



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:46 PM UTC

PDB ID : 4Q2E / pdb_00004q2e
Title : CRYSTAL STRUCTURE OF AN INTRAMEMBRANE CDP-DAG
SYNTHETASE CENTRAL FOR PHOSPHOLIPID BIOSYNTHESIS
(S200C/S258C, active mutant)
Authors : Liu, X.; Yin, Y.; Wu, J.; Liu, Z.
Deposited on : 2014-04-08
Resolution : 3.40 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
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

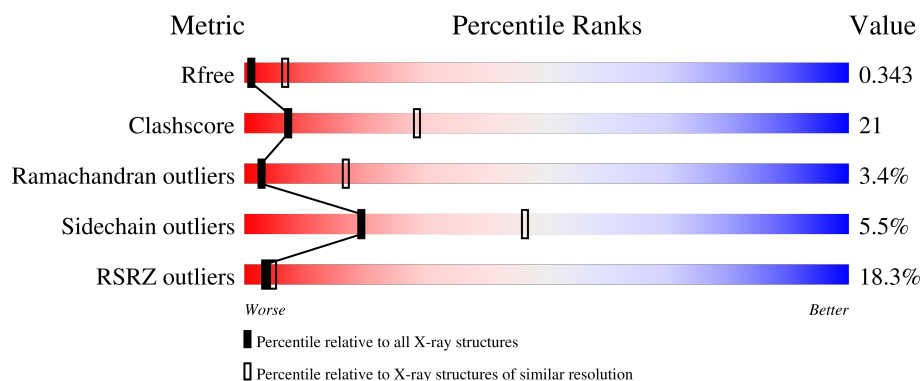
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	290	
1	B	290	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4190 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 Phosphatidate cytidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2069	1392	317	354	6			
1	B	267	Total	C	N	O	S	0	0	0
			2111	1419	326	360	6			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9X1B7
A	2	GLY	-	expression tag	UNP Q9X1B7
A	3	SER	-	expression tag	UNP Q9X1B7
A	4	SER	-	expression tag	UNP Q9X1B7
A	5	HIS	-	expression tag	UNP Q9X1B7
A	6	HIS	-	expression tag	UNP Q9X1B7
A	7	HIS	-	expression tag	UNP Q9X1B7
A	8	HIS	-	expression tag	UNP Q9X1B7
A	9	HIS	-	expression tag	UNP Q9X1B7
A	10	HIS	-	expression tag	UNP Q9X1B7
A	11	SER	-	expression tag	UNP Q9X1B7
A	12	SER	-	expression tag	UNP Q9X1B7
A	13	GLY	-	expression tag	UNP Q9X1B7
A	14	LEU	-	expression tag	UNP Q9X1B7
A	15	VAL	-	expression tag	UNP Q9X1B7
A	16	PRO	-	expression tag	UNP Q9X1B7
A	17	ARG	-	expression tag	UNP Q9X1B7
A	18	GLY	-	expression tag	UNP Q9X1B7
A	19	SER	-	expression tag	UNP Q9X1B7
A	20	HIS	-	expression tag	UNP Q9X1B7
A	220	CYS	SER	engineered mutation	UNP Q9X1B7
A	243	CYS	SER	engineered mutation	UNP Q9X1B7
B	1	MET	-	expression tag	UNP Q9X1B7
B	2	GLY	-	expression tag	UNP Q9X1B7
B	3	SER	-	expression tag	UNP Q9X1B7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	SER	-	expression tag	UNP Q9X1B7
B	5	HIS	-	expression tag	UNP Q9X1B7
B	6	HIS	-	expression tag	UNP Q9X1B7
B	7	HIS	-	expression tag	UNP Q9X1B7
B	8	HIS	-	expression tag	UNP Q9X1B7
B	9	HIS	-	expression tag	UNP Q9X1B7
B	10	HIS	-	expression tag	UNP Q9X1B7
B	11	SER	-	expression tag	UNP Q9X1B7
B	12	SER	-	expression tag	UNP Q9X1B7
B	13	GLY	-	expression tag	UNP Q9X1B7
