



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 05:36 PM EST

PDB ID : 2I44
Title : Crystal structure of serine-threonine phosphatase 2C from *Toxoplasma gondii*
Authors : Eswaramoorthy, S.; Burley, S.K.; Swamianthan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-08-21
Resolution : 2.04 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) : 1.13
EDS : 2.16
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.16

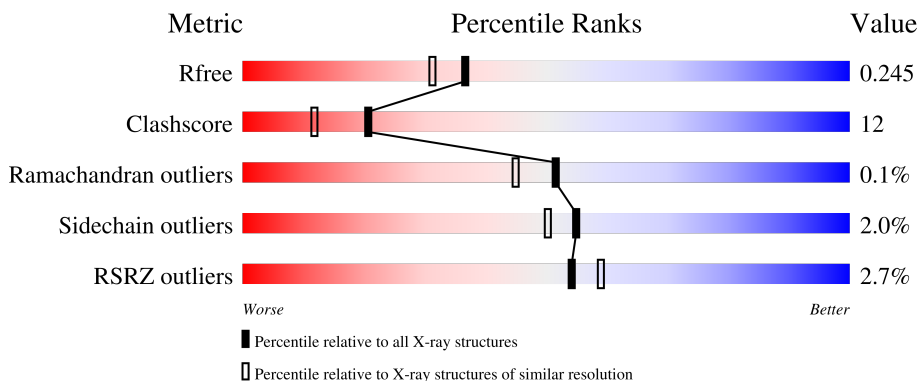
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

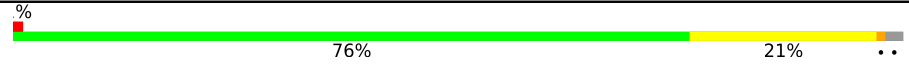
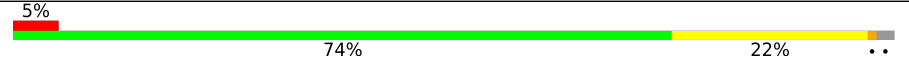

The reported resolution of this entry is 2.04 Å.

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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (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	324	
1	B	324	
1	C	324	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7746 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 phosphatase 2C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	317	2465	1542	433	473	4	13	0	0	0
1	B	316	2457	1538	432	470	4	13	0	0	0
1	C	317	2465	1542	433	473	4	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	SER	-	expression tag	UNP Q8WPN9
A	9	LEU	-	expression tag	UNP Q8WPN9
B	8	SER	-	expression tag	UNP Q8WPN9
B	9	LEU	-	expression tag	UNP Q8WPN9
C	8	SER	-	expression tag	UNP Q8WPN9
C	9	LEU	-	expression tag	UNP Q8WPN9

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	126	Total 126	O 126	0	0

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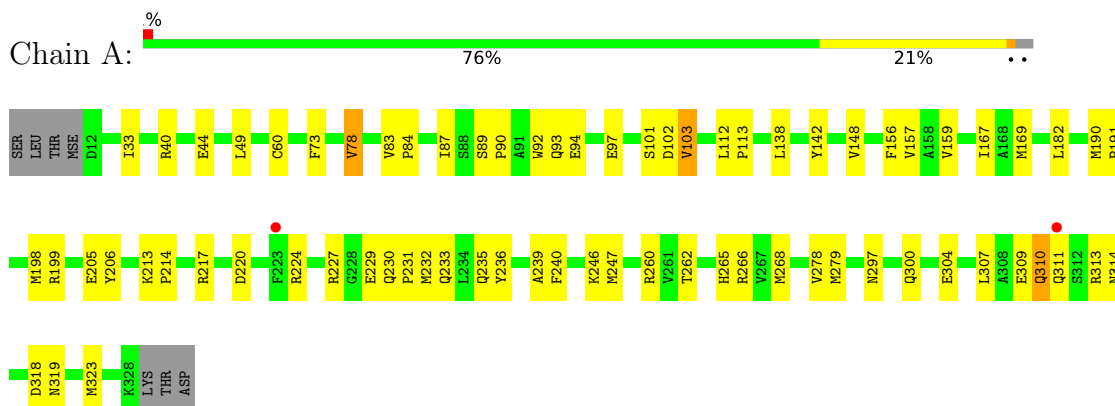
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	91	Total 91	O 91	0	0
3	C	136	Total 136	O 136	0	0

