



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:14 AM EDT

PDB ID : 1TRE / pdb_00001tre
Title : THE STRUCTURE OF TRIOSEPHOSPHATE ISOMERASE FROM ES-
CHERICHIA COLI DETERMINED AT 2.6 ANGSTROM RESOLUTION
Authors : Noble, M.E.M.; Wierenga, R.K.
Deposited on : 1992-10-12
Resolution : 2.60 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

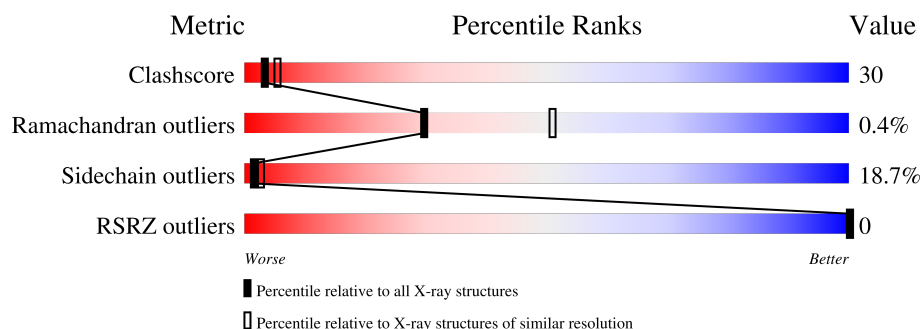
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	255	
1	B	255	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3943 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	255	Total	C	N	O	S	0	0	0
			1893	1187	334	362	10			
1	B	253	Total	C	N	O	S	0	0	0
			1878	1179	331	358	10			

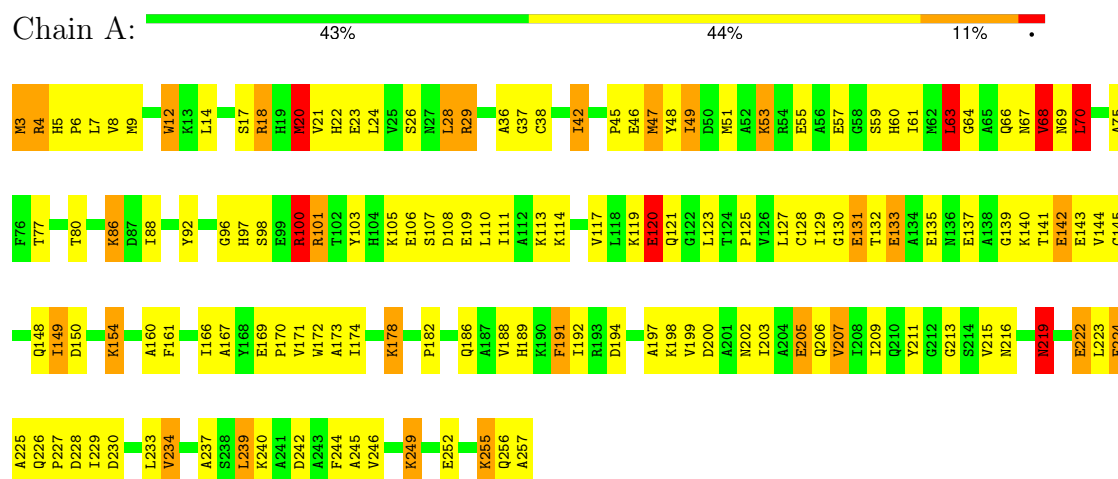
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	94	Total	O	0	0
			94	94		

