Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:04 AM GMT

PDB ID	:	2FIQ
Title	:	Crystal structure of putative tagatose 6-phosphate kinase
Authors	:	Ramagopal, U.A.; Fedorov, E.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2005-12-30
Resolution	:	2.25 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:

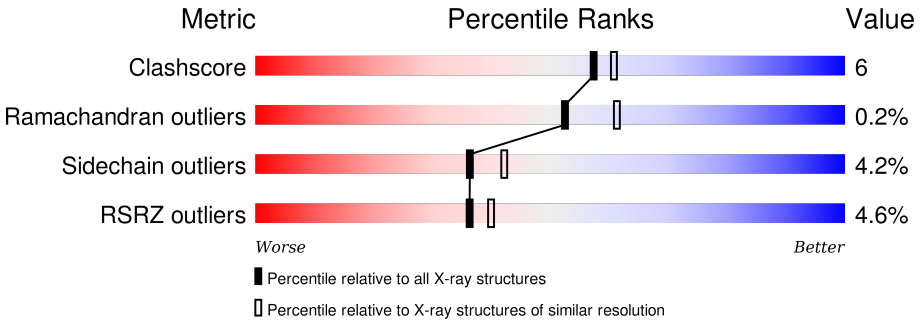
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.25 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	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	420	3% 84% 12%
1	B	420	8% 81% 14%
1	C	420	4% 86% 10%
1	D	420	2% 82% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13793 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 putative tagatose 6-phosphate kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	Se	0	3	0
			3270	2074	570	607	9	10			
1	B	408	Total	C	N	O	S	Se	0	3	0
			3242	2058	565	601	8	10			
1	C	410	Total	C	N	O	S	Se	0	7	0
			3285	2084	576	606	9	10			
1	D	409	Total	C	N	O	S	Se	4	4	0
			3272	2075	572	606	9	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P37191
A	59	MSE	MET	MODIFIED RESIDUE	UNP P37191
A	103	MSE	MET	MODIFIED RESIDUE	UNP P37191
A	127	MSE	MET	MODIFIED RESIDUE	UNP P37191
A	252	MSE	MET	MODIFIED RESIDUE	UNP P37191
A	319	MSE	MET	MODIFIED RESIDUE	UNP P37191
A	365	MSE	MET	MODIFIED RESIDUE	UNP P37191
A	366	MSE	MET	MODIFIED RESIDUE	UNP P37191
A	378	MSE	MET	MODIFIED RESIDUE	UNP P37191
A	404	MSE	MET	MODIFIED RESIDUE	UNP P37191
B	1	MSE	MET	MODIFIED RESIDUE	UNP P37191
B	59	MSE	MET	MODIFIED RESIDUE	UNP P37191
B	103	MSE	MET	MODIFIED RESIDUE	UNP P37191
B	127	MSE	MET	MODIFIED RESIDUE	UNP P37191
B	252	MSE	MET	MODIFIED RESIDUE	UNP P37191
B	319	MSE	MET	MODIFIED RESIDUE	UNP P37191
B	365	MSE	MET	MODIFIED RESIDUE	UNP P37191
B	366	MSE	MET	MODIFIED RESIDUE	UNP P37191
B	378	MSE	MET	MODIFIED RESIDUE	UNP P37191
B	404	MSE	MET	MODIFIED RESIDUE	UNP P37191
C	1	MSE	MET	MODIFIED RESIDUE	UNP P37191

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Chain	Residue	Modelled	Actual	Comment	Reference
C	59	MSE	MET	MODIFIED RESIDUE	UNP P37191
C	103	MSE	MET	MODIFIED RESIDUE	UNP P37191
C	127	MSE	MET	MODIFIED RESIDUE	UNP P37191
C	252	MSE	MET	MODIFIED RESIDUE	UNP P37191
C	319	MSE	MET	MODIFIED RESIDUE	UNP P37191
C	365	MSE	MET	MODIFIED RESIDUE	UNP P37191
C	366	MSE	MET	MODIFIED RESIDUE	UNP P37191
C	378	MSE	MET	MODIFIED RESIDUE	UNP P37191
C	404	MSE	MET	MODIFIED RESIDUE	UNP P37191
D	1	MSE	MET	MODIFIED RESIDUE	UNP P37191
D	59	MSE	MET	MODIFIED RESIDUE	UNP P37191
D	103	MSE	MET	MODIFIED RESIDUE	UNP P37191
D	127	MSE	MET	MODIFIED RESIDUE	UNP P37191
D	252	MSE	MET	MODIFIED RESIDUE	UNP P37191
D	319	MSE	MET	MODIFIED RESIDUE	UNP P37191
D	365	MSE	MET	MODIFIED RESIDUE	UNP P37191
D	366	MSE	MET	MODIFIED RESIDUE	UNP P37191
D	378	MSE	MET	MODIFIED RESIDUE	UNP P37191
D	404	MSE	MET	MODIFIED RESIDUE	UNP P37191

- Molecule 2 is water.

