



Full wwPDB X-ray Structure Validation Report i

May 29, 2023 – 05:03 PM JST

PDB ID : 7XPC
Title : Complex structure of D-glycerate-3-kinase(GLYK) and AVRvnt1
Authors : Hu, Q.; Zhou, J.; Yao, D.; Xing, W.
Deposited on : 2022-05-04
Resolution : 3.31 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 i 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](#) i) 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 : 2.33
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) : 2.33

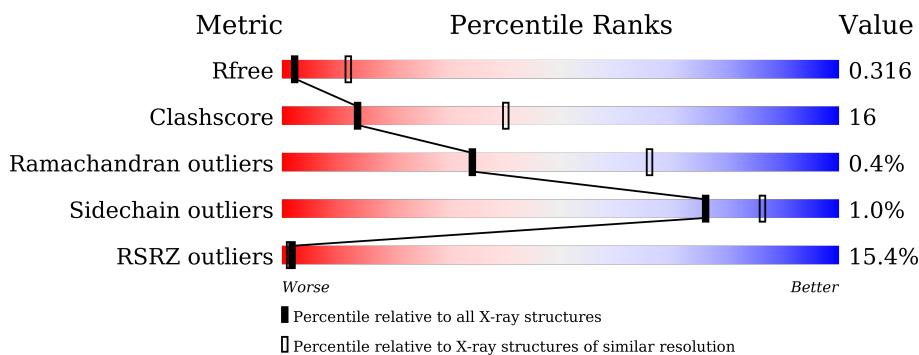
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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.



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6550 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 D-glycerate-3-kinase (GLYK).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	Se	0	0	0
			2701	1742	436	509	5	9			
1	C	337	Total	C	N	O	S	Se	0	0	0
			2701	1742	436	509	5	9			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	MSE	LEU	engineered mutation	UNP A0A3Q7FWS2
A	183	MSE	LEU	engineered mutation	UNP A0A3Q7FWS2
A	238	MSE	VAL	engineered mutation	UNP A0A3Q7FWS2
A	281	MSE	LEU	engineered mutation	UNP A0A3Q7FWS2
A	?	-	ALA	deletion	UNP A0A3Q7FWS2
A	?	-	SER	deletion	UNP A0A3Q7FWS2
A	?	-	ALA	deletion	UNP A0A3Q7FWS2
A	?	-	THR	deletion	UNP A0A3Q7FWS2
A	?	-	PHE	deletion	UNP A0A3Q7FWS2
A	?	-	GLY	deletion	UNP A0A3Q7FWS2
A	?	-	THR	deletion	UNP A0A3Q7FWS2
A	?	-	ALA	deletion	UNP A0A3Q7FWS2
A	?	-	PRO	deletion	UNP A0A3Q7FWS2
A	?	-	ILE	deletion	UNP A0A3Q7FWS2
A	?	-	CYS	deletion	UNP A0A3Q7FWS2
A	?	-	LEU	deletion	UNP A0A3Q7FWS2
A	?	-	THR	deletion	UNP A0A3Q7FWS2
A	?	-	ASN	deletion	UNP A0A3Q7FWS2
A	?	-	ILE	deletion	UNP A0A3Q7FWS2
A	?	-	GLN	deletion	UNP A0A3Q7FWS2
A	?	-	LEU	deletion	UNP A0A3Q7FWS2
A	?	-	HIS	deletion	UNP A0A3Q7FWS2
A	?	-	PRO	deletion	UNP A0A3Q7FWS2
A	357	MSE	LEU	engineered mutation	UNP A0A3Q7FWS2
A	414	MSE	LEU	engineered mutation	UNP A0A3Q7FWS2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	121	MSE	LEU	engineered mutation	UNP A0A3Q7FWS2
C	183	MSE	LEU	engineered mutation	UNP A0A3Q7FWS2
C	238	MSE	VAL	engineered mutation	UNP A0A3Q7FWS2
C	281	MSE	LEU	engineered mutation	UNP A0A3Q7FWS2
C	?	-	ALA	deletion	UNP A0A3Q7FWS2
C	?	-	SER	deletion	UNP A0A3Q7FWS2
C	?	-	ALA	deletion	UNP A0A3Q7FWS2
C	?	-	THR	deletion	UNP A0A3Q7FWS2
C	?	-	PHE	deletion	UNP A0A3Q7FWS2
C	?	-	GLY	deletion	UNP A0A3Q7FWS2
C	?	-	THR	deletion	UNP A0A3Q7FWS2
C	?	-	ALA	deletion	UNP A0A3Q7FWS2
C	?	-	PRO	deletion	UNP A0A3Q7FWS2
C	?	-	ILE	deletion	UNP A0A3Q7FWS2
C	?	-	CYS	deletion	UNP A0A3Q7FWS2
C	?	-	LEU	deletion	UNP A0A3Q7FWS2
C	?	-	THR	deletion	UNP A0A3Q7FWS2
C	?	-	ASN	deletion	UNP A0A3Q7FWS2
C	?	-	ILE	deletion	UNP A0A3Q7FWS2
C	?	-	GLN	deletion	UNP A0A3Q7FWS2
C	?	-	LEU	deletion	UNP A0A3Q7FWS2
C	?	-	HIS	deletion	UNP A0A3Q7FWS2
C	?	-	PRO	deletion	UNP A0A3Q7FWS2
C	357	MSE	LEU	engineered mutation	UNP A0A3Q7FWS2
C	414	MSE	LEU	engineered mutation	UNP A0A3Q7FWS2

