



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:58 PM UTC

PDB ID : 7XPC / pdb_00007xpc
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 ⓘ 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
Mogul : 2022.3.0, CSD as543be (2022)
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

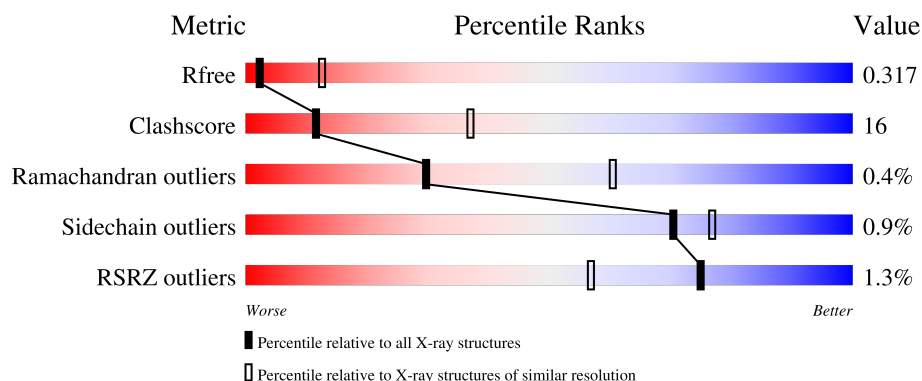
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	337	2% 68% 31% .
1	C	337	% 71% 27% .
2	B	84	56% 29% 15%
2	D	84	73% 12% 15%

2 Entry composition

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

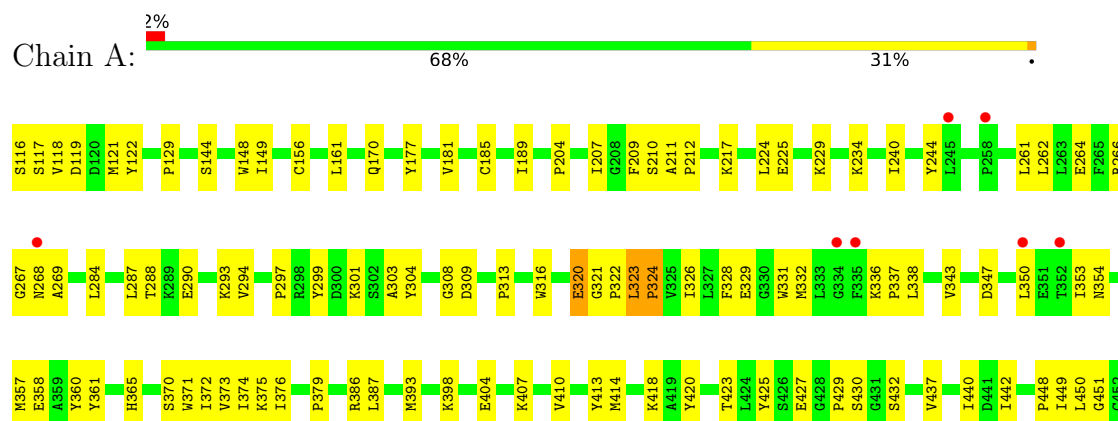
- Molecule 2 is a protein called RxLR effector protein Avr-vnt11.

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			

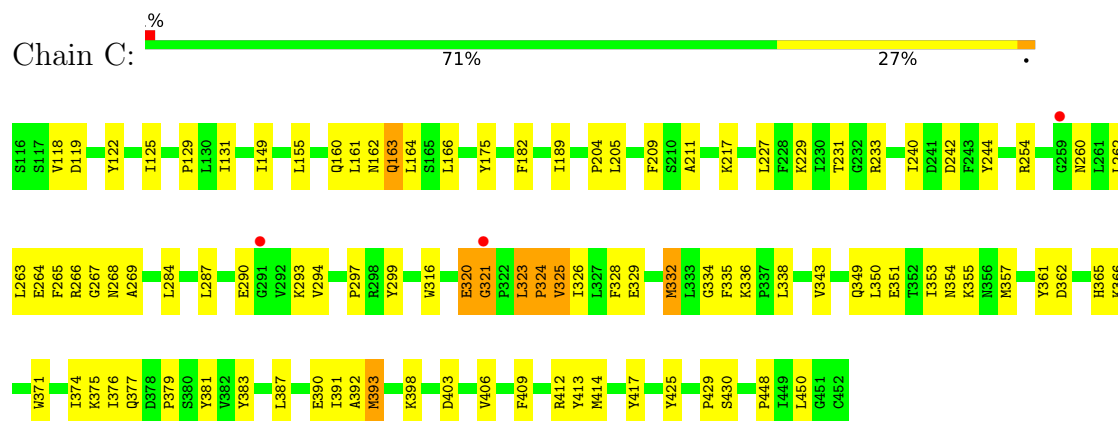
3 Residue-property plots

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.

