



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:49 am BST

PDB ID : 5Y6L
Title : A subcomplex crystal structure of human cytosolic aspartyl-tRNA synthetase and heterotetrameric glutathione transferase-homology domains in multi-tRNA synthetase complex
Authors : Cho, H.Y.; Lee, H.J.; Kang, B.S.
Deposited on : 2017-08-12
Resolution : 2.90 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	:	2.11
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)	:	2.11

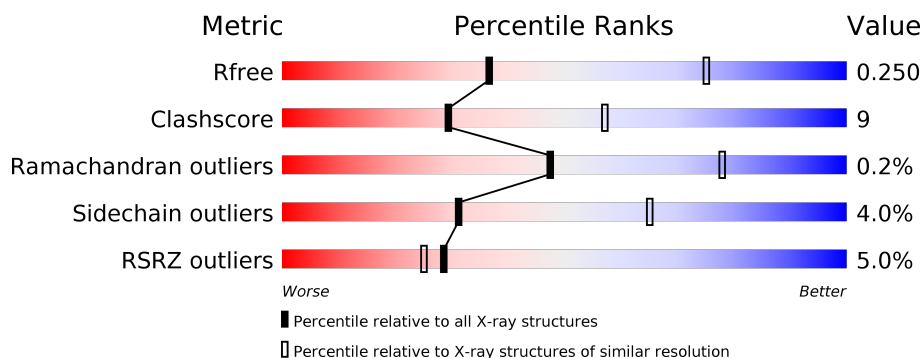
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 $\leq 5\%$. 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	232	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>• 9%</div> </div> </div>
2	B	186	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>• 7%</div> </div> </div>
3	C	175	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</div> </div> </div>
4	D	240	<div> <div>9%</div> <div> <div></div> <div>61%</div> <div>26%</div> <div>• 11%</div> </div> </div>
5	E	521	<div> <div>9%</div> <div> <div></div> <div>89%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6458 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 Methionine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1612	1039	268	299	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ARG	SER	engineered mutation	UNP P56192
A	225	LEU	-	expression tag	UNP P56192
A	226	GLU	-	expression tag	UNP P56192
A	227	HIS	-	expression tag	UNP P56192
A	228	HIS	-	expression tag	UNP P56192
A	229	HIS	-	expression tag	UNP P56192
A	230	HIS	-	expression tag	UNP P56192
A	231	HIS	-	expression tag	UNP P56192
A	232	HIS	-	expression tag	UNP P56192

- Molecule 2 is a protein called Eukaryotic translation elongation factor 1 epsilon-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1374	878	236	259	1			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	initiating methionine	UNP O43324
B	-10	ARG	-	expression tag	UNP O43324
B	-9	GLY	-	expression tag	UNP O43324
B	-8	SER	-	expression tag	UNP O43324
B	-7	HIS	-	expression tag	UNP O43324
B	-6	HIS	-	expression tag	UNP O43324
B	-5	HIS	-	expression tag	UNP O43324

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP O43324
B	-3	HIS	-	expression tag	UNP O43324
B	-2	HIS	-	expression tag	UNP O43324
B	-1	GLY	-	expression tag	UNP O43324
B	0	SER	-	expression tag	UNP O43324
B	147	SER	CYS	engineered mutation	UNP O43324

- Molecule 3 is a protein called Bifunctional glutamate/proline--tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	170	Total	C	N	O	S	0	0	0
			1299	826	220	252	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	92	SER	CYS	engineered mutation	UNP P07814
C	105	SER	CYS	engineered mutation	UNP P07814
C	123	SER	CYS	engineered mutation	UNP P07814

- Molecule 4 is a protein called Aminoacyl tRNA synthase complex-interacting multifunctional protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	213	Total	C	N	O	S	0	0	0
			1620	1042	277	292	9			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	89	MET	-	initiating methionine	UNP Q13155
D	321	LEU	-	expression tag	UNP Q13155
D	322	GLU	-	expression tag	UNP Q13155
D	323	HIS	-	expression tag	UNP Q13155
D	324	HIS	-	expression tag	UNP Q13155
D	325	HIS	-	expression tag	UNP Q13155
D	326	HIS	-	expression tag	UNP Q13155
D	327	HIS	-	expression tag	UNP Q13155
D	328	HIS	-	expression tag	UNP Q13155