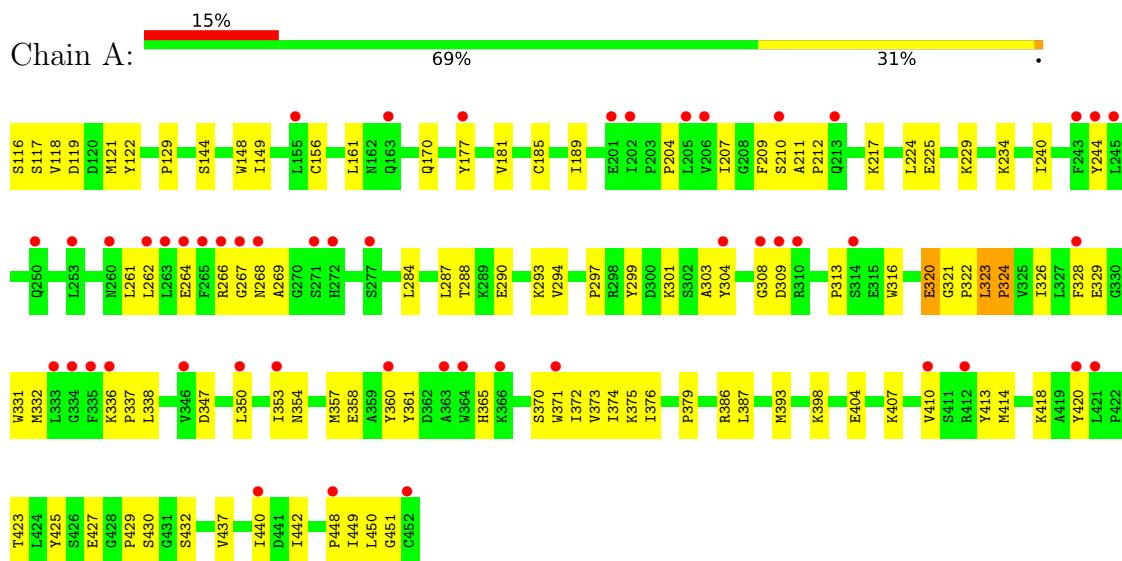
- Molecule 2 is a protein called RxLR effector protein Avr-vnt11.

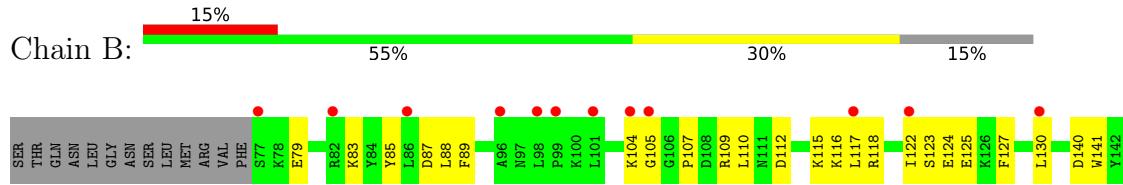
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	71	Total	C	N	O	0	0	0
			574	370	102	102			
2	D	71	Total	C	N	O	0	0	0
			574	370	102	102			