B	14	LEU	-	expression tag	UNP Q9X1B7
B	15	VAL	-	expression tag	UNP Q9X1B7
B	16	PRO	-	expression tag	UNP Q9X1B7
B	17	ARG	-	expression tag	UNP Q9X1B7
B	18	GLY	-	expression tag	UNP Q9X1B7
B	19	SER	-	expression tag	UNP Q9X1B7
B	20	HIS	-	expression tag	UNP Q9X1B7
B	220	CYS	SER	engineered mutation	UNP Q9X1B7
B	243	CYS	SER	engineered mutation	UNP Q9X1B7

- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Hg 3 3	0	0
2	B	3	Total Hg 3 3	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0

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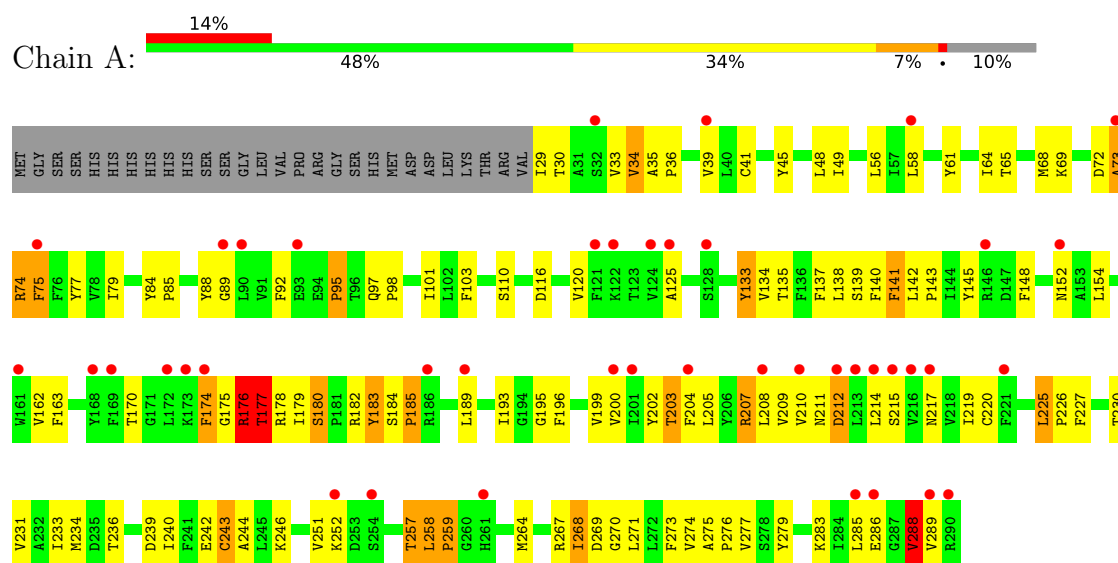
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		

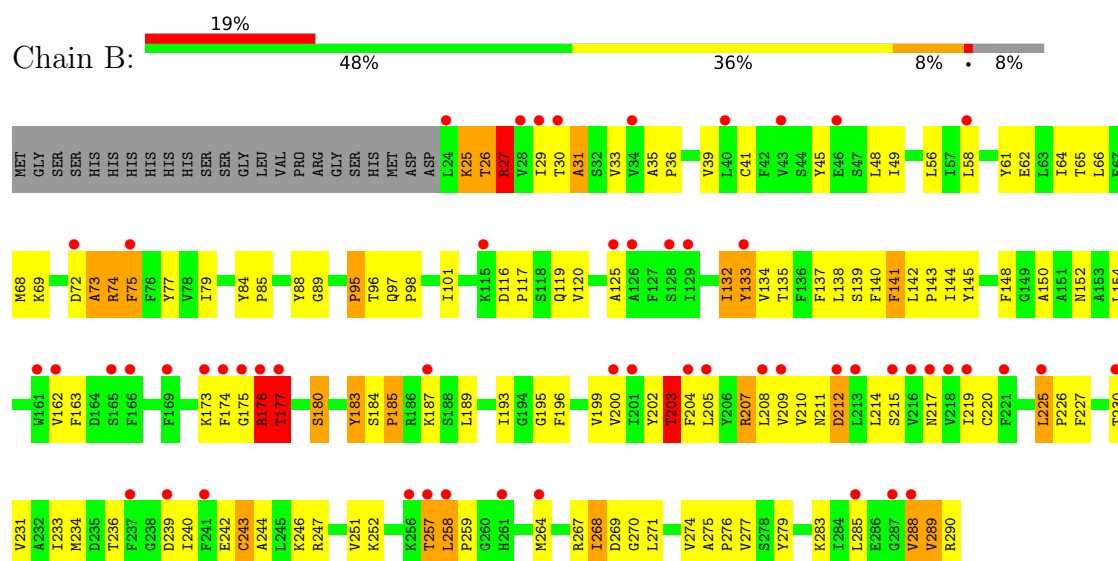
3 Residue-property plots [i](#)

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: Phosphatidate cytidyltransferase



• Molecule 1: Phosphatidate cytidyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	142.08Å 142.08Å 198.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.00 – 3.40 45.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (45.00-3.40) 98.2 (45.00-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.299 , 0.338 0.302 , 0.343	Depositor DCC
R_{free} test set	854 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	112.9	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4190	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: MG, K, HG

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	0.64	0/2123	1.32	27/2888 (0.9%)
1	B	0.62	0/2165	1.29	32/2944 (1.1%)
All	All	0.63	0/4288	1.30	59/5832 (1.0%)

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	PHE	N-CA-C	-11.96	98.23	111.14
1	B	26	THR	N-CA-C	10.83	123.16	111.36
1	A	176	ARG	N-CA-C	9.82	125.98	110.17
1	A	174	PHE	CA-CB-CG	-9.55	104.25	113.80
1	B	289	VAL	N-CA-C	-9.14	94.82	108.17
1	B	204	PHE	N-CA-C	-9.00	101.44	111.07
1	B	258	LEU	N-CA-C	8.53	121.48	110.39
1	B	135	THR	N-CA-C	8.38	120.04	111.07
1	A	176	ARG	CA-C-N	8.30	137.39	121.54
1	A	176	ARG	C-N-CA	8.30	137.39	121.54
1	A	258	LEU	N-CA-C	8.20	121.05	110.39
1	A	34	VAL	N-CA-C	8.11	118.67	110.23
1	A	135	THR	N-CA-C	8.05	119.69	111.07
1	B	176	ARG	CA-C-N	7.94	136.71	121.54
1	B	176	ARG	C-N-CA	7.94	136.71	121.54
