



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:16 AM GMT

PDB ID : 2GCD
Title : TAO2 kinase domain-staurosporine structure
Authors : Zhou, T.; Sun, L.; Gao, Y.; Earnest, S.; Cobb, M.H.; Goldsmith, E.J.
Deposited on : 2006-03-14
Resolution : 2.55 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

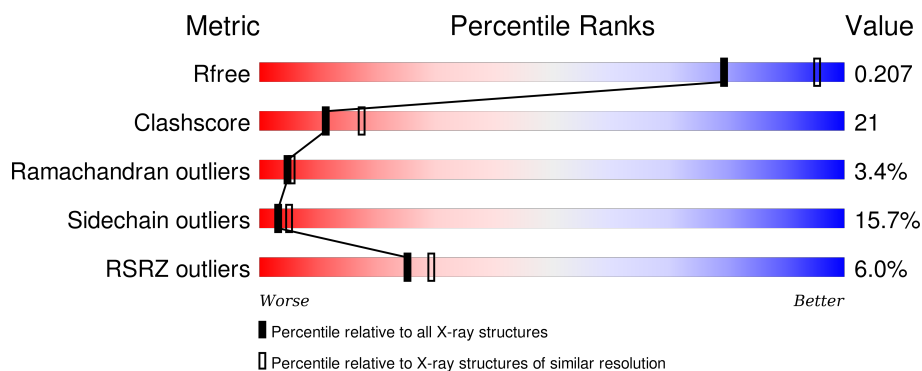
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	<div> <div>6%</div> <div>50%</div> <div>39%</div> <div>11%</div> <div>.</div> </div>
1	B	309	<div> <div>6%</div> <div>55%</div> <div>32%</div> <div>10%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5327 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.

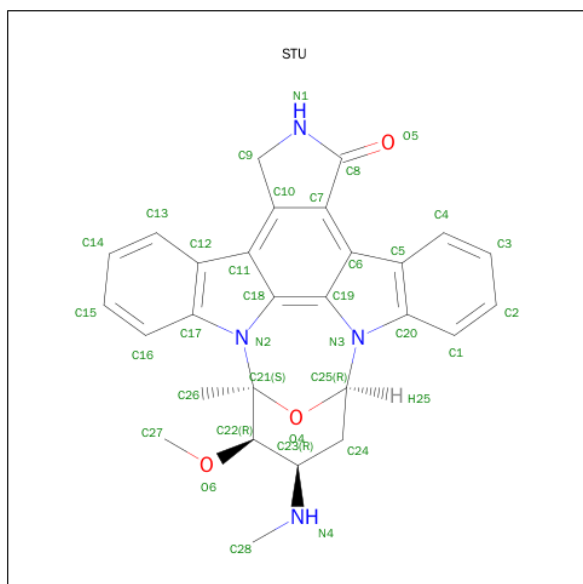
- Molecule 1 is a protein called Serine/threonine-protein kinase TAO2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	P	S	0	0	0
			2490	1586	432	457	1	14			
1	B	309	Total	C	N	O	P	S	0	0	0
			2490	1586	432	457	1	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	SEP	SER	MODIFIED RESIDUE	UNP Q9JLS3
B	181	SEP	SER	MODIFIED RESIDUE	UNP Q9JLS3

- Molecule 2 is STAUROSPORINE (three-letter code: STU) (formula: C₂₈H₂₆N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	28	4	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			35	28	4	3		

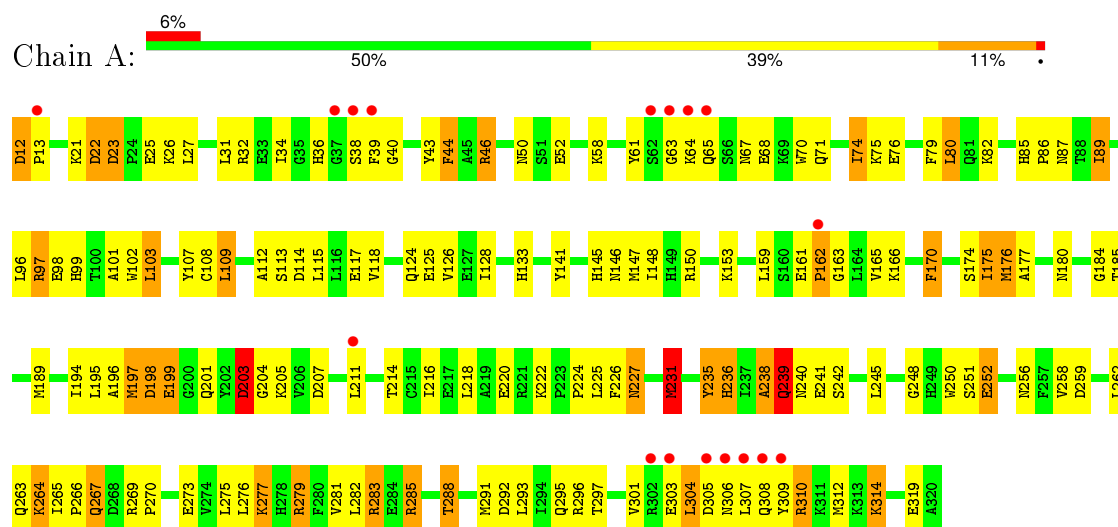
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	135	Total	O	0	0
			135	135		

