



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:48 AM EDT

PDB ID : 1VGA / pdb_00001vga
Title : Structures of unligated and inhibitor complexes of W168F mutant of
Triosephosphate Isomerase from Plasmodium falciparum
Authors : Eaazhisai, K.; Balaram, H.; Balaram, P.; Murthy, M.R.N.
Deposited on : 2004-04-23
Resolution : 1.80 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

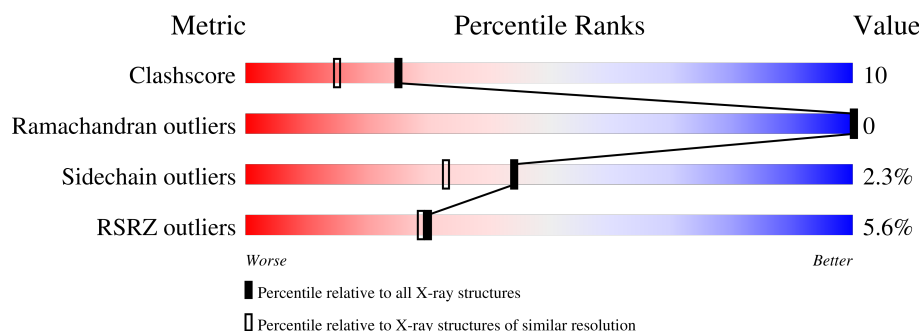
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	248	4% 77% 21% ..
1	B	248	6% 73% 24% ..
1	C	248	7% 81% 17% ..
1	D	248	5% 75% 24% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8374 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 Triosephosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1954	1237	332	380	5			
1	B	246	Total	C	N	O	S	0	0	0
			1954	1237	332	380	5			
1	C	246	Total	C	N	O	S	0	0	0
			1954	1237	332	380	5			
1	D	246	Total	C	N	O	S	0	0	0
			1954	1237	332	380	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	VAL	ALA	engineered mutation	UNP Q07412
A	168	PHE	TRP	engineered mutation	UNP Q07412
B	163	VAL	ALA	engineered mutation	UNP Q07412
B	168	PHE	TRP	engineered mutation	UNP Q07412
C	163	VAL	ALA	engineered mutation	UNP Q07412
C	168	PHE	TRP	engineered mutation	UNP Q07412
D	163	VAL	ALA	engineered mutation	UNP Q07412
D	168	PHE	TRP	engineered mutation	UNP Q07412

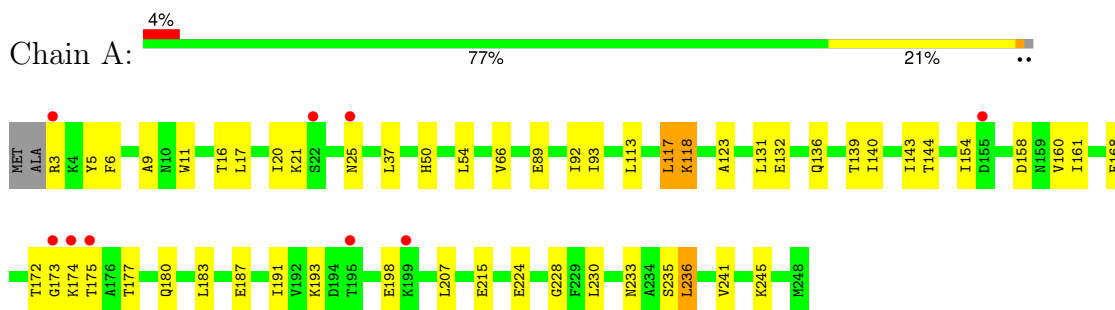
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	172	Total	O	0	0
			172	172		
2	B	144	Total	O	0	0
			144	144		
2	C	111	Total	O	0	0
			111	111		
2	D	131	Total	O	0	0
			131	131		

