



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:24 PM UTC

PDB ID : 5E9F / pdb_00005e9f
Title : Structural insights of isocitrate lyases from *Magnaporthe oryzae*
Authors : Park, Y.; Cho, Y.; Lee, Y.-H.; Lee, Y.-W.; Rhee, S.
Deposited on : 2015-10-15
Resolution : 2.80 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

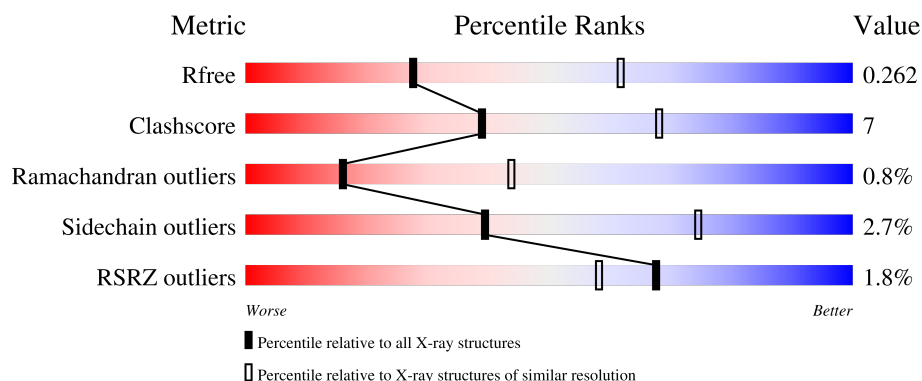
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	560	0% 76% 14% • 9%
1	B	560	0% 76% 12% • 11%
1	C	560	2% 71% 16% • 11%
1	D	560	3% 63% 16% • 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14983 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 Isocitrate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			3851	2440	662	731	18			
1	B	501	Total	C	N	O	S	0	0	0
			3853	2444	662	729	18			
1	C	496	Total	C	N	O	S	0	0	0
			3736	2368	642	709	17			
1	D	453	Total	C	N	O	S	0	0	0
			3474	2200	597	662	15			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	548	ALA	-	expression tag	UNP P0CT06
A	549	ALA	-	expression tag	UNP P0CT06
A	550	ALA	-	expression tag	UNP P0CT06
A	551	LEU	-	expression tag	UNP P0CT06
A	552	GLU	-	expression tag	UNP P0CT06
A	553	HIS	-	expression tag	UNP P0CT06
A	554	HIS	-	expression tag	UNP P0CT06
A	555	HIS	-	expression tag	UNP P0CT06
A	556	HIS	-	expression tag	UNP P0CT06
A	557	HIS	-	expression tag	UNP P0CT06
A	558	HIS	-	expression tag	UNP P0CT06
A	559	HIS	-	expression tag	UNP P0CT06
A	560	HIS	-	expression tag	UNP P0CT06
B	548	ALA	-	expression tag	UNP P0CT06
B	549	ALA	-	expression tag	UNP P0CT06
B	550	ALA	-	expression tag	UNP P0CT06
B	551	LEU	-	expression tag	UNP P0CT06
B	552	GLU	-	expression tag	UNP P0CT06
B	553	HIS	-	expression tag	UNP P0CT06
B	554	HIS	-	expression tag	UNP P0CT06
B	555	HIS	-	expression tag	UNP P0CT06