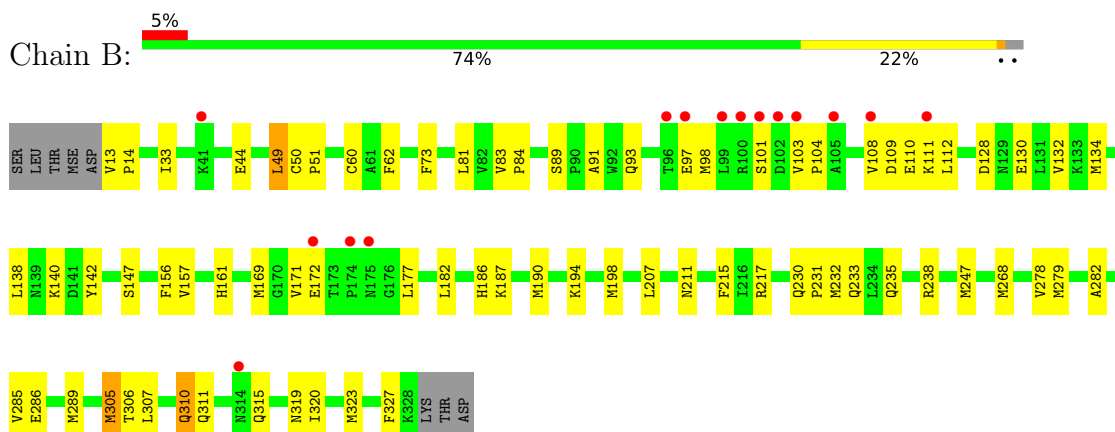
3 Residue-property plots [i](#)

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.

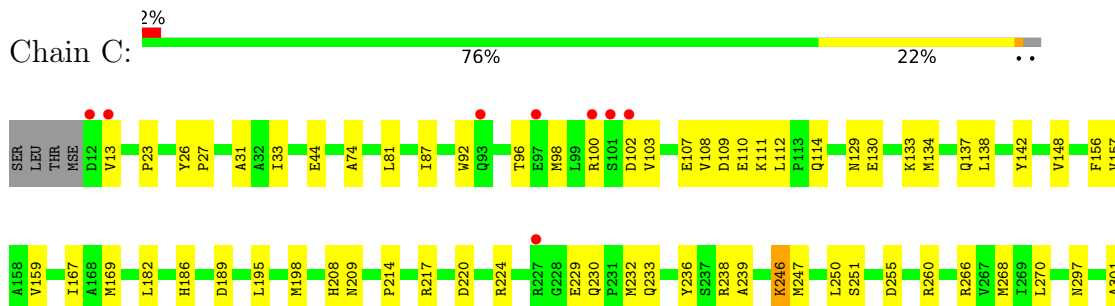
- Molecule 1: Serine-threonine phosphatase 2C



- Molecule 1: Serine-threonine phosphatase 2C



- Molecule 1: Serine-threonine phosphatase 2C





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.40Å 192.96Å 61.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.04 48.24 – 2.04	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.04) 85.9 (48.24-2.04)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.05Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.244 0.219 , 0.245	Depositor DCC
R_{free} test set	2696 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtrriage
Anisotropy	0.126	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7746	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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

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	0.33	0/2504	0.61	0/3374
1	B	0.32	0/2496	0.60	0/3363
1	C	0.34	0/2504	0.61	0/3374
All	All	0.33	0/7504	0.61	0/10111

There are no bond length outliers.