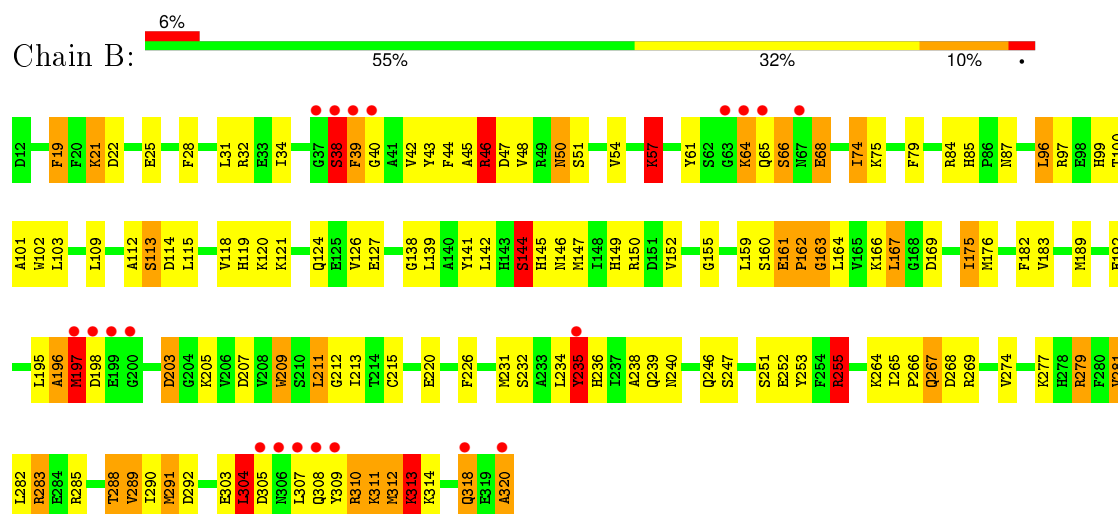
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Serine/threonine-protein kinase TAO2



• Molecule 1: Serine/threonine-protein kinase TAO2



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	186.02Å 186.02Å 94.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	160.13 – 2.55 24.89 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.8 (160.13-2.55) 92.3 (24.89-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.53Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.199 , 0.261 0.198 , 0.207	Depositor DCC
R_{free} test set	1548 reflections (5.53%)	DCC
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 31260 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5327	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 3.64% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: STU, SEP