1	A	175	GLY	N-CA-C	7.87	125.34	111.73
1	A	204	PHE	CB-CA-C	-7.65	98.81	110.90
1	B	176	ARG	N-CA-C	7.49	121.68	109.85
1	B	75	PHE	N-CA-C	7.01	119.81	111.33
1	B	175	GLY	N-CA-C	6.91	123.35	111.47
1	A	212	ASP	N-CA-C	-6.85	103.89	111.36
1	A	75	PHE	N-CA-C	6.77	119.52	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	ILE	N-CA-C	6.66	120.45	112.80
1	A	268	ILE	N-CA-C	6.61	120.40	112.80
1	A	133	TYR	N-CA-C	6.55	118.08	111.07
1	B	258	LEU	CA-C-N	6.47	127.93	119.84
1	B	258	LEU	C-N-CA	6.47	127.93	119.84
1	B	183	TYR	N-CA-C	6.43	119.98	111.75
1	A	258	LEU	CA-C-N	6.39	127.83	119.84
1	A	258	LEU	C-N-CA	6.39	127.83	119.84
1	B	173	LYS	N-CA-C	6.33	121.09	113.23
1	B	177	THR	N-CA-C	-6.25	97.50	110.80
1	B	204	PHE	CB-CA-C	-6.23	101.10	110.88
1	B	31	ALA	N-CA-C	-6.09	105.34	112.89
1	B	203	THR	N-CA-C	6.08	120.70	113.28
1	B	133	TYR	N-CA-C	6.05	117.54	111.07
1	B	212	ASP	N-CA-C	-5.95	104.38	111.69
1	A	257	THR	N-CA-C	-5.87	106.67	113.88
1	B	132	ILE	N-CA-C	5.85	115.97	110.30
1	B	285	LEU	N-CA-C	5.82	121.29	113.72
1	A	285	LEU	N-CA-C	5.80	121.26	113.72
1	B	204	PHE	CA-CB-CG	5.79	119.58	113.80
1	B	257	THR	N-CA-C	-5.63	106.95	113.88
1	A	141	PHE	N-CA-C	-5.57	105.36	111.82
1	A	180	SER	N-CA-C	5.54	116.67	109.64
1	B	89	GLY	N-CA-C	5.54	119.19	112.49
1	B	141	PHE	N-CA-C	-5.41	105.55	111.82
1	A	89	GLY	N-CA-C	5.41	119.03	112.49
1	A	180	SER	CA-C-N	5.38	126.57	119.84
1	A	180	SER	C-N-CA	5.38	126.57	119.84
1	B	27	ARG	N-CA-C	5.23	117.38	111.11
1	A	177	THR	N-CA-C	-5.21	99.70	110.80
1	B	252	LYS	N-CA-C	-5.21	105.67	112.23
1	B	132	ILE	CB-CA-C	-5.14	105.38	111.81
1	A	252	LYS	N-CA-C	-5.11	105.79	112.23
1	A	183	TYR	N-CA-C	5.06	121.58	110.80
1	A	288	VAL	N-CA-C	5.05	116.13	108.96
1	B	25	LYS	CA-C-N	5.01	127.40	120.29
1	B	25	LYS	C-N-CA	5.01	127.40	120.29

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	2069	0	2137	86	0
1	B	2111	0	2190	94	0
2	A	3	0	0	3	0
2	B	3	0	0	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	4190	0	4327	176	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 (176) 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:183:TYR:HB2	1:B:247:ARG:HG3	1.42	1.00
1:B:288:VAL:HG12	1:B:290:ARG:HD3	1.61	0.81
1:B:64:ILE:HG23	1:B:68:MET:HE3	1.63	0.80