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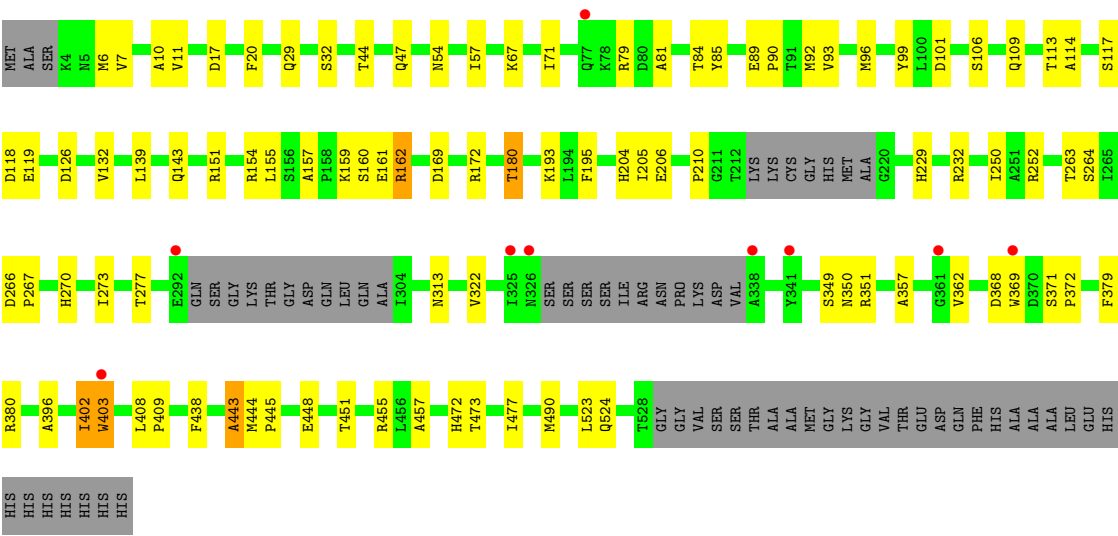
Chain	Residue	Modelled	Actual	Comment	Reference
B	556	HIS	-	expression tag	UNP P0CT06
B	557	HIS	-	expression tag	UNP P0CT06
B	558	HIS	-	expression tag	UNP P0CT06
B	559	HIS	-	expression tag	UNP P0CT06
B	560	HIS	-	expression tag	UNP P0CT06
C	548	ALA	-	expression tag	UNP P0CT06
C	549	ALA	-	expression tag	UNP P0CT06
C	550	ALA	-	expression tag	UNP P0CT06
C	551	LEU	-	expression tag	UNP P0CT06
C	552	GLU	-	expression tag	UNP P0CT06
C	553	HIS	-	expression tag	UNP P0CT06
C	554	HIS	-	expression tag	UNP P0CT06
C	555	HIS	-	expression tag	UNP P0CT06
C	556	HIS	-	expression tag	UNP P0CT06
C	557	HIS	-	expression tag	UNP P0CT06
C	558	HIS	-	expression tag	UNP P0CT06
C	559	HIS	-	expression tag	UNP P0CT06
C	560	HIS	-	expression tag	UNP P0CT06
D	548	ALA	-	expression tag	UNP P0CT06
D	549	ALA	-	expression tag	UNP P0CT06
D	550	ALA	-	expression tag	UNP P0CT06
D	551	LEU	-	expression tag	UNP P0CT06
D	552	GLU	-	expression tag	UNP P0CT06
D	553	HIS	-	expression tag	UNP P0CT06
D	554	HIS	-	expression tag	UNP P0CT06
D	555	HIS	-	expression tag	UNP P0CT06
D	556	HIS	-	expression tag	UNP P0CT06
D	557	HIS	-	expression tag	UNP P0CT06
D	558	HIS	-	expression tag	UNP P0CT06
D	559	HIS	-	expression tag	UNP P0CT06
D	560	HIS	-	expression tag	UNP P0CT06

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

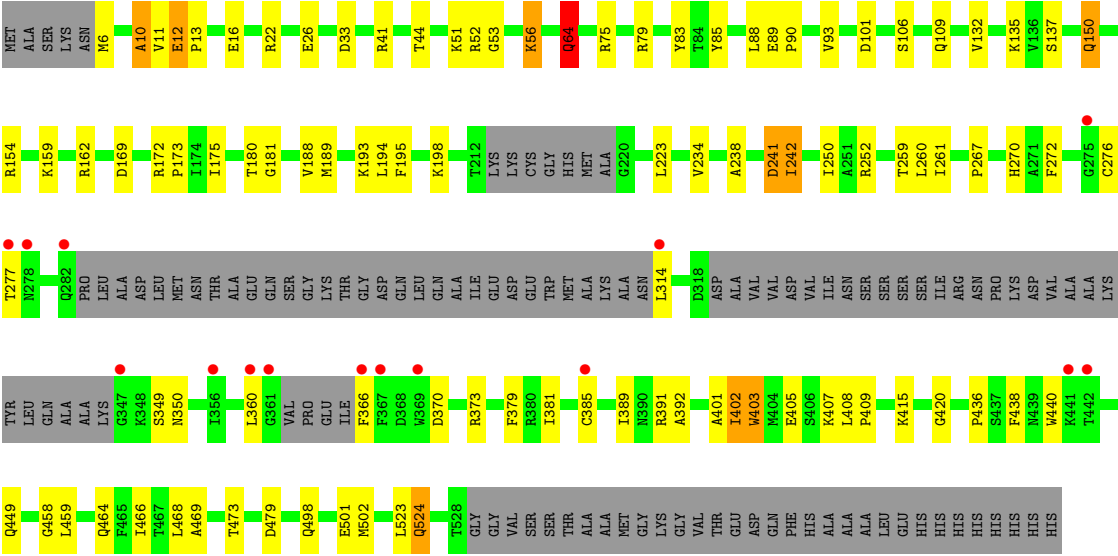
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total 20	O 20	0	0
3	B	16	Total 16	O 16	0	0
3	C	17	Total 17	O 17	0	0
3	D	12	Total 12	O 12	0	0