3 Residue-property plots

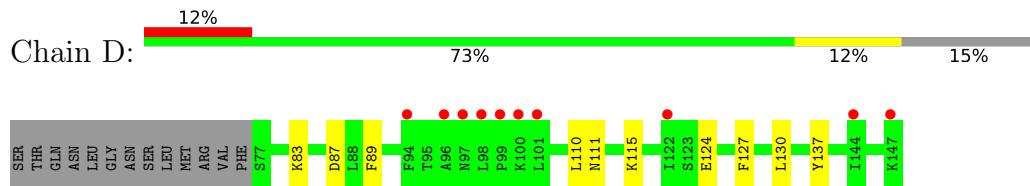
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: D-glycerate-3-kinase (GLYK)





- Molecule 2: RxLR effector protein Avr-vnt11



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	131.28Å 131.28Å 121.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.97 – 3.31 44.68 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.97-3.31) 93.4 (44.68-3.31)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	0.93 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R , R_{free}	0.293 , 0.317 0.290 , 0.316	Depositor DCC
R_{free} test set	1802 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	122.8	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 155.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.219 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6550	wwPDB-VP
Average B, all atoms (Å ²)	185.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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 [\(i\)](#)

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	0.29	0/2765	0.53	0/3734
1	C	0.28	0/2765	0.53	0/3734
2	B	0.30	0/585	0.58	0/779
2	D	0.28	0/585	0.56	0/779
All	All	0.29	0/6700	0.54	0/9026

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 [\(i\)](#)

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	2701	0	2661	108	0
1	C	2701	0	2661	86	0
2	B	574	0	593	19	0
2	D	574	0	593	5	0
All	All	6550	0	6508	209	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 16.

