



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:36 PM UTC

PDB ID : 1AI7 / pdb_00001ai7
Title : PENICILLIN ACYLASE COMPLEXED WITH PHENOL
Authors : Done, S.H.
Deposited on : 1997-05-01
Resolution : 2.50 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

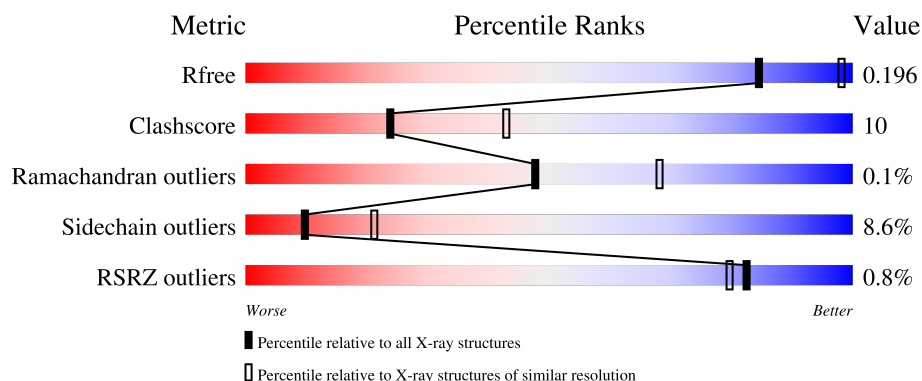
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	209	
2	B	557	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6715 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 PENICILLIN AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1656	1058	278	312	8			

- Molecule 2 is a protein called PENICILLIN AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	557	Total	C	N	O	S	0	0	0
			4415	2805	767	833	10			

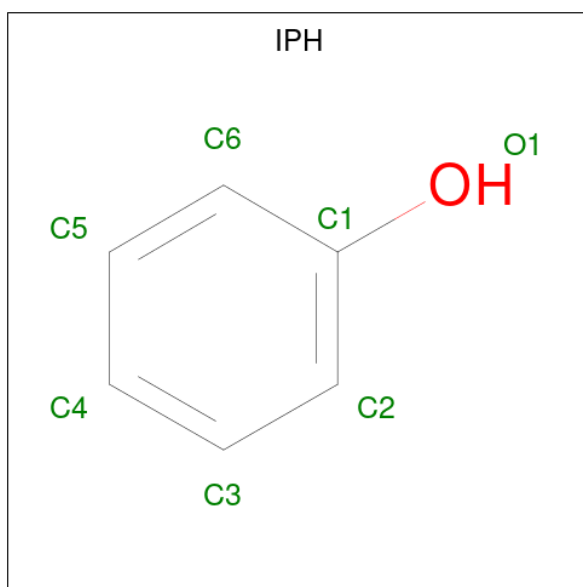
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	165	GLN	GLU	conflict	UNP P06875

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is PHENOL (CCD ID: IPH) (formula: C₆H₆O).



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

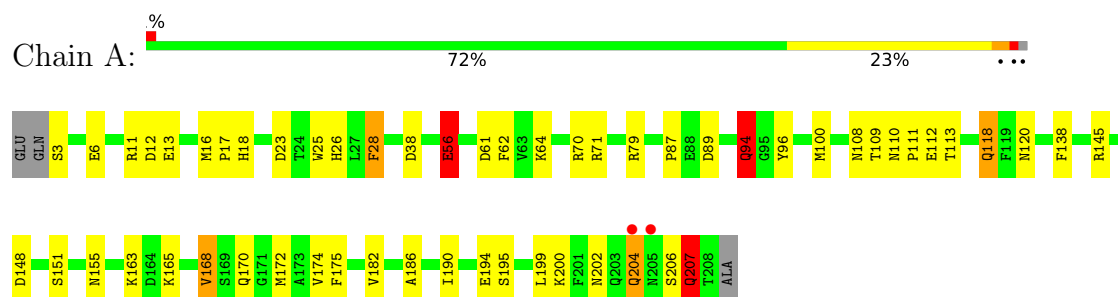
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total	O	0	0
			172	172		
5	B	464	Total	O	0	0
			464	464		

