



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:15 PM EDT

PDB ID : 1AJQ / pdb_00001ajq
Title : PENICILLIN ACYLASE COMPLEXED WITH THIOPHENEACETIC ACID
Authors : Done, S.H.
Deposited on : 1997-05-07
Resolution : 2.05 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

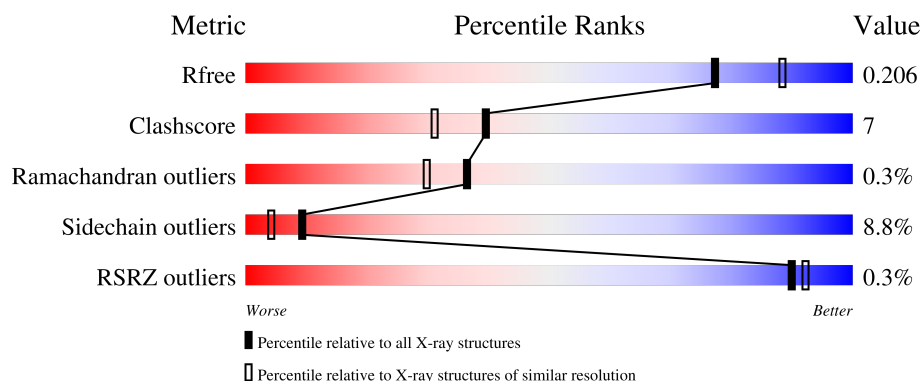
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	 65% 27% 6% •
2	B	557	 63% 29% 7% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6768 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	3	0
			4438	2818	773	837	10			

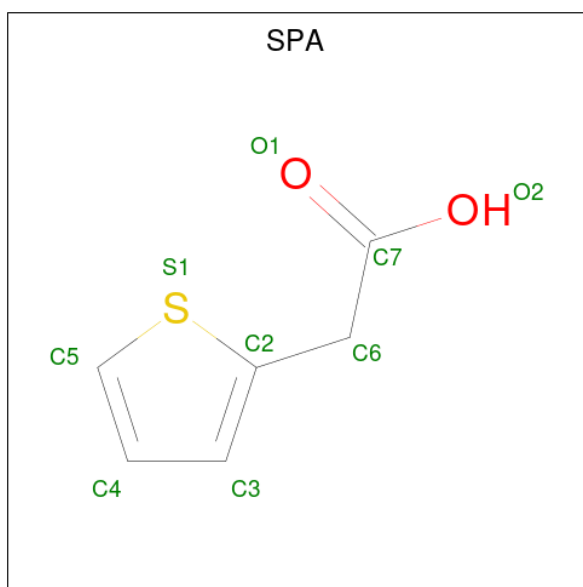
There is a discrepancy between the modelled and reference sequences:

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 THIOPHENEACETIC ACID (CCD ID: SPA) (formula: C₆H₆O₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	1
			13	9	2	2		

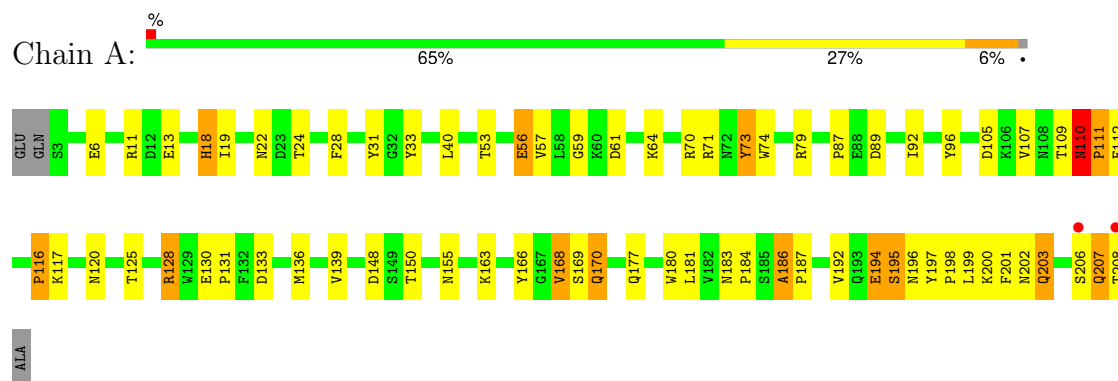
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	168	Total	O	0	0
			168	168		
5	B	492	Total	O	0	0
			492	492		

