Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2020 – 02:49 pm BST

PDB ID	:	1U5Q
Title	:	Crystal Structure of the TAO2 Kinase Domain: Activation and Specifity of a Ste20p MAP3K
Authors	:	Zhou, T.; Raman, M.; Gao, Y.; Earnest, S.; Chen, Z.; Machius, M.; Cobb, M.H.; Goldsmith, E.J.
Deposited on	:	2004-07-28
Resolution	:	2.10 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 following versions of software and data (see references ⓘ) were used in the production of this report:

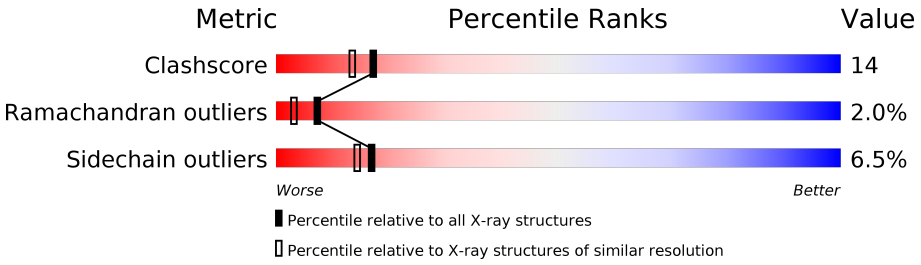
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	348	64% 21% • 11%
1	B	348	66% 21% • 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	B	181	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5416 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 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	CLONING ARTIFACT	UNP Q9JLS3
A	-26	SER	-	CLONING ARTIFACT	UNP Q9JLS3
A	-25	TYR	-	CLONING ARTIFACT	UNP Q9JLS3
A	-24	TYR	-	CLONING ARTIFACT	UNP Q9JLS3
A	-23	HIS	-	EXPRESSION TAG	UNP Q9JLS3
A	-22	HIS	-	EXPRESSION TAG	UNP Q9JLS3
A	-21	HIS	-	EXPRESSION TAG	UNP Q9JLS3
A	-20	HIS	-	EXPRESSION TAG	UNP Q9JLS3
A	-19	HIS	-	EXPRESSION TAG	UNP Q9JLS3
A	-18	HIS	-	EXPRESSION TAG	UNP Q9JLS3
A	-17	ASP	-	CLONING ARTIFACT	UNP Q9JLS3
A	-16	TYR	-	CLONING ARTIFACT	UNP Q9JLS3
A	-15	ASP	-	CLONING ARTIFACT	UNP Q9JLS3
A	-14	ILE	-	CLONING ARTIFACT	UNP Q9JLS3
A	-13	PRO	-	CLONING ARTIFACT	UNP Q9JLS3
A	-12	THR	-	CLONING ARTIFACT	UNP Q9JLS3
A	-11	THR	-	CLONING ARTIFACT	UNP Q9JLS3
A	-10	GLU	-	CLONING ARTIFACT	UNP Q9JLS3
A	-9	ASN	-	CLONING ARTIFACT	UNP Q9JLS3
A	-8	LEU	-	CLONING ARTIFACT	UNP Q9JLS3
A	-7	TYR	-	CLONING ARTIFACT	UNP Q9JLS3
A	-6	PHE	-	CLONING ARTIFACT	UNP Q9JLS3
A	-5	GLN	-	CLONING ARTIFACT	UNP Q9JLS3
A	-4	GLY	-	CLONING ARTIFACT	UNP Q9JLS3
A	-3	ALA	-	CLONING ARTIFACT	UNP Q9JLS3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	CLONING ARTIFACT	UNP Q9JLS3
A	-1	ASP	-	CLONING ARTIFACT	UNP Q9JLS3
A	0	PRO	-	CLONING ARTIFACT	UNP Q9JLS3
A	181	SEP	SER	MODIFIED RESIDUE	UNP Q9JLS3
B	-27	MET	-	CLONING ARTIFACT	UNP Q9JLS3
B	-26	SER	-	CLONING ARTIFACT	UNP Q9JLS3
B	-25	TYR	-	CLONING ARTIFACT	UNP Q9JLS3
B	-24	TYR	-	CLONING ARTIFACT	UNP Q9JLS3
B	-23	HIS	-	EXPRESSION TAG	UNP Q9JLS3
B	-22	HIS	-	EXPRESSION TAG	UNP Q9JLS3
B	-21	HIS	-	EXPRESSION TAG	UNP Q9JLS3
B	-20	HIS	-	EXPRESSION TAG	UNP Q9JLS3
B	-19	HIS	-	EXPRESSION TAG	UNP Q9JLS3
B	-18	HIS	-	EXPRESSION TAG	UNP Q9JLS3
B	-17	ASP	-	CLONING ARTIFACT	UNP Q9JLS3
B	-16	TYR	-	CLONING ARTIFACT	UNP Q9JLS3
B	-15	ASP	-	CLONING ARTIFACT	UNP Q9JLS3
B	-14	ILE	-	CLONING ARTIFACT	UNP Q9JLS3
B	-13	PRO	-	CLONING ARTIFACT	UNP Q9JLS3
B	-12	THR	-	CLONING ARTIFACT	UNP Q9JLS3
B	-11	THR	-	CLONING ARTIFACT	UNP Q9JLS3
B	-10	GLU	-	CLONING ARTIFACT	UNP Q9JLS3
B	-9	ASN	-	CLONING ARTIFACT	UNP Q9JLS3
B	-8	LEU	-	CLONING ARTIFACT	UNP Q9JLS3
B	-7	TYR	-	CLONING ARTIFACT	UNP Q9JLS3
B	-6	PHE	-	CLONING ARTIFACT	UNP Q9JLS3
B	-5	GLN	-	CLONING ARTIFACT	UNP Q9JLS3
B	-4	GLY	-	CLONING ARTIFACT	UNP Q9JLS3
B	-3	ALA	-	CLONING ARTIFACT	UNP Q9JLS3
B	-2	MET	-	CLONING ARTIFACT	UNP Q9JLS3
B	-1	ASP	-	CLONING ARTIFACT	UNP Q9JLS3
B	0	PRO	-	CLONING ARTIFACT	UNP Q9JLS3
B	181	SEP	SER	MODIFIED RESIDUE	UNP Q9JLS3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	197	Total O 197 197	0	0
3	B	237	Total O 237 237	0	0