• Molecule 1: Isocitrate lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.58Å 135.31Å 158.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.40 – 2.80 32.40 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.40-2.80) 95.2 (32.40-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.186 , 0.226 0.209 , 0.262	Depositor DCC
R_{free} test set	2000 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.5	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	0.92	EDS
Total number of atoms	14983	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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

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	0.59	0/3942	0.88	6/5371 (0.1%)
1	B	0.56	0/3942	0.91	8/5361 (0.1%)
1	C	0.56	0/3822	0.89	4/5213 (0.1%)
1	D	0.56	0/3556	0.90	11/4840 (0.2%)
All	All	0.57	0/15262	0.90	29/20785 (0.1%)

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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	266	ASP	CA-C-N	7.12	127.44	119.32
1	C	266	ASP	C-N-CA	7.12	127.44	119.32
1	B	292	GLU	N-CA-C	7.06	125.85	110.80
1	A	425	TYR	CA-C-N	6.93	126.63	119.56
1	A	425	TYR	C-N-CA	6.93	126.63	119.56
1	D	33	ASP	CA-C-N	6.90	128.47	119.84
1	D	33	ASP	C-N-CA	6.90	128.47	119.84
1	D	241	ASP	N-CA-C	-6.49	101.52	110.35
1	A	403	TRP	N-CA-C	6.32	118.78	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	ASP	N-CA-C	-6.06	102.11	110.35
1	D	150	GLN	N-CA-C	-5.86	104.31	112.45
1	D	524	GLN	N-CA-C	-5.83	104.52	111.69
1	A	89	GLU	N-CA-C	5.69	113.25	108.13
1	C	403	TRP	N-CA-C	5.58	117.75	108.99
1	D	41	ARG	CA-C-N	5.58	126.81	119.84
1	D	41	ARG	C-N-CA	5.58	126.81	119.84
1	B	371	SER	CA-C-N	-5.55	112.90	119.84
1	B	371	SER	C-N-CA	-5.55	112.90	119.84
1	B	403	TRP	N-CA-C	5.42	117.64	109.23
1	A	330	SER	CA-C-N	5.27	131.19	121.70
1	A	330	SER	C-N-CA	5.27	131.19	121.70
1	D	403	TRP	N-CA-C	5.26	117.26	108.99
1	B	403	TRP	CA-CB-CG	5.26	123.60	113.60
1	B	435	SER	CA-C-N	5.26	125.72	120.04
1	B	435	SER	C-N-CA	5.26	125.72	120.04
1	D	64	GLN	N-CA-C	5.22	116.97	111.28
1	C	114	ALA	N-CA-C	5.17	118.81	112.03
1	D	12	GLU	CA-C-N	5.11	125.40	119.47
1	D	12	GLU	C-N-CA	5.11	125.40	119.47

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	293	GLN	Peptide
1	C	443	ALA	Peptide
1	D	88	LEU	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	3851	0	3626	62	0
1	B	3853	0	3687	52	0
1	C	3736	0	3502	60	0
1	D	3474	0	3268	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	20	0	0	0	0
3	B	16	0	0	0	0
3	C	17	0	0	1	0
3	D	12	0	0	0	0
All	All	14983	0	14083	198	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 7.

