Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:02 AM GMT

PDB ID	:	2VOM
Title	:	STRUCTURAL BASIS OF HUMAN TRIOSEPHOSPHATE ISOMERASE DEFICIENCY. MUTATION E104D AND CORRELATION TO SOLVENT PERTURBATION.
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Deposited on	:	2008-02-19
Resolution	:	1.85 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

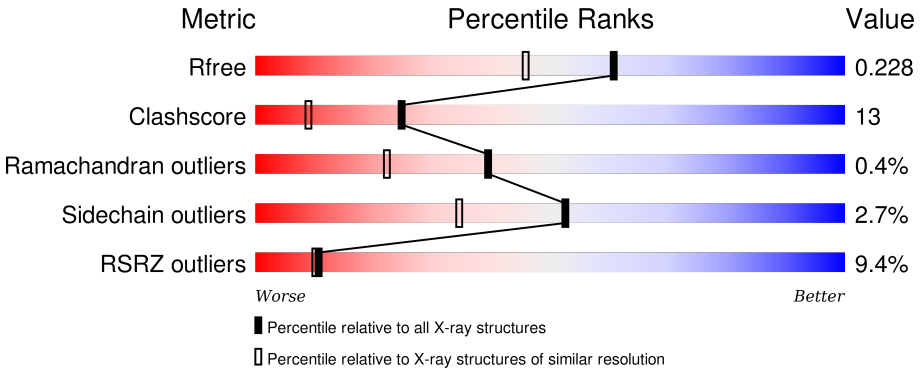
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	250	2% 79% 17%
1	B	250	6% 74% 24%
1	C	250	3% 77% 18%
1	D	250	26% 68% 27%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7983 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	245	Total	C	N	O	S	0	0	0
			1848	1169	321	351	7			
1	B	246	Total	C	N	O	S	0	0	0
			1854	1172	322	353	7			
1	C	245	Total	C	N	O	S	0	0	0
			1845	1167	320	351	7			
1	D	242	Total	C	N	O	S	0	0	0
			1825	1155	316	347	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	ASP	GLU	ENGINEERED MUTATION	UNP P60174
B	104	ASP	GLU	ENGINEERED MUTATION	UNP P60174
C	104	ASP	GLU	ENGINEERED MUTATION	UNP P60174
D	104	ASP	GLU	ENGINEERED MUTATION	UNP P60174

- Molecule 2 is water.

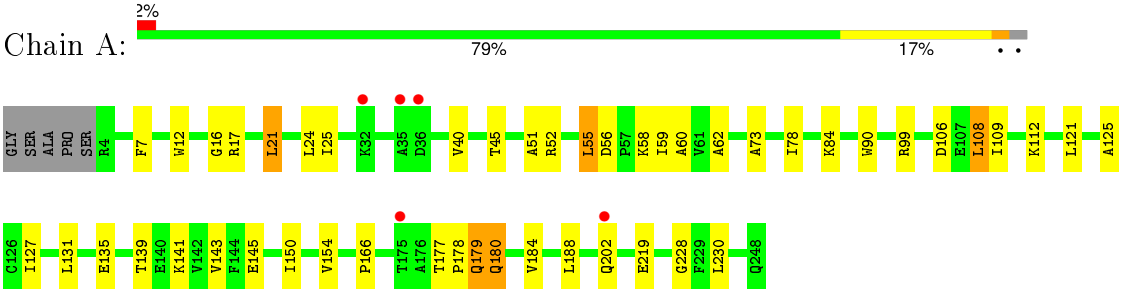
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	169	Total	O	0	0
			169	169		
2	B	181	Total	O	0	0
			181	181		
2	C	198	Total	O	0	0
			198	198		
2	D	63	Total	O	0	0
			63	63		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

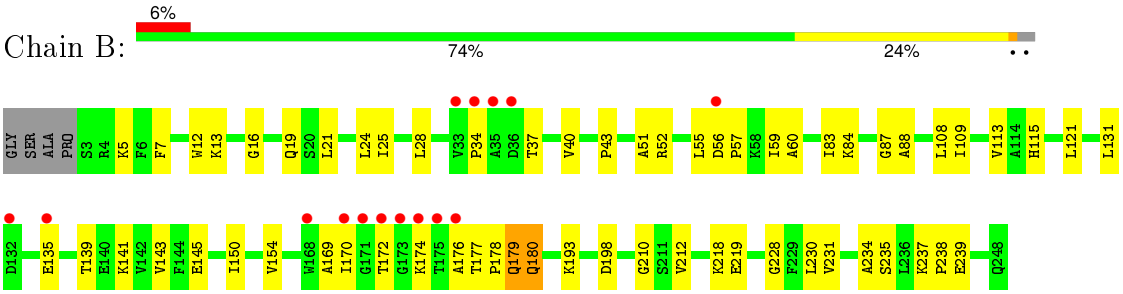
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A:



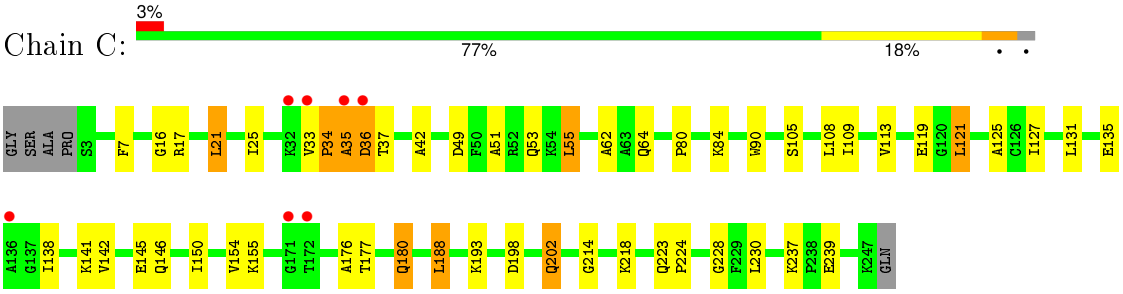
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B:



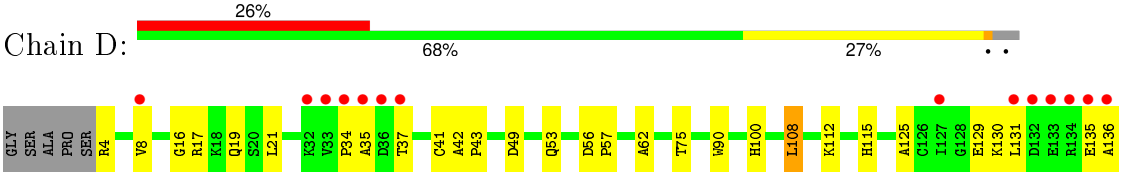
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

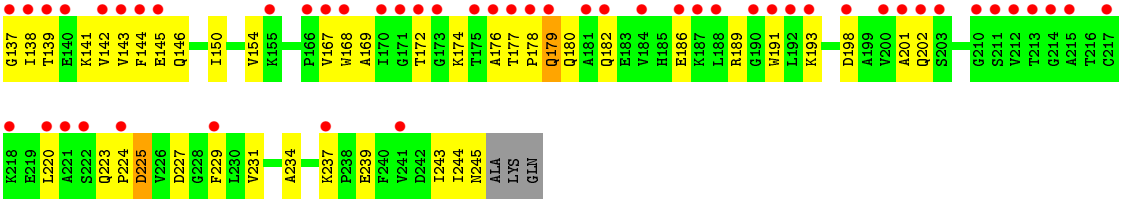
Chain C:



- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain D:




G137
I138
T139
E140
K141
V142