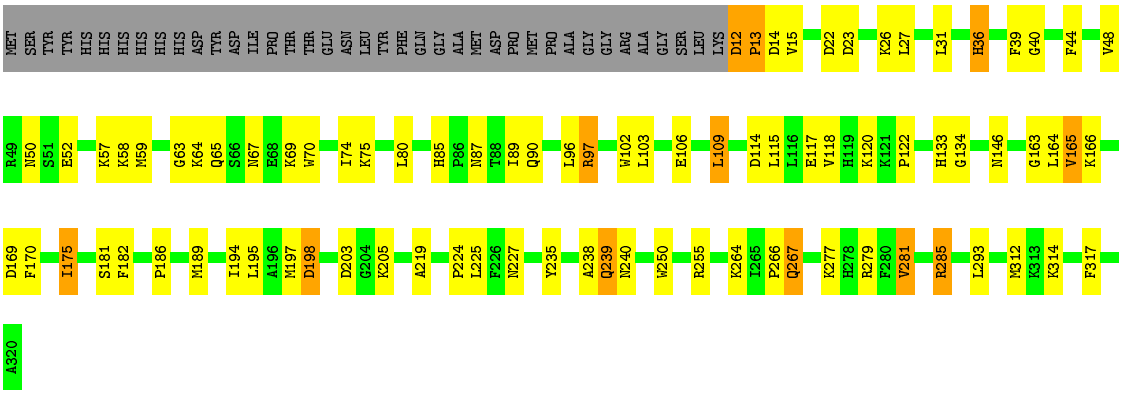
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