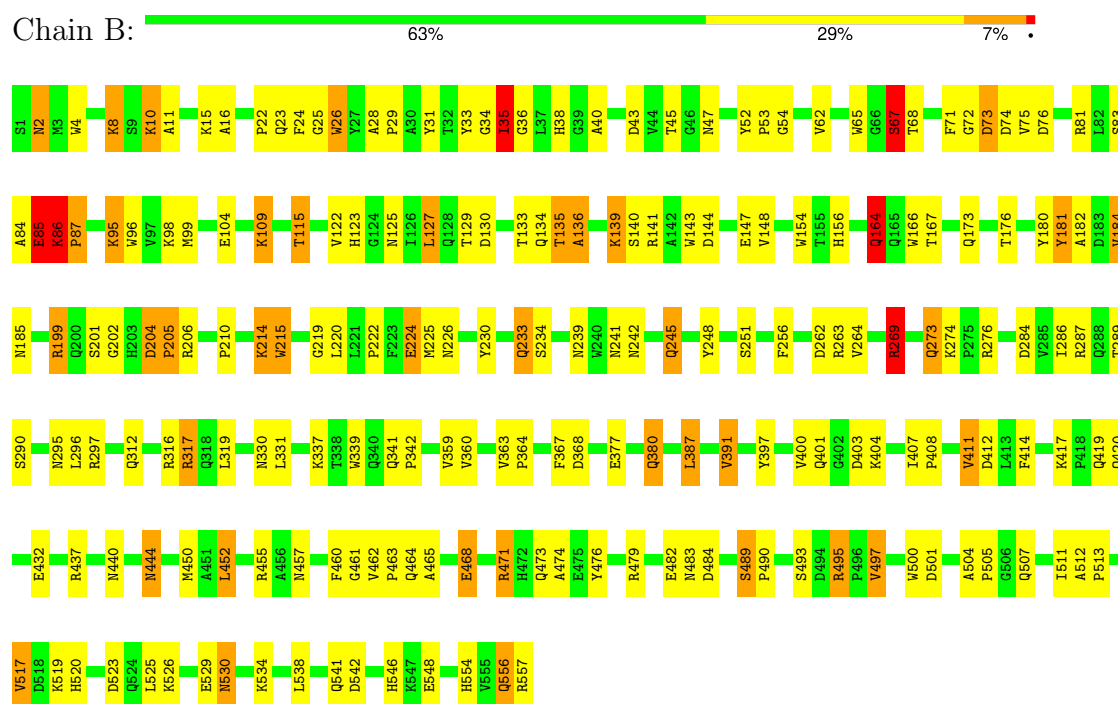
3 Residue-property plots

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: 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)	19.85 – 2.05 19.85 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.85-2.05) 97.2 (19.85-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.03Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.165 , 0.233 0.147 , 0.206	Depositor DCC
R_{free} test set	3707 reflections (7.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 66.4	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	0.97	EDS
Total number of atoms	6768	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% 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, SPA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.11	1/1698 (0.1%)	2.08	58/2305 (2.5%)
2	B	1.19	13/4569 (0.3%)	2.05	175/6230 (2.8%)
All	All	1.17	14/6267 (0.2%)	2.06	233/8535 (2.7%)

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	17

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	34	GLY	CA-C	8.12	1.60	1.52
2	B	25	GLY	N-CA	7.27	1.54	1.45
2	B	45	THR	CA-C	6.63	1.60	1.52
2	B	54	GLY	CA-C	6.16	1.56	1.52
2	B	36	GLY	CA-C	5.99	1.56	1.52
2	B	173	GLN	N-CA	5.67	1.53	1.46
2	B	484	ASP	N-CA	5.43	1.52	1.46
2	B	538	LEU	CA-C	5.25	1.57	1.52
2	B	483	ASN	CA-C	5.25	1.58	1.52
1	A	125	THR	N-CA	5.09	1.50	1.45
2	B	452	LEU	N-CA	5.08	1.52	1.46
2	B	140	SER	N-CA	-5.03	1.40	1.46
2	B	148	VAL	CA-C	-5.03	1.46	1.52
2	B	264	VAL	C-N	5.03	1.40	1.34