There are no bond angle outliers.

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	2465	0	2407	58	0
1	B	2457	0	2403	64	0
1	C	2465	0	2407	58	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	126	0	0	6	0
3	B	91	0	0	6	0
3	C	136	0	0	4	0
All	All	7746	0	7217	180	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 12.

All (180) 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:B:268:MSE:HE3	1:B:327:PHE:HZ	1.43	0.83
1:B:282:ALA:O	1:B:286:GLU:HG2	1.79	0.81
1:B:169:MSE:HE1	1:B:268:MSE:HE2	1.62	0.81
1:B:93:GLN:O	1:B:97:GLU:HG3	1.79	0.81
1:A:169:MSE:HE2	1:A:182:LEU:HD11	1.65	0.78
1:B:217:ARG:HE	1:B:233:GLN:NE2	1.81	0.78
1:B:310:GLN:HE21	1:B:310:GLN:HA	1.48	0.78
1:A:310:GLN:HA	1:A:310:GLN:HE21	1.50	0.76
1:C:217:ARG:HH21	1:C:233:GLN:HE22	1.32	0.74
1:A:44:GLU:H	1:A:319:ASN:ND2	1.86	0.74
1:C:169:MSE:HE2	1:C:182:LEU:HD11	1.70	0.73
1:A:278:VAL:HG12	1:A:279:MSE:HE2	1.71	0.73
1:A:217:ARG:HH21	1:A:233:GLN:HE22	1.37	0.72
1:B:278:VAL:HG12	1:B:279:MSE:HE2	1.71	0.72
1:A:266:ARG:HD3	3:A:495:HOH:O	1.90	0.72
1:A:157:VAL:HG11	1:A:268:MSE:HE1	1.73	0.71
1:C:310:GLN:HE21	1:C:310:GLN:HA	1.54	0.71
1:B:231:PRO:O	1:B:232:MSE:HE2	1.90	0.71
1:B:305:MSE:HA	1:B:305:MSE:HE3	1.72	0.70
1:C:81:LEU:HD11	1:C:134:MSE:HE1	1.72	0.70
1:C:130:GLU:HG2	1:C:134:MSE:CE	2.22	0.70
1:C:236:TYR:HE1	1:C:239:ALA:HB2	1.58	0.69
1:C:169:MSE:CE	1:C:268:MSE:HE3	2.21	0.69
1:A:190:MSE:HE3	1:A:191:PRO:HD2	1.75	0.68
1:C:169:MSE:HE1	1:C:268:MSE:HE3	1.75	0.68
1:B:230:GLN:O	1:B:232:MSE:HE3	1.93	0.67
1:B:101:SER:OG	1:B:103:VAL:HG23	1.95	0.66
1:C:98:MSE:HE1	1:C:111:LYS:HD3	1.78	0.65
1:A:89:SER:HB2	3:A:467:HOH:O	1.97	0.65
1:C:157:VAL:HG11	1:C:268:MSE:HE1	1.77	0.65
1:B:44:GLU:H	1:B:319:ASN:ND2	1.95	0.65
1:C:156:PHE:CE1	1:C:260:ARG:HG2	2.32	0.64
1:A:198:MSE:HE3	3:A:424:HOH:O	1.98	0.63
1:A:231:PRO:O	1:A:232:MSE:HE2	1.98	0.63
1:A:93:GLN:O	1:A:97:GLU:HG3	1.99	0.63
1:B:83:VAL:HB	1:B:84:PRO:HD3	1.81	0.63
1:C:236:TYR:CE1	1:C:239:ALA:HB2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:MSE:CE	1:B:268:MSE:HE2	2.28	0.62
1:B:157:VAL:HG11	1:B:268:MSE:HE1	1.81	0.62