V143
F144
E145
Q146
I150
V154
K155
P166
V167
W168
A169
I170
G171
T172
G173
K174
T175
A176
T177
P178
Q179
Q180
A181
Q182
E183
V184
H185
E186
K187
L188
R189
G190
W191
L192
K193
D198
A199
V200
A201
Q202
S203
G210
S211
V212
T213
G214
A215
T216
C217
K218
E219
L220
A221
S222
Q223
P224
D225
V226
D227
G228
F229
L230
V231
A234
K237
P238
E239
F240
V241
D242
I243
I244
N245
ALA
LYS
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	320.52Å 47.29Å 68.96Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	50.00 – 1.85 48.91 – 1.85	Depositor EDS
% Data completeness (in resolution range)	92.8 (50.00-1.85) 92.8 (48.91-1.85)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 1.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.253 0.222 , 0.228	Depositor DCC
R_{free} test set	4102 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	18.7	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 81962 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7983	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 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.30	0/1882	0.59	1/2549 (0.0%)
1	B	0.30	0/1888	0.60	1/2557 (0.0%)
1	C	0.31	0/1879	0.62	1/2545 (0.0%)
1	D	0.28	0/1859	0.58	0/2519
All	All	0.30	0/7508	0.60	3/10170 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	230	LEU	N-CA-C	-5.84	95.23	111.00
1	B	230	LEU	N-CA-C	-5.44	96.31	111.00
1	A	230	LEU	N-CA-C	-5.31	96.65	111.00

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	1848	0	1857	37	0
1	B	1854	0	1862	49	0
1	C	1845	0	1854	41	0
1	D	1825	0	1831	64	0
2	A	169	0	0	3	0
2	B	181	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	198	0	0	5	0
2	D	63	0	0	2	0
All	All	7983	0	7404	189	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 13.

All (189) 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:125:ALA:HB1	1:D:150:ILE:HD13	1.55	0.86