All (233) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ARG	CD-NE-CZ	16.00	146.80	124.40
2	B	471	ARG	CD-NE-CZ	14.07	144.10	124.40
2	B	363	VAL	CA-C-O	12.99	128.21	119.38
2	B	391	VAL	CB-CA-C	-12.09	95.82	112.14
2	B	495	ARG	CD-NE-CZ	11.15	140.01	124.40
2	B	269	ARG	CD-NE-CZ	10.70	139.38	124.40
2	B	75	VAL	CA-C-O	-10.67	109.05	120.36
2	B	287	ARG	CD-NE-CZ	10.25	138.74	124.40
2	B	199	ARG	CD-NE-CZ	-9.59	110.97	124.40
1	A	28	PHE	CA-CB-CG	-9.55	104.25	113.80
2	B	455	ARG	NE-CZ-NH1	9.48	130.98	121.50
2	B	287	ARG	CA-C-O	-9.29	110.95	120.90
2	B	455	ARG	CD-NE-CZ	9.00	137.00	124.40
2	B	76	ASP	CA-CB-CG	8.95	121.55	112.60
2	B	34	GLY	CA-C-O	-8.84	113.40	121.18
2	B	263	ARG	NE-CZ-NH1	8.63	130.13	121.50
2	B	241	ASN	CA-CB-CG	8.46	121.06	112.60
2	B	412	ASP	CA-C-O	8.09	129.49	120.43
2	B	233	GLN	CB-CG-CD	8.06	126.31	112.60
2	B	184	VAL	CB-CA-C	-8.02	99.73	112.16
1	A	168	VAL	N-CA-C	8.00	118.55	110.23
2	B	182	ALA	CA-C-O	-7.98	112.71	121.33
1	A	96	TYR	O-C-N	-7.96	113.87	122.07
2	B	554	HIS	CA-CB-CG	-7.89	105.91	113.80
2	B	290	SER	CB-CA-C	-7.85	97.33	110.68
1	A	110	ASN	CA-CB-CG	7.80	120.40	112.60
1	A	139	VAL	CA-C-N	7.63	129.68	120.14
1	A	139	VAL	C-N-CA	7.63	129.68	120.14
2	B	31	TYR	CA-C-O	-7.63	112.47	120.55
2	B	296	LEU	CA-C-O	7.63	129.46	121.07
2	B	71	PHE	CA-CB-CG	-7.52	106.28	113.80
1	A	61	ASP	CA-CB-CG	7.51	120.11	112.60
2	B	263	ARG	NE-CZ-NH2	-7.45	112.49	119.20
1	A	31	TYR	CA-C-N	7.41	128.37	119.99
1	A	31	TYR	C-N-CA	7.41	128.37	119.99
2	B	68	THR	CA-C-O	-7.35	113.10	121.40
1	A	22	ASN	CA-CB-CG	-7.33	105.27	112.60
2	B	330	ASN	CB-CG-ND2	7.29	127.34	116.40
2	B	34	GLY	O-C-N	7.28	130.63	123.35
2	B	482	GLU	CA-C-O	-7.25	113.20	121.40
2	B	419	GLN	OE1-CD-NE2	7.22	129.82	122.60
1	A	155	ASN	OD1-CG-ND2	7.22	129.82	122.60
2	B	239	ASN	OD1-CG-ND2	-7.21	115.39	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	464	GLN	OE1-CD-NE2	-7.18	115.42	122.60
2	B	220	LEU	CA-C-O	-7.16	112.97	120.70
2	B	367	PHE	CA-CB-CG	-7.10	106.70	113.80
2	B	29	PRO	CA-C-N	7.08	130.88	120.90
2	B	29	PRO	C-N-CA	7.08	130.88	120.90
2	B	62	VAL	O-C-N	7.06	127.41	121.98
2	B	460	PHE	CA-CB-CG	7.04	120.84	113.80
2	B	166	TRP	O-C-N	-6.98	114.72	122.12
2	B	457	ASN	CA-C-O	-6.95	112.92	120.92
1	A	70	ARG	NE-CZ-NH2	-6.93	112.97	119.20
2	B	148	VAL	CA-C-O	6.91	128.18	120.85
2	B	248	TYR	CA-C-N	6.89	127.43	119.99
2	B	248	TYR	C-N-CA	6.89	127.43	119.99
2	B	16	ALA	CA-C-O	6.83	128.40	120.89