1:C:198:MSE:HE3	3:C:475:HOH:O	1.99	0.62
1:A:169:MSE:HE1	1:A:268:MSE:HE3	1.81	0.62
1:B:310:GLN:HA	1:B:310:GLN:NE2	2.15	0.61
1:B:103:VAL:HB	3:B:447:HOH:O	2.00	0.61
1:C:138:LEU:N	1:C:138:LEU:HD12	2.16	0.61
1:A:169:MSE:CE	1:A:268:MSE:HE3	2.31	0.61
1:A:159:VAL:HG13	1:A:167:ILE:HD12	1.83	0.61
1:A:33:ILE:HG12	1:A:323:MSE:HG3	1.83	0.60
1:A:44:GLU:H	1:A:319:ASN:HD21	1.50	0.59
1:B:211:ASN:N	1:B:211:ASN:HD22	2.00	0.58
1:B:217:ARG:HH21	1:B:233:GLN:HE22	1.52	0.58
1:A:217:ARG:HH21	1:A:233:GLN:NE2	2.00	0.58
1:C:44:GLU:H	1:C:319:ASN:ND2	2.02	0.58
1:A:40:ARG:NH1	3:A:473:HOH:O	2.37	0.58
1:A:262:THR:H	1:A:265:HIS:CD2	2.22	0.57
1:B:187:LYS:O	1:B:190:MSE:HG3	2.04	0.57
1:B:305:MSE:HA	1:B:305:MSE:CE	2.34	0.57
1:C:156:PHE:HE1	1:C:260:ARG:HG2	1.70	0.56
1:A:156:PHE:CE1	1:A:260:ARG:HG2	2.40	0.56
1:B:247:MSE:SE	1:B:247:MSE:H	2.39	0.56
1:A:262:THR:OG1	1:A:265:HIS:HD2	1.88	0.56
1:B:103:VAL:HG12	1:B:108:VAL:HG23	1.88	0.55
1:B:268:MSE:HE3	1:B:327:PHE:CZ	2.32	0.55
1:B:110:GLU:HB2	3:B:491:HOH:O	2.07	0.55
1:C:189:ASP:HB3	1:C:214:PRO:HG3	1.89	0.54
1:B:98:MSE:HE1	1:B:111:LYS:HD3	1.89	0.54
1:A:217:ARG:HE	1:A:233:GLN:NE2	2.05	0.54
1:C:33:ILE:CD1	1:C:323:MSE:HE2	2.37	0.54
1:A:102:ASP:O	1:A:103:VAL:C	2.47	0.53
1:A:33:ILE:HD13	1:A:323:MSE:HE2	1.90	0.53
1:C:130:GLU:HG2	1:C:134:MSE:HE3	1.89	0.53
1:B:211:ASN:ND2	1:B:211:ASN:N	2.57	0.53
1:A:33:ILE:CD1	1:A:323:MSE:HE2	2.39	0.53
1:A:60:CYS:HB2	3:A:423:HOH:O	2.08	0.53
1:B:171:VAL:O	1:B:177:LEU:HD12	2.09	0.53
1:C:103:VAL:HG12	1:C:107:GLU:HB3	1.90	0.52
1:B:169:MSE:HE1	1:B:268:MSE:CE	2.37	0.52
1:C:224:ARG:O	1:C:229:GLU:HB2	2.10	0.52
1:A:278:VAL:CG1	1:A:279:MSE:HE2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:LEU:HD11	1:B:134:MSE:HE1	1.92	0.52
1:B:73:PHE:CG	1:B:140:LYS:HD3	2.45	0.52
1:C:81:LEU:HD11	1:C:134:MSE:CE	2.40	0.52
1:C:137:GLN:HB3	1:C:138:LEU:HD12	1.92	0.52
1:B:217:ARG:HE	1:B:233:GLN:HE21	1.56	0.52
1:B:171:VAL:HG12	1:B:172:GLU:N	2.25	0.51
1:B:103:VAL:HG13	1:B:104:PRO:HD2	1.93	0.50
1:B:285:VAL:O	1:B:289:MSE:HG2	2.11	0.50
1:C:230:GLN:O	1:C:232:MSE:HE2	2.12	0.50
1:C:112:LEU:HD23	1:C:156:PHE:CD2	2.47	0.50