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	1.58	21/2538 (0.8%)	1.38	24/3428 (0.7%)
1	B	1.57	19/2538 (0.7%)	1.37	16/3428 (0.5%)
All	All	1.58	40/5076 (0.8%)	1.37	40/6856 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	GLU	CG-CD	12.50	1.70	1.51
1	A	98	GLU	CG-CD	9.10	1.65	1.51
1	A	68	GLU	CB-CG	8.90	1.69	1.52
1	B	192	GLU	CB-CG	-8.76	1.35	1.52
1	A	199	GLU	CG-CD	8.49	1.64	1.51
1	A	68	GLU	CG-CD	8.39	1.64	1.51
1	B	252	GLU	CG-CD	8.15	1.64	1.51
1	A	117	GLU	CG-CD	7.63	1.63	1.51
1	A	235	TYR	CB-CG	7.33	1.62	1.51
1	A	252	GLU	CB-CG	7.00	1.65	1.52
1	A	117	GLU	CD-OE2	6.72	1.33	1.25
1	A	199	GLU	CB-CG	6.70	1.64	1.52
1	A	170	PHE	CD1-CE1	6.63	1.52	1.39
1	B	281	VAL	CB-CG1	-6.58	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	SER	CB-OG	-6.50	1.33	1.42
1	A	235	TYR	CE1-CZ	6.49	1.47	1.38
1	B	226	PHE	CD2-CE2	6.31	1.51	1.39
1	B	48	VAL	CB-CG2	6.20	1.65	1.52
1	B	101	ALA	CA-CB	-6.14	1.39	1.52
1	B	235	TYR	CG-CD2	5.99	1.47	1.39
1	B	182	PHE	CE1-CZ	5.95	1.48	1.37
1	A	98	GLU	CD-OE2	5.79	1.32	1.25
1	B	57	LYS	CB-CG	5.78	1.68	1.52
1	B	235	TYR	CE1-CZ	5.66	1.46	1.38
1	B	246	GLN	CB-CG	-5.55	1.37	1.52
1	A	101	ALA	CA-CB	-5.52	1.40	1.52
1	A	211	LEU	C-O	5.48	1.33	1.23
1	A	319	GLU	CB-CG	5.38	1.62	1.52
1	B	213	ILE	CA-CB	-5.37	1.42	1.54
1	B	267	GLN	CG-CD	5.36	1.63	1.51
1	B	48	VAL	CB-CG1	5.33	1.64	1.52
1	A	113	SER	CB-OG	-5.32	1.35	1.42
1	A	231	MET	CB-CG	5.24	1.68	1.51
1	B	289	VAL	CB-CG2	-5.24	1.41	1.52
1	B	21	LYS	CD-CE	5.23	1.64	1.51
1	B	209	TRP	CB-CG	-5.22	1.40	1.50
1	A	107	TYR	CB-CG	-5.17	1.43	1.51
1	A	26	LYS	CB-CG	5.15	1.66	1.52
1	A	102	TRP	CG-CD1	5.12	1.44	1.36
1	B	19	PHE	CE2-CZ	5.12	1.47	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ASP	CB-CG-OD2	8.70	126.13	118.30
1	A	89	ILE	CG1-CB-CG2	-7.95	93.91	111.40
1	A	207	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	32	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	A	264	LYS	CD-CE-NZ	7.18	128.21	111.70
1	B	96	LEU	CB-CG-CD2	-7.09	98.94	111.00
1	B	207	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	283	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	B	32	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	150	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	A	203	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	248	GLY	N-CA-C	-6.33	97.26	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	268	ASP	CB-CG-OD1	-6.20	112.72	118.30
1	A	184	GLY	N-CA-C	-6.11	97.84	113.10
1	A	22	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	B	211	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	113	SER	CB-CA-C	-6.03	98.64	110.10
1	B	255	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	46	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	285	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	B	197	MET	CG-SD-CE	5.69	109.30	100.20
1	A	26	LYS	CD-CE-NZ	5.63	124.64	111.70
1	A	252	GLU	OE1-CD-OE2	-5.62	116.55	123.30
1	B	320	ALA	N-CA-C	5.56	126.02	111.00
1	A	307	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	203	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	46	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	189	MET	CG-SD-CE	5.46	108.94	100.20
1	B	203	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	259	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	222	LYS	CD-CE-NZ	5.41	124.14	111.70
1	A	176	MET	CG-SD-CE	5.40	108.84	100.20
1	B	207	ASP	CB-CG-OD2	-5.39	113.44	118.30
1	A	231	MET	CG-SD-CE	5.37	108.79	100.20
1	B	291	MET	CG-SD-CE	5.16	108.45	100.20
1	A	293	LEU	CB-CG-CD2	-5.10	102.32	111.00
1	B	192	GLU	CB-CA-C	-5.10	100.20	110.40
1	A	283	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	283	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	MET	Peptide
1	B	196	ALA	Peptide
1	B	313	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2490	0	2468	107	0
1	B	2490	0	2468	91	0
2	A	35	0	26	3	0
2	B	35	0	26	7	0
3	A	142	0	0	14	0
3	B	135	0	0	6	0
All	All	5327	0	4988	207	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 21.