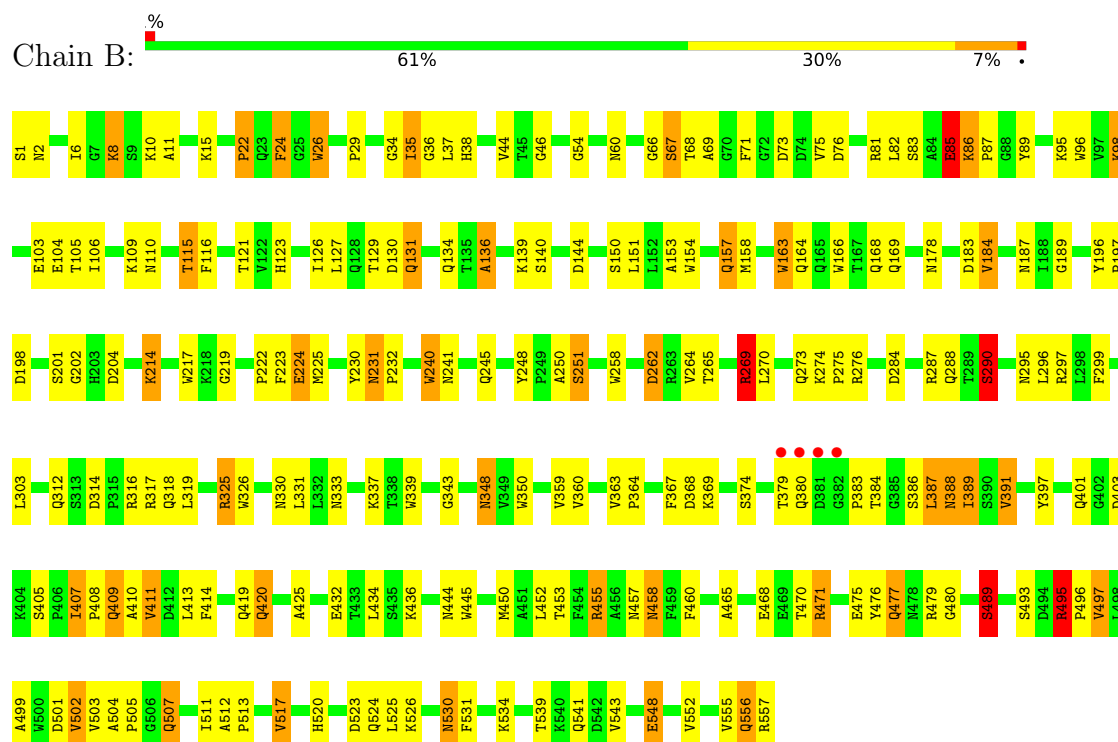
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PENICILLIN AMIDOHYDROLASE



• Molecule 2: PENICILLIN AMIDOHYDROLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.12Å 65.08Å 76.30Å 100.20° 111.44° 105.81°	Depositor
Resolution (Å)	24.97 – 2.50 24.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (24.97-2.50) 95.1 (24.97-2.50)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.24 (at 2.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.139 , 0.217 0.138 , 0.196	Depositor DCC
R_{free} test set	2023 reflections (7.19%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 77.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6715	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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, IPH

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	0.90	1/1698 (0.1%)	1.92	46/2305 (2.0%)
2	B	0.91	3/4541 (0.1%)	1.99	152/6192 (2.5%)
All	All	0.91	4/6239 (0.1%)	1.97	198/8497 (2.3%)

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
2	B	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	445	TRP	NE1-CE2	10.49	1.49	1.37
2	B	240	TRP	NE1-CE2	10.35	1.48	1.37
2	B	163	TRP	NE1-CE2	10.04	1.48	1.37
1	A	25	TRP	NE1-CE2	9.96	1.48	1.37