1:A:25:ILE:HG23	1:A:55:LEU:HD13	1.62	0.82
1:D:179:GLN:HE21	1:D:179:GLN:H	1.27	0.80
1:B:179:GLN:H	1:B:179:GLN:NE2	1.83	0.77
1:A:84:LYS:HG3	1:A:121:LEU:HD13	1.67	0.77
1:D:8:VAL:HG21	1:D:244:ILE:HA	1.69	0.75
1:C:202:GLN:HG3	2:C:2172:HOH:O	1.86	0.75
1:D:131:LEU:HD22	1:D:172:THR:HB	1.69	0.74
1:D:150:ILE:O	1:D:154:VAL:HG23	1.89	0.73
1:A:131:LEU:O	1:A:135:GLU:HG2	1.90	0.72
1:D:179:GLN:NE2	1:D:179:GLN:H	1.87	0.71
1:A:179:GLN:H	1:A:179:GLN:NE2	1.87	0.71
1:A:177:THR:OG1	1:A:180:GLN:HG2	1.91	0.71
1:C:218:LYS:HB2	2:C:2183:HOH:O	1.90	0.71
1:B:131:LEU:HD11	1:B:174:LYS:HE3	1.74	0.69
1:B:25:ILE:HG12	1:B:55:LEU:HD13	1.75	0.69
1:B:177:THR:OG1	1:B:180:GLN:HG2	1.94	0.68
1:B:169:ALA:HA	1:B:174:LYS:HB2	1.74	0.68
1:C:141:LYS:O	1:C:145:GLU:HG3	1.94	0.68
1:B:239:GLU:HB2	2:B:2173:HOH:O	1.93	0.67
1:A:141:LYS:O	1:A:145:GLU:HG3	1.95	0.66
1:C:25:ILE:HG23	1:C:55:LEU:HD13	1.75	0.66
1:B:131:LEU:O	1:B:135:GLU:HG2	1.97	0.65
1:C:25:ILE:HG23	1:C:55:LEU:CD1	2.27	0.64
1:D:182:GLN:OE1	1:D:223:GLN:HB3	1.98	0.64
1:C:155:LYS:HG2	2:C:2134:HOH:O	1.98	0.62
1:A:25:ILE:HG23	1:A:55:LEU:CD1	2.29	0.62
1:D:129:GLU:O	1:D:167:VAL:HB	2.00	0.62
1:D:62:ALA:HB2	1:D:90:TRP:HB2	1.81	0.62
1:B:24:LEU:HD21	1:B:235:SER:O	2.00	0.61
1:D:176:ALA:HA	1:D:180:GLN:OE1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LYS:HG3	1:C:121:LEU:HD13	1.83	0.61
1:B:28:LEU:HB3	1:B:59:ILE:CD1	2.31	0.60
1:B:12:TRP:CZ3	1:B:43:PRO:HB3	2.36	0.60
1:D:179:GLN:NE2	1:D:179:GLN:N	2.50	0.60
1:B:51:ALA:O	1:B:55:LEU:HB2	2.02	0.60
1:D:179:GLN:N	1:D:179:GLN:HE21	2.00	0.60
1:D:49:ASP:O	1:D:53:GLN:HG3	2.01	0.59
1:D:193:LYS:HE2	1:D:198:ASP:OD2	2.03	0.59
1:D:16:GLY:HA3	1:D:21:LEU:CD1	2.33	0.58
1:A:62:ALA:HB2	1:A:90:TRP:HB2	1.84	0.58
1:D:100:HIS:CD2	1:D:130:LYS:HD2	2.39	0.58
1:C:84:LYS:HG3	1:C:121:LEU:CD1	2.33	0.58
1:B:56:ASP:CG	1:B:57:PRO:HD2	2.24	0.58
1:A:177:THR:HB	1:A:179:GLN:NE2	2.19	0.57