1:B:30:THR:HA	1:B:33:VAL:HG23	1.63	0.79
1:A:64:ILE:HG23	1:A:68:MET:HE3	1.65	0.78
1:B:58:LEU:HD12	1:B:264:MET:HE2	1.66	0.76
1:B:205:LEU:O	1:B:209:VAL:HB	1.86	0.75
1:A:58:LEU:HD12	1:A:264:MET:HE2	1.68	0.74
1:B:58:LEU:HD22	1:B:257:THR:HG21	1.70	0.73
1:A:179:ILE:HD11	1:A:189:LEU:HA	1.72	0.71
1:A:205:LEU:O	1:A:209:VAL:HB	1.89	0.71
1:A:49:ILE:HG12	1:A:142:LEU:HD11	1.72	0.71
1:A:243:CYS:SG	2:A:303:HG:HG	2.08	0.70
1:A:41:CYS:SG	2:A:302:HG:HG	2.09	0.70
1:B:176:ARG:O	1:B:177:THR:HG23	1.92	0.70
1:A:195:GLY:O	1:A:199:VAL:HG23	1.92	0.69
1:B:49:ILE:HG12	1:B:142:LEU:HD11	1.73	0.69
1:B:95:PRO:O	1:B:98:PRO:HD2	1.92	0.68
1:A:196:PHE:O	1:A:200:VAL:HG23	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:CYS:SG	2:A:301:HG:HG	2.12	0.67
1:B:243:CYS:SG	2:B:303:HG:HG	2.12	0.67
1:A:39:VAL:HG13	1:A:154:LEU:HD11	1.76	0.67
1:B:41:CYS:SG	2:B:302:HG:HG	2.13	0.67
1:B:195:GLY:O	1:B:199:VAL:HG23	1.95	0.67
1:A:35:ALA:HB3	1:A:36:PRO:HD3	1.78	0.66
1:B:35:ALA:HB3	1:B:36:PRO:HD3	1.78	0.66
1:B:184:SER:HA	1:B:243:CYS:SG	2.35	0.66
1:B:220:CYS:SG	2:B:301:HG:HG	2.12	0.66
1:B:65:THR:OG1	1:B:74:ARG:HD2	1.95	0.66
1:B:39:VAL:HG13	1:B:154:LEU:HD11	1.78	0.65
1:A:125:ALA:HB1	1:B:125:ALA:HB1	1.79	0.65
1:B:180:SER:HB3	1:B:187:LYS:H	1.63	0.64
1:B:196:PHE:O	1:B:200:VAL:HG23	1.98	0.64
1:A:227:PHE:O	1:A:231:VAL:HG23	1.98	0.64
1:B:227:PHE:O	1:B:231:VAL:HG23	1.99	0.63
1:A:65:THR:OG1	1:A:74:ARG:HD2	1.99	0.63
1:A:95:PRO:O	1:A:98:PRO:HD2	1.99	0.63
1:A:176:ARG:O	1:A:177:THR:HG23	2.00	0.62
1:A:58:LEU:HD22	1:A:257:THR:HG21	1.82	0.61
1:A:189:LEU:O	1:A:193:ILE:HG13	2.01	0.61
1:B:225:LEU:HB2	1:B:226:PRO:HD3	1.83	0.59
1:B:97:GLN:O	1:B:101:ILE:HG13	2.03	0.58
1:B:140:PHE:CD1	1:B:276:PRO:HA	2.38	0.58
1:B:275:ALA:HB3	1:B:276:PRO:HD3	1.85	0.58
1:B:26:THR:O	1:B:29:ILE:HG22	2.04	0.58
1:B:183:TYR:CB	1:B:247:ARG:HG3	2.27	0.58
1:A:140:PHE:CD1	1:A:276:PRO:HA	2.39	0.58
1:A:75:PHE:O	1:A:79:ILE:HG13	2.03	0.57
1:A:288:VAL:HG12	1:A:289:VAL:H	1.70	0.57
1:A:180:SER:HB2	1:A:184:SER:OG	2.04	0.56
1:A:242:GLU:OE1	1:A:269:ASP:HB3	2.04	0.56
1:B:64:ILE:HG23	1:B:68:MET:CE	2.34	0.56
1:A:288:VAL:HG12	1:A:289:VAL:N	2.19	0.56
1:A:97:GLN:O	1:A:101:ILE:HG13	2.06	0.56
1:B:189:LEU:O	1:B:193:ILE:HG13	2.06	0.56