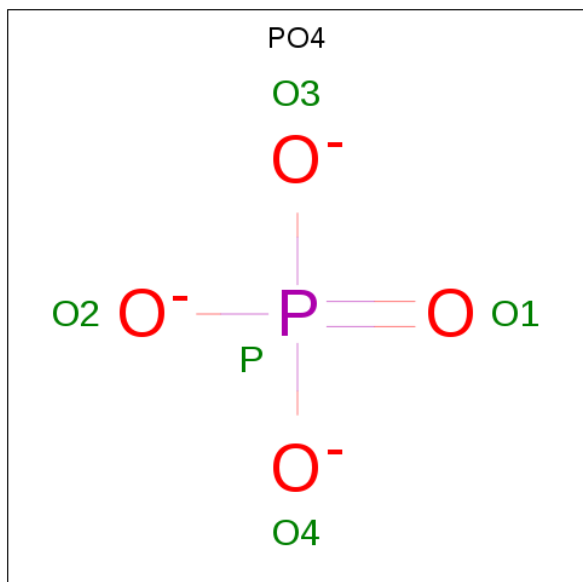
- Molecule 5 is a protein called Aspartate-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	58	Total	C	N	O	S	0	0	0
			465	300	72	90	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	MET	-	initiating methionine	UNP P14868
E	-18	GLY	-	expression tag	UNP P14868
E	-17	SER	-	expression tag	UNP P14868
E	-16	SER	-	expression tag	UNP P14868
E	-15	HIS	-	expression tag	UNP P14868
E	-14	HIS	-	expression tag	UNP P14868
E	-13	HIS	-	expression tag	UNP P14868
E	-12	HIS	-	expression tag	UNP P14868
E	-11	HIS	-	expression tag	UNP P14868
E	-10	HIS	-	expression tag	UNP P14868
E	-9	SER	-	expression tag	UNP P14868
E	-8	SER	-	expression tag	UNP P14868
E	-7	GLY	-	expression tag	UNP P14868
E	-6	LEU	-	expression tag	UNP P14868
E	-5	VAL	-	expression tag	UNP P14868
E	-4	PRO	-	expression tag	UNP P14868
E	-3	ARG	-	expression tag	UNP P14868
E	-2	GLY	-	expression tag	UNP P14868
E	-1	SER	-	expression tag	UNP P14868
E	0	HIS	-	expression tag	UNP P14868

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

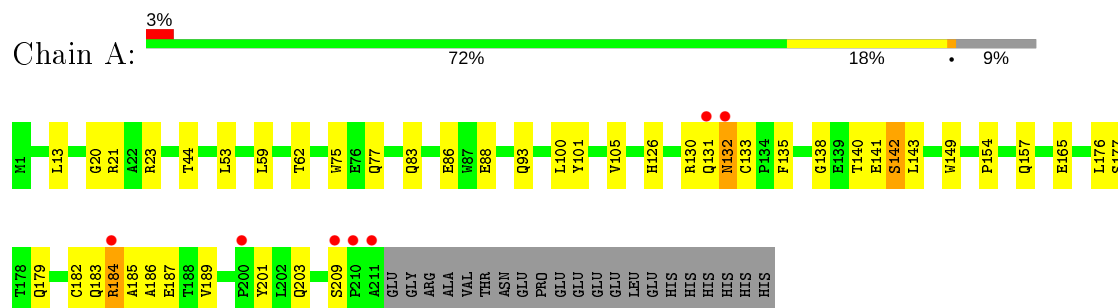
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	12	Total	O	0	0
			12	12		
7	B	30	Total	O	0	0
			30	30		
7	C	10	Total	O	0	0
			10	10		
7	D	16	Total	O	0	0
			16	16		
7	E	10	Total	O	0	0
			10	10		

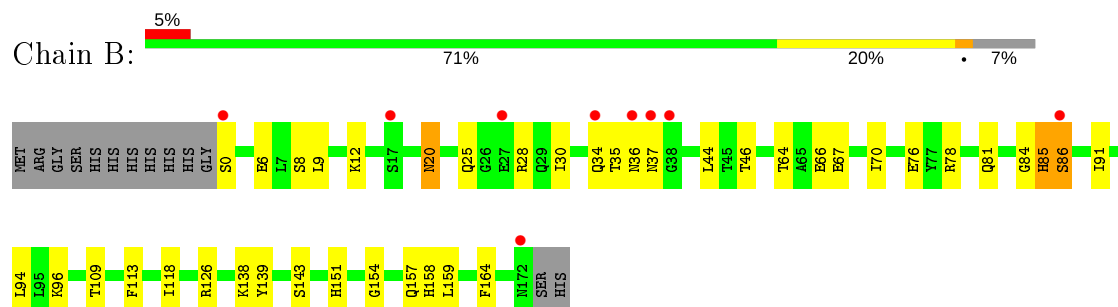
3 Residue-property plots [i](#)

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 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.