1:A:127:ILE:HD11	1:A:188:LEU:HD21	1.86	0.57
1:C:237:LYS:HG3	1:C:239:GLU:HB3	1.87	0.57
1:C:125:ALA:HB1	1:C:150:ILE:HD13	1.87	0.57
1:A:125:ALA:HB1	1:A:150:ILE:HD13	1.87	0.56
1:B:150:ILE:O	1:B:154:VAL:HG23	2.05	0.56
1:C:177:THR:OG1	1:C:180:GLN:HG2	2.04	0.56
1:D:186:GLU:HA	1:D:225:ASP:OD2	2.06	0.56
1:B:40:VAL:HG22	1:B:60:ALA:HB3	1.86	0.56
1:B:193:LYS:HE2	1:B:198:ASP:OD2	2.06	0.56
1:A:7:PHE:O	1:A:228:GLY:HA3	2.07	0.55
1:D:108:LEU:HD22	1:D:112:LYS:HE3	1.88	0.55
1:D:142:VAL:O	1:D:146:GLN:HG3	2.06	0.55
1:B:177:THR:HB	1:B:179:GLN:HE22	1.72	0.55
1:D:231:VAL:CG1	1:D:234:ALA:HB3	2.36	0.55
1:D:177:THR:H	1:D:180:GLN:CG	2.21	0.54
1:B:177:THR:HB	1:B:179:GLN:NE2	2.23	0.54
1:C:127:ILE:HD11	1:C:188:LEU:HD21	1.88	0.54
1:C:7:PHE:O	1:C:228:GLY:HA3	2.08	0.54
1:C:150:ILE:O	1:C:154:VAL:HG23	2.06	0.54
1:A:56:ASP:OD2	1:A:58:LYS:HG2	2.08	0.53
1:A:166:PRO:HG2	2:A:2123:HOH:O	2.07	0.53
1:B:177:THR:H	1:B:180:GLN:CG	2.22	0.53
1:D:139:THR:O	1:D:143:VAL:HG22	2.08	0.53
1:B:16:GLY:HA2	2:B:2017:HOH:O	2.10	0.52
1:A:145:GLU:HG3	2:A:2100:HOH:O	2.09	0.52
1:C:176:ALA:HA	1:C:180:GLN:OE1	2.09	0.52
1:B:19:GLN:HB3	2:B:2016:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LYS:O	1:B:145:GLU:HG3	2.09	0.52
1:C:34:PRO:O	1:C:37:THR:N	2.42	0.52
1:D:16:GLY:HA3	1:D:21:LEU:HD13	1.91	0.51
1:C:34:PRO:O	1:C:36:ASP:N	2.43	0.51
1:D:131:LEU:N	1:D:168:TRP:HA	2.25	0.51
1:D:193:LYS:N	1:D:201:ALA:HB2	2.26	0.51
1:B:218:LYS:HB2	2:B:2160:HOH:O	2.11	0.51
1:B:16:GLY:HA3	1:B:21:LEU:HD11	1.93	0.50
1:C:214:GLY:H	1:C:239:GLU:CD	2.15	0.50
1:C:80:PRO:HB2	1:C:119:GLU:HG3	1.92	0.50
1:B:56:ASP:OD1	1:B:57:PRO:HD2	2.11	0.50
1:A:40:VAL:HG22	1:A:60:ALA:HB3	1.92	0.50
1:D:4:ARG:HD2	1:D:227:ASP:CG	2.32	0.50
1:B:16:GLY:HA3	1:B:21:LEU:CD1	2.42	0.50
1:D:189:ARG:NH2	1:D:227:ASP:OD2	2.45	0.50
1:D:135:GLU:C	1:D:137:GLY:H	2.15	0.49
1:D:169:ALA:HA	1:D:174:LYS:HB2	1.93	0.49