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	ARG	CD-NE-CZ	16.34	147.27	124.40
2	B	541	GLN	CG-CD-NE2	-12.75	97.27	116.40
1	A	94	GLN	CG-CD-NE2	-12.75	97.28	116.40
2	B	409	GLN	CG-CD-NE2	-12.50	97.65	116.40
2	B	287	ARG	CD-NE-CZ	12.20	141.47	124.40
1	A	170	GLN	CG-CD-NE2	-12.14	98.19	116.40
2	B	420	GLN	CG-CD-NE2	-11.65	98.92	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	ASN	CB-CG-ND2	-11.62	98.97	116.40
2	B	455	ARG	CD-NE-CZ	11.28	140.19	124.40
2	B	444	ASN	CA-CB-CG	11.22	123.82	112.60
1	A	79	ARG	CD-NE-CZ	10.91	139.68	124.40
2	B	168	GLN	CG-CD-NE2	-10.82	100.17	116.40
2	B	333	ASN	CA-CB-CG	10.79	123.39	112.60
2	B	391	VAL	CB-CA-C	-10.77	98.18	111.97
2	B	131	GLN	CG-CD-NE2	-10.10	101.24	116.40
2	B	295	ASN	CB-CG-ND2	-9.98	101.43	116.40
2	B	530	ASN	CA-CB-CG	9.78	122.38	112.60
1	A	204	GLN	CB-CG-CD	-9.76	96.01	112.60
2	B	556	GLN	CA-CB-CG	-9.27	95.57	114.10
2	B	409	GLN	CG-CD-OE1	8.96	138.73	120.80
2	B	465	ALA	CA-C-O	-8.94	111.27	121.10
1	A	170	GLN	CG-CD-OE1	8.76	138.32	120.80
1	A	94	GLN	CG-CD-OE1	8.74	138.29	120.80
2	B	541	GLN	CG-CD-OE1	8.73	138.25	120.80
1	A	170	GLN	CB-CG-CD	8.57	127.18	112.60
2	B	2	ASN	CB-CG-OD1	8.56	137.91	120.80
1	A	204	GLN	CG-CD-NE2	8.54	129.22	116.40
2	B	420	GLN	CG-CD-OE1	8.52	137.83	120.80
2	B	389	ILE	CA-C-O	-8.41	111.27	120.85
2	B	269	ARG	CA-CB-CG	8.36	130.81	114.10
2	B	231	ASN	CA-C-N	7.90	127.95	119.89
2	B	231	ASN	C-N-CA	7.90	127.95	119.89
2	B	460	PHE	CA-CB-CG	7.89	121.69	113.80
2	B	168	GLN	CG-CD-OE1	7.88	136.55	120.80
2	B	477	GLN	CB-CG-CD	7.86	125.96	112.60
2	B	407	ILE	CA-C-O	7.84	123.51	119.12
1	A	118	GLN	CB-CG-CD	7.79	125.84	112.60
2	B	270	LEU	CA-C-O	-7.72	112.23	120.42
2	B	144	ASP	CA-CB-CG	7.71	120.31	112.60
2	B	556	GLN	CG-CD-NE2	7.48	127.61	116.40
1	A	168	VAL	CA-C-O	-7.43	113.68	121.41
2	B	420	GLN	CA-CB-CG	7.41	128.93	114.10
2	B	131	GLN	CG-CD-OE1	7.32	135.43	120.80
2	B	386	SER	O-C-N	-7.32	114.23	122.86
2	B	495	ARG	CA-C-N	7.31	126.94	119.19
2	B	495	ARG	C-N-CA	7.31	126.94	119.19
2	B	409	GLN	CA-CB-CG	-7.23	99.64	114.10
1	A	204	GLN	CG-CD-OE1	-7.19	106.43	120.80
2	B	295	ASN	CB-CG-OD1	7.17	135.15	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	VAL	N-CA-C	7.14	117.66	110.23
2	B	131	GLN	CB-CG-CD	7.11	124.68	112.60
2	B	71	PHE	CA-CB-CG	-7.10	106.70	113.80
2	B	269	ARG	N-CA-CB	7.02	120.40	109.94
2	B	409	GLN	CB-CG-CD	6.99	124.48	112.60
2	B	457	ASN	CA-C-O	-6.98	113.05	120.80
2	B	556	GLN	CB-CG-CD	-6.98	100.73	112.60
1	A	62	PHE	CA-CB-CG	-6.89	106.91	113.80
2	B	34	GLY	CA-C-O	-6.82	115.37	121.64
2	B	269	ARG	NE-CZ-NH1	6.80	128.31	121.50
1	A	94	GLN	CB-CG-CD	6.79	124.14	112.60
1	A	11	ARG	CD-NE-CZ	6.75	133.85	124.40
2	B	245	GLN	N-CA-CB	-6.75	101.10	111.56
2	B	284	ASP	CA-CB-CG	-6.71	105.89	112.60
2	B	420	GLN	CB-CG-CD	6.66	123.93	112.60
2	B	86	LYS	CA-CB-CG	6.65	127.41	114.10
2	B	76	ASP	CA-CB-CG	6.63	119.23	112.60
2	B	85	GLU	CA-C-O	-6.61	113.46	120.80