1:A:40:ARG:HD3	1:A:318:ASP:HA	1.94	0.49
1:A:148:VAL:HG23	1:A:148:VAL:O	2.13	0.49
1:B:307:LEU:O	1:B:311:GLN:HG3	2.13	0.49
1:A:90:PRO:O	1:A:94:GLU:HG3	2.12	0.48
1:C:142:TYR:CG	1:C:232:MSE:HB2	2.49	0.48
1:B:112:LEU:HD23	1:B:156:PHE:CD2	2.48	0.48
1:C:33:ILE:HD13	1:C:323:MSE:HE2	1.95	0.48
1:A:230:GLN:O	1:A:232:MSE:HE3	2.13	0.48
1:A:73:PHE:CE1	1:A:138:LEU:HD12	2.49	0.48
1:C:148:VAL:HG23	1:C:148:VAL:O	2.14	0.47
1:B:130:GLU:HG2	1:B:134:MSE:CE	2.44	0.47
1:B:128:ASP:O	1:B:132:VAL:HG23	2.14	0.47
1:B:81:LEU:HD22	1:B:130:GLU:OE2	2.14	0.47
1:A:199:ARG:NH1	3:A:409:HOH:O	2.48	0.47
1:C:23:PRO:HD3	1:C:297:ASN:ND2	2.30	0.47
1:B:147:SER:O	1:B:161:HIS:HB2	2.15	0.46
1:C:208:HIS:O	1:C:209:ASN:HB2	2.15	0.46
1:B:207:LEU:HG	1:B:215:PHE:CD2	2.50	0.46
1:B:50:CYS:HB3	1:B:62:PHE:HB3	1.98	0.46
1:A:49:LEU:HD23	1:A:49:LEU:C	2.36	0.46
1:A:87:ILE:HA	1:A:92:TRP:CD1	2.50	0.46
1:A:313:ARG:O	1:A:314:ASN:HB2	2.14	0.46
1:C:266:ARG:HD3	3:C:521:HOH:O	2.15	0.46
1:A:78:VAL:HG21	1:A:240:PHE:CG	2.51	0.45
1:C:232:MSE:HE1	3:C:466:HOH:O	2.15	0.45
1:B:157:VAL:HG21	1:B:268:MSE:HE1	1.98	0.45
1:A:102:ASP:O	1:A:103:VAL:O	2.35	0.45
1:A:78:VAL:HG21	1:A:240:PHE:CD2	2.52	0.45
1:A:213:LYS:HB3	1:A:235:GLN:NE2	2.32	0.45
1:A:224:ARG:O	1:A:229:GLU:HB2	2.16	0.45
1:C:108:VAL:O	1:C:112:LEU:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LYS:HB2	1:B:190:MSE:HG3	1.98	0.45
1:B:89:SER:OG	1:B:91:ALA:HB3	2.17	0.45
1:C:230:GLN:HB3	1:C:232:MSE:CE	2.47	0.45
1:B:112:LEU:HD23	1:B:156:PHE:HD2	1.82	0.45
1:B:230:GLN:HB3	1:B:232:MSE:HE3	1.99	0.45
1:C:236:TYR:HE1	1:C:239:ALA:CB	2.29	0.44
1:C:138:LEU:N	1:C:138:LEU:CD1	2.80	0.44
1:A:220:ASP:OD2	1:A:224:ARG:HD2	2.17	0.44
1:C:247:MSE:SE	1:C:247:MSE:H	2.51	0.44
1:B:142:TYR:CG	1:B:232:MSE:HB2	2.51	0.44
1:B:235:GLN:HG2	3:B:490:HOH:O	2.16	0.44
1:C:112:LEU:HD23	1:C:156:PHE:HD2	1.83	0.43
1:C:96:THR:CG2	1:C:100:ARG:NH1	2.81	0.43
1:B:49:LEU:HD23	1:B:51:PRO:HD3	1.99	0.43
1:C:74:ALA:HB3	3:C:424:HOH:O	2.17	0.43
1:A:300:GLN:O	1:A:304:GLU:HG3	2.18	0.43
1:C:13:VAL:HG22	1:C:87:ILE:HD11	2.00	0.43
1:C:159:VAL:HG13	1:C:167:ILE:HD12	2.01	0.43
1:C:246:LYS:HD2	1:C:250:LEU:O	2.18	0.43