All (207) 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:175:ILE:CG1	1:A:175:ILE:CD1	1.74	1.58
2:B:500:STU:H261	2:B:500:STU:H16	1.23	1.10
1:A:65:GLN:HE21	1:A:67:ASN:HB2	1.16	1.08
1:A:65:GLN:NE2	1:A:67:ASN:HB2	1.73	1.02
1:B:46:ARG:HH11	1:B:46:ARG:HG2	1.25	0.98
1:A:85:HIS:CD2	1:A:87:ASN:H	1.86	0.93
1:A:203:ASP:HB3	1:A:205:LYS:H	1.32	0.92
1:A:85:HIS:HD2	1:A:87:ASN:H	1.13	0.92
1:A:65:GLN:HE21	1:A:67:ASN:CB	1.84	0.90
1:A:96:LEU:O	1:A:97:ARG:HD3	1.72	0.89
1:A:279:ARG:HG2	3:A:420:HOH:O	1.72	0.88
1:A:175:ILE:N	1:A:175:ILE:HD12	1.89	0.87
1:A:133:HIS:CD2	1:A:285:ARG:HH22	1.92	0.87
1:B:85:HIS:HD2	1:B:87:ASN:H	1.22	0.86
1:B:85:HIS:CD2	1:B:87:ASN:H	1.96	0.83
1:B:39:PHE:CD1	1:B:40:GLY:N	2.46	0.83
1:A:175:ILE:H	1:A:175:ILE:CD1	1.93	0.81
1:A:108:CYS:HB3	1:A:159:LEU:O	1.80	0.81
1:B:235:TYR:CE1	1:B:239:GLN:HG3	2.16	0.80
2:B:500:STU:C26	2:B:500:STU:H16	2.08	0.80
1:A:114:ASP:HB3	1:A:312:MET:HE1	1.63	0.79
1:B:61:TYR:CE2	1:B:99:HIS:HA	2.19	0.78
1:A:175:ILE:HD12	1:A:175:ILE:H	1.48	0.76
2:B:500:STU:H261	2:B:500:STU:C16	2.04	0.75
1:A:175:ILE:N	1:A:175:ILE:CD1	2.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:O	1:A:89:ILE:HG22	1.86	0.75
1:B:61:TYR:CZ	1:B:99:HIS:HA	2.22	0.74
1:B:288:THR:HB	1:B:292:ASP:OD2	1.87	0.73
1:B:96:LEU:HD23	1:B:96:LEU:C	2.09	0.72
1:A:306:ASN:OD1	1:A:309:TYR:HB2	1.90	0.72
1:A:124:GLN:HG2	3:A:461:HOH:O	1.90	0.72
1:B:46:ARG:HH11	1:B:46:ARG:CG	2.01	0.71
1:A:36:HIS:HE1	3:A:518:HOH:O	1.73	0.70
1:A:240:ASN:O	1:A:264:LYS:HE3	1.93	0.69
1:A:161:GLU:HA	1:A:162:PRO:C	2.14	0.69
2:B:500:STU:C17	2:B:500:STU:H273	2.23	0.68
1:A:12:ASP:N	1:A:13:PRO:HD2	2.09	0.67
1:A:85:HIS:HD2	1:A:87:ASN:N	1.91	0.67
1:B:96:LEU:HD23	1:B:97:ARG:N	2.10	0.67
1:B:310:ARG:HH21	1:B:311:LYS:HD3	1.60	0.67
1:B:68:GLU:N	1:B:68:GLU:CD	2.48	0.67
1:B:79:PHE:CE1	1:B:147:MET:HE2	2.29	0.67
1:B:312:MET:HA	1:B:312:MET:HE3	1.77	0.66
1:A:50:ASN:OD1	1:A:52:GLU:HB2	1.96	0.65
1:A:224:PRO:O	1:A:225:LEU:CB	2.41	0.65
1:B:161:GLU:HA	1:B:162:PRO:C	2.17	0.65
1:A:194:ILE:O	1:A:197:MET:HG3	1.98	0.64
1:B:68:GLU:H	1:B:68:GLU:CD	2.01	0.64
1:A:89:ILE:O	1:A:89:ILE:CG2	2.47	0.63
1:A:23:ASP:HB2	1:A:97:ARG:NH2	2.14	0.63
1:A:310:ARG:CZ	1:A:310:ARG:HA	2.29	0.63
1:B:196:ALA:C	1:B:197:MET:O	2.36	0.62
1:B:265:ILE:O	1:B:266:PRO:C	2.34	0.62
1:A:133:HIS:HD2	1:A:285:ARG:HH22	1.46	0.61
1:B:145:HIS:O	1:B:146:ASN:CB	2.46	0.61
1:A:238:ALA:O	1:A:264:LYS:NZ	2.23	0.61
1:A:270:PRO:HG2	1:A:275:LEU:HD11	1.83	0.60
1:A:114:ASP:HB3	1:A:312:MET:CE	2.31	0.60
1:B:46:ARG:NH1	1:B:46:ARG:HG2	2.05	0.60
1:A:270:PRO:HG3	1:A:275:LEU:HD21	1.83	0.60
1:A:180:ASN:ND2	3:A:510:HOH:O	2.32	0.60
1:A:224:PRO:O	1:A:225:LEU:HB2	2.01	0.60
1:A:203:ASP:HB3	1:A:205:LYS:N	2.13	0.59
1:A:231:MET:HB2	3:A:404:HOH:O	2.02	0.59
1:A:288:THR:HB	1:A:292:ASP:OD2	2.03	0.58
1:B:318:GLN:HB3	3:B:580:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:TYR:CE1	1:A:58:LYS:HG3	2.39	0.58
1:B:114:ASP:O	1:B:118:VAL:HG23	2.03	0.58
1:B:79:PHE:CZ	1:B:147:MET:HE1	2.39	0.57