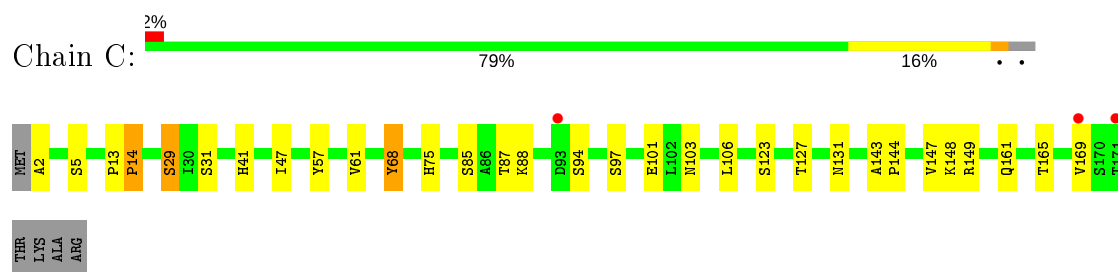
- Molecule 1: Methionine-tRNA ligase, cytoplasmic



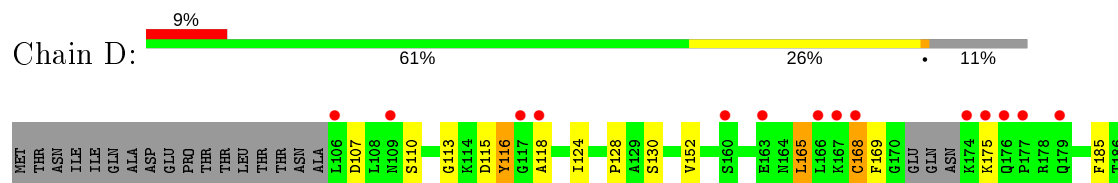
- Molecule 2: Eukaryotic translation elongation factor 1 epsilon-1



- Molecule 3: Bifunctional glutamate/proline--tRNA ligase



- Molecule 4: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.53Å 98.41Å 125.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.90 29.87 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.87-2.90) 99.7 (29.87-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.176 , 0.252 0.178 , 0.250	Depositor DCC
R_{free} test set	1962 reflections (8.23%)	wwPDB-VP
Wilson B-factor (Å ²)	67.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6458	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.55	0/1654	0.63	0/2268
2	B	0.60	0/1402	0.62	0/1904
3	C	0.54	0/1326	0.65	0/1809
4	D	0.53	0/1655	0.63	0/2252
5	E	0.55	0/474	0.61	0/638
All	All	0.55	0/6511	0.63	0/8871

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	SER	Peptide

5.2 Too-close contacts [i](#)

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	1612	0	1576	25	0
2	B	1374	0	1362	36	0
3	C	1299	0	1266	17	0
4	D	1620	0	1608	43	0
5	E	465	0	455	6	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	12	0	0	1	0
7	B	30	0	0	0	0
7	C	10	0	0	1	0
7	D	16	0	0	0	0
7	E	10	0	0	0	0
All	All	6458	0	6267	120	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 9.