All (209) 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:332:MSE:CE	1:A:357:MSE:CG	2.31	1.07
1:A:204:PRO:HB3	1:A:323:LEU:CD2	1.90	1.01
1:A:393:MSE:HE3	1:A:398:LYS:HB3	1.42	1.01
1:A:332:MSE:HE3	1:A:357:MSE:SE	2.11	0.99
1:A:204:PRO:HB3	1:A:323:LEU:HD21	1.44	0.96
1:A:332:MSE:CE	1:A:357:MSE:HG2	2.02	0.87
1:A:393:MSE:HE2	1:C:398:LYS:NZ	1.92	0.84
1:A:204:PRO:CB	1:A:323:LEU:CD2	2.56	0.84
1:A:393:MSE:HE3	1:A:398:LYS:CB	2.08	0.84
1:A:332:MSE:HE2	1:A:357:MSE:HG2	1.58	0.83
1:A:204:PRO:CG	1:A:323:LEU:CD2	2.60	0.80
1:A:323:LEU:HD23	1:A:323:LEU:O	1.82	0.80
1:A:204:PRO:HG3	1:A:323:LEU:HD23	1.62	0.79
1:A:269:ALA:HB2	1:A:332:MSE:HE1	1.64	0.79
1:C:267:GLY:HA3	1:C:413:TYR:HE1	1.47	0.78
1:A:290:GLU:HA	1:A:321:GLY:HA2	1.66	0.78
1:C:336:LYS:HD3	1:C:430:SER:HB2	1.65	0.78
1:A:204:PRO:HB3	1:A:323:LEU:HD23	1.67	0.77
1:A:204:PRO:CB	1:A:323:LEU:HD21	2.14	0.77
1:A:338:LEU:HD21	1:A:423:THR:HG21	1.67	0.76
1:A:204:PRO:CG	1:A:323:LEU:HD23	2.14	0.76
1:A:404:GLU:OE1	1:A:407:LYS:NZ	2.20	0.75
1:A:393:MSE:CE	1:C:398:LYS:HZ3	2.00	0.74
1:A:332:MSE:CE	1:A:357:MSE:HG3	2.16	0.74
1:A:323:LEU:HD11	1:A:326:ILE:HG12	1.69	0.73
1:A:332:MSE:HE1	1:A:357:MSE:HG3	1.68	0.73
1:C:393:MSE:HB2	1:C:398:LYS:HB3	1.70	0.73
1:A:398:LYS:HE3	1:A:398:LYS:HA	1.70	0.72
1:C:211:ALA:HB3	1:C:217:LYS:HD3	1.69	0.72
1:A:332:MSE:CE	1:A:357:MSE:SE	2.87	0.71
1:A:204:PRO:CB	1:A:323:LEU:HD23	2.21	0.69
1:A:393:MSE:CE	1:A:398:LYS:HB3	2.18	0.69
1:C:375:LYS:HE3	1:C:425:TYR:HB2	1.75	0.69
1:A:332:MSE:HE1	1:A:357:MSE:CG	2.18	0.68
1:A:117:SER:HB2	2:B:105:GLY:HA2	1.76	0.68
1:A:211:ALA:HB3	1:A:217:LYS:HD3	1.76	0.67
1:A:393:MSE:HE2	1:C:398:LYS:HZ1	1.60	0.67
1:A:267:GLY:HA3	1:A:413:TYR:HE1	1.60	0.66
1:A:393:MSE:CE	1:C:398:LYS:NZ	2.57	0.65
1:A:266:ARG:NE	1:A:299:TYR:OH	2.30	0.64
1:C:118:VAL:HG22	1:C:149:ILE:HD13	1.80	0.63
2:B:112:ASP:HA	2:B:115:LYS:HG3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:PRO:HG3	1:A:323:LEU:CD2	2.28	0.62
1:A:332:MSE:HE3	1:A:357:MSE:CG	2.15	0.62
1:C:332:MSE:HE1	1:C:357:MSE:SE	2.51	0.60
1:C:182:PHE:HZ	1:C:231:THR:HG21	1.65	0.60
2:D:110:LEU:HD22	2:D:137:TYR:HB3	1.84	0.60
1:A:374:ILE:HD13	1:A:440:ILE:HB	1.84	0.59
1:A:357:MSE:HE1	1:A:420:TYR:CE1	2.38	0.59
1:C:204:PRO:HG3	1:C:323:LEU:HB3	1.84	0.59
1:C:390:GLU:HG3	1:C:406:VAL:HG21	1.85	0.59
1:A:357:MSE:HA	1:A:360:TYR:CD1	2.38	0.59
1:C:332:MSE:CE	1:C:357:MSE:SE	3.01	0.58
1:C:406:VAL:O	1:C:409:PHE:HB3	2.03	0.58
1:A:414:MSE:HE3	1:A:418:LYS:HE3	1.85	0.58
1:A:207:ILE:HG12	1:A:370:SER:HB2	1.85	0.58
1:C:323:LEU:CD1	1:C:326:ILE:HG13	2.34	0.58