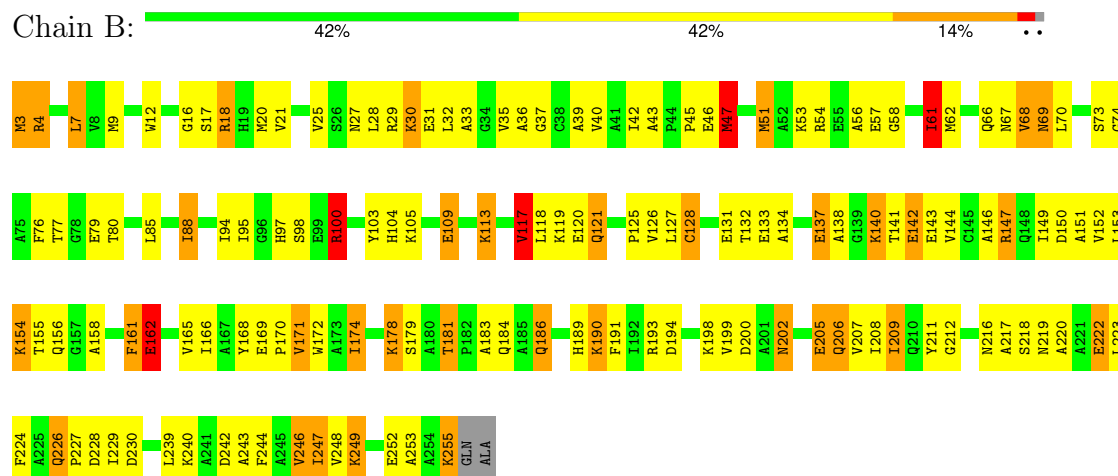
3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.69Å 46.78Å 151.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60 75.66 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60) 89.8 (75.66-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.60Å)	Xtriage
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.119 , (Not available) 0.124 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 141.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3943	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% 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	1.44	4/1922 (0.2%)	1.86	36/2597 (1.4%)
1	B	1.46	7/1907 (0.4%)	1.76	31/2578 (1.2%)
All	All	1.45	11/3829 (0.3%)	1.81	67/5175 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	6
All	All	0	7

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	CYS	N-CA	-8.19	1.36	1.46
1	A	75	ALA	CA-C	-7.18	1.44	1.53
1	B	199	VAL	CA-CB	-5.83	1.48	1.55
1	B	127	LEU	C-N	-5.66	1.25	1.33
1	A	167	ALA	C-O	5.51	1.30	1.24
1	A	61	ILE	CA-C	-5.47	1.46	1.52
1	B	200	ASP	CA-C	-5.42	1.46	1.52
1	B	33	ALA	C-O	5.42	1.30	1.23
1	B	121	GLN	CA-C	-5.14	1.45	1.52
1	A	7	LEU	CA-C	-5.12	1.46	1.52
1	B	30	LYS	N-CA	-5.09	1.40	1.46