All (120) 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)
4:D:285:LEU:O	4:D:288:ILE:HG13	1.13	1.30
4:D:285:LEU:O	4:D:288:ILE:CG1	1.95	1.13
4:D:288:ILE:HD12	4:D:289:GLY:N	1.81	0.96
2:B:70:ILE:HD11	2:B:109:THR:HA	1.49	0.95
4:D:280:VAL:O	4:D:284:VAL:HG23	1.69	0.91
4:D:198:LYS:HE2	5:E:382:GLU:O	1.81	0.80
4:D:295:VAL:HG23	4:D:300:GLN:HE21	1.49	0.77
2:B:64:THR:HG23	2:B:67:GLU:H	1.49	0.77
4:D:190:LYS:HG2	4:D:192:VAL:HG13	1.69	0.74
4:D:200:SER:HB3	4:D:204:MET:HG3	1.68	0.74
2:B:84:GLY:C	2:B:85:HIS:ND1	2.42	0.72
4:D:116:TYR:HB3	4:D:118:ALA:H	1.55	0.71
2:B:158:HIS:CD2	2:B:158:HIS:H	2.08	0.71
4:D:107:ASP:O	4:D:110:SER:OG	2.09	0.70
4:D:288:ILE:HD12	4:D:288:ILE:C	2.15	0.67
1:A:88:GLU:OE1	1:A:93:GLN:HG2	1.94	0.66
3:C:123:SER:O	3:C:127:THR:HG23	1.97	0.65
3:C:2:ALA:HA	3:C:29:SER:HB3	1.78	0.65
4:D:293:VAL:HG12	4:D:294:THR:H	1.61	0.65
1:A:53:LEU:HD13	2:B:66:GLU:HG2	1.80	0.64
2:B:9:LEU:HD21	2:B:158:HIS:NE2	2.13	0.63
2:B:64:THR:CG2	2:B:67:GLU:HB2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:115:ASP:O	4:D:116:TYR:HB2	1.98	0.63
1:A:133:CYS:HB3	1:A:138:GLY:HA2	1.81	0.63
4:D:274:LEU:CD1	4:D:278:ASP:HB2	2.29	0.62
3:C:87:THR:OG1	3:C:88:LYS:N	2.32	0.61
2:B:64:THR:HG23	2:B:67:GLU:HB2	1.82	0.60
5:E:356:ARG:NH1	5:E:362:MET:O	2.34	0.60
1:A:83:GLN:HA	2:B:46:THR:HG21	1.83	0.59
2:B:154:GLY:O	2:B:157:GLN:NE2	2.36	0.59
4:D:201:ILE:HD12	5:E:382:GLU:HG3	1.86	0.58
1:A:100:LEU:HD11	1:A:154:PRO:HB2	1.86	0.58
2:B:9:LEU:HD22	2:B:157:GLN:HG3	1.86	0.58
3:C:161:GLN:O	3:C:165:THR:HG23	2.05	0.57
2:B:9:LEU:HD21	2:B:158:HIS:CD2	2.40	0.57
4:D:244:LEU:HD11	4:D:285:LEU:HD21	1.86	0.56
1:A:86:GLU:OE2	2:B:46:THR:HG23	2.06	0.55
3:C:5:SER:HG	3:C:31:SER:HG	1.53	0.55
2:B:6:GLU:OE2	2:B:78:ARG:NH1	2.33	0.55
4:D:288:ILE:HD12	4:D:289:GLY:CA	2.37	0.54
1:A:101:TYR:O	1:A:105:VAL:HG12	2.08	0.54
4:D:253:ALA:HA	4:D:256:PHE:HD2	1.74	0.53
4:D:250:LYS:HG3	4:D:251:GLU:H	1.73	0.53
3:C:103:ASN:HA	3:C:147:VAL:HG13	1.91	0.52
5:E:350:GLU:O	5:E:354:MET:HG3	2.09	0.52
1:A:135:PHE:HE1	1:A:176:LEU:HD21	1.73	0.52
2:B:84:GLY:O	2:B:85:HIS:ND1	2.42	0.52
1:A:21:ARG:HH11	1:A:21:ARG:HG3	1.73	0.52
4:D:128:PRO:HG3	4:D:189:TRP:HB3	1.90	0.52
1:A:177:SER:O	1:A:183:GLN:HG3	2.11	0.50
4:D:282:TRP:CE3	4:D:312:PHE:HD2	2.30	0.50
1:A:126:HIS:HB3	1:A:130:ARG:NH1	2.26	0.50
2:B:20:ASN:N	2:B:20:ASN:ND2	2.60	0.49
4:D:310:ALA:O	4:D:314:THR:HG23	2.11	0.49
2:B:138:LYS:HD3	2:B:139:TYR:CZ	2.48	0.49
1:A:75:TRP:CH2	1:A:77:GLN:HA	2.47	0.49
2:B:158:HIS:H	2:B:158:HIS:HD2	1.57	0.49
2:B:28:ARG:NH2	2:B:30:ILE:HD11	2.28	0.49
3:C:143:ALA:HB3	3:C:148:LYS:HD2	1.95	0.48
2:B:85:HIS:ND1	2:B:85:HIS:N	2.60	0.48
4:D:238:ASP:O	4:D:242:PHE:HD1	1.95	0.48
4:D:248:SER:HB2	4:D:251:GLU:HG3	1.96	0.47
1:A:59:LEU:HD21	2:B:70:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:PRO:CD	3:C:169:VAL:HG11	2.44	0.47