1:A:336:LYS:NZ	1:A:427:GLU:OE1	2.35	0.57
1:A:149:ILE:HG21	2:B:104:LYS:NZ	2.20	0.57
1:A:149:ILE:HG21	2:B:104:LYS:HZ2	1.70	0.57
1:A:284:LEU:HD23	1:A:294:VAL:HG11	1.87	0.56
1:A:288:THR:O	1:A:322:PRO:HB3	2.06	0.56
1:A:429:PRO:HB2	1:A:432:SER:HB3	1.86	0.56
1:C:338:LEU:N	1:C:354:ASN:OD1	2.37	0.56
1:A:337:PRO:HB3	1:A:358:GLU:HG2	1.89	0.55
1:C:323:LEU:HD11	1:C:326:ILE:CG1	2.36	0.55
1:A:313:PRO:HA	1:A:316:TRP:CE2	2.42	0.55
1:C:362:ASP:OD1	1:C:366:LYS:NZ	2.35	0.54
1:A:185:CYS:O	1:A:189:ILE:HG13	2.07	0.54
1:A:376:ILE:HG22	1:A:442:ILE:HD11	1.89	0.54
1:C:162:ASN:H	1:C:166:LEU:HD21	1.73	0.54
1:C:155:LEU:HD11	1:C:227:LEU:HD11	1.89	0.54
2:B:89:PHE:CD1	2:B:110:LEU:HD23	2.42	0.54
2:B:88:LEU:HD11	2:B:109:ARG:HH21	1.72	0.54
1:A:177:TYR:HD1	1:A:448:PRO:HG3	1.73	0.54
1:C:383:TYR:CZ	1:C:387:LEU:HD11	2.43	0.54
1:A:323:LEU:HD11	1:A:326:ILE:CG1	2.37	0.53
1:C:361:TYR:HE1	1:C:430:SER:HB3	1.73	0.53
1:A:393:MSE:HE2	1:C:398:LYS:HZ3	1.59	0.53
1:C:293:LYS:HG2	1:C:320:GLU:CB	2.39	0.53
1:C:267:GLY:HA3	1:C:413:TYR:CE1	2.37	0.53
1:C:375:LYS:HG2	1:C:425:TYR:CD1	2.43	0.53
1:C:242:ASP:HA	1:C:299:TYR:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ASN:O	1:C:164:LEU:N	2.42	0.53
1:C:323:LEU:CD1	1:C:326:ILE:CG1	2.86	0.53
1:C:189:ILE:HG21	1:C:233:ARG:HE	1.73	0.52
1:A:211:ALA:O	1:A:331:TRP:HA	2.10	0.52
1:C:403:ASP:O	1:C:406:VAL:HB	2.09	0.51
1:A:119:ASP:O	1:A:122:TYR:HB3	2.11	0.51
1:A:240:ILE:HG23	1:A:329:GLU:O	2.11	0.51
1:A:350:LEU:O	1:A:354:ASN:N	2.37	0.51
1:A:244:TYR:HB3	1:A:266:ARG:NH1	2.26	0.51
1:C:377:GLN:HB3	1:C:381:TYR:HE2	1.76	0.51
1:A:209:PHE:CE2	1:A:372:ILE:HD12	2.46	0.51
1:A:336:LYS:HG2	1:A:430:SER:HB2	1.93	0.50
1:C:377:GLN:HB3	1:C:381:TYR:CE2	2.46	0.50
2:B:118:ARG:HD3	2:B:127:PHE:HE2	1.76	0.50
1:A:181:VAL:HG12	1:A:224:LEU:HD21	1.93	0.50
2:B:107:PRO:HB3	2:B:141:TRP:CE3	2.46	0.50
1:C:129:PRO:HG2	1:C:448:PRO:HB2	1.94	0.50
1:C:182:PHE:CZ	1:C:231:THR:HG21	2.47	0.50
1:A:379:PRO:HB2	1:A:414:MSE:HE1	1.94	0.49
1:A:287:LEU:O	1:A:322:PRO:HA	2.11	0.49
1:C:211:ALA:CB	1:C:374:ILE:HB	2.43	0.49
1:A:375:LYS:HG2	1:A:425:TYR:CD1	2.48	0.49
1:C:240:ILE:HG23	1:C:329:GLU:O	2.13	0.49
1:C:119:ASP:O	1:C:122:TYR:HB3	2.13	0.49
1:C:390:GLU:HG3	1:C:406:VAL:CG2	2.42	0.49
1:C:323:LEU:HD11	1:C:326:ILE:HG12	1.94	0.48
2:B:83:LYS:O	2:B:87:ASP:HB2	2.13	0.48
1:A:269:ALA:HB2	1:A:357:MSE:HG3	1.94	0.48
1:C:293:LYS:HG2	1:C:320:GLU:HB2	1.94	0.48
2:B:117:LEU:HD22	2:B:122:ILE:HD12	1.96	0.48
1:A:116:SER:HB3	1:A:121:MSE:SE	2.64	0.48
1:C:338:LEU:O	1:C:354:ASN:ND2	2.42	0.48
1:A:234:LYS:O	1:A:324:PRO:HD2	2.14	0.47