2	B	73	ASP	CA-CB-CG	-6.82	105.78	112.60
1	A	133	ASP	CA-C-O	-6.82	113.33	120.55
1	A	186	ALA	CA-C-N	6.78	127.15	119.83
1	A	186	ALA	C-N-CA	6.78	127.15	119.83
2	B	497	VAL	CB-CA-C	-6.74	98.65	110.71
1	A	11	ARG	CD-NE-CZ	6.73	133.82	124.40
2	B	67	SER	N-CA-CB	-6.72	100.00	111.69
1	A	194	GLU	CA-C-O	-6.71	112.44	120.56
2	B	205	PRO	O-C-N	-6.69	113.61	122.64
2	B	296	LEU	O-C-N	-6.67	114.95	122.08
1	A	56	GLU	N-CA-CB	6.65	119.90	110.12
2	B	269	ARG	CA-CB-CG	6.64	127.39	114.10
2	B	245	GLN	N-CA-CB	-6.63	101.28	111.56
2	B	341	GLN	CA-C-O	-6.61	112.99	120.46
2	B	173	GLN	OE1-CD-NE2	6.59	129.19	122.60
2	B	411	VAL	CB-CA-C	-6.58	100.35	110.95
1	A	183	ASN	CA-C-N	6.57	126.19	119.56
1	A	183	ASN	C-N-CA	6.57	126.19	119.56
2	B	495	ARG	NE-CZ-NH1	6.55	128.06	121.50
2	B	148	VAL	O-C-N	-6.54	115.09	121.83
2	B	465	ALA	CA-C-O	-6.53	113.91	121.10
2	B	495	ARG	CA-C-N	6.46	126.08	119.56
2	B	495	ARG	C-N-CA	6.46	126.08	119.56
2	B	455	ARG	NE-CZ-NH2	-6.45	113.40	119.20
2	B	62	VAL	N-CA-C	-6.43	106.54	111.62
1	A	107	VAL	CB-CA-C	-6.42	103.75	111.97
2	B	86	LYS	CA-CB-CG	6.41	126.91	114.10
2	B	87	PRO	N-CA-CB	6.40	109.28	103.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ARG	CD-NE-CZ	6.38	133.33	124.40
2	B	295	ASN	OD1-CG-ND2	6.37	128.97	122.60
2	B	471	ARG	CG-CD-NE	6.37	126.01	112.00
2	B	35	ILE	O-C-N	-6.35	117.09	123.19
2	B	359	VAL	CB-CA-C	-6.35	103.84	111.97
2	B	233	GLN	OE1-CD-NE2	-6.34	116.26	122.60
1	A	120	ASN	CA-CB-CG	-6.31	106.29	112.60
2	B	24	PHE	N-CA-CB	-6.30	100.59	110.98
2	B	242	ASN	OD1-CG-ND2	-6.29	116.31	122.60
2	B	500	TRP	CA-C-O	-6.29	114.30	121.40
2	B	391	VAL	CG1-CB-CG2	6.29	124.63	110.80
2	B	546	HIS	CA-CB-CG	-6.27	107.53	113.80
2	B	99	MET	CA-C-O	-6.24	114.30	121.47
2	B	530	ASN	CA-CB-CG	6.22	118.82	112.60
2	B	297	ARG	NE-CZ-NH2	6.17	124.76	119.20
1	A	28	PHE	CA-C-O	6.15	126.93	119.31
2	B	269	ARG	N-CA-CB	6.12	119.11	110.12
2	B	483	ASN	CA-C-N	-6.10	111.87	122.37
2	B	483	ASN	C-N-CA	-6.10	111.87	122.37
2	B	319	LEU	CA-C-O	-6.06	114.08	120.63
2	B	76	ASP	OD1-CG-OD2	-6.05	108.37	122.90
2	B	414	PHE	CA-C-N	6.05	130.99	122.46
2	B	414	PHE	C-N-CA	6.05	130.99	122.46
2	B	53	PRO	N-CA-CB	6.05	109.98	103.33
2	B	74	ASP	CA-C-O	6.02	127.23	119.95
2	B	256	PHE	O-C-N	-6.01	116.30	123.27
1	A	195	SER	CA-C-O	-5.98	114.88	121.28
1	A	184	PRO	N-CA-CB	5.95	109.22	103.51
2	B	47	ASN	OD1-CG-ND2	5.95	128.55	122.60
1	A	57	VAL	CA-C-O	-5.95	113.67	118.90
1	A	59	GLY	CA-C-N	5.94	128.83	120.28