3:C:14:PRO:HG2	3:C:14:PRO:O	2.15	0.47
4:D:277:ALA:O	4:D:281:LEU:HB2	2.13	0.47
1:A:131:GLN:O	1:A:132:ASN:ND2	2.47	0.47
1:A:131:GLN:NE2	7:A:401:HOH:O	2.41	0.46
1:A:20:GLY:HA2	1:A:23:ARG:HD2	1.96	0.46
3:C:106:LEU:O	3:C:149:ARG:NH2	2.48	0.46
1:A:105:VAL:HG23	1:A:203:GLN:CD	2.36	0.45
4:D:168:CYS:HB3	4:D:318:LEU:HD23	1.98	0.45
1:A:13:LEU:HD21	1:A:186:ALA:HA	1.99	0.45
4:D:124:ILE:HD12	4:D:185:PHE:CZ	2.52	0.45
3:C:97:SER:O	3:C:101:GLU:HG3	2.16	0.45
3:C:144:PRO:HB2	3:C:147:VAL:HG22	1.98	0.45
4:D:236:TRP:CE3	4:D:239:ILE:HD11	2.52	0.45
4:D:187:LEU:HD21	4:D:189:TRP:CZ2	2.53	0.44
2:B:81:GLN:HB3	2:B:94:LEU:HD21	2.00	0.44
2:B:0:SER:HA	2:B:126:ARG:HD2	1.98	0.44
4:D:218:PHE:CG	4:D:276:VAL:HG13	2.52	0.44
1:A:184:ARG:NH1	1:A:187:GLU:HG3	2.33	0.43
4:D:292:SER:O	4:D:293:VAL:HG22	2.18	0.43
1:A:142:SER:HB3	1:A:143:LEU:H	1.72	0.43
3:C:57:TYR:CZ	3:C:61:VAL:HG11	2.54	0.43
3:C:106:LEU:HD12	3:C:147:VAL:HG12	1.99	0.43
2:B:8:SER:O	2:B:12:LYS:HG2	2.19	0.43
2:B:143:SER:HB3	2:B:164:PHE:CD1	2.54	0.43
2:B:159:LEU:HD23	2:B:159:LEU:HA	1.86	0.42
4:D:175:LYS:HB2	4:D:175:LYS:HE3	1.76	0.42
4:D:240:ALA:HB2	4:D:281:LEU:HG	2.01	0.42
4:D:254:ALA:HA	4:D:257:ARG:HD2	2.02	0.42
4:D:255:VAL:O	4:D:259:MET:HG3	2.19	0.42
5:E:340:LEU:HD12	5:E:344:LEU:HB2	2.01	0.42
3:C:68:TYR:CZ	3:C:75:HIS:CE1	3.07	0.42
1:A:149:TRP:CH2	1:A:182:CYS:HB3	2.55	0.42
1:A:185:ALA:O	1:A:189:VAL:HG23	2.19	0.42
1:A:165:GLU:HG2	1:A:165:GLU:H	1.51	0.42
2:B:143:SER:HB3	2:B:164:PHE:CE1	2.55	0.42
3:C:131:ASN:HA	7:C:206:HOH:O	2.20	0.42
1:A:44:THR:HG21	2:B:96:LYS:HE3	2.00	0.42
2:B:20:ASN:N	2:B:20:ASN:HD22	2.17	0.42
2:B:35:THR:HG22	2:B:36:ASN:O	2.19	0.42
2:B:9:LEU:HD23	2:B:9:LEU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:218:PHE:CB	4:D:276:VAL:HG13	2.49	0.42
2:B:91:ILE:H	2:B:91:ILE:HG13	1.64	0.41
4:D:245:LYS:O	4:D:245:LYS:HG2	2.20	0.41
2:B:86:SER:O	2:B:91:ILE:HD11	2.21	0.41
3:C:41:HIS:HA	3:C:47:ILE:HG22	2.02	0.41
2:B:64:THR:HG22	2:B:67:GLU:HB2	1.98	0.41
2:B:44:LEU:HA	2:B:44:LEU:HD12	1.75	0.41
4:D:269:LEU:CD2	4:D:281:LEU:HD12	2.51	0.41
5:E:352:LEU:O	5:E:356:ARG:HG3	2.21	0.41
4:D:299:VAL:O	4:D:303:MET:HG3	2.21	0.41
4:D:169:PHE:CD1	4:D:169:PHE:N	2.89	0.40
1:A:141:GLU:CD	1:A:179:GLN:HE22	2.25	0.40
4:D:288:ILE:CD1	4:D:293:VAL:HG21	2.51	0.40
4:D:152:VAL:HG11	4:D:165:LEU:O	2.20	0.40
2:B:113:PHE:CZ	2:B:118:ILE:HG12	2.57	0.40
4:D:218:PHE:HB2	4:D:276:VAL:CG1	2.52	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	209/232 (90%)	202 (97%)	7 (3%)	0	100	100
2	B	171/186 (92%)	163 (95%)	8 (5%)	0	100	100
3	C	168/175 (96%)	160 (95%)	8 (5%)	0	100	100
4	D	209/240 (87%)	192 (92%)	15 (7%)	2 (1%)	15	45
5	E	56/521 (11%)	56 (100%)	0	0	100	100
All	All	813/1354 (60%)	773 (95%)	38 (5%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	165	LEU
4	D	113	GLY