1:C:265:PHE:HZ	1:C:412:ARG:HD3	1.79	0.47
1:C:284:LEU:HD23	1:C:294:VAL:HG11	1.95	0.47
1:A:304:TYR:HE2	1:A:309:ASP:HB2	1.79	0.47
1:A:357:MSE:HE1	1:A:420:TYR:CZ	2.50	0.47
1:C:320:GLU:O	1:C:320:GLU:HG3	2.10	0.47
1:C:343:VAL:HG11	1:C:354:ASN:HB2	1.96	0.47
1:A:371:TRP:HB2	1:A:437:VAL:HG22	1.96	0.47
1:C:263:LEU:HD21	1:C:353:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:PHE:CZ	1:C:412:ARG:HD3	2.50	0.46
1:A:177:TYR:CD1	1:A:448:PRO:HG3	2.51	0.46
1:C:376:ILE:HD11	1:C:379:PRO:HA	1.98	0.46
2:D:111:ASN:O	2:D:115:LYS:HG3	2.16	0.46
1:A:240:ILE:HG22	1:A:328:PHE:CZ	2.51	0.46
1:A:297:PRO:HA	1:A:316:TRP:CD2	2.51	0.46
1:A:386:ARG:HD2	1:A:386:ARG:HA	1.76	0.46
1:C:334:GLY:HA2	1:C:429:PRO:HB3	1.99	0.45
1:C:338:LEU:HB2	1:C:343:VAL:CG2	2.46	0.45
1:C:163:GLN:OE1	1:C:175:TYR:OH	2.32	0.45
2:D:83:LYS:NZ	2:D:87:ASP:OD1	2.48	0.45
1:A:261:LEU:HA	1:A:264:GLU:HG3	1.98	0.45
1:A:347:ASP:HB3	1:A:350:LEU:HG	1.98	0.45
1:C:343:VAL:HG21	1:C:354:ASN:CG	2.37	0.45
1:A:303:ALA:HB3	1:A:309:ASP:N	2.32	0.45
1:A:304:TYR:CE2	1:A:309:ASP:HB2	2.52	0.45
1:A:303:ALA:O	1:A:308:GLY:N	2.49	0.44
1:A:410:VAL:O	1:A:414:MSE:HG2	2.17	0.44
1:C:211:ALA:HB2	1:C:374:ILE:HB	1.99	0.44
1:A:144:SER:O	1:A:148:TRP:HD1	2.00	0.44
1:C:161:LEU:HB3	1:C:166:LEU:HD21	1.99	0.44
1:C:262:LEU:HB3	1:C:268:ASN:ND2	2.32	0.44
1:C:350:LEU:HD23	1:C:353:ILE:HD12	1.98	0.44
2:B:85:TYR:CE2	2:B:116:LYS:HD2	2.52	0.44
1:C:338:LEU:HB2	1:C:343:VAL:HG23	2.00	0.44
1:A:129:PRO:HB3	1:A:450:LEU:HA	2.00	0.43
1:C:125:ILE:O	1:C:131:ILE:HG13	2.18	0.43
1:C:129:PRO:CG	1:C:448:PRO:HB2	2.48	0.43
1:C:244:TYR:HB3	1:C:266:ARG:NH1	2.32	0.43
1:C:290:GLU:HA	1:C:321:GLY:HA2	1.99	0.43
1:C:371:TRP:CD2	1:C:429:PRO:HG2	2.53	0.43
1:A:267:GLY:HA3	1:A:413:TYR:CE1	2.45	0.43
1:C:129:PRO:HB3	1:C:450:LEU:HD12	2.00	0.43
1:A:161:LEU:HD22	1:A:170:GLN:NE2	2.33	0.43
1:A:212:PRO:O	1:A:217:LYS:NZ	2.48	0.43
1:C:260:ASN:ND2	1:C:349:GLN:HB3	2.33	0.43
1:C:287:LEU:HB3	1:C:323:LEU:HB2	2.01	0.43
1:A:117:SER:O	1:A:121:MSE:HG2	2.18	0.43
1:A:210:SER:HB3	1:A:373:VAL:HG22	1.99	0.43
1:A:293:LYS:HE2	1:A:320:GLU:HG3	2.00	0.43
1:C:351:GLU:HG2	1:C:355:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:GLU:O	2:B:83:LYS:HB2	2.19	0.43
1:C:262:LEU:O	1:C:268:ASN:ND2	2.49	0.43
1:A:225:GLU:HG2	1:A:229:LYS:HE3	2.00	0.43
2:B:140:ASP:OD1	2:B:143:ARG:NH1	2.49	0.42
1:C:269:ALA:HB2	1:C:357:MSE:SE	2.68	0.42
1:C:323:LEU:HD12	1:C:326:ILE:HD11	2.01	0.42
1:A:393:MSE:CE	1:A:398:LYS:CB	2.88	0.42
1:A:211:ALA:CB	1:A:374:ILE:HB	2.49	0.42
1:A:337:PRO:HG3	1:A:358:GLU:HA	2.00	0.42