All (198) 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:101:ASP:H	1:C:6:MET:HE2	1.35	0.90
1:D:159:LYS:HA	1:D:162:ARG:HG3	1.58	0.84
1:A:127:TYR:OH	1:A:179:ASP:OD2	1.96	0.82
1:C:444:MET:HG2	1:C:448:GLU:HB2	1.63	0.81
1:D:64:GLN:N	1:D:64:GLN:HE21	1.79	0.80
1:A:6:MET:HE2	1:D:101:ASP:H	1.48	0.78
1:D:389:ILE:HD13	1:D:420:GLY:HA3	1.68	0.76
1:C:157:ALA:O	1:C:162:ARG:NH1	2.21	0.74
1:B:440:TRP:O	1:B:449:GLN:NE2	2.20	0.73
1:D:370:ASP:HB3	1:D:373:ARG:HH21	1.54	0.72
1:C:349:SER:O	1:C:351:ARG:N	2.24	0.69
1:A:193:LYS:NZ	1:C:119:GLU:OE1	2.26	0.69
1:C:277:THR:OG1	1:C:313:ASN:O	2.16	0.63
1:B:10:ALA:HB2	1:C:169:ASP:HA	1.81	0.63
1:B:274:LEU:HD21	1:B:382:LYS:HB2	1.78	0.63
1:D:64:GLN:HE21	1:D:64:GLN:CA	2.12	0.62
1:B:84:THR:OG1	1:B:85:TYR:N	2.28	0.61
1:B:89:GLU:HG2	1:B:90:PRO:HD2	1.82	0.61
1:D:498:GLN:HG2	1:D:502:MET:HE2	1.81	0.61
1:B:289:ASN:C	1:B:291:ALA:H	2.11	0.58
1:B:87:CYS:SG	1:B:93:VAL:HG23	2.44	0.58
1:A:403:TRP:HB3	1:A:431:ALA:O	2.03	0.58
1:B:185:LEU:O	1:B:189:MET:HG3	2.03	0.58
1:A:523:LEU:HG	1:D:189:MET:HE1	1.85	0.58
1:A:108:TRP:CH2	1:B:511:HIS:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:GLU:O	1:C:232:ARG:NH1	2.37	0.57
1:A:83:TYR:O	1:D:6:MET:HE1	2.04	0.57
1:B:261:ILE:HB	1:B:381:ILE:HD12	1.87	0.57
1:C:472:HIS:ND1	1:D:501:GLU:OE2	2.38	0.57
1:A:89:GLU:OE2	1:A:91:THR:OG1	2.19	0.56
1:A:110:SER:HA	1:A:114:ALA:HB3	1.86	0.56
1:A:119:GLU:OE1	1:C:193:LYS:NZ	2.38	0.56
1:C:159:LYS:HA	1:C:162:ARG:HG3	1.88	0.56
1:D:440:TRP:O	1:D:449:GLN:NE2	2.38	0.56
1:D:276:CYS:HA	1:D:314:LEU:HD23	1.87	0.55
1:B:75:ARG:HB3	1:B:462:CYS:HB2	1.89	0.55
1:B:289:ASN:O	1:B:291:ALA:N	2.39	0.55
1:D:349:SER:OG	1:D:350:ASN:N	2.40	0.55
1:C:229:HIS:HA	1:C:232:ARG:HD2	1.90	0.54
1:A:151:ARG:HD3	1:D:52:ARG:O	2.07	0.54
1:D:64:GLN:CA	1:D:64:GLN:NE2	2.70	0.53
1:A:137:SER:HB2	1:A:198:LYS:HB3	1.89	0.53
1:A:89:GLU:OE1	1:B:88:LEU:HD13	2.08	0.53
1:A:83:TYR:HA	1:A:464:GLN:O	2.09	0.53
1:A:177:ASP:OD1	1:A:179:ASP:N	2.38	0.52
1:B:157:ALA:O	1:B:162:ARG:NH1	2.43	0.52
1:B:317:PHE:CZ	1:B:354:ARG:HG2	2.45	0.52
1:A:527:VAL:HG13	1:D:234:VAL:HG12	1.92	0.52
1:B:62:ASN:HB2	1:B:245:VAL:HG12	1.92	0.52
1:C:252:ARG:HD2	1:C:403:TRP:CZ2	2.45	0.52
1:A:6:MET:HE1	1:D:83:TYR:O	2.10	0.51