1:A:225:LEU:HB2	1:A:226:PRO:HD3	1.88	0.55
1:B:288:VAL:CG1	1:B:290:ARG:HD3	2.35	0.55
1:B:242:GLU:OE1	1:B:269:ASP:HB3	2.06	0.55
1:B:162:VAL:HG21	1:B:202:TYR:CD1	2.42	0.55
1:B:75:PHE:O	1:B:79:ILE:HG13	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:THR:HA	1:B:33:VAL:CG2	2.34	0.54
1:B:133:TYR:O	1:B:137:PHE:HB2	2.07	0.54
1:A:162:VAL:HG21	1:A:202:TYR:CD1	2.42	0.54
1:B:116:ASP:O	1:B:120:VAL:HG23	2.06	0.54
1:B:68:MET:SD	1:B:73:ALA:HB1	2.48	0.53
1:B:140:PHE:HD1	1:B:276:PRO:HA	1.74	0.53
1:A:84:TYR:HB3	1:A:85:PRO:HD3	1.90	0.52
1:A:97:GLN:HB2	1:A:98:PRO:HD3	1.91	0.52
1:B:69:LYS:HA	1:B:74:ARG:HH11	1.74	0.52
1:A:69:LYS:HA	1:A:74:ARG:HH11	1.75	0.51
1:A:275:ALA:HB3	1:A:276:PRO:HD3	1.93	0.51
1:B:26:THR:HA	1:B:29:ILE:HG22	1.91	0.51
1:A:64:ILE:HG23	1:A:68:MET:CE	2.37	0.51
1:A:143:PRO:HB2	1:A:279:TYR:CE1	2.46	0.51
1:A:140:PHE:HD1	1:A:276:PRO:HA	1.75	0.51
1:B:29:ILE:HG23	1:B:30:THR:HG23	1.92	0.51
1:B:69:LYS:HA	1:B:74:ARG:NH1	2.25	0.51
1:B:210:VAL:O	1:B:214:LEU:O	2.28	0.50
1:A:48:LEU:HD21	1:A:141:PHE:HB3	1.92	0.50
1:A:184:SER:HB2	1:A:185:PRO:HD2	1.94	0.50
1:B:270:GLY:O	1:B:274:VAL:HG23	2.11	0.50
1:B:234:MET:SD	1:B:277:VAL:HG21	2.52	0.50
1:A:68:MET:SD	1:A:73:ALA:HB1	2.51	0.50
1:B:185:PRO:HD3	1:B:243:CYS:SG	2.52	0.49
1:A:69:LYS:HA	1:A:74:ARG:NH1	2.27	0.49
1:B:64:ILE:HD13	1:B:77:TYR:HB2	1.95	0.49
1:B:84:TYR:HB3	1:B:85:PRO:HD3	1.95	0.49
1:A:273:PHE:O	1:A:276:PRO:HD2	2.13	0.49
1:B:56:LEU:HG	1:B:138:LEU:HD23	1.95	0.49
1:B:140:PHE:HD1	1:B:276:PRO:CA	2.26	0.48
1:A:258:LEU:HD13	1:A:267:ARG:NE	2.28	0.48
1:A:56:LEU:CD2	1:A:134:VAL:HG12	2.42	0.48
1:A:33:VAL:O	1:A:36:PRO:HD2	2.14	0.48
1:A:185:PRO:HD3	1:A:243:CYS:SG	2.53	0.48
1:A:116:ASP:O	1:A:120:VAL:HG23	2.13	0.48
1:B:88:TYR:C	1:B:88:TYR:CD1	2.92	0.48
1:A:139:SER:O	1:A:142:LEU:HB2	2.13	0.48
1:B:184:SER:HB2	1:B:185:PRO:HD2	1.94	0.48
1:A:270:GLY:O	1:A:274:VAL:HG23	2.13	0.48
1:A:148:PHE:HZ	1:A:283:LYS:HA	1.79	0.48
1:A:140:PHE:HD1	1:A:276:PRO:CA	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:VAL:O	1:A:214:LEU:O	2.32	0.47
1:B:48:LEU:HD21	1:B:141:PHE:HB3	1.95	0.47
1:B:97:GLN:HB2	1:B:98:PRO:HD3	1.95	0.47
1:A:233:ILE:HG22	1:A:234:MET:HE2	1.96	0.47
1:A:45:TYR:HD1	1:A:145:TYR:CD2	2.33	0.47