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	LEU	O-C-N	10.23	134.84	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	PHE	CA-CB-CG	-9.53	104.27	113.80
1	A	68	VAL	CB-CA-C	-8.33	99.67	111.34
1	A	4	ARG	N-CA-C	7.56	121.25	108.02
1	A	103	TYR	N-CA-CB	7.51	120.96	110.07
1	A	29	ARG	N-CA-CB	7.07	120.47	109.94
1	A	101	ARG	NE-CZ-NH1	6.45	127.95	121.50
1	B	61	ILE	N-CA-CB	6.45	117.98	110.82
1	B	126	VAL	CA-C-N	-6.38	113.92	122.72
1	B	126	VAL	C-N-CA	-6.38	113.92	122.72
1	A	120	GLU	N-CA-C	-6.36	104.39	111.71
1	A	70	LEU	CA-C-N	-6.28	111.33	122.07
1	A	70	LEU	C-N-CA	-6.28	111.33	122.07
1	A	61	ILE	CB-CA-C	-6.15	103.89	111.08
1	B	69	ASN	CA-CB-CG	-6.12	106.48	112.60
1	A	191	PHE	N-CA-C	-6.10	104.71	111.36
1	A	5	HIS	CA-C-N	5.92	125.83	119.85
1	A	5	HIS	C-N-CA	5.92	125.83	119.85
1	B	226	GLN	CA-C-O	5.91	124.01	119.46
1	B	100	ARG	N-CA-CB	5.88	119.16	110.33
1	B	149	ILE	CB-CA-C	-5.87	104.37	112.24
1	A	20	MET	N-CA-CB	5.85	118.72	110.12
1	A	207	VAL	N-CA-C	5.77	117.02	109.58
1	A	101	ARG	CD-NE-CZ	5.74	132.44	124.40
1	A	103	TYR	N-CA-C	5.74	117.34	111.14
1	A	61	ILE	O-C-N	5.72	129.24	122.83
1	A	100	ARG	CA-C-N	5.67	128.67	120.79
1	A	100	ARG	C-N-CA	5.67	128.67	120.79
1	A	63	LEU	N-CA-C	5.63	118.91	109.95
1	B	131	GLU	N-CA-C	5.63	118.91	109.95
1	A	199	VAL	N-CA-C	5.63	116.41	110.72
1	B	161	PHE	CA-C-N	-5.63	114.70	122.30
1	B	161	PHE	C-N-CA	-5.63	114.70	122.30
1	B	4	ARG	CD-NE-CZ	-5.62	116.53	124.40
1	B	162	GLU	CB-CA-C	5.59	119.56	110.22
1	B	7	LEU	CA-C-N	-5.56	115.08	122.98
1	B	7	LEU	C-N-CA	-5.56	115.08	122.98
1	A	70	LEU	N-CA-CB	5.56	119.12	110.44
1	B	248	VAL	N-CA-C	5.48	115.68	110.42
1	A	68	VAL	N-CA-CB	5.46	118.57	112.45
1	B	244	PHE	CA-CB-CG	-5.45	108.35	113.80
1	B	146	ALA	N-CA-CB	-5.45	102.11	110.12
1	B	205	GLU	CB-CA-C	-5.43	100.58	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	GLU	CB-CA-C	-5.40	102.40	110.88
1	B	117	VAL	N-CA-C	5.38	115.59	110.42
1	B	79	GLU	CA-C-O	-5.35	115.78	121.94
1	B	61	ILE	CA-CB-CG2	5.31	119.52	110.50
1	B	151	ALA	CB-CA-C	5.30	119.69	110.68
1	A	144	VAL	N-CA-C	5.29	115.50	110.42
1	A	224	PHE	CA-CB-CG	-5.29	108.51	113.80
1	A	234	VAL	CB-CA-C	-5.28	103.53	110.98
1	A	101	ARG	NE-CZ-NH2	-5.28	114.45	119.20
1	A	67	ASN	CA-CB-CG	5.28	117.88	112.60
1	B	40	VAL	N-CA-CB	-5.23	104.71	111.82
1	A	228	ASP	CA-CB-CG	-5.22	107.38	112.60
1	B	47	MET	CA-C-N	-5.22	114.30	122.65
1	B	47	MET	C-N-CA	-5.22	114.30	122.65
1	A	244	PHE	CA-CB-CG	-5.21	108.59	113.80
1	B	25	VAL	N-CA-CB	5.19	116.95	110.47
1	A	7	LEU	N-CA-CB	5.18	118.90	110.77
1	A	219	ASN	CA-CB-CG	-5.15	107.45	112.60
1	B	162	GLU	N-CA-CB	5.12	118.78	110.17
1	B	183	ALA	CB-CA-C	-5.11	102.00	110.68
1	A	188	VAL	O-C-N	5.09	127.07	121.83
1	A	12	TRP	N-CA-CB	5.07	118.02	110.22
1	B	76	PHE	CA-CB-CG	-5.04	108.76	113.80
1	B	142	GLU	N-CA-C	5.02	117.40	111.33

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	ARG	Mainchain
1	B	121	GLN	Mainchain
1	B	162	GLU	Mainchain
1	B	181	THR	Mainchain
1	B	186	GLN	Mainchain
1	B	220	ALA	Mainchain
1	B	97	HIS	Mainchain

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	1893	0	1899	124	0
1	B	1878	0	1886	121	0
2	A	78	0	0	5	0
2	B	94	0	0	7	0
All	All	3943	0	3785	229	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 30.