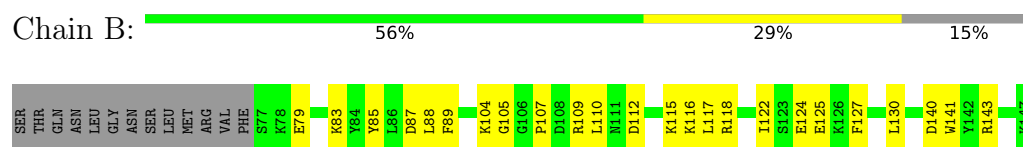
• Molecule 1: D-glycerate-3-kinase (GLYK)



• Molecule 1: D-glycerate-3-kinase (GLYK)



• Molecule 2: RxLR effector protein Avr-vnt11



• Molecule 2: RxLR effector protein Avr-vnt11



SER	THR	GLN	ASN	LEU	GLY	ASN	SER	LEU	MET	ARG	VAL	PHE	S77
													K83
													D87
													I88
													F89
													L110
													N111
													K115
													E124
													F127
													L130
													Y137
													K147

4 Data and refinement statistics

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 42.97 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.97-3.31) 93.5 (42.97-3.31)	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 0.292 , 0.317	Depositor DCC
R_{free} test set	1802 reflections (10.03%)	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)	0.37 , 406.8	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

5.1 Standard geometry

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	0.20	0/2765	0.46	0/3734
1	C	0.23	0/2765	0.49	3/3734 (0.1%)
2	B	0.23	0/585	0.49	0/779
2	D	0.18	0/585	0.48	0/779
All	All	0.22	0/6700	0.48	3/9026 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	GLY	CA-C-N	5.52	126.39	119.98
1	C	321	GLY	C-N-CA	5.52	126.39	119.98
1	C	325	VAL	N-CA-C	5.22	116.18	108.45

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	2701	0	2661	109	0
1	C	2701	0	2661	85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:336:LYS:NZ	1:A:427:GLU:OE1	2.35	0.58
1:C:323:LEU:CD1	1:C:326:ILE:HG13	2.34	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:343:VAL:HG21	1:C:354:ASN:CG	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:265:PHE:CZ	1:C:412:ARG:HD3	2.50	0.46
1:C:391:ILE:O	1:C:392:ALA:C	2.58	0.46
1:A:177:TYR:CD1	1:A:448:PRO:HG3	2.51	0.46
2:B:124:GLU:CD	2:B:124:GLU:H	2.24	0.46
1:C:376:ILE:HD11	1:C:379:PRO:HA	1.98	0.46
2:B:125:GLU:H	2:B:125:GLU:CD	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:343:VAL:HG21	1:A:354:ASN:CG	2.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:TYR:CE2	1:A:301:LYS:HG2	2.56	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: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
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%)	36	66
1	C	335/337 (99%)	321 (96%)	12 (4%)	2 (1%)	21	52
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%)	30	60

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%)	76	79
1	C	295/286 (103%)	291 (99%)	4 (1%)	59	72
2	B	55/67 (82%)	55 (100%)	0	100	100
2	D	55/67 (82%)	55 (100%)	0	100	100
All	All	700/706 (99%)	694 (99%)	6 (1%)	70	77

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	GLU
1	A	323	LEU
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	268	ASN
1	A	272	HIS
1	A	365	HIS
1	A	384	GLN
1	C	163	GLN
1	C	377	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](#)

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%)	-0.09	7 (2%) 63 44	106, 165, 280, 325	0
1	C	328/337 (97%)	0.03	3 (0%) 81 66	109, 184, 277, 322	0
2	B	71/84 (84%)	-0.22	0 100 100	110, 171, 237, 260	0
2	D	71/84 (84%)	-0.04	0 100 100	135, 203, 256, 284	0
All	All	798/842 (94%)	-0.05	10 (1%) 75 57	106, 177, 273, 325	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	259	GLY	4.2
1	A	352	THR	3.3
1	A	334	GLY	2.8
1	A	258	PRO	2.7
1	A	245	LEU	2.4
1	A	335	PHE	2.3
1	C	291	GLY	2.2
1	A	268	ASN	2.2
1	C	321	GLY	2.2
1	A	350	LEU	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.