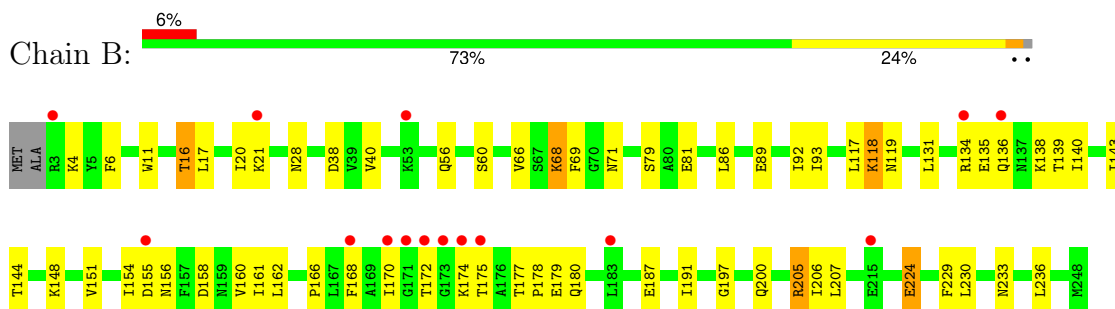
3 Residue-property plots

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.

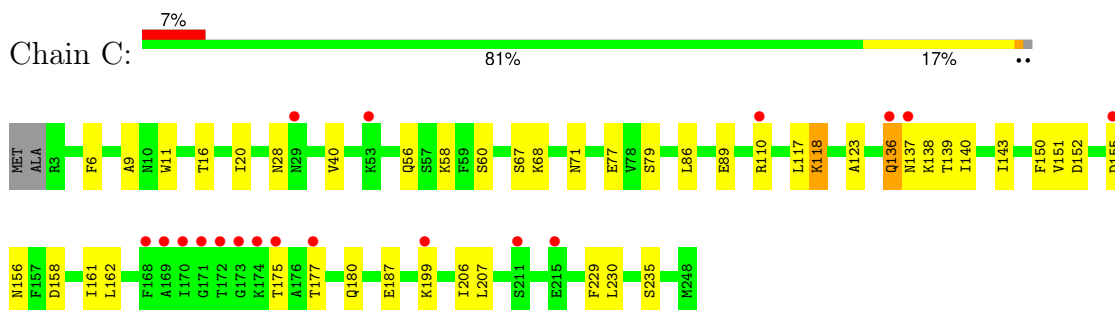
- Molecule 1: Triosephosphate isomerase



- Molecule 1: Triosephosphate isomerase

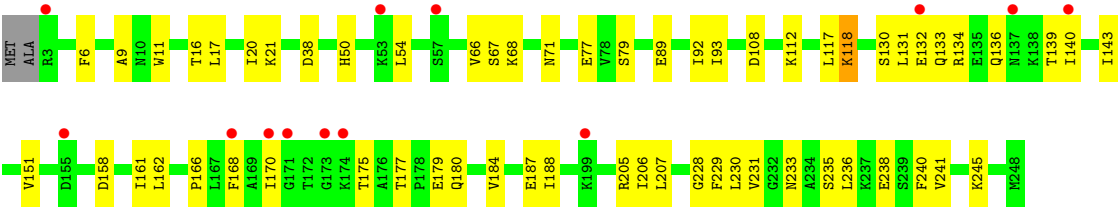


- Molecule 1: Triosephosphate isomerase



- Molecule 1: Triosephosphate isomerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.73Å 106.16Å 89.53Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	17.20 – 1.80 17.20 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (17.20-1.80) 93.7 (17.20-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 1.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.229 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8374	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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	0.34	0/1985	0.89	6/2675 (0.2%)
1	B	0.35	0/1985	0.86	7/2675 (0.3%)
1	C	0.34	0/1985	0.88	6/2675 (0.2%)
1	D	0.34	0/1985	0.89	7/2675 (0.3%)
All	All	0.34	0/7940	0.88	26/10700 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	89	GLU	N-CA-C	7.04	119.03	111.36
1	A	89	GLU	N-CA-C	6.86	118.84	111.36
1	D	158	ASP	N-CA-C	-6.51	105.64	113.97