1	A	182	VAL	O-C-N	-6.51	115.66	123.02
2	B	391	VAL	N-CA-CB	6.48	118.14	110.55
2	B	75	VAL	CA-C-O	-6.47	113.50	120.36
2	B	386	SER	CA-C-N	6.42	129.99	120.87
2	B	386	SER	C-N-CA	6.42	129.99	120.87
1	A	186	ALA	CA-C-O	6.42	125.78	119.75
2	B	29	PRO	CA-C-N	6.40	129.93	120.90
2	B	29	PRO	C-N-CA	6.40	129.93	120.90
2	B	541	GLN	CA-CB-CG	6.40	126.90	114.10
2	B	410	ALA	O-C-N	-6.38	115.35	122.12
2	B	296	LEU	CA-C-N	6.33	129.05	120.38
2	B	296	LEU	C-N-CA	6.33	129.05	120.38
2	B	367	PHE	CA-CB-CG	-6.33	107.47	113.80
2	B	183	ASP	CA-CB-CG	6.29	118.89	112.60
2	B	555	VAL	CA-C-N	-6.29	112.55	122.73
2	B	555	VAL	C-N-CA	-6.29	112.55	122.73
2	B	184	VAL	CB-CA-C	-6.27	99.81	111.79
2	B	497	VAL	CB-CA-C	-6.26	100.67	110.69
1	A	56	GLU	N-CA-CB	6.25	119.85	110.22
2	B	290	SER	CB-CA-C	-6.25	100.41	110.79
2	B	331	LEU	CA-C-O	-6.25	114.05	121.11
2	B	453	THR	O-C-N	-6.25	115.91	123.29
2	B	383	PRO	CA-C-O	6.24	128.45	121.34
2	B	66	GLY	CA-C-O	-6.21	114.92	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	PHE	CA-C-O	-6.19	113.95	120.63
2	B	411	VAL	N-CA-CB	6.14	122.58	111.21
1	A	70	ARG	NE-CZ-NH2	-6.12	113.69	119.20
2	B	287	ARG	NE-CZ-NH1	6.10	127.60	121.50
2	B	224	GLU	CB-CG-CD	6.09	122.96	112.60
2	B	144	ASP	CB-CG-OD1	6.08	132.38	118.40
1	A	89	ASP	CA-CB-CG	-6.08	106.53	112.60
2	B	312	GLN	CA-CB-CG	6.06	126.23	114.10
2	B	477	GLN	CA-CB-CG	6.05	126.20	114.10
1	A	111	PRO	N-CA-CB	6.04	109.92	103.52
2	B	54	GLY	O-C-N	-5.97	117.38	123.35
2	B	363	VAL	CA-C-O	5.95	123.43	119.38
2	B	480	GLY	CA-C-N	5.94	128.52	120.38
2	B	480	GLY	C-N-CA	5.94	128.52	120.38
2	B	541	GLN	CB-CG-CD	5.93	122.68	112.60
2	B	548	GLU	N-CA-CB	5.93	118.91	110.67
2	B	232	PRO	N-CA-CB	5.91	108.28	103.32
2	B	24	PHE	CA-CB-CG	5.91	119.71	113.80
2	B	556	GLN	CG-CD-OE1	-5.89	109.01	120.80
1	A	186	ALA	O-C-N	-5.88	116.06	121.30
1	A	138	PHE	O-C-N	-5.88	115.89	122.12
2	B	22	PRO	CA-C-O	-5.87	114.95	121.23
2	B	530	ASN	CB-CG-ND2	-5.84	107.65	116.40
1	A	61	ASP	CA-CB-CG	5.82	118.42	112.60
2	B	219	GLY	CA-C-O	-5.80	116.91	120.91
2	B	364	PRO	N-CA-CB	5.80	108.40	103.35
2	B	287	ARG	NE-CZ-NH2	-5.79	113.98	119.20
2	B	408	PRO	N-CA-CB	5.79	108.32	103.17
2	B	475	GLU	OE1-CD-OE2	-5.73	109.15	122.90
2	B	312	GLN	CB-CG-CD	5.70	122.29	112.60
2	B	69	ALA	CA-C-O	-5.69	114.43	120.92
2	B	330	ASN	CB-CG-ND2	5.67	124.91	116.40
1	A	155	ASN	CA-CB-CG	-5.66	106.94	112.60
1	A	155	ASN	CB-CG-ND2	5.66	124.89	116.40
2	B	425	ALA	O-C-N	-5.63	116.15	122.12
2	B	136	ALA	CA-C-O	-5.61	114.20	120.66
2	B	489	SER	CA-C-O	5.58	124.73	120.26
2	B	552	VAL	O-C-N	-5.58	117.45	123.14
2	B	457	ASN	CA-C-N	-5.57	111.50	122.02
2	B	457	ASN	C-N-CA	-5.57	111.50	122.02
2	B	248	TYR	CA-C-O	5.53	124.19	119.66
2	B	223	PHE	O-C-N	-5.52	115.76	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASP	CA-C-O	-5.52	112.81	119.49
2	B	548	GLU	CA-CB-CG	5.52	125.13	114.10
1	A	16	MET	CA-C-N	5.51	126.36	120.13
1	A	16	MET	C-N-CA	5.51	126.36	120.13
2	B	319	LEU	CA-C-O	-5.50	114.71	120.55