All (229) 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:171:VAL:HA	1:B:174:ILE:HD12	1.27	1.09
1:A:150:ASP:HB3	1:A:154:LYS:HG2	1.40	1.03
1:B:3:MET:HE2	1:B:4:ARG:HG3	1.51	0.92
1:B:69:ASN:HD22	1:B:80:THR:H	0.99	0.92
1:A:129:ILE:HB	1:A:148:GLN:NE2	1.89	0.88
1:B:42:ILE:HG12	1:B:61:ILE:CD1	2.04	0.88
1:B:42:ILE:HG12	1:B:61:ILE:HD11	1.59	0.83
1:A:129:ILE:HB	1:A:148:GLN:HE21	1.41	0.83
1:A:189:HIS:CE1	1:A:209:ILE:HG22	2.14	0.83
1:B:166:ILE:HD12	1:B:207:VAL:HG11	1.59	0.83
1:B:147:ARG:HG3	1:B:147:ARG:HH11	1.44	0.82
1:A:130:GLY:H	1:A:148:GLN:HE22	1.23	0.82
1:B:171:VAL:CA	1:B:174:ILE:HD12	2.09	0.81
1:A:66:GLN:HG2	1:B:77:THR:HG23	1.61	0.81
1:B:3:MET:HE2	1:B:4:ARG:CG	2.10	0.81
1:A:239:LEU:C	1:A:240:LYS:HD2	2.05	0.81
1:A:53:LYS:NZ	1:B:18:ARG:HH22	1.79	0.80
1:A:53:LYS:NZ	1:B:18:ARG:NH2	2.29	0.80
1:A:60:HIS:HA	2:A:499:HOH:O	1.82	0.80
1:B:132:THR:HG22	1:B:134:ALA:H	1.45	0.79
1:A:186:GLN:CD	1:A:227:PRO:HD2	2.08	0.79
1:B:69:ASN:ND2	1:B:80:THR:H	1.79	0.79
1:A:53:LYS:CE	1:B:18:ARG:HH22	1.97	0.77
1:A:178:LYS:HD2	1:A:178:LYS:N	2.01	0.76
1:A:45:PRO:HB2	1:A:47:MET:HE3	1.68	0.75
1:A:96:GLY:O	1:A:101:ARG:HD2	1.87	0.74
1:A:182:PRO:HB2	1:A:226:GLN:HE21	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ALA:O	1:B:247:ILE:HD13	1.88	0.73
1:B:109:GLU:O	1:B:113:LYS:HD3	1.90	0.71
1:B:17:SER:O	1:B:21:VAL:HG23	1.91	0.71
1:B:138:ALA:HB3	1:B:140:LYS:HG3	1.71	0.71
1:B:37:GLY:HA3	1:B:252:GLU:HG3	1.73	0.69
1:A:178:LYS:HD2	1:A:178:LYS:H	1.55	0.69
1:B:45:PRO:HB2	1:B:47:MET:HE3	1.73	0.69
1:A:182:PRO:CB	1:A:226:GLN:HE21	2.05	0.69
1:A:9:MET:HG2	1:A:233:LEU:CD1	2.23	0.69
1:A:182:PRO:HB2	1:A:226:GLN:NE2	2.08	0.68
1:A:132:THR:HG23	1:A:135:GLU:OE1	1.94	0.68
1:B:69:ASN:HD22	1:B:80:THR:N	1.84	0.68
1:A:53:LYS:HE3	1:A:88:ILE:O	1.95	0.66
1:A:101:ARG:NH2	1:A:108:ASP:OD1	2.29	0.66
1:A:216:ASN:H	1:A:219:ASN:HB2	1.60	0.66
1:B:193:ARG:NH2	1:B:209:ILE:HG13	2.11	0.65
1:A:198:LYS:NZ	2:A:413:HOH:O	2.29	0.65
1:A:120:GLU:HG2	1:A:121:GLN:N	2.10	0.65
1:B:3:MET:N	2:B:481:HOH:O	2.30	0.65
1:A:123:LEU:O	1:A:125:PRO:HD3	1.97	0.64
1:A:4:ARG:HD3	1:A:205:GLU:O	1.96	0.64
1:A:36:ALA:N	1:A:252:GLU:OE2	2.29	0.64
1:A:131:GLU:OE2	1:A:141:THR:HG23	1.98	0.64
1:A:229:ILE:O	1:A:255:LYS:NZ	2.30	0.64
1:A:120:GLU:HG2	1:A:121:GLN:HG2	1.79	0.64
1:B:37:GLY:CA	1:B:252:GLU:HG3	2.28	0.64
1:B:181:THR:OG1	1:B:184:GLN:HG3	1.99	0.63
1:B:132:THR:HG22	1:B:134:ALA:N	2.14	0.63
1:B:95:ILE:O	1:B:128:CYS:HB2	1.99	0.62
1:A:142:GLU:HB3	1:A:191:PHE:CZ	2.35	0.62