1	B	158	ASP	N-CA-C	-6.29	105.76	113.50
1	A	158	ASP	N-CA-C	-6.16	105.92	113.50
1	A	173	GLY	N-CA-C	-6.10	106.32	114.25
1	C	158	ASP	N-CA-C	-6.10	106.00	113.50
1	B	68	LYS	N-CA-C	-5.99	105.98	113.28
1	C	89	GLU	N-CA-C	5.92	118.97	111.69
1	D	240	PHE	N-CA-C	-5.86	104.97	111.71
1	C	230	LEU	N-CA-C	-5.86	97.62	107.99
1	C	151	VAL	N-CA-C	5.78	119.14	111.17
1	D	230	LEU	N-CA-C	-5.61	96.42	107.69
1	B	230	LEU	N-CA-C	-5.58	98.11	107.99
1	B	16	THR	N-CA-C	-5.57	100.95	109.41
1	D	68	LYS	N-CA-C	-5.51	106.56	113.28
1	B	89	GLU	N-CA-C	5.50	118.46	111.69
1	C	123	ALA	N-CA-C	5.48	117.90	109.07
1	C	68	LYS	N-CA-C	-5.48	106.59	113.28
1	A	230	LEU	N-CA-C	-5.47	96.69	107.69
1	A	224	GLU	N-CA-C	5.44	117.21	111.28
1	A	123	ALA	N-CA-C	5.40	117.70	108.90
1	D	151	VAL	N-CA-C	5.35	118.56	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	VAL	N-CA-C	5.35	118.55	111.17
1	D	231	VAL	N-CA-C	5.29	115.92	108.36
1	B	224	GLU	N-CA-C	5.09	118.26	111.75

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	1954	0	1952	44	0
1	B	1954	0	1952	42	0
1	C	1954	0	1952	38	0
1	D	1954	0	1952	36	0
2	A	172	0	0	5	0
2	B	144	0	0	0	0
2	C	111	0	0	2	0
2	D	131	0	0	2	0
All	All	8374	0	7808	152	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 10.

