN:HA	2.17	0.45
1:A:682:GLU:OE1	1:A:684:ARG:HG3	2.16	0.45
1:B:706:ILE:HG21	4:B:1662:HOH:O	2.15	0.45
1:A:220:ILE:HD13	1:A:474:MET:SD	2.57	0.45
1:A:696:ARG:O	1:A:697:PRO:C	2.58	0.45
1:A:727:ARG:HA	1:A:727:ARG:NH1	2.29	0.45
1:A:549:ILE:CG2	1:A:610:ALA:HB1	2.47	0.45
1:B:48:THR:O	1:B:49:SER:HB3	2.16	0.45
1:B:538:THR:HG21	1:B:584:LYS:HZ2	1.82	0.45
1:B:709:MET:HE3	1:B:717:VAL:HB	1.99	0.44
1:A:559[A]:PHE:CZ	1:A:599:LEU:HD13	2.52	0.44
1:B:12[A]:ARG:NH2	4:B:1503:HOH:O	2.49	0.44
1:B:553:LEU:O	1:B:570:LYS:HD2	2.17	0.44
1:A:30:GLU:HB2	1:A:169:VAL:HB	2.00	0.44
1:B:339:PHE:HA	1:B:370:TRP:O	2.17	0.44
1:A:231:GLU:OE1	1:A:231:GLU:HA	2.18	0.44
1:A:629:ILE:HD12	1:A:630:PRO:HG2	1.98	0.44
1:B:529:LEU:CD2	1:B:656:LEU:HD21	2.47	0.44
1:A:29:VAL:HG23	1:A:29:VAL:O	2.18	0.44
1:A:569:LYS:HD2	1:A:593:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:MET:HE1	1:A:258:VAL:CG2	2.45	0.43
1:A:598:LEU:HD11	1:A:627:LEU:HD13	2.00	0.43
1:B:52:LEU:O	1:B:53:PHE:C	2.60	0.43
1:B:443:THR:HB	1:B:451:VAL:CG1	2.34	0.43
1:A:1:SAC:O	1:A:2:GLU:CB	2.67	0.43
1:A:44:PHE:CZ	1:A:166:PRO:HD2	2.53	0.43
1:A:674:ARG:HG3	1:A:674:ARG:HH11	1.84	0.43
1:A:189:GLU:HA	1:A:194:TYR:CD1	2.53	0.43
1:A:310:ARG:HA	1:A:311:TYR:HA	1.72	0.43
1:A:491:ARG:HD2	4:A:1658:HOH:O	2.18	0.43
1:B:428:ALA:N	1:B:429:PRO:CD	2.82	0.43
1:A:569:LYS:HE2	1:A:589:ILE:HG13	2.01	0.43
1:A:629:ILE:HD13	1:A:714:LEU:HD11	1.99	0.43
1:A:634:ILE:HD12	1:A:720:GLU:HA	2.00	0.43
1:B:130:TRP:HA	1:B:147:GLN:O	2.18	0.43
1:A:663:VAL:HG13	1:A:709:MET:SD	2.59	0.43
1:B:377:GLU:HA	1:B:393:GLN:O	2.19	0.43
1:A:283:TYR:O	1:A:284:ALA:C	2.62	0.43
1:A:683:ILE:HG12	1:A:689:VAL:HG13	2.01	0.43
1:B:42:GLN:O	1:B:43:GLU:OE1	2.36	0.43
1:A:667:LEU:HD23	1:A:676:MET:CE	2.48	0.42
1:A:684:ARG:O	1:A:685:PRO:C	2.60	0.42
1:B:88:PHE:O	1:B:140:ARG:HB3	2.19	0.42
1:B:56:ARG:CD	1:B:67:ASP:O	2.67	0.42
1:B:439:LEU:HB2	1:B:456:ASP:HB3	2.02	0.42
1:B:573:PHE:CZ	1:B:585:GLU:HG2	2.54	0.42
1:B:264:ALA:HA	1:B:408:ARG:HG2	2.02	0.42
1:B:117:ILE:HG21	1:B:130:TRP:CE2	2.55	0.42
1:B:611:ARG:HE	1:B:611:ARG:HB3	1.66	0.42
1:B:629:ILE:CG2	1:B:717:VAL:HG22	2.50	0.42
1:B:184:PHE:HB3	1:B:193:VAL:HG11	2.02	0.42
1:B:538:THR:HG21	1:B:584:LYS:HZ3	1.82	0.42
1:B:310[B]:ARG:HA	1:B:311:TYR:HA	1.62	0.42
1:A:173:SER:HA	4:A:1500:HOH:O	2.19	0.42
1:A:194:TYR:CE2	1:A:196:ASP:HB3	2.55	0.42
1:A:428:ALA:N	1:A:429:PRO:CD	2.83	0.42
1:A:425:GLN:HB2	1:A:426:PHE:CD2	2.54	0.42
1:B:72:ASN:ND2	4:B:1789:HOH:O	2.53	0.41
1:A:485:GLU:HA	1:A:490:GLU:CD	2.45	0.41
1:B:100:ARG:HG2	1:B:119:VAL:O	2.20	0.41
1:B:310[A]:ARG:HA	1:B:311:TYR:HA	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:GLY:O	1:B:670:PRO:C	2.63	0.41
1:A:559[A]:PHE:CD2	1:B:10:GLY:CA	3.03	0.41
1:A:661:ARG:HH12	1:A:681:ARG:HG2	1.85	0.41
1:B:475:MET:HE2	4:B:1355:HOH:O	2.20	0.41
1:A:541:ASN:CB	1:A:577:LEU:HD22	2.51	0.41
1:A:606:PHE:HE2	1:A:625:THR:HB	1.85	0.41
1:A:659:THR:HG22	1:A:685:PRO:HD3	2.02	0.41
1:B:90:ARG:HB2	1:B:91:PRO:HD2	2.03	0.41
1:B:538:THR:CG2	4:B:1495:HOH:O	2.69	0.41
1:B:156:LYS:HD2	1:B:181:TYR:CE2	2.55	0.41
1:B:664:TRP:CE3	1:B:677:LYS:HD2	2.55	0.41
1:A:361:ASN:ND2	1:A:364:LEU:HD22	2.36	0.41
1:B:237:THR:HG21	1:B:299:LEU:HB3	2.02	0.41
1:B:634:ILE:HD11	1:B:707:ALA:HB2	2.02	0.41
1:B:516:SER:HB3	1:B:617:ASP:OD2	2.21	0.40
1:A:181:TYR:CD2	1:A:235:LEU:HD21	2.56	0.40
1:A:525:GLU:HB3	1:A:533:PHE:HB2	2.03	0.40
1:B:350:MET:HE2	1:B:350:MET:HB2	1.87	0.40
1:B:418:LYS:NZ	1:B:479:ASP:O	2.41	0.40
1:B:523:GLU:O	1:B:535:LEU:HA	2.21	0.40
1:A:77:ARG:HB3	1:A:185:ASN:HB2	2.02	0.40
1:A:81:SER:HA	1:A:146:ILE:O	2.21	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	705/731 (96%)	668 (95%)	34 (5%)	3 (0%)	30	27
1	B	706/731 (97%)	676 (96%)	28 (4%)	2 (0%)	36	35
All	All	1411/1462 (96%)	1344 (95%)	62 (4%)	5 (0%)	30	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	B	45	LEU
1	A	580	LEU
1	A	292	TRP
1	B	669	GLY