2:B:500:STU:C26	2:B:500:STU:C16	2.73	0.57
1:A:203:ASP:CB	1:A:205:LYS:H	2.11	0.57
1:B:145:HIS:O	1:B:146:ASN:HB2	2.04	0.57
1:A:231:MET:HG3	3:A:418:HOH:O	2.04	0.57
1:B:79:PHE:HE1	1:B:147:MET:HG2	1.70	0.57
1:B:31:LEU:HD22	1:B:45:ALA:HB2	1.87	0.56
1:B:161:GLU:HA	1:B:162:PRO:O	2.05	0.56
1:A:270:PRO:CG	1:A:275:LEU:HD21	2.36	0.56
1:A:236:HIS:O	1:A:240:ASN:HB2	2.06	0.56
1:B:46:ARG:HH21	1:B:320:ALA:HB2	1.71	0.55
1:B:79:PHE:CE1	1:B:147:MET:CE	2.89	0.55
1:B:212:GLY:O	1:B:215:CYS:HB2	2.06	0.55
1:B:39:PHE:HD1	1:B:40:GLY:N	2.03	0.55
1:A:304:LEU:HD22	1:A:310:ARG:HD2	1.88	0.55
1:A:34:ILE:HA	1:A:314:LYS:HD3	1.89	0.54
1:A:25:GLU:HG3	3:A:470:HOH:O	2.07	0.54
1:A:196:ALA:C	1:A:198:ASP:O	2.46	0.54
2:A:400:STU:H16	2:A:400:STU:H261	1.90	0.54
1:B:236:HIS:HB3	3:B:543:HOH:O	2.07	0.54
1:A:76:GLU:HG2	1:A:80:LEU:HD22	1.90	0.54
1:B:113:SER:HB3	1:B:155:GLY:HA2	1.90	0.54
1:B:79:PHE:CE1	1:B:147:MET:HG2	2.42	0.54
1:B:46:ARG:NH1	1:B:46:ARG:CG	2.65	0.53
1:A:85:HIS:CD2	1:A:86:PRO:HD2	2.43	0.53
1:A:205:LYS:HE2	1:A:269:ARG:O	2.08	0.53
1:A:146:ASN:ND2	1:A:177:ALA:HB3	2.24	0.53
1:A:70:TRP:CZ2	1:A:74:ILE:HD11	2.43	0.53
1:A:235:TYR:CE1	1:A:239:GLN:HG3	2.44	0.53
1:B:175:ILE:HD12	1:B:176:MET:H	1.73	0.53
1:B:267:GLN:N	1:B:267:GLN:OE1	2.41	0.52
1:B:43:TYR:N	1:B:43:TYR:CD1	2.78	0.52
1:A:231:MET:CG	3:A:418:HOH:O	2.56	0.52
1:A:258:VAL:CG1	1:A:262:LEU:HD12	2.39	0.52
1:A:185:THR:O	1:A:189:MET:HG3	2.10	0.52
1:B:238:ALA:O	1:B:264:LYS:NZ	2.40	0.52
1:B:209:TRP:CD1	1:B:209:TRP:C	2.83	0.52
1:B:19:PHE:CD2	1:B:96:LEU:HB2	2.45	0.51
1:B:119:HIS:O	1:B:120:LYS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:THR:O	1:A:218:LEU:HG	2.10	0.51
1:A:227:ASN:HD22	1:A:227:ASN:C	2.13	0.51
1:A:310:ARG:NE	1:A:310:ARG:HA	2.25	0.51
1:B:100:THR:O	1:B:102:TRP:HD1	1.94	0.51
1:A:277:LYS:O	1:A:282:LEU:HD12	2.10	0.51
1:B:103:LEU:HD23	1:B:103:LEU:N	2.27	0.50
1:B:85:HIS:HD2	1:B:87:ASN:N	2.00	0.50
1:A:235:TYR:CD1	1:A:239:GLN:HG3	2.47	0.50
1:A:196:ALA:O	1:A:198:ASP:O	2.30	0.49
1:A:241:GLU:HG2	1:A:242:SER:H	1.76	0.49
1:B:308:GLN:HB2	1:B:309:TYR:CD2	2.47	0.49
1:B:39:PHE:CG	1:B:57:LYS:HE3	2.47	0.49
1:B:96:LEU:CD2	1:B:96:LEU:C	2.80	0.49
1:B:160:SER:O	1:B:163:GLY:HA2	2.12	0.49
1:A:79:PHE:HE2	1:A:170:PHE:CD2	2.31	0.48
1:B:220:GLU:OE1	3:B:553:HOH:O	2.20	0.48
1:A:258:VAL:HG12	1:A:262:LEU:HD12	1.94	0.48
1:B:149:HIS:O	1:B:150:ARG:HB2	2.13	0.48
1:A:118:VAL:HG23	1:A:312:MET:CE	2.44	0.48
1:A:273:GLU:O	1:A:276:LEU:HB2	2.13	0.48
1:B:159:LEU:HD22	1:B:159:LEU:N	2.29	0.48
1:A:245:LEU:HD13	1:A:250:TRP:CD1	2.49	0.48
1:B:247:SER:O	1:B:255:ARG:NH2	2.47	0.48
1:B:282:LEU:O	1:B:283:ARG:C	2.53	0.47
1:A:252:GLU:OE2	1:A:256:ASN:HB2	2.14	0.47
1:A:266:PRO:HB2	1:A:267:GLN:OE1	2.13	0.47
1:A:147:MET:HG3	3:A:494:HOH:O	2.15	0.47
2:A:400:STU:H4	2:A:400:STU:O5	2.15	0.47
1:A:34:ILE:CA	1:A:314:LYS:HD3	2.45	0.46
1:B:79:PHE:CZ	1:B:147:MET:CE	2.98	0.46
1:A:301:VAL:O	1:A:304:LEU:HB2	2.16	0.46
1:B:290:ILE:HA	1:B:290:ILE:HD13	1.59	0.46
1:A:44:PHE:CD2	1:A:44:PHE:C	2.89	0.46
1:A:205:LYS:NZ	3:A:416:HOH:O	2.34	0.46