All (152) 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:D:140:ILE:HD12	1:D:187:GLU:HG2	1.45	0.98
1:A:154:ILE:HD12	1:A:160:VAL:HG21	1.46	0.94
1:B:177:THR:HB	1:C:136:GLN:OE1	1.74	0.88
1:C:177:THR:HG22	1:C:180:GLN:HG3	1.60	0.82
1:A:233:ASN:HA	1:A:236:LEU:HD23	1.65	0.77
1:B:154:ILE:HD12	1:B:160:VAL:HG21	1.66	0.75
1:C:136:GLN:CB	1:C:138:LYS:HE2	2.17	0.74
1:B:233:ASN:HA	1:B:236:LEU:HD23	1.75	0.69
1:C:140:ILE:HD12	1:C:187:GLU:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:CD1	1:A:160:VAL:HG21	2.24	0.67
1:C:86:LEU:HD21	1:D:17:LEU:HD21	1.77	0.66
1:D:11:TRP:CZ3	1:D:20:ILE:HD12	2.31	0.66
1:B:177:THR:OG1	1:B:180:GLN:HG3	1.96	0.65
1:C:16:THR:O	1:C:20:ILE:HG12	1.96	0.65
1:D:132:GLU:O	1:D:136:GLN:HG3	1.95	0.65
1:B:177:THR:HB	1:C:136:GLN:CD	2.21	0.65
1:A:154:ILE:HD12	1:A:160:VAL:CG2	2.24	0.64
1:C:177:THR:HG22	1:C:180:GLN:CG	2.28	0.63
1:B:11:TRP:CZ3	1:B:20:ILE:HD12	2.33	0.63
1:A:236:LEU:HD21	2:A:360:HOH:O	1.98	0.63
1:B:178:PRO:HD2	1:C:136:GLN:OE1	2.01	0.61
1:C:136:GLN:HB3	1:C:138:LYS:HE2	1.83	0.61
1:B:38:ASP:OD2	1:B:205:ARG:NH2	2.34	0.61
1:D:38:ASP:OD2	1:D:205:ARG:NH2	2.30	0.61
1:B:144:THR:O	1:B:148:LYS:HG3	2.01	0.60
1:D:162:LEU:HD12	1:D:206:ILE:HD12	1.84	0.59
1:A:11:TRP:CZ3	1:A:20:ILE:HD12	2.39	0.58
1:B:162:LEU:HD12	1:B:206:ILE:HD12	1.86	0.58
1:B:140:ILE:HD12	1:B:187:GLU:HG2	1.85	0.57
1:D:16:THR:O	1:D:20:ILE:HG12	2.04	0.57
1:C:136:GLN:HE21	1:C:136:GLN:HA	1.69	0.57
1:D:92:ILE:O	1:D:93:ILE:HD13	2.04	0.57
1:A:113:LEU:CD1	1:A:117:LEU:HD22	2.35	0.57
1:D:162:LEU:HD12	1:D:206:ILE:CD1	2.35	0.56
1:A:66:VAL:HG12	1:A:93:ILE:HD11	1.87	0.56
1:A:50:HIS:HD2	2:A:380:HOH:O	1.88	0.56
1:B:131:LEU:O	1:B:135:GLU:HG3	2.06	0.56
1:C:162:LEU:HD12	1:C:206:ILE:HD12	1.86	0.56
1:A:236:LEU:N	1:A:236:LEU:HD22	2.22	0.55
1:C:199:LYS:HE2	2:C:296:HOH:O	2.05	0.55
1:C:58:LYS:HD2	2:C:328:HOH:O	2.06	0.55
1:C:136:GLN:HB2	1:C:138:LYS:HE2	1.89	0.55
1:C:110:ARG:NH1	1:C:152:ASP:OD1	2.40	0.55
1:C:177:THR:CG2	1:C:180:GLN:HG3	2.35	0.55
1:B:205:ARG:O	1:B:206:ILE:HD13	2.07	0.55
1:C:6:PHE:HB3	1:C:207:LEU:HD21	1.89	0.55
1:A:172:THR:OG1	1:A:174:LYS:HB2	2.08	0.54
1:B:236:LEU:HD22	1:B:236:LEU:N	2.22	0.54
1:B:16:THR:O	1:B:20:ILE:HG12	2.07	0.54
1:B:136:GLN:CB	1:B:138:LYS:HE2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:THR:HG23	1:C:180:GLN:H	1.72	0.54
1:B:66:VAL:HG12	1:B:93:ILE:CD1	2.38	0.54
1:D:130:SER:OG	1:D:133:GLN:HG3	2.08	0.53