1:D:178:PRO:HB3	1:D:220:LEU:HD23	1.95	0.49
1:A:58:LYS:HG3	1:A:59:ILE:HG13	1.93	0.49
1:A:127:ILE:HD11	1:A:188:LEU:CD2	2.42	0.49
1:B:109:ILE:O	1:B:113:VAL:HG23	2.12	0.49
1:D:17:ARG:O	1:D:21:LEU:HB2	2.12	0.49
1:A:184:VAL:O	1:A:188:LEU:HD13	2.13	0.49
1:D:19:GLN:HB3	2:D:2009:HOH:O	2.13	0.49
1:C:105:SER:O	1:C:109:ILE:HG13	2.13	0.49
1:C:177:THR:H	1:C:180:GLN:CG	2.26	0.48
1:B:84:LYS:CG	1:B:121:LEU:HD13	2.43	0.48
1:D:237:LYS:HG3	1:D:239:GLU:HB3	1.94	0.48
1:C:155:LYS:HD3	2:C:2133:HOH:O	2.13	0.48
1:B:25:ILE:HG23	1:B:55:LEU:CD1	2.43	0.48
1:A:177:THR:HB	1:A:179:GLN:HE22	1.77	0.47
1:C:34:PRO:O	1:C:35:ALA:C	2.52	0.47
1:D:141:LYS:O	1:D:145:GLU:HG3	2.14	0.47
1:B:84:LYS:HG2	1:B:121:LEU:HD13	1.96	0.47
1:D:177:THR:H	1:D:180:GLN:HG2	1.79	0.47
1:A:17:ARG:O	1:A:21:LEU:HB2	2.14	0.47
1:C:16:GLY:HA3	1:C:21:LEU:HD13	1.96	0.47
1:A:24:LEU:HD12	2:A:2024:HOH:O	2.13	0.47
1:C:109:ILE:O	1:C:113:VAL:HG23	2.15	0.47
1:C:62:ALA:HB2	1:C:90:TRP:HB2	1.96	0.47
1:B:131:LEU:HD22	1:B:172:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ILE:HA	2:C:2120:HOH:O	2.16	0.46
1:B:12:TRP:CZ3	1:B:21:LEU:HG	2.51	0.46
1:A:12:TRP:CZ3	1:A:21:LEU:HG	2.50	0.46
1:B:178:PRO:HG3	1:B:219:GLU:OE2	2.15	0.46
1:B:237:LYS:HB2	1:B:238:PRO:HD2	1.98	0.45
1:D:244:ILE:HG22	1:D:244:ILE:O	2.15	0.45
1:A:108:LEU:HD22	1:A:112:LYS:HE3	1.98	0.45
1:C:33:VAL:O	1:C:33:VAL:HG13	2.15	0.45
1:A:51:ALA:O	1:A:55:LEU:HB2	2.16	0.45
1:D:177:THR:HG23	1:D:180:GLN:OE1	2.17	0.45
1:B:139:THR:O	1:B:143:VAL:HG22	2.16	0.45
1:D:131:LEU:O	1:D:135:GLU:HG2	2.17	0.45
1:D:125:ALA:HB1	1:D:150:ILE:CD1	2.37	0.45
1:B:179:GLN:H	1:B:179:GLN:HE21	1.62	0.45
1:D:144:PHE:CE1	1:D:191:TRP:HB2	2.52	0.45
1:B:170:ILE:O	1:B:172:THR:HG23	2.17	0.45
1:D:16:GLY:HA3	1:D:21:LEU:HD11	1.99	0.44
1:D:56:ASP:CG	1:D:57:PRO:HD2	2.37	0.44
1:A:16:GLY:HA3	1:A:21:LEU:HD13	1.99	0.44