1:B:45:PRO:CB	1:B:47:MET:HE3	2.29	0.62
1:B:70:LEU:HD22	1:B:113:LYS:HB3	1.82	0.61
1:A:53:LYS:HZ1	1:B:18:ARG:NH2	1.97	0.61
1:B:165:VAL:HG22	1:B:208:ILE:HB	1.82	0.61
1:B:154:LYS:NZ	1:B:155:THR:HG22	2.15	0.61
1:B:222:GLU:HB2	2:B:387:HOH:O	2.00	0.60
1:B:117:VAL:HG12	1:B:118:LEU:N	2.14	0.60
1:B:226:GLN:O	1:B:255:LYS:NZ	2.34	0.60
1:B:153:LEU:HD13	1:B:161:PHE:CE2	2.36	0.60
1:B:57:GLU:OE2	1:B:58:GLY:N	2.36	0.59
1:B:29:ARG:NH1	1:B:57:GLU:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:THR:C	1:A:172:TRP:HB3	2.29	0.57
1:B:30:LYS:HG3	1:B:31:GLU:N	2.19	0.57
1:A:29:ARG:NH1	1:A:57:GLU:O	2.38	0.57
1:A:106:GLU:CD	1:A:114:LYS:HZ2	2.11	0.57
1:A:53:LYS:HE2	1:B:18:ARG:HH22	1.69	0.56
1:A:96:GLY:O	1:A:128:CYS:HB2	2.06	0.55
1:A:130:GLY:H	1:A:148:GLN:NE2	1.98	0.55
1:A:234:VAL:HG11	1:A:237:ALA:HB3	1.88	0.55
1:B:193:ARG:NE	1:B:228:ASP:OD2	2.36	0.55
1:A:86:LYS:HE2	1:A:121:GLN:O	2.07	0.55
1:A:186:GLN:HB2	1:A:226:GLN:HB3	1.88	0.55
1:B:29:ARG:HH12	1:B:57:GLU:C	2.14	0.55
1:B:70:LEU:CD2	1:B:113:LYS:HB3	2.37	0.55
1:A:194:ASP:HA	1:A:197:ALA:HB3	1.89	0.54
1:A:18:ARG:O	1:A:51:MET:HE1	2.07	0.54
1:B:144:VAL:O	1:B:147:ARG:HB3	2.07	0.54
1:B:242:ASP:OD1	1:B:242:ASP:N	2.39	0.54
1:A:46:GLU:OE2	1:B:46:GLU:HB3	2.07	0.54
1:A:70:LEU:HD11	1:A:110:LEU:HD12	1.89	0.54
1:A:100:ARG:HB3	1:A:106:GLU:HG3	1.90	0.53
1:A:239:LEU:O	1:A:240:LYS:HD2	2.08	0.53
1:A:242:ASP:O	1:A:246:VAL:HG23	2.09	0.53
1:A:69:ASN:OD1	1:A:80:THR:N	2.40	0.53
1:B:7:LEU:HD12	1:B:39:ALA:O	2.08	0.53
1:A:53:LYS:HZ3	1:B:18:ARG:NH2	2.06	0.53
1:A:68:VAL:HG12	1:A:69:ASN:H	1.74	0.53
1:B:21:VAL:HG11	1:B:51:MET:HG2	1.90	0.53
1:B:27:ASN:O	1:B:31:GLU:HG2	2.09	0.53
1:A:211:TYR:CZ	1:A:213:GLY:HA3	2.43	0.53
1:B:103:TYR:HB2	1:B:104:HIS:CD2	2.45	0.52
1:A:189:HIS:O	1:A:192:ILE:HB	2.10	0.51
1:B:4:ARG:HB2	1:B:4:ARG:NH1	2.24	0.51
1:A:186:GLN:NE2	1:A:227:PRO:HD2	2.25	0.51
1:B:42:ILE:HG12	1:B:61:ILE:HD13	1.89	0.51
1:A:53:LYS:HA	1:A:63:LEU:HD13	1.91	0.51
1:B:147:ARG:HH11	1:B:147:ARG:CG	2.18	0.51
1:B:186:GLN:HB2	1:B:226:GLN:CB	2.40	0.51
1:A:107:SER:O	1:A:111:ILE:HG13	2.11	0.51
1:A:59:SER:HB2	2:A:332:HOH:O	2.10	0.51
1:B:4:ARG:NH1	1:B:230:ASP:OD1	2.44	0.51
1:A:145:CYS:O	1:A:149:ILE:HD12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:HE2	1:A:160:ALA:O	2.12	0.50
1:A:182:PRO:HG3	1:A:222:GLU:HB3	1.94	0.50
1:B:152:VAL:O	1:B:156:GLN:N	2.43	0.50
1:B:190:LYS:HD3	1:B:194:ASP:OD2	2.11	0.50
1:A:48:TYR:CE1	1:B:88:ILE:HD12	2.46	0.50
1:B:4:ARG:NE	1:B:205:GLU:O	2.45	0.49
1:B:154:LYS:HZ2	1:B:155:THR:HG22	1.76	0.49