1	A	59	GLY	C-N-CA	5.94	128.83	120.28
2	B	287	ARG	O-C-N	5.92	128.25	122.09
2	B	224	GLU	CB-CG-CD	5.91	122.64	112.60
2	B	22	PRO	N-CA-CB	5.90	108.55	103.36
2	B	109	LYS	O-C-N	-5.88	115.66	122.95
2	B	144	ASP	CA-C-O	-5.88	114.45	120.80
2	B	557	ARG	NE-CZ-NH2	-5.86	113.93	119.20
2	B	364	PRO	N-CA-CB	5.84	108.51	103.31
1	A	170	GLN	CA-C-N	5.82	126.44	119.98
1	A	170	GLN	C-N-CA	5.82	126.44	119.98
1	A	125	THR	CA-C-N	5.80	125.70	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	THR	C-N-CA	5.80	125.70	119.85
2	B	136	ALA	CA-C-N	-5.70	114.16	122.65
2	B	136	ALA	C-N-CA	-5.70	114.16	122.65
2	B	474	ALA	CA-C-O	-5.68	114.40	120.42
1	A	24	THR	CA-CB-OG1	-5.65	101.12	109.60
2	B	476	TYR	N-CA-CB	5.64	118.32	109.69
2	B	219	GLY	CA-C-O	-5.60	117.05	120.91
2	B	262	ASP	CA-CB-CG	-5.59	107.01	112.60
2	B	342	PRO	CA-C-N	5.58	126.28	120.03
2	B	342	PRO	C-N-CA	5.58	126.28	120.03
1	A	40	LEU	CA-C-O	-5.58	114.97	120.82
1	A	111	PRO	N-CA-CB	5.57	108.86	103.51
2	B	479	ARG	CA-C-N	-5.57	115.05	120.34
2	B	479	ARG	C-N-CA	-5.57	115.05	120.34
2	B	139	LYS	CA-C-N	5.56	131.19	123.07
2	B	139	LYS	C-N-CA	5.56	131.19	123.07
1	A	183	ASN	OD1-CG-ND2	5.55	128.15	122.60
2	B	29	PRO	N-CA-CB	5.54	108.70	102.60
2	B	525	LEU	N-CA-C	5.53	116.99	111.07
2	B	2	ASN	OD1-CG-ND2	-5.52	117.08	122.60
2	B	143	TRP	CB-CG-CD2	5.52	134.53	126.80
2	B	95	LYS	CA-C-O	-5.50	115.03	121.46
1	A	53	THR	CA-C-O	5.48	127.00	120.53
2	B	8	LYS	CB-CA-C	-5.46	102.08	110.81
2	B	181	TYR	CA-C-O	-5.45	114.39	120.66
1	A	33	TYR	CA-C-O	-5.44	115.10	120.82
1	A	128	ARG	NE-CZ-NH2	5.43	124.08	119.20
2	B	144	ASP	CA-CB-CG	5.43	118.03	112.60
2	B	164	GLN	O-C-N	-5.42	116.37	122.12
2	B	176	THR	O-C-N	-5.42	114.93	122.41
1	A	150	THR	CA-C-O	-5.40	114.95	120.99
2	B	463	PRO	N-CA-CB	5.37	108.10	103.27
1	A	73	TYR	CB-CG-CD1	5.36	128.84	120.80
2	B	226	ASN	CB-CG-ND2	5.36	124.44	116.40
2	B	464	GLN	CG-CD-NE2	5.35	124.42	116.40
2	B	440	ASN	CA-CB-CG	-5.34	107.25	112.60
2	B	363	VAL	O-C-N	-5.34	116.60	121.41
1	A	168	VAL	O-C-N	-5.34	116.19	121.96
2	B	377	GLU	CA-C-O	-5.33	114.56	120.70
2	B	28	ALA	CA-C-O	-5.33	115.43	119.59
2	B	135	THR	CA-C-N	-5.33	114.10	122.73
2	B	135	THR	C-N-CA	-5.33	114.10	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	206	ARG	NE-CZ-NH2	5.32	123.98	119.20
2	B	210	PRO	N-CA-CB	5.31	108.28	103.34
1	A	148	ASP	CA-C-N	-5.29	115.42	122.72
1	A	148	ASP	C-N-CA	-5.29	115.42	122.72
2	B	156	HIS	O-C-N	-5.28	116.52	122.12