1:A:45:THR:HG23	1:A:78:ILE:HD13	1.99	0.44
1:C:51:ALA:O	1:C:55:LEU:HB2	2.18	0.44
1:A:178:PRO:HG3	1:A:219:GLU:OE2	2.18	0.44
1:B:25:ILE:HG23	1:B:55:LEU:HD13	2.00	0.44
1:D:177:THR:HB	1:D:179:GLN:NE2	2.33	0.44
1:D:237:LYS:HB3	1:D:237:LYS:HE2	1.84	0.44
1:D:41:CYS:O	1:D:43:PRO:HD3	2.17	0.44
1:A:125:ALA:HB1	1:A:150:ILE:CD1	2.48	0.43
1:C:25:ILE:HG12	1:C:55:LEU:HD13	2.00	0.43
1:C:35:ALA:C	1:C:37:THR:H	2.21	0.43
1:D:34:PRO:O	1:D:37:THR:N	2.50	0.43
1:B:210:GLY:O	1:B:212:VAL:HG23	2.18	0.43
1:D:62:ALA:CB	1:D:90:TRP:HB2	2.48	0.43
1:B:52:ARG:HG2	1:B:87:GLY:HA3	2.00	0.43
1:C:17:ARG:O	1:C:21:LEU:HB2	2.18	0.43
1:B:34:PRO:HB2	1:B:37:THR:OG1	2.19	0.43
1:D:177:THR:C	1:D:179:GLN:N	2.71	0.43
1:D:35:ALA:C	1:D:37:THR:H	2.22	0.43
1:B:115:HIS:HD2	2:B:2046:HOH:O	2.02	0.43
1:C:180:GLN:HE21	1:C:180:GLN:HB3	1.61	0.42
1:D:220:LEU:HB3	1:D:229:PHE:HE1	1.85	0.42
1:D:138:ILE:HB	1:D:141:LYS:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:THR:OG1	1:D:180:GLN:HG2	2.19	0.42
1:B:28:LEU:HB3	1:B:59:ILE:HD11	1.98	0.42
1:D:223:GLN:HA	1:D:224:PRO:HD3	1.84	0.42
1:D:129:GLU:OE2	1:D:139:THR:HG23	2.20	0.42
1:D:115:HIS:HD2	2:D:2017:HOH:O	2.01	0.42
1:D:177:THR:C	1:D:179:GLN:H	2.22	0.42
1:B:176:ALA:HA	1:B:180:GLN:OE1	2.20	0.42
1:A:99:ARG:HG2	1:A:109:ILE:HD11	2.00	0.42
1:A:84:LYS:CG	1:A:121:LEU:HD13	2.44	0.42
1:D:220:LEU:HB3	1:D:229:PHE:CE1	2.55	0.42
1:C:142:VAL:O	1:C:146:GLN:HG3	2.20	0.42
1:A:180:GLN:H	1:A:180:GLN:HG2	1.70	0.42
1:B:7:PHE:O	1:B:228:GLY:HA3	2.20	0.41
1:D:42:ALA:HA	1:D:62:ALA:O	2.20	0.41
1:D:231:VAL:HG11	1:D:234:ALA:HB3	2.02	0.41
1:A:139:THR:O	1:A:143:VAL:HG22	2.20	0.41
1:B:83:ILE:CG2	1:B:88:ALA:HB3	2.50	0.41
1:C:131:LEU:O	1:C:135:GLU:HG3	2.20	0.41
1:D:177:THR:O	1:D:179:GLN:N	2.54	0.41
1:D:4:ARG:HD2	1:D:227:ASP:OD1	2.21	0.41
1:B:52:ARG:HA	1:B:52:ARG:NE	2.36	0.41
1:C:49:ASP:O	1:C:53:GLN:HG3	2.20	0.41
1:A:179:GLN:HE21	1:A:179:GLN:H	1.66	0.41