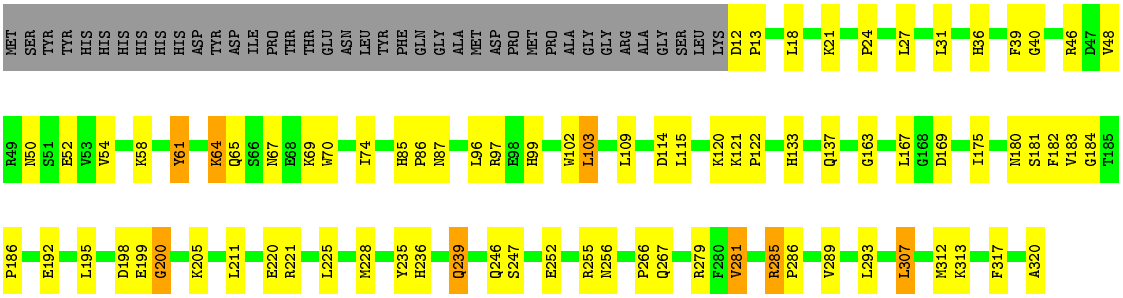
- Molecule 1: serine/threonine protein kinase TAO2

Chain A:



- Molecule 1: serine/threonine protein kinase TAO2

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	186.22Å 186.22Å 94.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.10	Depositor
% Data completeness (in resolution range)	97.3 (50.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5416	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.61	0/2538	0.77	2/3428 (0.1%)
1	B	0.60	0/2538	0.79	1/3428 (0.0%)
All	All	0.61	0/5076	0.78	3/6856 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	ASP	N-CA-C	-5.85	95.20	111.00
1	B	200	GLY	N-CA-C	-5.30	99.86	113.10
1	A	109	LEU	CA-CB-CG	5.23	127.33	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2467	76	1
1	B	2490	0	2467	63	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	197	0	0	9	1
3	B	237	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5416	0	4934	138	2

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 14.