2	B	316	ARG	NE-CZ-NH2	5.28	123.95	119.20
2	B	507	GLN	CA-C-O	5.26	126.00	120.42
2	B	489	SER	O-C-N	-5.23	119.12	121.53
1	A	89	ASP	CA-CB-CG	-5.23	107.37	112.60
2	B	417	LYS	CA-C-N	5.23	125.14	119.76
2	B	417	LYS	C-N-CA	5.23	125.14	119.76
2	B	72	GLY	N-CA-C	-5.22	104.21	112.66
1	A	180	TRP	CA-CB-CG	5.21	123.51	113.60
2	B	164	GLN	CB-CG-CD	5.21	121.45	112.60
2	B	140	SER	CA-C-O	5.20	125.86	120.40
2	B	408	PRO	O-C-N	-5.19	117.28	123.10
2	B	215	TRP	CA-CB-CG	-5.18	103.75	113.60
2	B	490	PRO	CA-C-O	-5.17	115.70	121.23
2	B	464	GLN	CA-C-O	-5.17	113.70	119.34
1	A	18	HIS	CE1-NE2-CD2	-5.16	103.84	109.00
2	B	33	TYR	CA-C-N	-5.16	116.57	121.57
2	B	33	TYR	C-N-CA	-5.16	116.57	121.57
2	B	173	GLN	CB-CG-CD	-5.15	103.85	112.60
2	B	490	PRO	N-CA-CB	5.15	107.90	103.27
2	B	23	GLN	CA-C-O	-5.14	114.95	120.46
2	B	331	LEU	CA-C-O	-5.14	114.43	120.60
1	A	177	GLN	N-CA-C	-5.14	106.17	112.90
2	B	407	ILE	CA-C-O	5.14	122.18	119.15
2	B	173	GLN	N-CA-C	-5.14	101.39	109.25
1	A	117	LYS	N-CA-C	5.13	117.54	111.33
2	B	123	HIS	CA-C-O	-5.13	113.27	119.27
2	B	440	ASN	OD1-CG-ND2	5.12	127.72	122.60
2	B	62	VAL	CA-C-O	-5.12	116.24	120.80
2	B	184	VAL	CA-C-O	-5.12	115.09	120.57
2	B	312	GLN	OE1-CD-NE2	5.12	127.72	122.60
2	B	417	LYS	CA-C-O	5.12	125.20	120.60
1	A	87	PRO	O-C-N	-5.11	116.36	122.24
2	B	462	VAL	CA-C-N	5.11	125.35	119.83
2	B	462	VAL	C-N-CA	5.11	125.35	119.83
2	B	529	GLU	CA-C-O	-5.10	115.12	120.63
2	B	363	VAL	N-CA-C	5.10	113.45	107.89
2	B	269	ARG	NH1-CZ-NH2	-5.10	112.67	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	289	THR	O-C-N	-5.09	116.26	122.22
2	B	457	ASN	CA-C-N	-5.09	113.46	121.86
2	B	457	ASN	C-N-CA	-5.09	113.46	121.86
2	B	226	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	116	PRO	CA-CB-CG	-5.07	94.88	104.50
2	B	125	ASN	OD1-CG-ND2	-5.06	117.54	122.60
2	B	22	PRO	N-CA-C	-5.05	103.17	110.80
2	B	287	ARG	NE-CZ-NH1	5.05	126.55	121.50
2	B	204	ASP	CA-C-O	-5.05	115.58	119.32
1	A	74	TRP	CA-C-N	5.04	124.49	119.24
1	A	74	TRP	C-N-CA	5.04	124.49	119.24
1	A	19	ILE	CA-CB-CG1	5.04	118.96	110.40
2	B	164	GLN	CA-C-O	5.03	125.89	120.55
2	B	284	ASP	CA-CB-CG	-5.03	107.57	112.60
1	A	33	TYR	O-C-N	5.03	127.25	122.07
2	B	28	ALA	CB-CA-C	-5.03	102.73	110.62
2	B	230	TYR	CA-C-N	-5.03	117.40	122.83
2	B	230	TYR	C-N-CA	-5.03	117.40	122.83
2	B	40	ALA	CA-C-O	-5.02	115.30	121.28
1	A	92	ILE	CA-CB-CG1	-5.02	101.87	110.40
2	B	297	ARG	CA-CB-CG	5.02	124.13	114.10
2	B	86	LYS	CA-C-O	5.00	127.01	120.16