1:A:140:ILE:HD12	1:A:187:GLU:HG2	1.90	0.53
1:A:66:VAL:HG12	1:A:93:ILE:CD1	2.39	0.53
1:B:68:LYS:HE3	1:B:69:PHE:CZ	2.44	0.52
1:A:241:VAL:O	1:A:245:LYS:HG3	2.10	0.52
1:C:139:THR:O	1:C:143:ILE:HG12	2.09	0.52
1:C:118:LYS:NZ	1:C:118:LYS:HB2	2.24	0.52
1:A:174:LYS:HD2	2:A:350:HOH:O	2.09	0.52
1:C:86:LEU:HD23	1:D:17:LEU:HD11	1.92	0.52
1:B:92:ILE:O	1:B:93:ILE:HD13	2.10	0.52
1:A:92:ILE:O	1:A:93:ILE:HD13	2.10	0.51
1:C:9:ALA:HB1	1:C:235:SER:HB2	1.91	0.51
1:A:131:LEU:HD13	1:A:168:PHE:HB2	1.91	0.51
1:C:136:GLN:HE21	1:C:136:GLN:CA	2.22	0.51
1:D:238:GLU:O	1:D:241:VAL:HG22	2.11	0.51
1:A:16:THR:O	1:A:20:ILE:HG12	2.09	0.51
1:B:155:ASP:OD1	1:B:156:ASN:N	2.43	0.51
1:B:161:ILE:HD12	1:B:161:ILE:N	2.26	0.50
1:C:162:LEU:HD12	1:C:206:ILE:CD1	2.41	0.50
1:D:118:LYS:NZ	1:D:118:LYS:HB2	2.25	0.50
1:D:179:GLU:HB2	2:D:350:HOH:O	2.11	0.50
1:D:6:PHE:HB3	1:D:207:LEU:HD21	1.94	0.50
1:B:6:PHE:HB3	1:B:207:LEU:HD21	1.93	0.49
1:D:139:THR:O	1:D:143:ILE:HG12	2.11	0.49
1:D:177:THR:OG1	1:D:180:GLN:HG3	2.12	0.49
1:A:118:LYS:HB2	1:A:118:LYS:NZ	2.26	0.49
1:B:71:ASN:ND2	1:B:79:SER:OG	2.46	0.49
1:D:175:THR:HG23	2:D:348:HOH:O	2.13	0.49
1:A:17:LEU:HD21	1:B:86:LEU:CD2	2.43	0.48
1:C:86:LEU:CD2	1:D:17:LEU:HD21	2.43	0.48
1:D:131:LEU:HD13	1:D:168:PHE:HB2	1.95	0.48
1:B:81:GLU:HG3	1:B:119:ASN:OD1	2.13	0.48
1:B:134:ARG:HD2	1:B:168:PHE:CD1	2.48	0.48
1:D:241:VAL:O	1:D:245:LYS:HG3	2.13	0.48
1:D:71:ASN:ND2	1:D:79:SER:OG	2.47	0.48
1:A:9:ALA:HB1	1:A:235:SER:HB2	1.95	0.47
1:B:118:LYS:HB2	1:B:118:LYS:NZ	2.29	0.47
1:A:161:ILE:HD12	1:A:161:ILE:N	2.30	0.47
1:A:113:LEU:HD11	1:A:117:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:GLN:N	1:B:200:GLN:OE1	2.46	0.47
1:D:166:PRO:O	1:D:170:ILE:HG13	2.14	0.47
1:A:6:PHE:HB3	1:A:207:LEU:HD21	1.95	0.47
1:B:179:GLU:OE1	1:C:136:GLN:OE1	2.33	0.47
1:B:187:GLU:O	1:B:191:ILE:HG13	2.15	0.47
1:B:166:PRO:HB2	1:B:168:PHE:CE1	2.50	0.47
1:B:17:LEU:O	1:B:21:LYS:HG3	2.14	0.46
1:C:177:THR:CG2	1:C:180:GLN:H	2.28	0.46
1:D:17:LEU:O	1:D:50:HIS:HE1	1.98	0.46
1:A:113:LEU:C	1:A:113:LEU:HD13	2.41	0.46
1:D:21:LYS:HA	1:D:54:LEU:HD13	1.96	0.46
1:C:71:ASN:ND2	1:C:79:SER:OG	2.49	0.46
1:A:21:LYS:HA	1:A:54:LEU:HD13	1.97	0.46
1:B:136:GLN:HB3	1:B:138:LYS:HE2	1.98	0.46
1:D:66:VAL:HG12	1:D:93:ILE:CD1	2.45	0.46
1:B:40:VAL:HG22	1:B:60:SER:HB2	1.99	0.45
1:A:21:LYS:O	1:A:25:ASN:ND2	2.50	0.45
1:C:11:TRP:CZ3	1:C:20:ILE:HD12	2.52	0.45