1:C:64:GLN:HB3	1:D:75:THR:CG2	2.51	0.41
1:C:177:THR:H	1:C:180:GLN:CD	2.23	0.41
1:B:5:LYS:NZ	1:B:5:LYS:HB2	2.34	0.41
1:A:52:ARG:HA	1:A:52:ARG:NE	2.35	0.41
1:C:42:ALA:HA	1:C:62:ALA:O	2.21	0.40
1:B:231:VAL:CG1	1:B:234:ALA:HB3	2.51	0.40
1:C:193:LYS:HG3	1:C:198:ASP:OD1	2.21	0.40
1:A:73:ALA:HA	1:B:13:LYS:HD3	2.04	0.40
1:A:150:ILE:O	1:A:154:VAL:HG23	2.21	0.40
1:C:223:GLN:HA	1:C:224:PRO:HD3	1.95	0.40
1:D:243:ILE:C	1:D:245:ASN:H	2.25	0.40
1:D:139:THR:O	1:D:143:VAL:HG13	2.21	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	243/250 (97%)	237 (98%)	6 (2%)	0	100 100
1	B	244/250 (98%)	234 (96%)	10 (4%)	0	100 100
1	C	243/250 (97%)	233 (96%)	7 (3%)	3 (1%)	16 4
1	D	240/250 (96%)	224 (93%)	15 (6%)	1 (0%)	39 22
All	All	970/1000 (97%)	928 (96%)	38 (4%)	4 (0%)	39 22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	35	ALA
1	D	136	ALA
1	C	36	ASP
1	C	34	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	193/196 (98%)	186 (96%)	7 (4%)	42 21
1	B	194/196 (99%)	191 (98%)	3 (2%)	72 60
1	C	193/196 (98%)	186 (96%)	7 (4%)	42 21
1	D	191/196 (97%)	187 (98%)	4 (2%)	61 45
All	All	771/784 (98%)	750 (97%)	21 (3%)	52 34

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	55	LEU
1	A	106	ASP
1	A	108	LEU
1	A	179	GLN
1	A	180	GLN
1	A	202	GLN
1	B	108	LEU
1	B	179	GLN
1	B	180	GLN
1	C	21	LEU
1	C	55	LEU
1	C	108	LEU
1	C	121	LEU
1	C	180	GLN
1	C	188	LEU
1	C	202	GLN
1	D	108	LEU
1	D	179	GLN
1	D	202	GLN
1	D	225	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	115	HIS
1	A	179	GLN
1	B	53	GLN
1	B	115	HIS
1	B	179	GLN
1	B	248	GLN
1	C	19	GLN
1	C	53	GLN
1	C	100	HIS
1	C	115	HIS
1	D	53	GLN
1	D	100	HIS
1	D	115	HIS
1	D	179	GLN
1	D	195	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	245/250 (98%)	0.02	5 (2%) 68 67	11, 20, 38, 50	0
1	B	246/250 (98%)	0.30	15 (6%) 25 23	10, 20, 38, 48	0
1	C	245/250 (98%)	0.25	7 (2%) 55 52	9, 18, 36, 48	0