2	B	499	ALA	CA-C-O	-5.50	115.18	121.40
1	A	28	PHE	CA-CB-CG	-5.50	108.30	113.80
2	B	105	THR	O-C-N	5.49	129.63	123.27
2	B	150	SER	CA-C-N	5.48	127.56	120.44
2	B	150	SER	C-N-CA	5.48	127.56	120.44
1	A	174	VAL	CA-C-N	5.47	127.88	120.38
1	A	174	VAL	C-N-CA	5.47	127.88	120.38
2	B	187	ASN	OD1-CG-ND2	5.45	128.05	122.60
2	B	407	ILE	N-CA-C	5.44	112.51	107.56
2	B	73	ASP	OD1-CG-OD2	-5.43	109.86	122.90
2	B	231	ASN	O-C-N	-5.43	119.03	121.53
2	B	1	SER	N-CA-CB	-5.41	101.30	110.50
2	B	8	LYS	CB-CA-C	-5.40	101.77	110.74
1	A	165	LYS	CA-C-O	-5.38	114.79	120.55
2	B	434	LEU	CA-C-O	-5.38	114.27	120.24
2	B	68	THR	CA-C-O	-5.38	114.82	121.06
2	B	269	ARG	NH1-CZ-NH2	-5.38	112.31	119.30
2	B	359	VAL	CB-CA-C	-5.38	105.09	111.97
1	A	17	PRO	N-CA-CB	5.38	107.82	103.36
1	A	182	VAL	CA-C-O	5.37	126.94	121.63
1	A	151	SER	CA-C-O	-5.36	114.86	120.32
2	B	196	TYR	CA-C-N	5.35	125.26	119.85
2	B	196	TYR	C-N-CA	5.35	125.26	119.85
2	B	316	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	A	207	GLN	O-C-N	-5.34	114.48	122.39
1	A	87	PRO	O-C-N	-5.33	115.83	122.23
2	B	46	GLY	CA-C-O	-5.33	117.23	120.91
1	A	100	MET	CA-C-O	5.32	126.05	120.42
2	B	477	GLN	CG-CD-NE2	-5.30	108.44	116.40
1	A	151	SER	O-C-N	5.30	128.78	122.21
2	B	411	VAL	CB-CA-C	-5.28	102.78	110.81
2	B	348	ASN	O-C-N	5.27	127.50	122.07
2	B	265	THR	CA-C-N	5.27	128.32	120.31
2	B	265	THR	C-N-CA	5.27	128.32	120.31
2	B	383	PRO	N-CA-CB	5.25	107.98	103.31
2	B	153	ALA	O-C-N	-5.25	116.56	122.12
2	B	248	TYR	CA-C-N	5.25	125.66	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	248	TYR	C-N-CA	5.25	125.66	119.99
2	B	383	PRO	O-C-N	-5.24	116.69	123.03
1	A	38	ASP	N-CA-C	5.23	118.12	111.69
2	B	314	ASP	O-C-N	5.22	125.75	121.31
2	B	262	ASP	O-C-N	-5.17	117.36	123.41
2	B	455	ARG	CA-C-N	5.16	130.75	121.66
2	B	455	ARG	C-N-CA	5.16	130.75	121.66
2	B	476	TYR	N-CA-CB	5.16	117.54	109.85
2	B	164	GLN	O-C-N	-5.15	116.77	122.07
2	B	110	ASN	CA-CB-CG	-5.13	107.47	112.60
1	A	190	ILE	O-C-N	-5.13	117.34	123.03
2	B	471	ARG	CD-NE-CZ	-5.12	117.23	124.40
2	B	525	LEU	N-CA-C	5.12	116.86	111.28
2	B	269	ARG	CG-CD-NE	5.10	123.22	112.00
1	A	71	ARG	CD-NE-CZ	-5.09	117.28	124.40
1	A	145	ARG	CD-NE-CZ	-5.08	117.29	124.40
2	B	325	ARG	CD-NE-CZ	-5.06	117.31	124.40
2	B	231	ASN	N-CA-CB	-5.06	106.05	111.66
2	B	29	PRO	N-CA-CB	5.05	108.16	102.60
2	B	73	ASP	CB-CG-OD2	5.05	130.01	118.40
2	B	391	VAL	CA-C-N	5.04	125.68	120.03
2	B	391	VAL	C-N-CA	5.04	125.68	120.03
1	A	3	SER	CA-C-O	5.04	129.37	120.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	169	GLN	Mainchain
2	B	198	ASP	Mainchain
2	B	222	PRO	Mainchain
2	B	251	SER	Mainchain
2	B	26	TRP	Mainchain
2	B	290	SER	Mainchain
2	B	299	PHE	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	1656	0	1604	22	0
2	B	4415	0	4244	108	0
3	B	1	0	0	0	0
4	B	7	0	6	0	0
5	A	172	0	0	2	0
5	B	464	0	0	4	0
All	All	6715	0	5854	120	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 10.