All (138) 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:181:SEP:C	1:A:182:PHE:N	2.10	1.15
1:B:181:SEP:C	1:B:182:PHE:N	2.28	0.97
1:B:46:ARG:HH21	1:B:320:ALA:HB2	1.28	0.97
1:B:85:HIS:HD2	1:B:87:ASN:H	1.28	0.82
1:A:70:TRP:NE1	1:A:74:ILE:HD11	1.94	0.82
1:B:181:SEP:HA	1:B:182:PHE:N	1.97	0.80
1:B:85:HIS:CD2	1:B:87:ASN:H	1.99	0.79
1:A:266:PRO:HB2	1:A:267:GLN:OE1	1.84	0.78
1:A:96:LEU:O	1:A:97:ARG:HD3	1.83	0.78
1:A:85:HIS:HD2	1:A:87:ASN:H	1.31	0.75
1:B:247:SER:O	1:B:255:ARG:NH2	2.20	0.73
1:A:85:HIS:CD2	1:A:87:ASN:H	2.07	0.73
1:B:64:LYS:O	1:B:69:LYS:HE3	1.91	0.71
1:A:114:ASP:HB3	1:A:312:MET:HE3	1.72	0.70
1:B:61:TYR:HA	1:B:69:LYS:HD3	1.75	0.69
1:A:181:SEP:C	1:A:182:PHE:CA	2.71	0.68
1:B:46:ARG:HH21	1:B:320:ALA:CB	2.05	0.68
1:B:50:ASN:OD1	1:B:52:GLU:HB2	1.94	0.68
1:A:114:ASP:HB3	1:A:312:MET:CE	2.23	0.67
1:B:181:SEP:CA	1:B:182:PHE:N	2.58	0.66
1:B:198:ASP:O	1:B:199:GLU:HG3	1.94	0.66
1:A:64:LYS:HG3	1:A:65:GLN:H	1.60	0.65
1:B:235:TYR:CE1	1:B:239:GLN:HG3	2.31	0.65
1:A:134:GLY:HA3	1:A:165:VAL:HG13	1.78	0.64
1:A:267:GLN:H	1:A:267:GLN:CD	2.01	0.64
1:B:46:ARG:NH2	1:B:320:ALA:HB2	2.07	0.62
1:B:181:SEP:O	1:B:182:PHE:N	2.32	0.62
1:A:203:ASP:HB3	1:A:205:LYS:H	1.65	0.61
1:A:165:VAL:HG12	3:A:563:HOH:O	2.00	0.61
1:A:239:GLN:HA	1:A:239:GLN:HE21	1.66	0.60
1:B:52:GLU:HG2	3:B:597:HOH:O	2.00	0.60
1:A:239:GLN:CA	1:A:239:GLN:HE21	2.15	0.60
1:A:27:LEU:O	1:A:48:VAL:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ASP:HB3	1:B:312:MET:CE	2.32	0.59
1:A:267:GLN:N	1:A:267:GLN:OE1	2.35	0.59
1:B:39:PHE:CD1	1:B:40:GLY:N	2.70	0.59
1:A:134:GLY:HA3	1:A:165:VAL:CG1	2.34	0.58
1:B:133:HIS:CE1	1:B:281:VAL:HG13	2.39	0.57
1:B:307:LEU:HD22	1:B:313:LYS:HB3	1.85	0.57
1:B:114:ASP:HB3	1:B:312:MET:HE2	1.84	0.57
1:A:70:TRP:HE1	1:A:74:ILE:HD11	1.70	0.56
1:B:27:LEU:O	1:B:48:VAL:HG22	2.05	0.56
1:A:133:HIS:CD2	1:A:285:ARG:HH22	2.24	0.55
1:A:65:GLN:HA	1:A:65:GLN:OE1	2.07	0.55
1:A:39:PHE:CD1	1:A:40:GLY:N	2.75	0.54
1:B:255:ARG:HD2	3:B:691:HOH:O	2.06	0.54
1:A:181:SEP:CA	1:A:182:PHE:N	2.70	0.54
1:B:70:TRP:CZ2	1:B:74:ILE:HD11	2.43	0.54
1:B:24:PRO:HB2	1:B:102:TRP:CE3	2.43	0.53
1:B:64:LYS:O	1:B:69:LYS:CE	2.55	0.53
1:B:21:LYS:O	1:B:21:LYS:HG2	2.08	0.53
1:A:120:LYS:NZ	3:A:665:HOH:O	2.42	0.53
1:B:181:SEP:C	1:B:183:VAL:HG12	2.39	0.53
1:B:235:TYR:CZ	1:B:239:GLN:HG3	2.44	0.52
1:B:121:LYS:HB3	1:B:122:PRO:HD2	1.90	0.52
1:B:286:PRO:O	1:B:289:VAL:HG23	2.09	0.52
1:A:224:PRO:O	1:A:225:LEU:HB2	2.10	0.52
1:B:61:TYR:HA	1:B:69:LYS:CD	2.39	0.52
1:A:164:LEU:HD23	1:A:166:LYS:HE2	1.92	0.51
1:A:194:ILE:O	1:A:197:MET:HB2	2.10	0.51
1:B:67:ASN:HB3	3:B:631:HOH:O	2.11	0.51
1:B:61:TYR:CE2	1:B:99:HIS:HA	2.45	0.51
1:A:12:ASP:HB2	1:A:15:VAL:HB	1.93	0.51
1:A:118:VAL:HG23	1:A:312:MET:CE	2.41	0.50
1:A:115:LEU:CD1	1:A:293:LEU:HD21	2.41	0.50
1:A:164:LEU:HD12	3:A:563:HOH:O	2.11	0.50
1:A:205:LYS:NZ	3:A:555:HOH:O	2.36	0.50
1:A:277:LYS:HE2	3:A:580:HOH:O	2.12	0.50
1:A:267:GLN:N	1:A:267:GLN:CD	2.66	0.49
1:A:12:ASP:O	1:A:15:VAL:HB	2.12	0.49