1:A:46:GLU:CD	1:B:46:GLU:HB3	2.37	0.49
1:B:3:MET:HE2	1:B:4:ARG:HG2	1.93	0.49
1:A:166:ILE:O	1:A:209:ILE:HA	2.13	0.49
1:A:234:VAL:CG1	1:A:237:ALA:HB3	2.42	0.49
1:A:98:SER:N	1:A:169:GLU:OE2	2.41	0.49
1:B:181:THR:HG1	1:B:184:GLN:HG3	1.78	0.49
1:A:133:GLU:HA	1:A:172:TRP:CB	2.43	0.49
1:A:12:TRP:CD1	1:A:12:TRP:N	2.80	0.49
1:A:12:TRP:CH2	1:A:24:LEU:HD23	2.48	0.49
1:A:92:TYR:N	1:A:92:TYR:CD1	2.81	0.49
1:A:133:GLU:HA	1:A:172:TRP:HB2	1.94	0.49
1:A:194:ASP:O	1:A:197:ALA:HB3	2.13	0.48
1:B:153:LEU:HD11	1:B:158:ALA:HA	1.95	0.48
1:A:101:ARG:O	1:A:105:LYS:HA	2.14	0.48
1:A:9:MET:HG2	1:A:233:LEU:HD11	1.94	0.48
1:A:45:PRO:HB2	1:A:47:MET:CE	2.42	0.48
1:A:96:GLY:C	1:A:101:ARG:HD2	2.38	0.48
1:A:14:LEU:O	1:B:73:SER:HA	2.14	0.48
1:B:68:VAL:HG13	1:B:85:LEU:CD1	2.43	0.48
1:A:66:GLN:OE1	1:B:77:THR:HA	2.13	0.48
1:A:70:LEU:HD11	1:A:110:LEU:CD1	2.44	0.48
1:A:45:PRO:CB	1:A:47:MET:HE3	2.42	0.47
1:A:143:GLU:HB2	2:A:331:HOH:O	2.14	0.47
1:B:36:ALA:N	1:B:252:GLU:OE2	2.45	0.47
1:A:17:SER:O	1:A:21:VAL:HG23	2.13	0.47
1:A:3:MET:O	1:A:3:MET:HG3	2.09	0.47
1:A:172:TRP:CZ3	1:A:173:ALA:HB2	2.49	0.47
1:B:28:LEU:O	1:B:32:LEU:HG	2.14	0.47
1:A:14:LEU:HG	1:B:73:SER:HA	1.96	0.47
1:A:77:THR:HG23	1:B:66:GLN:HB3	1.96	0.47
1:B:66:GLN:O	1:B:67:ASN:HB2	2.13	0.47
1:B:168:TYR:O	1:B:212:GLY:N	2.43	0.47
1:A:60:HIS:HD2	2:A:499:HOH:O	1.97	0.47
1:A:170:PRO:HD2	1:A:213:GLY:CA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:HD13	1:B:161:PHE:HE2	1.80	0.46
1:B:35:VAL:HG12	1:B:36:ALA:N	2.30	0.46
1:B:118:LEU:HD12	1:B:125:PRO:HB3	1.98	0.46
1:A:256:GLN:O	1:A:257:ALA:HB3	2.16	0.46
1:B:4:ARG:HG2	2:B:441:HOH:O	2.16	0.46
1:A:22:HIS:HD2	1:A:55:GLU:OE2	1.99	0.45
1:B:103:TYR:HB2	1:B:104:HIS:HD2	1.81	0.45
1:A:154:LYS:N	1:A:154:LYS:HD2	2.30	0.45
1:B:223:LEU:HD12	1:B:223:LEU:HA	1.74	0.45
1:A:142:GLU:HB3	1:A:191:PHE:CE2	2.51	0.45
1:B:45:PRO:HB2	1:B:47:MET:CE	2.44	0.45
1:B:132:THR:CG2	1:B:133:GLU:N	2.80	0.45
1:B:154:LYS:NZ	1:B:155:THR:CG2	2.79	0.45
1:A:203:ILE:O	1:A:206:GLN:HB2	2.16	0.45
1:A:245:ALA:O	1:A:249:LYS:HG3	2.17	0.45
1:B:51:MET:HA	1:B:54:ARG:CZ	2.47	0.45
1:B:132:THR:HG22	1:B:133:GLU:N	2.32	0.45
1:A:224:PHE:O	1:A:255:LYS:HE3	2.17	0.44
1:B:16:GLY:HA2	1:B:20:MET:CE	2.48	0.44
1:A:37:GLY:N	1:A:252:GLU:OE2	2.48	0.44
1:A:28:LEU:HD12	1:A:28:LEU:HA	1.78	0.44
1:A:200:ASP:CG	1:A:203:ILE:HG12	2.42	0.44
1:B:189:HIS:ND1	1:B:229:ILE:HG12	2.33	0.44
1:A:130:GLY:HA3	1:A:169:GLU:O	2.17	0.44
1:B:170:PRO:O	1:B:174:ILE:HG13	2.18	0.44
1:B:224:PHE:O	1:B:255:LYS:HE3	2.18	0.43