1:A:73:ALA:O	1:A:74:ARG:C	2.58	0.47
1:B:45:TYR:HD1	1:B:145:TYR:CD2	2.33	0.47
1:B:268:ILE:O	1:B:271:LEU:HB3	2.15	0.47
1:A:162:VAL:HG21	1:A:202:TYR:CE1	2.50	0.46
1:A:236:THR:O	1:A:240:ILE:HG13	2.16	0.46
1:B:236:THR:O	1:B:240:ILE:HG13	2.14	0.46
1:A:110:SER:OG	1:A:120:VAL:HG13	2.15	0.46
1:A:133:TYR:O	1:A:137:PHE:HB2	2.15	0.46
1:B:73:ALA:O	1:B:74:ARG:C	2.57	0.46
1:B:226:PRO:O	1:B:230:THR:HG23	2.15	0.46
1:A:30:THR:O	1:A:34:VAL:HG23	2.16	0.46
1:B:148:PHE:HZ	1:B:283:LYS:HA	1.80	0.46
1:A:152:ASN:OD1	1:A:219:ILE:HG23	2.15	0.45
1:A:178:ARG:O	1:A:178:ARG:HG3	2.16	0.45
1:B:33:VAL:O	1:B:36:PRO:HD2	2.15	0.45
1:A:61:TYR:CD2	1:A:61:TYR:C	2.94	0.45
1:A:92:PHE:CD2	1:A:98:PRO:HG3	2.51	0.45
1:B:193:ILE:O	1:B:196:PHE:HB3	2.16	0.45
1:B:233:ILE:HG22	1:B:234:MET:HE2	1.99	0.45
1:A:29:ILE:HG22	1:A:29:ILE:O	2.17	0.45
1:A:140:PHE:HD1	1:A:276:PRO:HG3	1.82	0.45
1:A:148:PHE:HE1	1:A:286:GLU:HB2	1.81	0.45
1:A:202:TYR:CD2	1:A:202:TYR:C	2.94	0.45
1:A:88:TYR:CD1	1:A:88:TYR:C	2.93	0.45
1:B:140:PHE:HD1	1:B:276:PRO:HG3	1.82	0.45
1:B:162:VAL:HG21	1:B:202:TYR:CE1	2.52	0.45
1:A:163:PHE:CD2	1:A:195:GLY:HA3	2.52	0.44
1:B:152:ASN:OD1	1:B:219:ILE:HG23	2.17	0.44
1:B:203:THR:O	1:B:207:ARG:CB	2.65	0.44
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.86	0.44
1:A:56:LEU:HG	1:A:138:LEU:HD23	1.99	0.43
1:B:143:PRO:HB2	1:B:279:TYR:CE1	2.53	0.43
1:B:56:LEU:CD2	1:B:134:VAL:HG12	2.49	0.43
1:B:202:TYR:CD2	1:B:202:TYR:C	2.95	0.43
1:A:234:MET:SD	1:A:277:VAL:HG21	2.57	0.43
1:A:183:TYR:CE1	1:A:244:ALA:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ILE:HG12	1:B:279:TYR:HD1	1.84	0.43
1:B:140:PHE:CD1	1:B:276:PRO:HG3	2.54	0.43
1:B:61:TYR:CD2	1:B:61:TYR:C	2.97	0.42
1:B:140:PHE:HD2	1:B:140:PHE:HA	1.68	0.42
1:A:64:ILE:HD13	1:A:77:TYR:HB2	2.01	0.42
1:B:116:ASP:HB3	1:B:119:GLN:HB3	2.01	0.42
1:A:140:PHE:CD1	1:A:276:PRO:HG3	2.54	0.42
1:A:203:THR:O	1:A:207:ARG:CB	2.67	0.42
1:A:103:PHE:CG	1:B:132:ILE:HG21	2.54	0.42
1:A:268:ILE:O	1:A:271:LEU:HB3	2.20	0.42
1:B:26:THR:HA	1:B:29:ILE:CG2	2.49	0.42
1:B:139:SER:O	1:B:142:LEU:HB2	2.18	0.42
1:B:258:LEU:HD13	1:B:267:ARG:NE	2.34	0.42
1:B:140:PHE:O	1:B:144:ILE:HG13	2.20	0.42
1:B:148:PHE:HA	1:B:289:VAL:HG23	2.02	0.42