All (120) 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)
2:B:318:GLN:HG2	5:B:847:HOH:O	1.54	1.06
1:A:207:GLN:HE22	2:B:204:ASP:H	1.06	0.99
2:B:397:TYR:O	2:B:401:GLN:HG2	1.64	0.96
2:B:458:ASN:C	2:B:458:ASN:HD22	1.68	0.96
2:B:269:ARG:HH21	2:B:297:ARG:HD3	1.31	0.94
2:B:317:ARG:HG3	2:B:317:ARG:HH11	1.29	0.92
2:B:318:GLN:CG	5:B:847:HOH:O	2.14	0.86
2:B:157:GLN:HE22	2:B:166:TRP:HE1	1.21	0.85
1:A:18:HIS:HD2	2:B:38:HIS:NE2	1.74	0.85
2:B:317:ARG:HG3	2:B:317:ARG:NH1	1.89	0.84
2:B:339:TRP:HH2	2:B:450:MET:HE2	1.46	0.81
2:B:157:GLN:NE2	2:B:166:TRP:HE1	1.79	0.80
2:B:384:THR:HG22	2:B:455:ARG:HH12	1.48	0.77
2:B:458:ASN:C	2:B:458:ASN:ND2	2.41	0.76
2:B:556:GLN:HG3	2:B:557:ARG:N	1.99	0.76
2:B:157:GLN:NE2	2:B:166:TRP:NE1	2.34	0.74
2:B:503:VAL:H	2:B:524:GLN:NE2	1.84	0.73
2:B:502:VAL:HA	2:B:524:GLN:HE22	1.55	0.71
1:A:172:MET:HG2	1:A:204:GLN:OE1	1.93	0.69
2:B:269:ARG:NH2	2:B:297:ARG:HD3	2.07	0.69
1:A:118:GLN:OE1	5:A:229:HOH:O	2.10	0.69
2:B:157:GLN:HE22	2:B:166:TRP:NE1	1.91	0.69
2:B:503:VAL:H	2:B:524:GLN:HE22	1.39	0.69
2:B:520:HIS:HE1	2:B:548:GLU:OE2	1.76	0.68
2:B:86:LYS:N	2:B:87:PRO:HD3	2.09	0.68
2:B:214:LYS:H	2:B:214:LYS:HD2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:ILE:O	2:B:409:GLN:NE2	2.28	0.67
2:B:240:TRP:O	2:B:241:ASN:HB2	1.96	0.65
1:A:207:GLN:NE2	2:B:204:ASP:H	1.87	0.65
2:B:269:ARG:HH21	2:B:297:ARG:CD	2.04	0.65
2:B:15:LYS:HG3	2:B:489:SER:HB2	1.77	0.64
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.33	0.63
1:A:23:ASP:CG	1:A:26:HIS:HD1	2.07	0.61
2:B:556:GLN:CG	2:B:557:ARG:N	2.64	0.60
2:B:388:ASN:HD22	2:B:389:ILE:H	1.51	0.59
2:B:89:TYR:CZ	2:B:98:LYS:HG3	2.38	0.58
2:B:288:GLN:HG2	5:B:727:HOH:O	2.02	0.58
2:B:83:SER:HB2	2:B:96:TRP:CH2	2.40	0.57
2:B:501:ASP:OD1	2:B:534:LYS:HE2	2.05	0.57
2:B:129:THR:HG22	2:B:136:ALA:CB	2.36	0.56
2:B:520:HIS:HD2	2:B:523:ASP:OD2	1.89	0.56
2:B:86:LYS:N	2:B:87:PRO:CD	2.69	0.55
2:B:384:THR:HG22	2:B:455:ARG:NH1	2.20	0.55
2:B:384:THR:CG2	2:B:455:ARG:HH12	2.17	0.55
2:B:82:LEU:HD11	2:B:136:ALA:HB2	1.88	0.54
2:B:214:LYS:H	2:B:214:LYS:CD	2.21	0.54
2:B:157:GLN:NE2	2:B:166:TRP:CD1	2.76	0.54
2:B:503:VAL:N	2:B:524:GLN:HE22	2.05	0.54
2:B:317:ARG:HH11	2:B:317:ARG:CG	2.04	0.53
2:B:106:ILE:HD11	2:B:116:PHE:HE1	1.74	0.53
1:A:18:HIS:CD2	2:B:38:HIS:NE2	2.65	0.53
1:A:12:ASP:O	2:B:548:GLU:HG2	2.09	0.53
1:A:23:ASP:OD1	1:A:23:ASP:C	2.51	0.52
2:B:512:ALA:HB1	2:B:513:PRO:HD2	1.92	0.52
2:B:86:LYS:H	2:B:87:PRO:HD3	1.76	0.51
2:B:11:ALA:O	2:B:276:ARG:NH1	2.42	0.51
2:B:37:LEU:HB2	2:B:44:VAL:HG22	1.92	0.51
2:B:348:ASN:ND2	2:B:374:SER:OG	2.43	0.51
1:A:199:LEU:HD21	2:B:225:MET:HE1	1.93	0.51
2:B:414:PHE:CZ	2:B:419:GLN:HG2	2.45	0.50
2:B:502:VAL:CA	2:B:524:GLN:HE22	2.23	0.50
2:B:388:ASN:ND2	2:B:389:ILE:H	2.08	0.50
2:B:530:ASN:O	2:B:531:PHE:HB2	2.11	0.50
2:B:121:THR:HG23	2:B:126:ILE:HD11	1.93	0.50
2:B:502:VAL:HA	2:B:524:GLN:NE2	2.23	0.50
1:A:23:ASP:OD1	1:A:26:HIS:ND1	2.41	0.50
2:B:556:GLN:CD	2:B:557:ARG:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASN:ND2	1:A:206:SER:OG	2.45	0.49
2:B:60:ASN:C	2:B:60:ASN:OD1	2.56	0.49
2:B:318:GLN:HG3	5:B:847:HOH:O	1.97	0.48
2:B:339:TRP:CH2	2:B:450:MET:HE2	2.36	0.48
2:B:387:LEU:HD21	2:B:450:MET:HE1	1.96	0.48
1:A:172:MET:HE2	1:A:204:GLN:HA	1.96	0.47
2:B:511:ILE:HG12	2:B:517:VAL:HG22	1.95	0.47
1:A:194:GLU:O	1:A:195:SER:HB3	2.14	0.47
2:B:504:ALA:HA	2:B:505:PRO:C	2.40	0.47
2:B:502:VAL:HG23	2:B:524:GLN:HE21	1.80	0.47
2:B:539:THR:O	2:B:543:VAL:HG23	2.15	0.47
2:B:317:ARG:NH1	2:B:317:ARG:CG	2.61	0.46
2:B:129:THR:HA	2:B:136:ALA:HA	1.97	0.46
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.96	0.46
2:B:130:ASP:O	2:B:134:GLN:N	2.48	0.46
2:B:262:ASP:OD1	2:B:264:VAL:HG12	2.15	0.46
2:B:470:THR:O	2:B:471:ARG:HD3	2.15	0.46
2:B:230:TYR:O	2:B:231:ASN:C	2.59	0.46
2:B:477:GLN:HE21	2:B:479:ARG:HD3	1.80	0.46
1:A:163:LYS:HG2	1:A:168:VAL:HA	1.98	0.45
1:A:206:SER:HB2	2:B:202:GLY:O	2.17	0.45
2:B:360:VAL:HG13	2:B:368:ASP:HB2	1.98	0.45
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.51	0.45
2:B:129:THR:HG22	2:B:136:ALA:HB2	1.99	0.45
2:B:157:GLN:HE21	2:B:157:GLN:HB2	1.47	0.45
2:B:495:ARG:HA	2:B:496:PRO:HD3	1.91	0.44
2:B:250:ALA:HB2	2:B:258:TRP:CE3	2.52	0.44
1:A:56:GLU:O	2:B:109:LYS:HB2	2.18	0.44
2:B:35:ILE:HG13	2:B:36:GLY:N	2.33	0.44
2:B:471:ARG:HD3	2:B:471:ARG:HH11	1.61	0.43
2:B:151:LEU:HD23	2:B:151:LEU:C	2.43	0.43
2:B:556:GLN:OE1	2:B:556:GLN:HA	2.12	0.42
2:B:384:THR:HG22	2:B:455:ARG:HH22	1.84	0.42
2:B:507:GLN:HE21	2:B:507:GLN:HB2	1.63	0.42
1:A:199:LEU:CD2	2:B:225:MET:HE1	2.49	0.42
2:B:104:GLU:O	2:B:115:THR:HA	2.20	0.42
2:B:85:GLU:O	2:B:86:LYS:HG2	2.19	0.42
2:B:326:TRP:CZ3	2:B:343:GLY:HA3	2.55	0.42
2:B:67:SER:HA	2:B:178:ASN:O	2.20	0.42
2:B:6:ILE:HG23	2:B:10:LYS:HB3	2.02	0.42
2:B:123:HIS:O	2:B:140:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:LYS:HA	2:B:275:PRO:HD3	1.93	0.42
2:B:163:TRP:CZ3	2:B:189:GLY:HA3	2.55	0.41
1:A:148:ASP:OD2	2:B:139:LYS:NZ	2.53	0.41
2:B:197:PRO:HB3	2:B:217:TRP:CD2	2.56	0.41
1:A:120:ASN:HD22	1:A:120:ASN:HA	1.65	0.41
2:B:503:VAL:N	2:B:524:GLN:NE2	2.60	0.41
1:A:94:GLN:NE2	5:A:321:HOH:O	2.54	0.40
2:B:413:LEU:HD23	2:B:413:LEU:HA	1.93	0.40
2:B:303:LEU:HD21	2:B:350:TRP:CE2	2.56	0.40
2:B:325:ARG:HH11	2:B:325:ARG:HD2	1.58	0.40
1:A:28:PHE:O	1:A:96:TYR:HA	2.22	0.40
2:B:388:ASN:HD22	2:B:389:ILE:N	2.16	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	204/209 (98%)	200 (98%)	4 (2%)	0	100	100
2	B	555/557 (100%)	541 (98%)	13 (2%)	1 (0%)	43	63
All	All	759/766 (99%)	741 (98%)	17 (2%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	251	SER