1:A:17:SER:HA	1:A:48:TYR:OH	2.18	0.43
1:B:211:TYR:CD2	1:B:223:LEU:HD21	2.53	0.43
1:A:142:GLU:H	1:A:142:GLU:HG3	1.56	0.43
1:B:253:ALA:HB3	2:B:505:HOH:O	2.18	0.43
1:A:142:GLU:CB	1:A:191:PHE:CZ	3.00	0.43
1:B:186:GLN:HB2	1:B:226:GLN:HB3	1.99	0.43
1:A:174:ILE:O	1:A:174:ILE:HG22	2.19	0.43
1:B:154:LYS:HB3	1:B:154:LYS:HE3	1.60	0.43
1:B:226:GLN:HA	1:B:227:PRO:HD3	1.89	0.43
1:A:14:LEU:HB3	1:B:74:GLY:O	2.17	0.43
1:B:98:SER:HB3	1:B:169:GLU:OE2	2.19	0.43
1:A:97:HIS:O	1:A:101:ARG:HG3	2.18	0.42
1:A:186:GLN:OE1	1:A:227:PRO:HD2	2.19	0.42
1:A:150:ASP:CB	1:A:154:LYS:HG2	2.28	0.42
1:B:137:GLU:HB3	2:B:522:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLY:CA	1:A:111:ILE:HD13	2.50	0.42
1:A:233:LEU:HA	1:A:233:LEU:HD12	1.80	0.42
1:A:240:LYS:HD2	1:A:240:LYS:N	2.33	0.42
1:B:4:ARG:HD3	1:B:206:GLN:HA	2.01	0.42
1:B:142:GLU:HB3	1:B:191:PHE:CZ	2.54	0.42
1:B:249:LYS:HB3	2:B:353:HOH:O	2.19	0.42
1:B:217:ALA:HB2	1:B:246:VAL:HG21	2.01	0.42
1:B:61:ILE:HD12	1:B:62:MET:O	2.19	0.42
1:B:158:ALA:O	1:B:161:PHE:HB2	2.20	0.42
1:B:9:MET:HE2	1:B:43:ALA:HB2	2.01	0.42
1:B:178:LYS:HD3	1:B:178:LYS:HA	1.54	0.42
1:B:216:ASN:N	1:B:219:ASN:OD1	2.30	0.42
1:A:64:GLY:HA2	1:A:92:TYR:O	2.20	0.42
1:B:153:LEU:HA	1:B:153:LEU:HD12	1.61	0.42
1:B:3:MET:HE3	1:B:3:MET:O	2.19	0.41
1:B:154:LYS:HZ1	1:B:155:THR:HG22	1.83	0.41
1:B:171:VAL:H	1:B:171:VAL:HG23	1.49	0.41
1:A:77:THR:O	1:B:100:ARG:HD2	2.19	0.41
1:A:42:ILE:O	1:A:64:GLY:N	2.54	0.41
1:B:132:THR:HG23	2:B:523:HOH:O	2.20	0.41
1:A:110:LEU:O	1:A:113:LYS:HB2	2.20	0.41
1:A:202:ASN:O	1:A:206:GLN:OE1	2.38	0.41
1:B:12:TRP:N	1:B:12:TRP:CD1	2.86	0.41
1:A:8:VAL:HG23	1:A:38:CYS:SG	2.60	0.41
1:B:98:SER:HB3	1:B:169:GLU:CD	2.46	0.41
1:B:150:ASP:O	1:B:154:LYS:HB2	2.19	0.41
1:B:207:VAL:HG12	1:B:208:ILE:N	2.36	0.41
1:A:20:MET:HB2	1:A:20:MET:HE2	1.78	0.41
1:A:45:PRO:CB	1:A:47:MET:CE	2.99	0.41
1:A:137:GLU:C	1:A:139:GLY:H	2.29	0.41
1:A:23:GLU:O	1:A:26:SER:HB2	2.21	0.41
1:B:29:ARG:NH1	1:B:56:ALA:C	2.79	0.40
1:B:133:GLU:HA	1:B:172:TRP:CB	2.52	0.40
1:B:202:ASN:ND2	1:B:202:ASN:C	2.79	0.40
1:A:6:PRO:HG3	1:A:255:LYS:HG3	2.04	0.40
1:A:49:ILE:O	1:A:53:LYS:N	2.55	0.40
1:A:223:LEU:C	1:A:225:ALA:N	2.79	0.40
1:B:98:SER:N	1:B:169:GLU:OE2	2.51	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	253/255 (99%)	232 (92%)	20 (8%)	1 (0%)	30	51
1	B	251/255 (98%)	243 (97%)	7 (3%)	1 (0%)	30	51
All	All	504/510 (99%)	475 (94%)	27 (5%)	2 (0%)	30	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	THR
1	A	49	ILE