1:B:58:LEU:HD22	1:B:257:THR:CG2	2.46	0.42
1:B:62:GLU:O	1:B:66:LEU:HG	2.19	0.42
1:B:203:THR:O	1:B:207:ARG:HB3	2.20	0.42
1:B:208:LEU:HD23	1:B:208:LEU:HA	1.84	0.42
1:B:25:LYS:HD2	1:B:25:LYS:HA	1.94	0.41
1:A:226:PRO:O	1:A:230:THR:HG23	2.20	0.41
1:A:163:PHE:CE2	1:A:195:GLY:HA3	2.56	0.41
1:B:58:LEU:HB2	1:B:264:MET:HG2	2.01	0.41
1:B:183:TYR:HE1	1:B:244:ALA:HB2	1.85	0.41
1:A:242:GLU:O	1:A:246:LYS:N	2.46	0.41
1:B:242:GLU:HG3	1:B:246:LYS:HG3	2.02	0.41
1:A:58:LEU:HB2	1:A:264:MET:HG2	2.02	0.41
1:A:170:THR:O	1:A:174:PHE:HB2	2.21	0.40
1:A:258:LEU:HA	1:A:259:PRO:HD3	1.75	0.40
1:B:163:PHE:CD2	1:B:195:GLY:HA3	2.56	0.40
1:A:140:PHE:HZ	1:B:96:THR:HB	1.87	0.40
1:A:183:TYR:CG	1:B:117:PRO:HB3	2.56	0.40
1:B:27:ARG:O	1:B:31:ALA:HB2	2.22	0.40
1:A:148:PHE:O	1:A:152:ASN:ND2	2.55	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	260/290 (90%)	232 (89%)	19 (7%)	9 (4%)	3	16
1	B	265/290 (91%)	237 (89%)	19 (7%)	9 (3%)	3	17
All	All	525/580 (90%)	469 (89%)	38 (7%)	18 (3%)	3	17

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	THR
1	A	185	PRO
1	B	73	ALA
1	B	177	THR
1	B	185	PRO
1	A	73	ALA
1	A	207	ARG
1	A	72	ASP
1	B	72	ASP
1	B	207	ARG
1	B	259	PRO
1	A	74	ARG
1	A	182	ARG
1	A	259	PRO
1	B	74	ARG
1	B	150	ALA
1	B	95	PRO
1	A	95	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	225/250 (90%)	214 (95%)	11 (5%)	22	49
1	B	230/250 (92%)	216 (94%)	14 (6%)	17	43
All	All	455/500 (91%)	430 (94%)	25 (6%)	19	46

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	ARG
1	A	203	THR
1	A	211	ASN
1	A	212	ASP
1	A	215	SER
1	A	217	ASN
1	A	225	LEU
1	A	239	ASP
1	A	243	CYS
1	A	251	VAL
1	A	288	VAL
1	B	27	ARG
1	B	174	PHE
1	B	176	ARG
1	B	180	SER
1	B	203	THR
1	B	211	ASN
1	B	212	ASP
1	B	215	SER
1	B	217	ASN
1	B	225	LEU
1	B	239	ASP
1	B	243	CYS
1	B	251	VAL
1	B	288	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	211	ASN
1	B	97	GLN

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 10 ligands modelled in this entry, 10 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	262/290 (90%)	0.94	42 (16%) 5 6	61, 111, 157, 174	0
1	B	267/290 (92%)	1.03	55 (20%) 2 4	62, 111, 161, 175	0
All	All	529/580 (91%)	0.98	97 (18%) 3 5	61, 111, 158, 175	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	TYR	10.3