1:A:115:LEU:HD13	1:A:293:LEU:HD21	1.93	0.49
1:A:12:ASP:N	1:A:13:PRO:HD3	2.28	0.49
1:A:39:PHE:CD1	1:A:57:LYS:HE3	2.47	0.49
1:A:117:GLU:HG2	3:A:550:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLU:CG	1:B:266:PRO:HG3	2.43	0.48
1:B:205:LYS:NZ	3:B:601:HOH:O	2.43	0.48
1:A:182:PHE:CE1	1:A:189:MET:HE1	2.48	0.47
1:A:189:MET:HE3	1:A:189:MET:HB3	1.66	0.47
1:B:180:ASN:CB	1:B:200:GLY:O	2.62	0.47
1:A:240:ASN:O	1:A:264:LYS:HE2	2.13	0.47
1:A:118:VAL:HG23	1:A:312:MET:HE2	1.97	0.47
1:A:50:ASN:OD1	1:A:52:GLU:HB2	2.15	0.46
1:A:120:LYS:HE3	1:B:52:GLU:HG3	1.96	0.46
1:B:58:LYS:HE2	1:B:102:TRP:CE2	2.50	0.46
1:B:312:MET:HB3	1:B:312:MET:HE3	1.89	0.46
1:B:133:HIS:CD2	1:B:285:ARG:HH22	2.34	0.46
1:B:120:LYS:HD2	1:B:221:ARG:NH2	2.31	0.46
1:B:24:PRO:HD2	1:B:97:ARG:CG	2.45	0.46
1:B:115:LEU:HD13	1:B:293:LEU:HD21	1.96	0.46
1:A:36:HIS:HD1	1:A:36:HIS:C	2.19	0.45
1:A:39:PHE:CG	1:A:57:LYS:HE3	2.50	0.45
1:B:198:ASP:C	1:B:199:GLU:HG3	2.37	0.45
1:A:89:ILE:HG22	1:A:170:PHE:HE1	1.82	0.45
1:A:312:MET:HE2	1:A:312:MET:HB3	1.88	0.45
1:B:133:HIS:O	1:B:137:GLN:HG3	2.17	0.45
1:A:175:ILE:HD12	3:A:688:HOH:O	2.16	0.45
1:A:12:ASP:OD1	1:A:12:ASP:N	2.49	0.45
1:B:220:GLU:OE2	1:B:246:GLN:HG2	2.17	0.44
1:B:85:HIS:HD2	1:B:87:ASN:N	2.06	0.44
1:A:58:LYS:HE2	1:A:102:TRP:CZ2	2.52	0.44
1:B:85:HIS:CD2	1:B:86:PRO:HD2	2.52	0.44
1:B:317:PHE:O	1:B:320:ALA:N	2.41	0.44
1:A:58:LYS:HE2	1:A:102:TRP:CE2	2.53	0.44
1:B:103:LEU:N	1:B:103:LEU:HD23	2.33	0.44
1:B:228:MET:SD	1:B:236:HIS:CD2	3.11	0.44
1:B:64:LYS:O	1:B:65:GLN:HB2	2.17	0.43
1:A:235:TYR:O	1:A:239:GLN:HG2	2.19	0.43
1:A:64:LYS:HE2	1:A:69:LYS:HE3	2.00	0.43
1:A:224:PRO:O	1:A:225:LEU:CB	2.63	0.43
1:A:267:GLN:HB3	3:A:553:HOH:O	2.19	0.43
1:B:183:VAL:HG23	3:B:704:HOH:O	2.18	0.43
1:A:122:PRO:HB3	1:A:219:ALA:O	2.19	0.42
1:B:252:GLU:OE2	1:B:256:ASN:HB2	2.18	0.42
1:A:250:TRP:O	1:A:255:ARG:NH2	2.52	0.42
1:A:238:ALA:O	1:A:264:LYS:NZ	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:CG2	1:A:312:MET:HE2	2.49	0.42
1:A:114:ASP:HB3	1:A:312:MET:HE1	1.99	0.42
1:A:64:LYS:H	1:A:69:LYS:HZ2	1.68	0.42
1:A:75:LYS:HE3	3:A:683:HOH:O	2.20	0.42
1:A:14:ASP:OD1	1:A:74:ILE:HD13	2.20	0.42
1:A:57:LYS:HE2	1:A:59:MET:SD	2.59	0.42
1:B:46:ARG:NH2	1:B:320:ALA:CB	2.76	0.42
1:A:90:GLN:N	1:A:106:GLU:OE1	2.44	0.41
1:A:314:LYS:HA	1:A:317:PHE:CE2	2.55	0.41
1:A:133:HIS:CE1	1:A:281:VAL:HG13	2.55	0.41
1:A:64:LYS:HG2	1:A:69:LYS:NZ	2.36	0.41
1:A:314:LYS:HA	1:A:317:PHE:CD2	2.56	0.41
1:A:23:ASP:HB2	1:A:97:ARG:HH21	1.85	0.41
1:B:225:LEU:HD22	1:B:228:MET:CE	2.50	0.41
1:A:23:ASP:HB3	1:A:26:LYS:CE	2.51	0.41
1:A:194:ILE:O	1:A:197:MET:CB	2.69	0.40
1:B:183:VAL:HG22	1:B:184:GLY:N	2.37	0.40
1:B:36:HIS:O	1:B:39:PHE:CZ	2.74	0.40
1:A:23:ASP:HB3	1:A:26:LYS:HE3	2.02	0.40
1:B:24:PRO:HD2	1:B:97:ARG:HG3	2.02	0.40
1:B:18:LEU:HA	3:B:681:HOH:O	2.20	0.40
1:B:267:GLN:CD	1:B:267:GLN:H	2.23	0.40
1:B:61:TYR:CD2	1:B:61:TYR:N	2.89	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:MET:CE	1:A:197:MET:CE[10_665]	1.80	0.40
3:A:666:HOH:O	3:A:666:HOH:O[7_555]	2.06	0.14