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	188/188 (100%)	157 (84%)	31 (16%)	2	4
1	B	187/188 (100%)	148 (79%)	39 (21%)	1	2
All	All	375/376 (100%)	305 (81%)	70 (19%)	1	3

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	20	MET
1	A	28	LEU
1	A	42	ILE

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Mol	Chain	Res	Type
1	A	47	MET
1	A	53	LYS
1	A	63	LEU
1	A	68	VAL
1	A	70	LEU
1	A	86	LYS
1	A	100	ARG
1	A	109	GLU
1	A	117	VAL
1	A	120	GLU
1	A	127	LEU
1	A	131	GLU
1	A	133	GLU
1	A	140	LYS
1	A	142	GLU
1	A	149	ILE
1	A	154	LYS
1	A	171	VAL
1	A	178	LYS
1	A	205	GLU
1	A	207	VAL
1	A	215	VAL
1	A	219	ASN
1	A	230	ASP
1	A	239	LEU
1	A	249	LYS
1	A	255	LYS
1	B	3	MET
1	B	18	ARG
1	B	47	MET
1	B	51	MET
1	B	53	LYS
1	B	61	ILE
1	B	68	VAL
1	B	88	ILE
1	B	94	ILE
1	B	100	ARG
1	B	105	LYS
1	B	109	GLU
1	B	113	LYS
1	B	117	VAL
1	B	119	LYS

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Mol	Chain	Res	Type
1	B	120	GLU
1	B	137	GLU
1	B	140	LYS
1	B	143	GLU
1	B	147	ARG
1	B	154	LYS
1	B	162	GLU
1	B	171	VAL
1	B	174	ILE
1	B	178	LYS
1	B	179	SER
1	B	190	LYS
1	B	198	LYS
1	B	202	ASN
1	B	206	GLN
1	B	209	ILE
1	B	218	SER
1	B	222	GLU
1	B	239	LEU
1	B	240	LYS
1	B	246	VAL
1	B	247	ILE
1	B	249	LYS
1	B	255	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	22	HIS
1	A	71	ASN
1	A	121	GLN
1	A	148	GLN
1	A	210	GLN
1	A	219	ASN
1	A	226	GLN
1	B	69	ASN
1	B	91	GLN
1	B	156	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	255/255 (100%)	-1.13	0 100 100	9, 29, 57, 94	0
1	B	253/255 (99%)	-1.17	0 100 100	11, 27, 57, 89	0
All	All	508/510 (99%)	-1.15	0 100 100	9, 28, 57, 94	0

There are no RSRZ outliers to report.

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.