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	169/197 (86%)	162 (96%)	7 (4%)	30	64
2	B	148/163 (91%)	140 (95%)	8 (5%)	22	54
3	C	141/151 (93%)	136 (96%)	5 (4%)	36	70
4	D	174/211 (82%)	168 (97%)	6 (3%)	37	71
5	E	50/456 (11%)	49 (98%)	1 (2%)	55	82
All	All	682/1178 (58%)	655 (96%)	27 (4%)	31	65

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	THR
1	A	132	ASN
1	A	140	THR
1	A	142	SER
1	A	157	GLN
1	A	184	ARG
1	A	201	TYR
2	B	20	ASN
2	B	25	GLN
2	B	34	GLN
2	B	37	ASN
2	B	76	GLU
2	B	85	HIS
2	B	86	SER
2	B	151	HIS
3	C	14	PRO
3	C	29	SER
3	C	68	TYR

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Mol	Chain	Res	Type
3	C	85	SER
3	C	94	SER
4	D	116	TYR
4	D	130	SER
4	D	168	CYS
4	D	202	GLN
4	D	301	ARG
4	D	305	SER
5	E	341	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	157	GLN
1	A	179	GLN
2	B	20	ASN
2	B	34	GLN
2	B	158	HIS
3	C	75	HIS
3	C	140	GLN
4	D	300	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
6	PO4	B	201	-	4,4,4	0.88	0	6,6,6	0.48	0
6	PO4	A	301	-	4,4,4	0.68	0	6,6,6	0.65	0

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	211/232 (90%)	0.04	7 (3%) 46 41	40, 62, 100, 125	0
2	B	173/186 (93%)	-0.12	9 (5%) 27 23	37, 53, 97, 123	0
3	C	170/175 (97%)	-0.17	3 (1%) 68 67	37, 56, 93, 116	0
4	D	213/240 (88%)	0.33	22 (10%) 6 5	40, 81, 114, 124	0
5	E	58/521 (11%)	-0.15	0 100 100	39, 56, 101, 113	0
All	All	825/1354 (60%)	0.02	41 (4%) 28 25	37, 62, 109, 125	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	171	THR	6.9
2	B	37	ASN	5.5
3	C	169	VAL	5.0
1	A	209	SER	4.2
4	D	321	LEU	3.9
4	D	291	CYS	3.8
4	D	265	LYS	3.5
4	D	175	LYS	3.5
4	D	174	LYS	3.3
4	D	319	LEU	3.3
1	A	210	PRO	3.2
2	B	36	ASN	3.2
4	D	109	ASN	3.2
2	B	172	ASN	3.1
4	D	163	GLU	3.1
4	D	168	CYS	3.1
4	D	118	ALA	3.1
1	A	131	GLN	2.9
4	D	166	LEU	2.9
4	D	167	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	27	GLU	2.9
4	D	177	PRO	2.9
2	B	0	SER	2.7
4	D	179	GLN	2.7
1	A	132	ASN	2.6
4	D	160	SER	2.6
3	C	93	ASP	2.6
4	D	176	GLN	2.5
2	B	17	SER	2.5
4	D	106	LEU	2.4
1	A	184	ARG	2.4
2	B	38	GLY	2.3
4	D	264	GLY	2.3
4	D	289	GLY	2.3
2	B	34	GLN	2.3
4	D	304	ARG	2.2
4	D	117	GLY	2.2
1	A	211	ALA	2.2
2	B	86	SER	2.2
1	A	200	PRO	2.1
4	D	259	MET	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
6	PO4	A	301	5/5	0.93	0.19	73,82,101,106	0
6	PO4	B	201	5/5	0.96	0.15	71,79,93,95	0

6.5 Other polymers

There are no such residues in this entry.