1:A:89:GLU:HG3	1:A:90:PRO:N	2.26	0.51
1:B:17:ASP:OD1	1:C:162:ARG:NH2	2.44	0.51
1:A:83:TYR:H	1:D:6:MET:HE1	1.76	0.51
1:C:89:GLU:HG2	1:C:90:PRO:HD2	1.91	0.51
1:C:263:THR:HA	1:C:379:PHE:CE1	2.45	0.51
1:A:17:ASP:OD1	1:D:162:ARG:NH2	2.44	0.51
1:D:22:ARG:O	1:D:26:GLU:HG3	2.11	0.51
1:D:154:ARG:O	1:D:162:ARG:HD3	2.10	0.51
1:D:267:PRO:HA	1:D:270:HIS:CE1	2.46	0.50
1:D:436:PRO:HG3	1:D:466:ILE:HG22	1.93	0.50
1:D:64:GLN:NE2	1:D:64:GLN:HA	2.26	0.50
1:A:190:LYS:NZ	1:C:126:ASP:OD1	2.44	0.50
1:B:241:ASP:O	1:B:242:ILE:HB	2.12	0.50
1:C:44:THR:OG1	1:C:47:GLN:HG3	2.11	0.50
1:C:205:ILE:HG23	1:C:229:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:THR:HG23	1:C:524:GLN:HE21	1.77	0.50
1:A:508:VAL:HG22	1:A:514:TRP:CE2	2.47	0.50
1:A:189:MET:HE1	1:D:523:LEU:HB3	1.94	0.49
1:C:490:MET:HE2	1:D:440:TRP:CE2	2.48	0.49
1:C:368:ASP:OD2	1:C:371:SER:OG	2.31	0.49
1:D:106:SER:HB3	1:D:109:GLN:HB2	1.94	0.49
1:D:83:TYR:HA	1:D:464:GLN:O	2.13	0.49
1:B:162:ARG:NH2	1:C:17:ASP:OD1	2.46	0.48
1:C:101:ASP:HA	1:C:172:ARG:HD2	1.95	0.48
1:C:477:ILE:HD13	1:D:473:THR:O	2.13	0.48
1:A:495:GLU:HB3	1:A:496:LEU:HD12	1.95	0.48
1:B:155:LEU:HD13	1:C:20:PHE:CD1	2.48	0.48
1:B:164:LYS:HA	1:B:164:LYS:HD2	1.61	0.48
1:A:409:PRO:HD3	1:A:438:PHE:CG	2.49	0.48
1:A:205:ILE:HD13	1:A:232:ARG:HB3	1.95	0.48
1:D:267:PRO:HA	1:D:270:HIS:ND1	2.28	0.48
1:A:490:MET:HE2	1:B:440:TRP:CZ2	2.49	0.48
1:A:519:TYR:OH	1:D:51:LYS:O	2.32	0.48
1:A:28:LYS:NZ	1:A:46:GLU:OE2	2.47	0.48
1:B:189:MET:HE1	1:C:523:LEU:HB3	1.96	0.48
1:C:109:GLN:O	1:C:113:THR:OG1	2.29	0.47
1:C:180:THR:HG21	1:C:210:PRO:HB3	1.94	0.47
1:A:8:ASN:ND2	1:D:169:ASP:OD2	2.47	0.47
1:B:278:ASN:OD1	1:B:280:SER:OG	2.31	0.47
1:B:385:CYS:O	1:B:389:ILE:HG13	2.15	0.47
1:D:385:CYS:O	1:D:389:ILE:HG13	2.15	0.47
1:B:500:PRO:O	1:B:504:LEU:HG	2.14	0.47
1:A:101:ASP:HA	1:A:172:ARG:HD2	1.97	0.47
1:B:147:ASP:OD1	1:C:54:ASN:ND2	2.47	0.47
1:C:372:PRO:HB2	1:C:380:ARG:HG3	1.96	0.47
1:A:5:ASN:O	1:D:75:ARG:NH2	2.44	0.47
1:A:89:GLU:CD	1:B:88:LEU:HD13	2.41	0.46
1:A:87:CYS:SG	1:A:93:VAL:HG23	2.55	0.46
1:C:451:THR:O	1:C:455:ARG:HG3	2.14	0.46
1:B:47:GLN:O	1:B:51:LYS:HG2	2.15	0.46
1:D:259:THR:O	1:D:260:LEU:HD23	2.16	0.46
1:D:89:GLU:HG2	1:D:90:PRO:HD2	1.97	0.46