1:D:233:ASN:HA	1:D:236:LEU:HD23	1.97	0.45
1:A:113:LEU:HD13	1:A:117:LEU:HD22	1.98	0.45
1:A:233:ASN:CA	1:A:236:LEU:HD23	2.40	0.45
1:B:205:ARG:C	1:B:206:ILE:HD13	2.43	0.44
1:A:132:GLU:HG2	1:A:136:GLN:NE2	2.33	0.44
1:B:172:THR:C	1:B:174:LYS:H	2.25	0.44
1:D:134:ARG:HD2	1:D:168:PHE:CD1	2.53	0.44
1:B:139:THR:O	1:B:143:ILE:HG12	2.17	0.44
1:A:118:LYS:HB2	1:A:118:LYS:HZ2	1.82	0.44
1:A:177:THR:OG1	1:A:180:GLN:HG3	2.18	0.44
1:A:233:ASN:O	1:A:236:LEU:HD23	2.18	0.44
1:B:28:ASN:HB3	1:B:56:GLN:NE2	2.33	0.43
1:A:6:PHE:O	1:A:228:GLY:HA3	2.17	0.43
1:C:136:GLN:HA	1:C:136:GLN:NE2	2.33	0.43
1:C:161:ILE:N	1:C:161:ILE:HD12	2.34	0.43
1:B:4:LYS:HB3	1:B:205:ARG:HH21	1.83	0.43
1:D:161:ILE:HD12	1:D:161:ILE:N	2.34	0.43
1:A:139:THR:O	1:A:143:ILE:HG12	2.18	0.43
1:A:154:ILE:CD1	1:A:160:VAL:HG11	2.49	0.43
1:A:233:ASN:HA	1:A:236:LEU:CD2	2.42	0.42
1:A:233:ASN:C	1:A:236:LEU:HD23	2.44	0.42
1:C:28:ASN:HB3	1:C:56:GLN:NE2	2.34	0.42
1:C:67:SER:HB2	1:C:77:GLU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:PRO:O	1:B:170:ILE:HG12	2.20	0.42
1:D:9:ALA:HB1	1:D:235:SER:HB2	2.01	0.42
1:D:67:SER:HB2	1:D:77:GLU:HB3	2.00	0.42
1:A:5:TYR:O	1:A:37:LEU:HD12	2.20	0.42
1:A:193:LYS:HG3	1:A:198:GLU:HA	2.02	0.42
1:D:184:VAL:O	1:D:188:ILE:HG13	2.19	0.42
1:D:236:LEU:HD22	1:D:236:LEU:N	2.35	0.41
1:A:236:LEU:N	1:A:236:LEU:CD2	2.83	0.41
1:D:6:PHE:O	1:D:228:GLY:HA3	2.20	0.41
1:A:3:ARG:NH2	2:A:307:HOH:O	2.52	0.41
1:A:183:LEU:HG	2:A:414:HOH:O	2.21	0.41
1:D:108:ASP:O	1:D:112:LYS:HG3	2.20	0.41
1:B:236:LEU:N	1:B:236:LEU:CD2	2.83	0.41
1:C:40:VAL:HG22	1:C:60:SER:HB2	2.02	0.41
1:A:144:THR:HA	1:A:191:ILE:HD13	2.01	0.41
1:C:150:PHE:CD1	1:C:150:PHE:C	2.98	0.41
1:C:155:ASP:OD1	1:C:156:ASN:N	2.54	0.41
1:D:131:LEU:CD1	1:D:168:PHE:HB2	2.51	0.41
1:B:197:GLY:HA3	1:B:200:GLN:NE2	2.36	0.40
1:C:28:ASN:HB3	1:C:56:GLN:HE21	1.86	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	244/248 (98%)	239 (98%)	5 (2%)	0	100	100
1	B	244/248 (98%)	236 (97%)	8 (3%)	0	100	100
1	C	244/248 (98%)	234 (96%)	10 (4%)	0	100	100
1	D	244/248 (98%)	237 (97%)	7 (3%)	0	100	100
All	All	976/992 (98%)	946 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	219/220 (100%)	214 (98%)	5 (2%)	44	33
1	B	219/220 (100%)	213 (97%)	6 (3%)	39	27
1	C	219/220 (100%)	213 (97%)	6 (3%)	39	27
1	D	219/220 (100%)	216 (99%)	3 (1%)	59	52
All	All	876/880 (100%)	856 (98%)	20 (2%)	44	33