1:A:262:LEU:HB3	1:A:268:ASN:ND2	2.34	0.42
1:C:335:PHE:HB3	1:C:357:MSE:HE2	2.01	0.42
2:D:124:GLU:HA	2:D:127:PHE:HB3	2.02	0.42
1:A:387:LEU:HD13	1:C:160:GLN:HG3	2.01	0.42
2:B:107:PRO:HB3	2:B:141:TRP:CD2	2.55	0.42
1:C:209:PHE:HB2	1:C:329:GLU:HA	2.01	0.42
1:C:361:TYR:HE1	1:C:430:SER:CB	2.32	0.42
1:C:323:LEU:HA	1:C:324:PRO:HD3	1.77	0.42
1:A:357:MSE:HA	1:A:360:TYR:HD1	1.85	0.41
1:A:375:LYS:HD2	1:A:375:LYS:HA	1.92	0.41
2:B:124:GLU:CD	2:B:124:GLU:H	2.24	0.41
1:C:391:ILE:O	1:C:392:ALA:C	2.58	0.41
1:A:118:VAL:HG13	1:A:149:ILE:HD11	2.01	0.41
2:B:83:LYS:NZ	2:B:87:ASP:OD2	2.39	0.41
2:B:89:PHE:CZ	2:B:130:LEU:HD22	2.55	0.41
1:C:297:PRO:HA	1:C:316:TRP:CD2	2.55	0.41
1:C:361:TYR:HA	1:C:365:HIS:HD1	1.84	0.41
1:C:414:MSE:HA	1:C:417:TYR:HB2	2.02	0.41
1:A:211:ALA:HB2	1:A:374:ILE:HB	2.02	0.41
1:C:240:ILE:HG22	1:C:328:PHE:CZ	2.55	0.41
1:C:254:ARG:HG3	1:C:264:GLU:HA	2.03	0.41
2:B:104:LYS:HB2	2:B:104:LYS:HE3	1.63	0.41
1:A:156:CYS:O	1:A:161:LEU:N	2.53	0.41
1:A:244:TYR:CD2	1:A:266:ARG:HD3	2.55	0.41
1:A:269:ALA:HB3	1:A:353:ILE:HG23	2.02	0.41
1:A:299:TYR:CE2	1:A:301:LYS:HG2	2.56	0.41
2:B:125:GLU:H	2:B:125:GLU:CD	2.23	0.41
1:C:229:LYS:HA	1:C:233:ARG:O	2.20	0.41
1:C:205:LEU:O	1:C:325:VAL:HA	2.21	0.41
1:C:325:VAL:O	1:C:325:VAL:HG13	2.20	0.41
1:A:129:PRO:HG2	1:A:448:PRO:HB2	2.03	0.40
1:A:332:MSE:O	1:A:332:MSE:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ILE:HG22	1:A:451:GLY:N	2.36	0.40
1:A:361:TYR:O	1:A:365:HIS:HB2	2.22	0.40
2:D:89:PHE:CD2	2:D:130:LEU:HD22	2.57	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	335/337 (99%)	318 (95%)	16 (5%)	1 (0%)	41 71
1	C	335/337 (99%)	321 (96%)	12 (4%)	2 (1%)	25 57
2	B	69/84 (82%)	67 (97%)	2 (3%)	0	100 100
2	D	69/84 (82%)	66 (96%)	3 (4%)	0	100 100
All	All	808/842 (96%)	772 (96%)	33 (4%)	3 (0%)	34 66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	163	GLN
1	C	324	PRO
1	A	324	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	295/286 (103%)	293 (99%)	2 (1%)	84	91
1	C	295/286 (103%)	291 (99%)	4 (1%)	67	82
2	B	55/67 (82%)	54 (98%)	1 (2%)	59	79
2	D	55/67 (82%)	55 (100%)	0	100	100
All	All	700/706 (99%)	693 (99%)	7 (1%)	76	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	GLU
1	A	323	LEU
2	B	123	SER
1	C	320	GLU
1	C	323	LEU
1	C	332	MSE
1	C	393	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	268	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 [\(i\)](#)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	328/337 (97%)	0.96	50 (15%) 2 1	106, 165, 280, 325	0
1	C	328/337 (97%)	0.98	50 (15%) 2 1	109, 184, 277, 322	0