1:B:13:VAL:HA	1:B:14:PRO:HD3	1.91	0.43
1:A:217:ARG:HE	1:A:233:GLN:HE21	1.66	0.42
1:A:297:ASN:HB3	1:A:300:GLN:HB3	2.00	0.42
1:B:194:LYS:NZ	1:B:198:MSE:SE	3.02	0.42
1:B:33:ILE:HG12	1:B:323:MSE:HG3	2.00	0.42
1:C:310:GLN:NE2	1:C:310:GLN:HA	2.29	0.42
1:A:142:TYR:CG	1:A:232:MSE:HB2	2.54	0.42
1:A:227:ARG:HG3	1:A:227:ARG:O	2.19	0.42
1:B:13:VAL:HA	3:B:437:HOH:O	2.18	0.42
1:B:169:MSE:HE2	1:B:182:LEU:HD11	2.01	0.42
1:C:301:ALA:O	1:C:305:MSE:HG2	2.20	0.42
1:A:205:GLU:HG3	1:A:217:ARG:CZ	2.49	0.42
1:B:60:CYS:HB2	3:B:452:HOH:O	2.20	0.42
1:B:194:LYS:O	1:B:198:MSE:HG3	2.20	0.42
1:C:318:ASP:O	1:C:320:ILE:HG13	2.20	0.42
1:C:87:ILE:HA	1:C:92:TRP:CD1	2.55	0.42
1:A:83:VAL:HB	1:A:84:PRO:HD3	2.01	0.42
1:B:217:ARG:NE	1:B:233:GLN:NE2	2.61	0.42
1:A:206:TYR:CD1	1:A:214:PRO:HB3	2.55	0.41
1:C:103:VAL:CG1	1:C:107:GLU:HB3	2.50	0.41
1:B:186:HIS:CE1	1:B:238:ARG:HD2	2.55	0.41
1:B:89:SER:CB	3:B:467:HOH:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LEU:HD21	1:C:134:MSE:HE1	2.02	0.41
1:B:194:LYS:HZ1	1:B:198:MSE:SE	2.53	0.41
1:C:130:GLU:HG2	1:C:134:MSE:HE2	2.02	0.41
1:A:89:SER:O	1:A:93:GLN:HG3	2.21	0.41
1:C:114:GLN:HA	1:C:114:GLN:OE1	2.19	0.41
1:A:112:LEU:HB3	1:A:113:PRO:HD3	2.03	0.41
1:A:236:TYR:HE1	1:A:239:ALA:HB2	1.85	0.41
1:C:270:LEU:N	1:C:270:LEU:HD12	2.36	0.41
1:A:307:LEU:O	1:A:311:GLN:HG3	2.21	0.41
1:C:129:ASN:O	1:C:133:LYS:HG3	2.21	0.41
1:C:238:ARG:HG2	1:C:251:SER:HB3	2.02	0.41
1:C:26:TYR:HB3	1:C:27:PRO:HD2	2.03	0.41
1:A:236:TYR:CE1	1:A:239:ALA:HB2	2.56	0.40
1:C:186:HIS:NE2	1:C:255:ASP:OD2	2.51	0.40
1:A:309:GLU:O	1:A:313:ARG:HG3	2.21	0.40
1:B:306:THR:HG21	1:B:320:ILE:HD13	2.02	0.40
1:A:101:SER:OG	1:A:103:VAL:HG23	2.22	0.40
1:B:306:THR:CG2	1:B:320:ILE:HD13	2.52	0.40
1:C:220:ASP:O	1:C:224:ARG:HG3	2.21	0.40
1:C:31:ALA:HA	1:C:324:THR:O	2.22	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	315/324 (97%)	303 (96%)	11 (4%)	1 (0%)	41	31
1	B	314/324 (97%)	305 (97%)	9 (3%)	0	100	100
1	C	315/324 (97%)	306 (97%)	9 (3%)	0	100	100
All	All	944/972 (97%)	914 (97%)	29 (3%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	VAL