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	178/180 (99%)	166 (93%)	12 (7%)	15	31
2	B	460/460 (100%)	417 (91%)	43 (9%)	8	18
All	All	638/640 (100%)	583 (91%)	55 (9%)	10	21

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	13	GLU
1	A	56	GLU
1	A	64	LYS
1	A	94	GLN
1	A	108	ASN
1	A	109	THR
1	A	110	ASN
1	A	112	GLU
1	A	113	THR
1	A	200	LYS
1	A	207	GLN
2	B	8	LYS
2	B	35	ILE
2	B	67	SER
2	B	81	ARG
2	B	85	GLU
2	B	95	LYS
2	B	98	LYS
2	B	103	GLU
2	B	115	THR
2	B	127	LEU
2	B	131	GLN
2	B	154	TRP
2	B	157	GLN
2	B	184	VAL
2	B	201	SER

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Mol	Chain	Res	Type
2	B	214	LYS
2	B	224	GLU
2	B	269	ARG
2	B	273	GLN
2	B	290	SER
2	B	337	LYS
2	B	369	LYS
2	B	379	THR
2	B	380	GLN
2	B	387	LEU
2	B	388	ASN
2	B	391	VAL
2	B	403	ASP
2	B	405	SER
2	B	411	VAL
2	B	420	GLN
2	B	432	GLU
2	B	436	LYS
2	B	458	ASN
2	B	468	GLU
2	B	489	SER
2	B	493	SER
2	B	495	ARG
2	B	497	VAL
2	B	502	VAL
2	B	507	GLN
2	B	517	VAL
2	B	526	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	22	ASN
1	A	94	GLN
1	A	108	ASN
1	A	120	ASN
1	A	155	ASN
1	A	170	GLN
1	A	207	GLN
2	B	93	ASN
2	B	110	ASN