2	B	71/84 (84%)	1.12	13 (18%) 1 1	110, 171, 237, 260	0
2	D	71/84 (84%)	1.15	10 (14%) 2 2	135, 203, 256, 284	0
All	All	798/842 (94%)	1.00	123 (15%) 2 1	106, 177, 273, 325	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	99	PRO	14.3
1	C	268	ASN	11.7
2	D	98	LEU	9.0
1	A	265	PHE	8.0
1	A	335	PHE	7.1
1	C	335	PHE	7.0
2	B	98	LEU	6.6
1	A	420	TYR	6.6
2	B	101	LEU	6.5
2	B	105	GLY	6.5
1	C	334	GLY	6.3
2	D	97	ASN	6.3
2	B	99	PRO	6.2
2	D	101	LEU	6.0
1	A	304	TYR	5.6
1	A	266	ARG	5.3
1	A	268	ASN	5.2
1	C	266	ARG	5.1
1	C	364	TRP	4.9
1	C	270	GLY	4.9
2	D	100	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	163	GLN	4.8
1	A	350	LEU	4.8
1	C	245	LEU	4.8
1	A	360	TYR	4.8
1	C	250	GLN	4.6
1	A	245	LEU	4.5
1	A	364	TRP	4.4
1	C	284	LEU	4.2
1	A	250	GLN	4.2
1	A	260	ASN	4.2
1	C	328	PHE	4.2
1	A	336	LYS	4.1
2	D	147	LYS	4.0
2	D	96	ALA	4.0
2	B	147	LYS	3.9
1	C	243	PHE	3.9
1	A	263	LEU	3.9
1	C	452	CYS	3.8
1	A	267	GLY	3.8
2	B	86	LEU	3.7
1	C	269	ALA	3.7
1	A	243	PHE	3.7
1	A	309	ASP	3.6
1	C	412	ARG	3.5
1	C	263	LEU	3.5
1	C	410	VAL	3.5
1	A	353	ILE	3.5
1	A	328	PHE	3.5
1	C	420	TYR	3.5
1	C	413	TYR	3.5
1	A	366	LYS	3.4
1	A	334	GLY	3.4
1	A	277	SER	3.3
2	D	94	PHE	3.2
1	C	203	PRO	3.1
1	C	267	GLY	3.1
1	A	253	LEU	3.1
1	A	410	VAL	3.1
1	A	244	TYR	3.0
1	A	371	TRP	3.0
1	C	298	ARG	3.0
1	C	233	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	163	GLN	3.0
1	A	202	ILE	3.0
1	A	346	VAL	2.9
2	B	96	ALA	2.8
1	A	210	SER	2.8
1	C	360	TYR	2.8
1	C	241	ASP	2.8
1	A	421	LEU	2.8
1	C	366	LYS	2.8
1	C	319	VAL	2.8
1	C	235	ALA	2.8
1	C	425	TYR	2.8
2	D	144	ILE	2.8
1	C	336	LYS	2.7
1	C	271	SER	2.7
1	A	205	LEU	2.6
1	A	271	SER	2.6
2	B	122	ILE	2.6
1	C	244	TYR	2.6
1	A	314	SER	2.6
1	C	450	LEU	2.6
1	C	197	LYS	2.6
1	A	308	GLY	2.5
1	C	297	PRO	2.5
1	A	177	TYR	2.5
2	B	130	LEU	2.5
1	C	257	ASN	2.5
1	C	309	ASP	2.5
1	A	310	ARG	2.5
1	C	331	TRP	2.4
1	C	275	PRO	2.4
1	A	264	GLU	2.4
1	C	246	THR	2.4
1	A	262	LEU	2.4
1	C	346	VAL	2.3
2	B	77	SER	2.3
1	C	202	ILE	2.3
1	A	201	GLU	2.3
1	C	159	PHE	2.3
2	D	122	ILE	2.3
1	A	363	ALA	2.3
1	C	272	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	452	CYS	2.2
1	A	155	LEU	2.2
1	A	448	PRO	2.2
1	A	272	HIS	2.2
1	A	333	LEU	2.2
1	A	206	VAL	2.1
1	A	440	ILE	2.1
1	C	156	CYS	2.1
1	A	213	GLN	2.1
2	B	82	ARG	2.1
2	B	117	LEU	2.1
1	C	182	PHE	2.1
1	C	130	LEU	2.1
2	B	104	LYS	2.0
1	C	326	ILE	2.0
1	C	160	GLN	2.0
1	A	412	ARG	2.0
1	C	390	GLU	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 [\(i\)](#)

There are no ligands in this entry.

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.