1	D	242/250 (96%)	1.25	65 (26%) 1 0	12, 26, 43, 49	0
All	All	978/1000 (97%)	0.45	92 (9%) 11 10	9, 21, 41, 50	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	THR	8.5
1	B	172	THR	7.1
1	D	170	ILE	7.1
1	D	172	THR	6.8
1	D	35	ALA	6.7
1	B	174	LYS	5.9
1	B	170	ILE	5.9
1	D	144	PHE	5.6
1	D	198	ASP	5.4
1	D	176	ALA	5.0
1	D	175	THR	5.0
1	B	171	GLY	4.9
1	A	35	ALA	4.8
1	C	35	ALA	4.8
1	B	33	VAL	4.7
1	D	177	THR	4.6
1	D	179	GLN	4.5
1	B	173	GLY	4.5
1	D	131	LEU	4.2
1	D	137	GLY	4.1
1	D	140	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	168	TRP	3.9
1	D	191	TRP	3.9
1	D	229	PHE	3.9
1	D	36	ASP	3.9
1	D	173	GLY	3.8
1	D	178	PRO	3.8
1	D	139	THR	3.8
1	D	213	THR	3.8
1	D	222	SER	3.7
1	D	33	VAL	3.7
1	D	143	VAL	3.7
1	D	212	VAL	3.7
1	D	215	ALA	3.7
1	D	145	GLU	3.7
1	D	202	GLN	3.6
1	D	37	THR	3.5
1	B	35	ALA	3.5
1	D	138	ILE	3.4
1	D	135	GLU	3.4
1	D	220	LEU	3.4
1	C	172	THR	3.4
1	A	36	ASP	3.1
1	D	193	LYS	3.1
1	D	32	LYS	3.1
1	B	168	TRP	3.1
1	D	200	VAL	3.1
1	D	217	CYS	3.1
1	D	188	LEU	3.0
1	B	56	ASP	3.0
1	D	136	ALA	2.9
1	D	127	ILE	2.9
1	B	34	PRO	2.9
1	D	142	VAL	2.9
1	A	32	LYS	2.9
1	D	171	GLY	2.8
1	C	33	VAL	2.8
1	B	36	ASP	2.8
1	D	210	GLY	2.8
1	D	184	VAL	2.7
1	C	171	GLY	2.7
1	D	221	ALA	2.6
1	D	186	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	211	SER	2.6
1	D	167	VAL	2.6
1	D	181	ALA	2.6
1	D	190	GLY	2.6
1	B	135	GLU	2.6
1	D	34	PRO	2.5
1	D	182	GLN	2.5
1	D	201	ALA	2.5
1	C	136	ALA	2.5
1	D	214	GLY	2.5
1	D	8	VAL	2.5
1	D	192	LEU	2.5
1	D	134	ARG	2.4
1	D	241	VAL	2.4
1	D	155	LYS	2.4
1	D	224	PRO	2.4
1	A	175	THR	2.3
1	D	187	LYS	2.3
1	D	132	ASP	2.3
1	D	203	SER	2.2
1	C	32	LYS	2.2
1	D	237	LYS	2.2
1	C	36	ASP	2.2
1	B	176	ALA	2.2
1	D	166	PRO	2.2
1	B	132	ASP	2.2
1	D	218	LYS	2.2
1	A	202	GLN	2.1
1	D	133	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates 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.