1:B:163:GLY:HA3	1:B:290:ILE:HG22	1.98	0.46
1:B:47:ASP:O	1:B:51:SER:N	2.49	0.46
1:A:97:ARG:HA	1:A:97:ARG:HD2	1.92	0.46
1:B:61:TYR:CE2	1:B:99:HIS:CA	2.95	0.46
1:A:216:ILE:O	1:A:220:GLU:N	2.46	0.46
1:A:279:ARG:CG	3:A:420:HOH:O	2.43	0.46
1:B:65:GLN:O	1:B:66:SER:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ALA:O	1:B:115:LEU:HB2	2.16	0.45
1:B:141:TYR:O	1:B:144:SER:HB2	2.16	0.45
1:A:279:ARG:NE	3:A:420:HOH:O	2.49	0.45
1:A:118:VAL:HG23	1:A:312:MET:HE2	1.99	0.45
1:B:68:GLU:N	1:B:68:GLU:OE2	2.50	0.45
1:B:239:GLN:C	1:B:240:ASN:HD22	2.20	0.45
1:B:203:ASP:C	1:B:203:ASP:OD1	2.54	0.45
1:B:304:LEU:HD21	1:B:310:ARG:NH1	2.32	0.45
1:B:50:ASN:O	1:B:51:SER:HB2	2.16	0.45
1:A:61:TYR:CE2	1:A:99:HIS:HA	2.51	0.45
1:A:75:LYS:NZ	1:A:175:ILE:HD11	2.31	0.45
1:A:23:ASP:HB2	1:A:97:ARG:HH21	1.82	0.45
1:A:252:GLU:OE2	1:A:279:ARG:NH1	2.43	0.44
1:B:100:THR:O	1:B:102:TRP:CD1	2.70	0.44
1:A:279:ARG:H	1:A:279:ARG:HG2	1.53	0.44
1:A:153:LYS:HA	1:A:214:THR:OG1	2.18	0.43
1:B:65:GLN:NE2	1:B:68:GLU:HG2	2.34	0.43
1:B:38:SER:CB	3:B:535:HOH:O	2.66	0.43
1:A:296:ARG:HB2	3:A:482:HOH:O	2.18	0.43
1:A:109:LEU:CD2	1:A:109:LEU:N	2.82	0.43
1:B:205:LYS:HE2	1:B:269:ARG:O	2.19	0.43
1:A:125:GLU:HA	1:A:128:ILE:HD12	2.00	0.43
1:B:235:TYR:CZ	1:B:239:GLN:HG3	2.53	0.43
2:B:500:STU:H25	2:B:500:STU:H1	1.84	0.43
1:B:163:GLY:HA3	1:B:290:ILE:CG2	2.49	0.43
1:A:197:MET:C	1:A:198:ASP:O	2.57	0.42
1:A:112:ALA:O	1:A:115:LEU:HB2	2.18	0.42
1:A:282:LEU:O	1:A:283:ARG:C	2.58	0.42
1:B:28:PHE:HA	1:B:46:ARG:O	2.20	0.42
1:A:148:ILE:HG23	1:A:204:GLY:HA2	2.01	0.42
1:B:34:ILE:HG12	1:B:42:VAL:O	2.20	0.42
1:A:263:GLN:HA	1:A:263:GLN:OE1	2.19	0.42
1:A:103:LEU:N	1:A:103:LEU:HD23	2.33	0.42
2:A:400:STU:H22	3:A:411:HOH:O	2.19	0.42
1:A:265:ILE:HA	1:A:265:ILE:HD13	1.70	0.42
1:A:141:TYR:CE1	1:A:145:HIS:HE1	2.38	0.42
1:B:161:GLU:N	3:B:521:HOH:O	2.38	0.41
1:B:138:GLY:HA3	1:B:167:LEU:HD22	2.02	0.41
1:B:96:LEU:O	1:B:97:ARG:HG2	2.20	0.41
1:A:176:MET:HG3	1:A:177:ALA:O	2.20	0.41
1:A:297:THR:O	1:A:301:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LYS:HB3	1:B:313:LYS:HE3	1.90	0.41
1:A:175:ILE:CB	1:A:175:ILE:CD1	2.82	0.41
1:B:169:ASP:C	1:B:169:ASP:OD1	2.58	0.41
1:A:79:PHE:CE2	1:A:170:PHE:CD2	3.09	0.40
1:B:141:TYR:O	1:B:142:LEU:C	2.60	0.40
1:B:166:LYS:NZ	3:B:600:HOH:O	2.50	0.40
1:A:39:PHE:CD1	1:A:40:GLY:N	2.88	0.40
1:B:307:LEU:O	1:B:313:LYS:HG3	2.21	0.40
1:B:74:ILE:O	1:B:75:LYS:C	2.59	0.40
1:B:274:VAL:O	1:B:277:LYS:HB2	2.22	0.40
1:B:34:ILE:HD12	2:B:500:STU:C5	2.52	0.40
1:A:85:HIS:CG	1:A:86:PRO:CD	3.05	0.40
1:A:252:GLU:OE1	1:A:279:ARG:NH1	2.53	0.40
1:B:124:GLN:HB2	1:B:127:GLU:HG3	2.04	0.40
1:A:85:HIS:CG	1:A:86:PRO:HD2	2.57	0.40
1:B:139:LEU:HG	1:B:167:LEU:HD21	2.03	0.40
1:B:253:TYR:CD2	1:B:279:ARG:HD2	2.57	0.40
1:B:234:LEU:HD23	1:B:234:LEU:HA	1.92	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	306/309 (99%)	269 (88%)	26 (8%)	11 (4%)	4	5
1	B	306/309 (99%)	266 (87%)	30 (10%)	10 (3%)	5	6
All	All	612/618 (99%)	535 (87%)	56 (9%)	21 (3%)	5	5