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	270/263 (103%)	266 (98%)	4 (2%)	65	63
1	B	269/263 (102%)	263 (98%)	6 (2%)	52	46
1	C	270/263 (103%)	264 (98%)	6 (2%)	52	46
All	All	809/789 (102%)	793 (98%)	16 (2%)	55	50

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	VAL
1	A	246	LYS
1	A	247	MSE
1	A	310	GLN
1	B	49	LEU
1	B	109	ASP
1	B	138	LEU
1	B	305	MSE
1	B	310	GLN
1	B	315	GLN
1	C	102	ASP
1	C	109	ASP
1	C	110	GLU
1	C	195	LEU
1	C	246	LYS
1	C	310	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	212	ASN
1	A	233	GLN
1	A	253	GLN
1	A	265	HIS
1	A	310	GLN
1	A	319	ASN
1	B	139	ASN
1	B	175	ASN
1	B	178	ASN
1	B	211	ASN
1	B	212	ASN
1	B	230	GLN
1	B	233	GLN
1	B	253	GLN
1	B	310	GLN
1	B	314	ASN
1	B	319	ASN
1	C	52	GLN
1	C	175	ASN
1	C	212	ASN
1	C	233	GLN
1	C	253	GLN
1	C	310	GLN
1	C	319	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [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	304/324 (93%)	0.00	2 (0%) 87 89	11, 22, 35, 40	0
1	B	303/324 (93%)	0.14	15 (4%) 28 31	14, 26, 40, 44	0
1	C	304/324 (93%)	0.02	8 (2%) 56 60	12, 21, 36, 44	0
All	All	911/972 (93%)	0.06	25 (2%) 54 59	11, 23, 37, 44	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	ARG	6.6
1	B	101	SER	5.4
1	B	108	VAL	5.4
1	B	102	ASP	4.6
1	B	103	VAL	4.5
1	B	97	GLU	3.8
1	B	175	ASN	3.6
1	C	102	ASP	3.5
1	B	111	LYS	3.2
1	B	174	PRO	3.1
1	C	97	GLU	2.9
1	C	13	VAL	2.8
1	C	100	ARG	2.6
1	B	41	LYS	2.6
1	C	12	ASP	2.5
1	B	314	ASN	2.4
1	A	223	PHE	2.4
1	B	96	THR	2.4
1	A	311	GLN	2.4
1	B	105	ALA	2.3
1	B	99	LEU	2.3
1	B	172	GLU	2.2
1	C	93	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	227	ARG	2.2
1	C	101	SER	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 monosaccharides 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
2	CA	C	406	1/1	0.96	0.09	27,27,27,27	0
2	CA	B	403	1/1	0.97	0.11	28,28,28,28	0
2	CA	B	404	1/1	0.98	0.05	37,37,37,37	0
2	CA	A	402	1/1	0.98	0.06	24,24,24,24	0
2	CA	C	405	1/1	0.98	0.04	26,26,26,26	0
2	CA	A	401	1/1	0.99	0.04	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.