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	122	VAL	Mainchain
2	B	141	ARG	Mainchain
2	B	147	GLU	Mainchain
2	B	167	THR	Mainchain
2	B	181	TYR	Mainchain
2	B	185	ASN	Mainchain
2	B	205	PRO	Mainchain
2	B	222	PRO	Mainchain
2	B	234	SER	Mainchain
2	B	26	TRP	Mainchain
2	B	286	ILE	Mainchain
2	B	35	ILE	Mainchain
2	B	380	GLN	Mainchain
2	B	43	ASP	Mainchain
2	B	461	GLY	Mainchain

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Mol	Chain	Res	Type	Group
2	B	52	TYR	Mainchain
2	B	85[B]	GLU	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	24	0
2	B	4438	0	4265	68	0
3	B	1	0	0	0	0
4	B	13	0	6	1	0
5	A	168	0	0	0	0
5	B	492	0	0	0	0
All	All	6768	0	5875	80	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 7.

All (80) 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:207:GLN:HE22	2:B:204:ASP:H	1.10	0.99
2:B:85[A]:GLU:OE1	2:B:85[A]:GLU:HA	1.63	0.95
2:B:269:ARG:HH21	2:B:273:GLN:HE22	1.16	0.88
2:B:85[B]:GLU:O	2:B:86:LYS:HB3	1.76	0.85
2:B:85[A]:GLU:O	2:B:86:LYS:HB3	1.75	0.85
1:A:18:HIS:HD2	2:B:38:HIS:NE2	1.81	0.78
2:B:15:LYS:HG3	2:B:489:SER:HB2	1.64	0.77
2:B:339:TRP:HH2	2:B:450:MET:HE2	1.49	0.77
2:B:269:ARG:HH21	2:B:273:GLN:NE2	1.81	0.77
2:B:444:ASN:C	2:B:444:ASN:HD22	1.95	0.73
2:B:387:LEU:HD21	2:B:450:MET:HE1	1.72	0.71
2:B:214:LYS:H	2:B:214:LYS:HD2	1.56	0.70
2:B:269:ARG:NH2	2:B:273:GLN:HE22	1.91	0.67
1:A:194:GLU:OE2	2:B:233:GLN:HG3	1.95	0.65
1:A:207:GLN:NE2	2:B:204:ASP:H	1.88	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:ALA:O	2:B:276:ARG:NH1	2.29	0.65
1:A:207:GLN:H	1:A:207:GLN:HE21	1.44	0.64
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.33	0.64
2:B:86:LYS:HG2	2:B:86:LYS:O	1.95	0.64
2:B:85[A]:GLU:OE1	2:B:85[A]:GLU:CA	2.40	0.62
2:B:317:ARG:HG3	2:B:317:ARG:HH11	1.66	0.61
2:B:520:HIS:HE1	2:B:548:GLU:OE1	1.85	0.59
2:B:511:ILE:HG12	2:B:517:VAL:HG22	1.84	0.59
2:B:85[B]:GLU:O	2:B:85[B]:GLU:HG3	2.03	0.58
2:B:67:SER:HB3	4:B:559[B]:SPA:H5	1.86	0.57
2:B:214:LYS:H	2:B:214:LYS:CD	2.18	0.57
2:B:85[A]:GLU:O	2:B:86:LYS:CB	2.52	0.56
2:B:130:ASP:CG	2:B:133:THR:HG22	2.30	0.56
2:B:520:HIS:HD2	2:B:523:ASP:OD2	1.89	0.55
2:B:84:ALA:HB2	2:B:134:GLN:NE2	2.21	0.55
1:A:206:SER:HB2	2:B:202:GLY:O	2.08	0.54
1:A:197:TYR:CD1	1:A:198:PRO:HD2	2.45	0.52
1:A:18:HIS:CD2	2:B:38:HIS:NE2	2.72	0.51
2:B:133:THR:HG23	2:B:135:THR:HB	1.93	0.50
2:B:556:GLN:HA	2:B:556:GLN:OE1	2.11	0.50
1:A:199:LEU:HG	2:B:225:MET:CE	2.43	0.48
2:B:495:ARG:NH2	2:B:542:ASP:OD1	2.45	0.48
1:A:199:LEU:HG	2:B:225:MET:HE1	1.95	0.48
2:B:83:SER:HB2	2:B:96:TRP:CH2	2.50	0.47
2:B:468:GLU:CD	2:B:468:GLU:H	2.23	0.47
1:A:56:GLU:O	2:B:109:LYS:HB2	2.14	0.47
1:A:105:ASP:OD1	1:A:128:ARG:NH1	2.48	0.47
1:A:163:LYS:HG2	1:A:168:VAL:HA	1.96	0.47
1:A:195:SER:OG	2:B:245:GLN:NE2	2.48	0.46
2:B:317:ARG:HG3	2:B:317:ARG:NH1	2.30	0.46
2:B:65:TRP:HA	2:B:180:TYR:O	2.16	0.46
2:B:127:LEU:HD11	2:B:139:LYS:HB2	1.97	0.46
2:B:133:THR:HG23	2:B:135:THR:CB	2.46	0.45
2:B:397:TYR:O	2:B:401:GLN:HG2	2.16	0.45
2:B:512:ALA:HB1	2:B:513:PRO:HD2	1.99	0.45
1:A:130:GLU:HB2	1:A:131:PRO:CD	2.47	0.44
2:B:339:TRP:CH2	2:B:450:MET:HE2	2.40	0.44
1:A:166:TYR:O	1:A:170:GLN:HB3	2.17	0.44
2:B:360:VAL:HG13	2:B:368:ASP:HB2	2.00	0.44
1:A:181:LEU:HD21	1:A:201:PHE:HB2	1.98	0.44
2:B:164:GLN:NE2	2:B:164:GLN:H	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:HB2	1:A:131:PRO:HD2	1.99	0.44
2:B:501:ASP:OD1	2:B:534:LYS:NZ	2.50	0.44
2:B:504:ALA:HA	2:B:505:PRO:C	2.43	0.44
2:B:511:ILE:HG12	2:B:517:VAL:CG2	2.48	0.43
2:B:84:ALA:HB2	2:B:134:GLN:HE21	1.84	0.43
1:A:203:GLN:HE21	1:A:203:GLN:HB2	1.50	0.42
2:B:73:ASP:OD1	2:B:73:ASP:C	2.59	0.42
2:B:452:LEU:HD23	2:B:473:GLN:NE2	2.35	0.42
2:B:129:THR:HG22	2:B:136:ALA:CB	2.50	0.42
2:B:85[B]:GLU:O	2:B:86:LYS:CB	2.56	0.42
1:A:202:ASN:HB2	2:B:202:GLY:HA2	2.02	0.41
2:B:471:ARG:HA	2:B:471:ARG:HD3	1.73	0.41
1:A:186:ALA:HA	1:A:187:PRO:HD3	1.86	0.41
2:B:127:LEU:CD1	2:B:139:LYS:HB2	2.50	0.41
2:B:199:ARG:HH11	2:B:199:ARG:HD2	1.47	0.41
1:A:110:ASN:N	1:A:111:PRO:HD3	2.35	0.41
1:A:73:TYR:CE2	1:A:136:MET:HE2	2.55	0.41
2:B:10:LYS:NZ	2:B:274:LYS:O	2.54	0.40
2:B:104:GLU:O	2:B:115:THR:HA	2.20	0.40
1:A:207:GLN:HA	2:B:215:TRP:CZ2	2.56	0.40
2:B:224:GLU:O	2:B:224:GLU:HG2	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	204/209 (98%)	200 (98%)	4 (2%)	0	100	100
2	B	558/557 (100%)	542 (97%)	14 (2%)	2 (0%)	30	22
All	All	762/766 (100%)	742 (97%)	18 (2%)	2 (0%)	36	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	86	LYS
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%)	164 (92%)	14 (8%)	11	5
2	B	463/460 (101%)	418 (90%)	45 (10%)	8	3
All	All	641/640 (100%)	582 (91%)	59 (9%)	9	4