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	305/348 (88%)	288 (94%)	10 (3%)	7 (2%)	6 2
1	B	305/348 (88%)	284 (93%)	16 (5%)	5 (2%)	9 5
All	All	610/696 (88%)	572 (94%)	26 (4%)	12 (2%)	7 3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	B	64	LYS
1	B	163	GLY
1	A	13	PRO
1	A	163	GLY
1	A	169	ASP
1	B	169	ASP
1	A	63	GLY
1	A	186	PRO
1	A	198	ASP
1	B	186	PRO
1	B	13	PRO

5.3.2 Protein sidechains (i)

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	268/300 (89%)	249 (93%)	19 (7%)	14 11
1	B	268/300 (89%)	252 (94%)	16 (6%)	19 16
All	All	536/600 (89%)	501 (94%)	35 (6%)	17 14

All (35) residues with a non-rotameric sidechain are listed below:

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

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Mol	Chain	Res	Type
1	A	31	LEU
1	A	36	HIS
1	A	44	PHE
1	A	80	LEU
1	A	97	ARG
1	A	103	LEU
1	A	109	LEU
1	A	146	ASN
1	A	165	VAL
1	A	175	ILE
1	A	195	LEU
1	A	227	ASN
1	A	239	GLN
1	A	267	GLN
1	A	279	ARG
1	A	281	VAL
1	A	285	ARG
1	B	12	ASP
1	B	31	LEU
1	B	54	VAL
1	B	61	TYR
1	B	96	LEU
1	B	103	LEU
1	B	109	LEU
1	B	167	LEU
1	B	175	ILE
1	B	195	LEU
1	B	211	LEU
1	B	239	GLN
1	B	279	ARG
1	B	281	VAL
1	B	285	ARG
1	B	307	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	81	GLN
1	A	85	HIS
1	A	133	HIS
1	A	137	GLN

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Mol	Chain	Res	Type
1	A	146	ASN
1	A	227	ASN
1	A	239	GLN
1	A	295	GLN
1	A	306	ASN
1	B	65	GLN
1	B	85	HIS
1	B	133	HIS
1	B	137	GLN
1	B	201	GLN
1	B	239	GLN

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	1,2	8,9,10	1.02	0	8,12,14	2.13	3 (37%)
1	SEP	B	181	1,2	8,9,10	1.06	0	8,12,14	2.99	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
1	SEP	A	181	1,2	-	4/5/8/10	-
1	SEP	B	181	1,2	-	2/5/8/10	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	181	SEP	OG-CB-CA	-5.99	102.31	108.14
1	B	181	SEP	O2P-P-OG	-4.35	95.16	106.73
1	A	181	SEP	O3P-P-OG	-4.28	95.36	106.73
1	B	181	SEP	O3P-P-O2P	2.51	117.22	107.64
1	A	181	SEP	O3P-P-O2P	2.43	116.93	107.64
1	A	181	SEP	O2P-P-OG	-2.11	101.13	106.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	181	SEP	N-CA-CB-OG
1	A	181	SEP	CB-OG-P-O1P
1	A	181	SEP	CB-OG-P-O2P
1	A	181	SEP	CB-OG-P-O3P
1	B	181	SEP	N-CA-CB-OG
1	B	181	SEP	CB-OG-P-O2P

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	181	SEP	3	0
1	B	181	SEP	5	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	181:SEP	C	182:PHE	N	2.28
1	A	181:SEP	C	182:PHE	N	2.10

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.