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Mol	Chain	Res	Type
2	B	157	GLN
2	B	168	GLN
2	B	233	GLN
2	B	241	ASN
2	B	245	GLN
2	B	288	GLN
2	B	348	ASN
2	B	388	ASN
2	B	440	ASN
2	B	458	ASN
2	B	473	GLN
2	B	477	GLN
2	B	507	GLN
2	B	520	HIS
2	B	524	GLN
2	B	546	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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
4	IPH	B	559	-	7,7,7	0.51	0	8,8,8	2.31	3 (37%)

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	IPH	B	559	-	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	559	IPH	C6-C1-C2	3.88	125.94	119.77
4	B	559	IPH	C3-C2-C1	-3.72	114.26	119.29
4	B	559	IPH	C5-C6-C1	-2.62	115.75	119.29

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	206/209 (98%)	-0.56	2 (0%) 79 76	22, 35, 66, 81	0
2	B	557/557 (100%)	-0.74	4 (0%) 84 81	19, 34, 66, 112	0
All	All	763/766 (99%)	-0.69	6 (0%) 82 80	19, 34, 66, 112	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	GLN	3.4
2	B	382	GLY	3.2
2	B	380	GLN	3.1
2	B	379	THR	2.1
2	B	381	ASP	2.0
1	A	205	ASN	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	IPH	B	559	7/7	0.95	0.09	26,30,36,43	0
3	CA	B	558	1/1	1.00	0.02	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.