1:A:396:ALA:HA	1:A:402:ILE:HD11	1.97	0.46
1:A:269:ASP:O	1:A:273:ILE:HG13	2.15	0.46
1:A:29:GLN:O	1:A:32:SER:OG	2.24	0.46
1:C:273:ILE:HG22	1:C:369:TRP:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:MET:HE2	1:B:440:TRP:CE2	2.52	0.45
1:B:159:LYS:HA	1:B:162:ARG:HG3	1.97	0.45
1:D:261:ILE:HG22	1:D:379:PHE:HB2	1.98	0.45
1:A:169:ASP:HA	1:D:10:ALA:HB2	1.97	0.45
1:A:444:MET:HE3	1:A:444:MET:HB2	1.76	0.45
1:C:99:TYR:OH	1:D:479:ASP:OD1	2.20	0.45
1:C:84:THR:OG1	1:C:85:TYR:N	2.48	0.45
1:C:132:VAL:HG12	1:C:195:PHE:HE1	1.82	0.45
1:B:83:TYR:O	1:C:6:MET:HE1	2.16	0.45
1:B:52:ARG:O	1:C:151:ARG:HD3	2.17	0.45
1:B:118:ASP:O	1:B:120:PRO:HD3	2.17	0.45
1:A:127:TYR:C	1:A:127:TYR:HD1	2.25	0.45
1:A:476:LEU:O	1:A:480:ARG:HG2	2.17	0.45
1:D:194:LEU:O	1:D:198:LYS:HG2	2.17	0.45
1:B:184:GLY:O	1:B:188:VAL:HG23	2.17	0.45
1:B:8:ASN:OD1	1:C:172:ARG:NH1	2.47	0.44
1:C:139:LEU:O	1:C:143:GLN:HG3	2.17	0.44
1:A:409:PRO:HD3	1:A:438:PHE:CD2	2.53	0.44
1:B:16:GLU:CD	1:C:154:ARG:HH21	2.23	0.44
1:B:403:TRP:HB3	1:B:431:ALA:O	2.16	0.44
1:C:396:ALA:HA	1:C:402:ILE:HD11	2.00	0.44
1:D:79:ARG:HB3	1:D:458:GLY:HA2	1.99	0.44
1:A:127:TYR:C	1:A:127:TYR:CD1	2.96	0.44
1:C:159:LYS:C	1:C:161:GLU:H	2.25	0.44
1:A:67:LYS:O	1:A:71:ILE:HG13	2.16	0.44
1:A:137:SER:HB2	1:A:198:LYS:HD2	1.99	0.44
1:A:345:ALA:HA	1:A:348:LYS:HG3	2.00	0.44
1:A:79:ARG:HD3	1:A:79:ARG:HA	1.78	0.44
1:A:101:ASP:H	1:D:6:MET:HE2	1.82	0.44
1:C:445:PRO:HD2	1:C:448:GLU:HG3	2.00	0.44
1:D:241:ASP:O	1:D:242:ILE:HB	2.17	0.43
1:D:392:ALA:HB1	1:D:402:ILE:HG21	2.01	0.43
1:A:432:TYR:HB3	1:A:464:GLN:HG2	1.99	0.43
1:C:357:ALA:HB1	1:C:362:VAL:HB	2.00	0.43
1:A:194:LEU:O	1:A:198:LYS:HG2	2.19	0.43
1:B:278:ASN:ND2	1:B:311:LYS:O	2.48	0.43
1:D:85:TYR:CD2	1:D:469:ALA:HB3	2.54	0.43
1:D:137:SER:HB2	1:D:198:LYS:HD2	2.00	0.43
1:A:127:TYR:HE1	1:A:182:HIS:CE1	2.36	0.43
1:C:263:THR:OG1	1:C:264:SER:N	2.51	0.43
1:A:185:LEU:O	1:A:189:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:TRP:CZ3	1:A:309:MET:HE2	2.54	0.43
1:C:29:GLN:O	1:C:32:SER:OG	2.34	0.43
1:D:272:PHE:O	1:D:381:ILE:HG13	2.19	0.43
1:C:79:ARG:NH1	3:C:701:HOH:O	2.52	0.42
1:D:172:ARG:HA	1:D:173:PRO:HD3	1.91	0.42
1:A:101:ASP:OD1	1:D:6:MET:HE3	2.19	0.42