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	625/643 (97%)	563 (90%)	62 (10%)	7	4
1	B	627/643 (98%)	576 (92%)	51 (8%)	11	7
All	All	1252/1286 (97%)	1139 (91%)	113 (9%)	9	6

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	12[A]	ARG
1	A	12[B]	ARG
1	A	14	VAL
1	A	18	ASN
1	A	45	LEU
1	A	86	ILE
1	A	95	ARG
1	A	96	ARG
1	A	104	VAL
1	A	107	ARG
1	A	127	SER
1	A	136	MET
1	A	177[A]	GLU
1	A	177[B]	GLU
1	A	193	VAL
1	A	195	LEU
1	A	211	VAL

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Mol	Chain	Res	Type
1	A	222	THR
1	A	224	SER
1	A	269	LYS
1	A	282	ILE
1	A	287	VAL
1	A	289	PRO
1	A	290	SER
1	A	293	THR
1	A	297	ASP
1	A	303	ARG
1	A	335	VAL
1	A	340	SER
1	A	359	ASN
1	A	364	LEU
1	A	366	LYS
1	A	369	VAL
1	A	455	VAL
1	A	482	LYS
1	A	485	GLU
1	A	487	GLN
1	A	503	LYS
1	A	516	SER
1	A	531	LYS
1	A	534	LYS
1	A	543	SER
1	A	545	ASN
1	A	572	THR
1	A	580	LEU
1	A	590	GLN
1	A	603	SER
1	A	618	VAL
1	A	625	THR
1	A	629	ILE
1	A	644	SER
1	A	674	ARG
1	A	675	PRO
1	A	678	LYS
1	A	681	ARG
1	A	684	ARG
1	A	692	GLU
1	A	702	HIS
1	A	704	LYS