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	118	LYS
1	A	175	THR
1	A	215	GLU
1	A	236	LEU
1	B	117	LEU
1	B	118	LYS
1	B	175	THR
1	B	205	ARG
1	B	224	GLU
1	B	229	PHE
1	C	117	LEU
1	C	118	LYS
1	C	136	GLN
1	C	137	ASN
1	C	175	THR
1	C	229	PHE
1	D	117	LEU
1	D	118	LYS
1	D	229	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	29	ASN
1	A	50	HIS
1	A	71	ASN
1	A	87	ASN
1	A	114	GLN
1	A	120	ASN
1	A	159	ASN
1	A	222	GLN
1	B	29	ASN
1	B	56	GLN
1	B	71	ASN
1	B	87	ASN
1	B	159	ASN
1	B	222	GLN
1	C	29	ASN
1	C	71	ASN
1	C	87	ASN
1	C	120	ASN
1	C	159	ASN
1	C	222	GLN
1	D	14	ASN
1	D	29	ASN
1	D	50	HIS
1	D	56	GLN
1	D	71	ASN
1	D	87	ASN
1	D	159	ASN
1	D	200	GLN
1	D	203	GLN
1	D	223	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 [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

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	246/248 (99%)	0.04	9 (3%) 45 45	13, 19, 38, 47	0
1	B	246/248 (99%)	0.18	15 (6%) 27 25	13, 20, 42, 61	0
1	C	246/248 (99%)	0.34	18 (7%) 21 19	14, 21, 47, 84	0
1	D	246/248 (99%)	0.12	13 (5%) 32 31	14, 20, 42, 64	0
All	All	984/992 (99%)	0.17	55 (5%) 30 29	13, 20, 43, 84	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	173	GLY	10.6
1	C	171	GLY	6.8
1	C	172	THR	5.7
1	C	168	PHE	5.1
1	C	170	ILE	4.1
1	D	171	GLY	4.1
1	C	136	GLN	3.8
1	C	174	LYS	3.8
1	B	171	GLY	3.8
1	D	199	LYS	3.8
1	B	172	THR	3.8
1	B	173	GLY	3.6
1	B	215	GLU	3.5
1	B	136	GLN	3.4
1	B	53	LYS	3.3
1	A	155	ASP	3.2
1	B	155	ASP	3.2
1	B	175	THR	3.2
1	C	215	GLU	3.2
1	A	25	ASN	3.1
1	C	175	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	168	PHE	3.1
1	B	174	LYS	3.0
1	D	170	ILE	2.9
1	B	21	LYS	2.8
1	A	175	THR	2.8
1	A	3	ARG	2.7
1	C	211	SER	2.7
1	D	137	ASN	2.7
1	B	170	ILE	2.5
1	D	140	ILE	2.5
1	B	183	LEU	2.5
1	B	134	ARG	2.4
1	C	169	ALA	2.4
1	C	155	ASP	2.4
1	C	53	LYS	2.4
1	D	173	GLY	2.4
1	D	53	LYS	2.3
1	D	155	ASP	2.3
1	C	177	THR	2.3
1	A	199	LYS	2.3
1	D	3	ARG	2.2
1	A	195	THR	2.2
1	A	174	LYS	2.2
1	A	173	GLY	2.2
1	C	137	ASN	2.1
1	D	174	LYS	2.1
1	D	168	PHE	2.1
1	B	3	ARG	2.1
1	D	132	GLU	2.1
1	C	29	ASN	2.1
1	A	22	SER	2.0
1	C	110	ARG	2.0
1	C	199	LYS	2.0
1	D	57	SER	2.0

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 [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.