1:B:252:ARG:HD2	1:B:403:TRP:CZ2	2.54	0.42
1:B:56:LYS:HE3	1:B:56:LYS:HB3	1.79	0.42
1:C:67:LYS:O	1:C:71:ILE:HG13	2.19	0.42
1:C:92:MET:O	1:C:96:MET:HG3	2.19	0.42
1:D:276:CYS:SG	1:D:277:THR:N	2.92	0.42
1:C:117:SER:O	1:C:118:ASP:HB2	2.19	0.42
1:D:52:ARG:HE	1:D:242:ILE:HA	1.85	0.42
1:D:252:ARG:HD2	1:D:403:TRP:CZ2	2.55	0.42
1:D:407:LYS:O	1:D:408:LEU:HD12	2.19	0.42
1:B:177:ASP:OD1	1:B:179:ASP:N	2.41	0.42
1:D:250:ILE:HG12	1:D:401:ALA:HB3	2.01	0.42
1:C:408:LEU:HD23	1:C:409:PRO:HD2	2.02	0.42
1:C:473:THR:O	1:C:477:ILE:HG12	2.20	0.42
1:A:175:ILE:HD12	1:A:463:TRP:CZ2	2.55	0.42
1:A:328:SER:O	1:A:330:SER:HA	2.20	0.42
1:D:238:ALA:O	1:D:242:ILE:HG13	2.19	0.42
1:A:273:ILE:HA	1:A:381:ILE:HG13	2.02	0.42
1:D:12:GLU:HA	1:D:13:PRO:HD3	1.94	0.41
1:D:409:PRO:HD3	1:D:438:PHE:CG	2.54	0.41
1:A:154:ARG:NE	1:D:16:GLU:OE2	2.38	0.41
1:A:392:ALA:HB1	1:A:402:ILE:HG21	2.02	0.41
1:C:154:ARG:O	1:C:162:ARG:HD3	2.19	0.41
1:D:436:PRO:HG2	1:D:468:LEU:HB2	2.02	0.41
1:B:278:ASN:HA	1:B:279:PRO:HD3	1.86	0.41
1:D:132:VAL:HG12	1:D:195:PHE:HE1	1.84	0.41
1:D:181:GLY:HA3	1:D:188:VAL:HG22	2.02	0.41
1:C:81:ALA:HB2	1:C:457:ALA:HB2	2.03	0.41
1:C:438:PHE:CE1	1:C:443:ALA:HB2	2.56	0.41
1:C:477:ILE:HD12	1:D:473:THR:HB	2.03	0.41
1:B:20:PHE:CD1	1:C:155:LEU:HD13	2.55	0.41
1:B:119:GLU:CD	1:D:193:LYS:HE2	2.46	0.41
1:B:289:ASN:C	1:B:291:ALA:N	2.79	0.41
1:D:223:LEU:HD13	1:D:391:ARG:NH1	2.36	0.41
1:C:267:PRO:HA	1:C:270:HIS:CE1	2.56	0.41
1:A:151:ARG:NH1	1:D:53:GLY:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:THR:HA	1:D:366:PHE:HE2	1.86	0.41
1:B:9:PRO:O	1:B:10:ALA:HB3	2.20	0.40
1:B:274:LEU:HD21	1:B:382:LYS:CB	2.47	0.40
1:D:56:LYS:HD3	1:D:56:LYS:HA	1.96	0.40
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.91	0.40
1:A:491:ARG:O	1:A:495:GLU:HB2	2.21	0.40
1:B:52:ARG:HE	1:B:242:ILE:HA	1.86	0.40
1:C:204:HIS:HB3	1:C:250:ILE:HB	2.04	0.40
1:D:415:LYS:HG3	1:D:459:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	501/560 (90%)	478 (95%)	18 (4%)	5 (1%)	12	38
1	B	493/560 (88%)	472 (96%)	17 (3%)	4 (1%)	16	44
1	C	488/560 (87%)	463 (95%)	21 (4%)	4 (1%)	16	44
1	D	443/560 (79%)	415 (94%)	25 (6%)	3 (1%)	18	47
All	All	1925/2240 (86%)	1828 (95%)	81 (4%)	16 (1%)	16	44