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Mol	Chain	Res	Type
1	A	706	ILE
1	A	727	ARG
1	B	14	VAL
1	B	25	ASP
1	B	32	GLN
1	B	43	GLU
1	B	47	VAL
1	B	104	VAL
1	B	126	GLN
1	B	127	SER
1	B	142	VAL
1	B	169	VAL
1	B	193	VAL
1	B	269	LYS
1	B	350	MET
1	B	354	LEU
1	B	445	LYS
1	B	446	LYS
1	B	451	VAL
1	B	455	VAL
1	B	462	LYS
1	B	463	LEU
1	B	465	VAL
1	B	482	LYS
1	B	484	GLN
1	B	489	GLU
1	B	492	LEU
1	B	494	LEU
1	B	498	LEU
1	B	507	ASN
1	B	519	ASP
1	B	528	VAL
1	B	534	LYS
1	B	538	THR
1	B	540	ARG
1	B	546	ARG
1	B	548	THR
1	B	553	LEU
1	B	572	THR
1	B	575	VAL
1	B	588	LEU
1	B	589	ILE

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Mol	Chain	Res	Type
1	B	595	MET
1	B	604	LEU
1	B	623	LYS
1	B	650	VAL
1	B	659	THR
1	B	661	ARG
1	B	676	MET
1	B	687	SER
1	B	694	VAL
1	B	704	LYS
1	B	721	LEU

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	18	ASN
1	A	46	ASN
1	A	267	ASN
1	A	313	GLN
1	A	415	GLN
1	A	421	HIS
1	A	526	ASN
1	A	541	ASN
1	A	545	ASN
1	A	601	GLN
1	A	662	ASN
1	A	686	ASN
1	B	42	GLN
1	B	51	HIS
1	B	65	HIS
1	B	110	GLN
1	B	112	ASN
1	B	267	ASN
1	B	347	ASN
1	B	425	GLN
1	B	544	HIS
1	B	613	ASN
1	B	686	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	SAC	A	1	1	7,8,9	0.85	0	7,9,11	2.76	4 (57%)

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
1	SAC	A	1	1	-	4/7/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	SAC	OAC-C1A-C2A	4.76	130.53	122.05
1	A	1	SAC	C2A-C1A-N	-3.48	110.35	116.12
1	A	1	SAC	OG-CB-CA	3.36	120.38	111.13
1	A	1	SAC	CB-CA-C	2.14	116.06	111.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	SAC	C2A-C1A-N-CA
1	A	1	SAC	OAC-C1A-N-CA

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Mol	Chain	Res	Type	Atoms
1	A	1	SAC	C-CA-CB-OG
1	A	1	SAC	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	SAC	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	PGO	B	1203	-	4,4,4	1.19	1 (25%)	4,4,4	1.85	2 (50%)

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	PGO	B	1203	-	-	0/2/2/2	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1203	PGO	C1-C2	2.16	1.57	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1203	PGO	O1-C1-C2	-2.52	101.17	114.54
3	B	1203	PGO	O2-C2-C3	-2.00	100.83	109.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	707/731 (96%)	0.34	27 (3%)	44 43	18, 43, 70, 91	7 (0%)
1	B	708/731 (96%)	0.02	19 (2%)	56 55	19, 37, 64, 86	5 (0%)
All	All	1415/1462 (96%)	0.18	46 (3%)	49 48	18, 40, 68, 91	12 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	THR	7.3
1	A	4	SER	7.2
1	B	8	PHE	7.1
1	A	5	ARG	5.7
1	B	33	GLY	4.4
1	A	284	ALA	3.9
1	B	35	VAL	3.4
1	B	34	VAL	3.0
1	A	573	PHE	3.0
1	B	582	PHE	2.9
1	A	2	GLU	2.9
1	A	164	TRP	2.9
1	A	683	ILE	2.8
1	B	686	ASN	2.8
1	A	572	THR	2.8
1	B	454[A]	ASN	2.8
1	A	516	SER	2.6
1	A	656	LEU	2.6
1	A	270	ASP	2.6
1	B	44	PHE	2.5
1	B	687	SER	2.4
1	A	96	ARG	2.4
1	A	508	THR	2.4
1	A	7	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	167	TYR	2.3
1	B	639	THR	2.3
1	A	43	GLU	2.3
1	A	642	VAL	2.3
1	B	32	GLN	2.3
1	B	630	PRO	2.2
1	A	674	ARG	2.2
1	B	547	TYR	2.2
1	B	674	ARG	2.2
1	A	579	PRO	2.1
1	B	680	PHE	2.1
1	A	663	VAL	2.1
1	A	359	ASN	2.1
1	B	164	TRP	2.1
1	A	680	PHE	2.1
1	B	489	GLU	2.1
1	A	577	LEU	2.1
1	A	687	SER	2.1
1	A	95	ARG	2.0
1	A	688	THR	2.0
1	A	704	LYS	2.0
1	B	285	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	SAC	A	1	9/10	0.82	0.26	53,59,68,71	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PGO	B	1203	5/5	0.92	0.10	39,42,46,47	0
2	CA	A	1201	1/1	0.96	0.05	57,57,57,57	0
2	CA	B	1202	1/1	0.97	0.05	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.