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	251	SER
1	B	39	PHE
1	B	64	LYS
1	B	162	PRO
1	B	197	MET
1	B	304	LEU
1	B	314	LYS
1	A	238	ALA
1	A	239	GLN
1	B	50	ASN
1	A	226	PHE
1	B	38	SER
1	A	203	ASP
1	A	303	GLU
1	A	314	LYS
1	A	63	GLY
1	A	163	GLY
1	B	289	VAL
1	B	163	GLY
1	A	162	PRO

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	268/268 (100%)	228 (85%)	40 (15%)	4	6
1	B	268/268 (100%)	224 (84%)	44 (16%)	3	4
All	All	536/536 (100%)	452 (84%)	84 (16%)	3	5

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	21	LYS
1	A	22	ASP

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Mol	Chain	Res	Type
1	A	27	LEU
1	A	31	LEU
1	A	38	SER
1	A	44	PHE
1	A	46	ARG
1	A	64	LYS
1	A	71	GLN
1	A	74	ILE
1	A	80	LEU
1	A	82	LYS
1	A	97	ARG
1	A	103	LEU
1	A	109	LEU
1	A	126	VAL
1	A	165	VAL
1	A	166	LYS
1	A	174	SER
1	A	175	ILE
1	A	195	LEU
1	A	199	GLU
1	A	201	GLN
1	A	227	ASN
1	A	231	MET
1	A	236	HIS
1	A	239	GLN
1	A	267	GLN
1	A	277	LYS
1	A	279	ARG
1	A	281	VAL
1	A	285	ARG
1	A	288	THR
1	A	291	MET
1	A	295	GLN
1	A	304	LEU
1	A	305	ASP
1	A	308	GLN
1	A	310	ARG
1	B	21	LYS
1	B	22	ASP
1	B	25	GLU
1	B	38	SER
1	B	44	PHE

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Mol	Chain	Res	Type
1	B	46	ARG
1	B	54	VAL
1	B	57	LYS
1	B	64	LYS
1	B	66	SER
1	B	68	GLU
1	B	74	ILE
1	B	84	ARG
1	B	109	LEU
1	B	113	SER
1	B	121	LYS
1	B	126	VAL
1	B	144	SER
1	B	152	VAL
1	B	161	GLU
1	B	164	LEU
1	B	167	LEU
1	B	175	ILE
1	B	183	VAL
1	B	195	LEU
1	B	198	ASP
1	B	211	LEU
1	B	231	MET
1	B	232	SER
1	B	235	TYR
1	B	251	SER
1	B	255	ARG
1	B	279	ARG
1	B	281	VAL
1	B	288	THR
1	B	291	MET
1	B	303	GLU
1	B	304	LEU
1	B	305	ASP
1	B	310	ARG
1	B	311	LYS
1	B	312	MET
1	B	313	LYS
1	B	318	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	81	GLN
1	A	85	HIS
1	A	133	HIS
1	A	145	HIS
1	A	146	ASN
1	A	227	ASN
1	A	236	HIS
1	B	85	HIS
1	B	240	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	SEP	A	181	1	8,9,10	1.81	3 (37%)	8,12,14	3.10	3 (37%)
1	SEP	B	181	1	8,9,10	1.75	3 (37%)	8,12,14	3.32	4 (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
1	SEP	A	181	1	-	0/6/8/10	0/0/0/0
1	SEP	B	181	1	-	0/6/8/10	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	SEP	O-C	2.04	1.29	1.19
1	A	181	SEP	P-O2P	2.38	1.63	1.54
1	B	181	SEP	P-O2P	2.43	1.63	1.54
1	B	181	SEP	P-O3P	2.57	1.64	1.54
1	B	181	SEP	P-O1P	2.59	1.59	1.51
1	A	181	SEP	P-O1P	3.67	1.63	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	SEP	O3P-P-OG	-5.88	89.63	106.56
1	B	181	SEP	O2P-P-OG	-5.16	91.72	106.56
1	A	181	SEP	OG-CB-CA	-4.79	104.19	108.27
1	B	181	SEP	OG-CB-CA	-3.30	105.45	108.27
1	A	181	SEP	O3P-P-O1P	3.49	121.82	110.58
1	B	181	SEP	OG-P-O1P	3.66	116.46	107.14
1	B	181	SEP	O3P-P-O2P	5.52	128.38	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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
2	STU	A	400	-	27,42,42	1.64	6 (22%)	23,68,68	1.77	6 (26%)
2	STU	B	500	-	27,42,42	3.21	13 (48%)	23,68,68	3.19	10 (43%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	STU	A	400	-	-	0/4/42/42	0/0/8/8
2	STU	B	500	-	-	0/4/42/42	0/0/8/8