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	242	ILE
1	B	292	GLU
1	C	350	ASN
1	A	10	ALA
1	B	242	ILE

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Mol	Chain	Res	Type
1	B	290	THR
1	A	434	LEU
1	D	10	ALA
1	B	11	VAL
1	C	10	ALA
1	C	160	SER
1	C	11	VAL
1	D	11	VAL
1	D	242	ILE
1	A	331	ILE

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	381/462 (82%)	370 (97%)	11 (3%)	37	73
1	B	389/462 (84%)	380 (98%)	9 (2%)	44	78
1	C	364/462 (79%)	356 (98%)	8 (2%)	45	78
1	D	347/462 (75%)	335 (96%)	12 (4%)	32	67
All	All	1481/1848 (80%)	1441 (97%)	40 (3%)	39	74

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	88	LEU
1	A	89	GLU
1	A	93	VAL
1	A	127	TYR
1	A	135	LYS
1	A	160	SER
1	A	206	GLU
1	A	381	ILE
1	A	413	GLN
1	A	471	LEU

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Mol	Chain	Res	Type
1	B	89	GLU
1	B	93	VAL
1	B	161	GLU
1	B	180	THR
1	B	293	GLN
1	B	307	GLU
1	B	381	ILE
1	B	447	ASP
1	B	524	GLN
1	C	7	VAL
1	C	57	ILE
1	C	93	VAL
1	C	106	SER
1	C	162	ARG
1	C	180	THR
1	C	322	VAL
1	C	402	ILE
1	D	44	THR
1	D	56	LYS
1	D	64	GLN
1	D	93	VAL
1	D	135	LYS
1	D	150	GLN
1	D	175	ILE
1	D	180	THR
1	D	360	LEU
1	D	402	ILE
1	D	405	GLU
1	D	524	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	143	GLN
1	A	150	GLN
1	A	333	ASN
1	B	152	HIS
1	B	166	GLN
1	B	293	GLN
1	B	524	GLN
1	C	413	GLN

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Mol	Chain	Res	Type
1	C	428	GLN
1	C	524	GLN
1	D	64	GLN
1	D	166	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 4 ligands modelled in this entry, 4 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	507/560 (90%)	-0.11	6 (1%) 76 68	20, 34, 53, 68	0
1	B	501/560 (89%)	0.00	6 (1%) 76 68	22, 39, 57, 82	0
1	C	496/560 (88%)	0.01	9 (1%) 67 58	22, 37, 67, 85	0
1	D	453/560 (80%)	0.06	15 (3%) 49 39	23, 38, 73, 93	0
All	All	1957/2240 (87%)	-0.01	36 (1%) 67 58	20, 37, 62, 93	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	369	TRP	5.1
1	D	366	PHE	4.1
1	A	369	TRP	3.8
1	A	289	ASN	3.7
1	D	385	CYS	3.5
1	B	294	SER	3.5
1	D	361	GLY	3.4
1	D	277	THR	3.3
1	A	292	GLU	3.2
1	B	369	TRP	3.1
1	A	89	GLU	3.0
1	B	292	GLU	3.0
1	C	325	ILE	2.9
1	A	304	ILE	2.9
1	D	282	GLN	2.8
1	C	326	ASN	2.6
1	D	278	ASN	2.6
1	B	5	ASN	2.5
1	A	306	ASP	2.5
1	C	369	TRP	2.5
1	C	338	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	293	GLN	2.4
1	C	403	TRP	2.4
1	B	304	ILE	2.4
1	D	360	LEU	2.4
1	D	275	GLY	2.3
1	D	367	PHE	2.3
1	D	314	LEU	2.2
1	C	77	GLN	2.2
1	D	441	LYS	2.2
1	D	442	THR	2.2
1	C	292	GLU	2.2
1	C	341	TYR	2.1
1	D	356	ILE	2.1
1	C	361	GLY	2.1
1	D	347	GLY	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](#)

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($\text{\AA}^2$)	Q<0.9
2	MG	D	601	1/1	0.80	0.30	36,36,36,36	0
2	MG	A	601	1/1	0.85	0.21	41,41,41,41	0
2	MG	C	601	1/1	0.87	0.15	28,28,28,28	0
2	MG	B	601	1/1	0.89	0.11	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.