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	13	GLU
1	A	64	LYS
1	A	109	THR
1	A	110	ASN
1	A	112	GLU
1	A	116	PRO
1	A	169	SER
1	A	192	VAL
1	A	196	ASN
1	A	200	LYS
1	A	203	GLN
1	A	207	GLN
1	A	208	THR
2	B	2	ASN
2	B	4	TRP
2	B	8	LYS
2	B	10	LYS
2	B	35	ILE
2	B	67	SER
2	B	81[A]	ARG

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Mol	Chain	Res	Type
2	B	81[B]	ARG
2	B	85[A]	GLU
2	B	85[B]	GLU
2	B	86	LYS
2	B	95	LYS
2	B	98	LYS
2	B	115	THR
2	B	127	LEU
2	B	154	TRP
2	B	164	GLN
2	B	184	VAL
2	B	201	SER
2	B	214	LYS
2	B	269	ARG
2	B	273	GLN
2	B	317	ARG
2	B	337	LYS
2	B	380	GLN
2	B	387	LEU
2	B	391	VAL
2	B	400	VAL
2	B	403	ASP
2	B	404	LYS
2	B	411	VAL
2	B	420	GLN
2	B	432	GLU
2	B	437	ARG
2	B	444	ASN
2	B	468	GLU
2	B	493	SER
2	B	497	VAL
2	B	517	VAL
2	B	519	LYS
2	B	526	LYS
2	B	530	ASN
2	B	541[A]	GLN
2	B	541[B]	GLN
2	B	556	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	110	ASN
1	A	196	ASN
1	A	203	GLN
1	A	204	GLN
1	A	207	GLN
2	B	2	ASN
2	B	93	ASN
2	B	110	ASN
2	B	131	GLN
2	B	164	GLN
2	B	245	GLN
2	B	273	GLN
2	B	288	GLN
2	B	292	GLN
2	B	341	GLN
2	B	348	ASN
2	B	441	ASN
2	B	444	ASN
2	B	473	GLN
2	B	520	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	SPA	B	559[B]	-	9,9,9	1.28	1 (11%)	10,11,11	1.41	2 (20%)
4	SPA	B	559[A]	-	9,9,9	1.30	1 (11%)	10,11,11	1.36	2 (20%)

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	SPA	B	559[B]	-	-	0/4/4/4	0/1/1/1
4	SPA	B	559[A]	-	-	0/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	559[A]	SPA	C6-C7	3.68	1.56	1.51
4	B	559[B]	SPA	C6-C7	3.68	1.56	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	559[A]	SPA	O2-C7-C6	-3.23	104.50	114.51
4	B	559[B]	SPA	O2-C7-C6	-3.23	104.50	114.51
4	B	559[A]	SPA	O1-C7-C6	2.39	128.91	122.11
4	B	559[B]	SPA	O1-C7-C6	2.39	128.91	122.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	559[B]	SPA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.61	2 (0%) 79 81	12, 23, 57, 87	0
2	B	557/557 (100%)	-0.73	0 100 100	9, 21, 49, 97	3 (0%)
All	All	763/766 (99%)	-0.70	2 (0%) 90 92	9, 22, 51, 97	3 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	SER	2.0
1	A	208	THR	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(Å ²)	Q<0.9
4	SPA	B	559[A]	9/9	0.98	0.05	14,15,18,19	4
4	SPA	B	559[B]	9/9	0.98	0.05	14,17,18,19	4
3	CA	B	558	1/1	0.99	0.02	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.