1	A	212	ASP	8.1
1	B	212	ASP	7.0
1	B	201	ILE	6.5
1	B	174	PHE	6.3
1	A	213	LEU	5.9
1	B	187	LYS	5.6
1	B	58	LEU	5.5
1	A	172	LEU	5.5
1	A	174	PHE	5.4
1	B	177	THR	5.3
1	B	264	MET	5.2
1	B	205	LEU	5.1
1	B	258	LEU	5.0
1	B	218	VAL	5.0
1	B	204	PHE	4.8
1	B	221	PHE	4.8
1	B	169	PHE	4.7
1	B	257	THR	4.4
1	A	252	LYS	4.4
1	B	165	SER	4.4
1	A	32	SER	4.3
1	B	217	ASN	4.1
1	A	125	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	285	LEU	4.0
1	B	24	LEU	3.9
1	B	126	ALA	3.9
1	B	241	PHE	3.8
1	A	216	VAL	3.8
1	B	219	ILE	3.7
1	A	210	VAL	3.7
1	B	175	GLY	3.7
1	B	225	LEU	3.6
1	A	73	ALA	3.6
1	A	214	LEU	3.5
1	B	129	ILE	3.5
1	B	28	VAL	3.4
1	A	128	SER	3.4
1	B	75	PHE	3.3
1	A	189	LEU	3.3
1	A	289	VAL	3.3
1	B	213	LEU	3.2
1	A	58	LEU	3.2
1	A	75	PHE	3.1
1	B	128	SER	3.0
1	A	89	GLY	3.0
1	B	161	TRP	3.0
1	A	121	PHE	3.0
1	A	208	LEU	2.9
1	A	161	TRP	2.9
1	B	200	VAL	2.9
1	B	288	VAL	2.9
1	B	166	PHE	2.9
1	A	169	PHE	2.9
1	A	122	LYS	2.9
1	B	209	VAL	2.8
1	B	173	LYS	2.8
1	A	290	ARG	2.8
1	B	40	LEU	2.8
1	B	216	VAL	2.8
1	B	287	GLY	2.8
1	A	186	ARG	2.8
1	A	124	VAL	2.8
1	B	43	VAL	2.7
1	A	90	LEU	2.7
1	B	176	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	93	GLU	2.7
1	B	29	ILE	2.6
1	B	285	LEU	2.6
1	A	286	GLU	2.5
1	B	30	THR	2.5
1	B	208	LEU	2.5
1	A	201	ILE	2.5
1	B	34	VAL	2.4
1	B	72	ASP	2.4
1	A	215	SER	2.4
1	B	230	THR	2.4
1	B	46	GLU	2.3
1	A	173	LYS	2.3
1	B	256	LYS	2.3
1	A	254	SER	2.2
1	A	200	VAL	2.2
1	A	39	VAL	2.2
1	B	115	LYS	2.2
1	A	217	ASN	2.2
1	B	239	ASP	2.2
1	B	261	HIS	2.2
1	B	162	VAL	2.1
1	A	261	HIS	2.1
1	B	215	SER	2.1
1	B	237	PHE	2.1
1	B	125	ALA	2.1
1	A	152	ASN	2.0
1	A	146	ARG	2.0
1	B	133	TYR	2.0
1	A	204	PHE	2.0
1	A	221	PHE	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
3	MG	A	304	1/1	0.62	0.14	101,101,101,101	0
3	MG	B	304	1/1	0.70	0.22	104,104,104,104	0
4	K	B	305	1/1	0.92	0.22	111,111,111,111	0
2	HG	B	301	1/1	0.93	0.19	234,234,234,234	0
4	K	A	305	1/1	0.95	0.07	113,113,113,113	0
2	HG	A	302	1/1	0.96	0.05	180,180,180,180	0
2	HG	A	301	1/1	0.97	0.20	230,230,230,230	0
2	HG	B	303	1/1	0.98	0.03	127,127,127,127	0
2	HG	B	302	1/1	0.99	0.02	169,169,169,169	0
2	HG	A	303	1/1	0.99	0.03	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.