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	STU	C10-C11	-4.79	1.34	1.42
2	B	500	STU	C19-C18	-2.51	1.35	1.41
2	A	400	STU	C6-C19	-2.32	1.39	1.42
2	A	400	STU	C28-N4	2.29	1.53	1.46
2	A	400	STU	C15-C16	2.30	1.42	1.36
2	A	400	STU	C26-C21	2.74	1.55	1.51
2	B	500	STU	C3-C2	2.82	1.45	1.38
2	B	500	STU	C1-C20	2.90	1.47	1.41
2	A	400	STU	C2-C1	2.94	1.43	1.36
2	B	500	STU	C28-N4	3.68	1.57	1.46
2	B	500	STU	C22-C23	3.83	1.56	1.52
2	B	500	STU	C24-C25	4.04	1.58	1.51
2	B	500	STU	C5-C20	4.06	1.48	1.41
2	B	500	STU	C2-C1	4.19	1.46	1.36
2	B	500	STU	C14-C15	4.79	1.50	1.38
2	A	400	STU	C22-C23	4.84	1.57	1.52
2	B	500	STU	C15-C16	5.78	1.49	1.36
2	B	500	STU	C13-C12	5.91	1.53	1.41
2	B	500	STU	C3-C4	6.57	1.51	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	STU	O5-C8-C7	-7.68	115.80	128.62
2	B	500	STU	C1-C20-N3	-7.19	123.53	132.18
2	B	500	STU	C2-C1-C20	-5.16	108.74	119.32
2	B	500	STU	C3-C4-C5	-4.01	113.88	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	STU	C3-C4-C5	-3.47	114.81	120.79
2	A	400	STU	C27-O6-C22	-3.10	108.46	114.39
2	B	500	STU	C24-C23-N4	-2.51	106.48	112.16
2	B	500	STU	C15-C14-C13	-2.39	116.98	120.45
2	B	500	STU	C11-C12-C17	-2.39	103.76	106.37
2	B	500	STU	C16-C17-N2	-2.36	129.33	132.22
2	A	400	STU	C6-C19-C18	-2.17	118.47	121.69
2	A	400	STU	C3-C2-C1	2.64	124.29	120.45
2	A	400	STU	C13-C12-C17	2.82	122.96	119.39
2	B	500	STU	C3-C2-C1	3.58	125.66	120.45
2	A	400	STU	C4-C5-C20	4.03	124.49	119.39
2	B	500	STU	C1-C20-C5	5.46	128.61	120.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	STU	3	0
2	B	500	STU	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	308/309 (99%)	0.00	17 (5%) 29 33	15, 37, 83, 117	0
1	B	308/309 (99%)	0.07	20 (6%) 22 25	16, 37, 84, 113	0
All	All	616/618 (99%)	0.03	37 (6%) 25 29	15, 37, 84, 117	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	TYR	9.2
1	A	63	GLY	8.1
1	B	308	GLN	6.7
1	A	305	ASP	6.2
1	A	309	TYR	5.8
1	A	306	ASN	5.6
1	B	307	LEU	5.4
1	B	38	SER	5.2
1	B	320	ALA	5.1
1	A	64	LYS	5.0
1	A	307	LEU	5.0
1	A	65	GLN	4.6
1	B	306	ASN	4.4
1	B	198	ASP	4.0
1	A	308	GLN	3.9
1	B	64	LYS	3.7
1	B	199	GLU	3.4
1	B	65	GLN	3.3
1	B	305	ASP	3.1
1	B	197	MET	3.1
1	B	40	GLY	2.8
1	B	67	ASN	2.7
1	B	39	PHE	2.6
1	A	303	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	200	GLY	2.5
1	B	235	TYR	2.5
1	A	162	PRO	2.4
1	A	13	PRO	2.4
1	A	37	GLY	2.3
1	B	37	GLY	2.3
1	A	38	SER	2.3
1	B	63	GLY	2.2
1	B	318	GLN	2.2
1	A	302	ARG	2.2
1	A	39	PHE	2.2
1	A	62	SER	2.1
1	A	211	LEU	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
1	SEP	A	181	10/11	0.98	0.09	-	36,37,40,46	0
1	SEP	B	181	10/11	0.96	0.09	-	33,37,41,43	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	STU	B	500	35/35	0.97	0.11	-0.39	18,22,24,29	0
2	STU	A	400	35/35	0.97	0.10	-0.64	27,29,34,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.