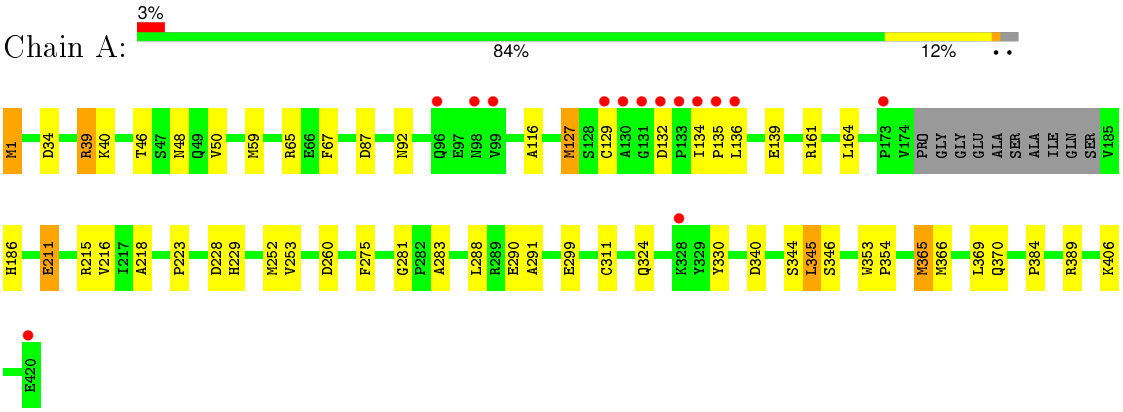
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	211	Total O 211 211	0	0
2	B	139	Total O 139 139	0	0
2	C	174	Total O 174 174	0	0
2	D	200	Total O 200 200	0	0

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.

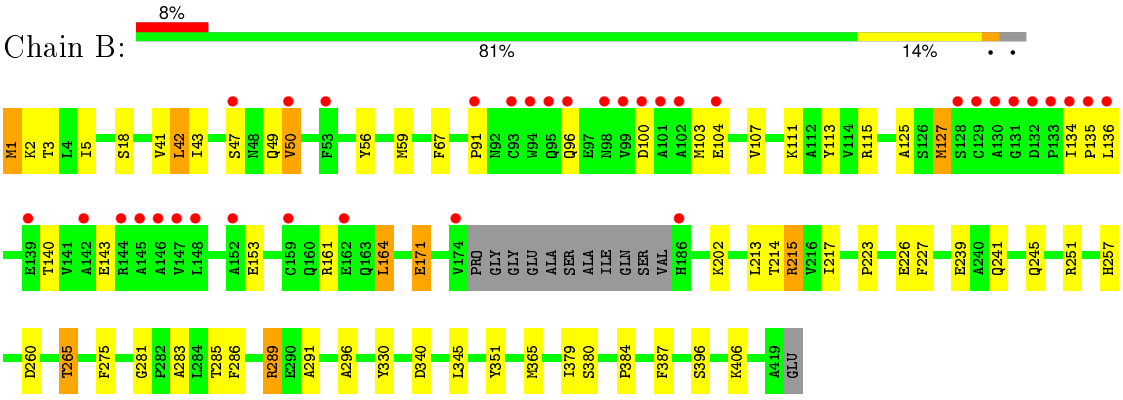
- Molecule 1: putative tagatose 6-phosphate kinase 1

Chain A:



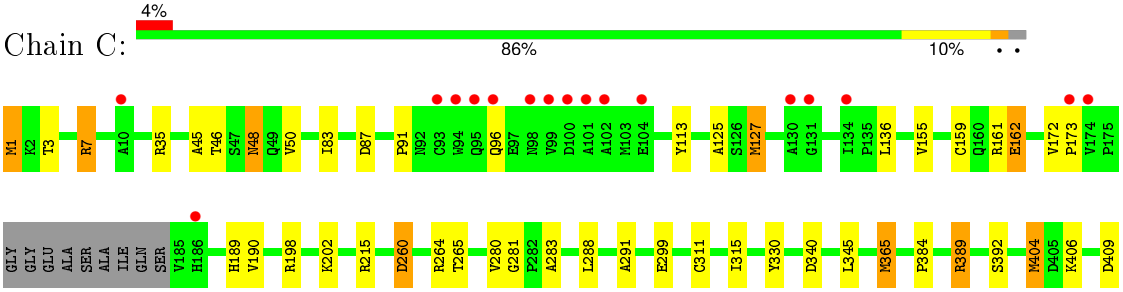
- Molecule 1: putative tagatose 6-phosphate kinase 1

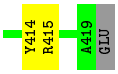
Chain B:



- Molecule 1: putative tagatose 6-phosphate kinase 1

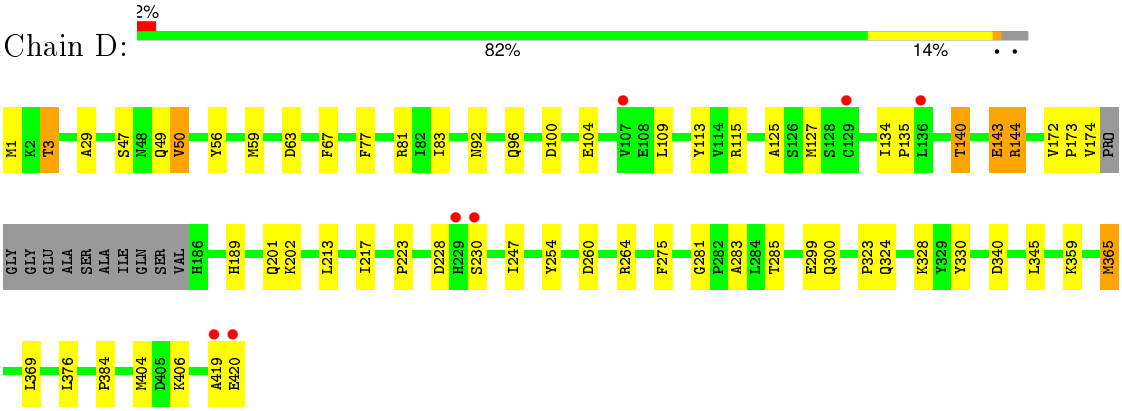
Chain C:





• Molecule 1: putative tagatose 6-phosphate kinase 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.35Å 100.00Å 206.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 48.60 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.25) 92.3 (48.60-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.90 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.187 , 0.233 0.185 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 89387 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13793	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.64	0/3331	0.68	4/4505 (0.1%)
1	B	0.61	0/3303	0.66	2/4468 (0.0%)
1	C	0.62	0/3347	0.69	5/4528 (0.1%)
1	D	0.65	1/3333 (0.0%)	0.69	5/4506 (0.1%)
All	All	0.63	1/13314 (0.0%)	0.68	16/18007 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	115	ARG	CZ-NH1	5.62	1.40	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	365	MSE	CG-SE-CE	-8.21	80.84	98.90
1	B	289	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	C	389	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	B	289	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	C	404	MSE	CG-SE-CE	6.85	113.98	98.90
1	C	215	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	C	7[A]	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	39	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	D	63	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	39	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	365	MSE	CG-SE-CE	-5.93	85.86	98.90
1	D	115	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	389	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	D	100	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	63	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	365	MSE	CG-SE-CE	-5.03	87.84	98.90

There are no chirality outliers.

There are no planarity outliers.

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	3270	0	3228	35	0
1	B	3242	0	3203	45	0
1	C	3285	0	3249	37	0
1	D	3272	0	3231	43	0
2	A	211	0	0	2	0
2	B	139	0	0	2	0
2	C	174	0	0	5	0
2	D	200	0	0	5	0
All	All	13793	0	12911	157	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 6.

All (157) 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:59:MSE:HE1	1:B:67:PHE:HB2	1.38	1.05
1:B:296:ALA:HA	1:B:365:MSE:HE2	1.42	1.00
1:D:59:MSE:HE1	1:D:67:PHE:CB	1.92	0.99
1:C:91:PRO:HD2	1:C:127:MSE:HE1	1.44	0.98
1:A:59:MSE:HE1	1:A:67:PHE:HB2	1.45	0.98
1:B:296:ALA:HA	1:B:365:MSE:CE	1.96	0.95
1:D:59:MSE:HE1	1:D:67:PHE:HB2	1.49	0.94
1:D:419:ALA:HA	1:D:420:GLU:OXT	1.68	0.93
1:C:91:PRO:HG2	1:C:127:MSE:HE3	1.49	0.92
1:C:125:ALA:HA	1:C:127:MSE:HE1	1.53	0.91
1:B:296:ALA:HB2	1:B:365:MSE:HE1	1.54	0.90
1:B:214:THR:HA	1:B:251:ARG:HH22	1.36	0.88
1:C:264[B]:ARG:NH2	2:C:556:HOH:O	1.70	0.87
1:B:296:ALA:CB	1:B:365:MSE:HE1	2.06	0.85
1:B:215:ARG:HH11	1:B:215:ARG:HG2	1.44	0.82
1:C:1:MSE:HG2	1:C:83:ILE:HD13	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:PRO:HD2	1:C:127:MSE:CE	2.13	0.76
1:D:323:PRO:HD2	1:D:324[A]:GLN:NE2	2.00	0.76
1:B:171:GLU:HG2	1:B:257:HIS:HB2	1.67	0.75
1:B:164:LEU:O	1:B:215:ARG:HG2	1.86	0.75
1:C:3[A]:THR:HG22	1:C:7[A]:ARG:HH11	1.50	0.74
1:B:59:MSE:HE1	1:B:67:PHE:CB	2.16	0.73
1:A:59:MSE:HE1	1:A:67:PHE:CB	2.20	0.71
1:B:296:ALA:CA	1:B:365:MSE:CE	2.69	0.71
1:B:127:MSE:SE	1:B:127:MSE:H	2.24	0.71
1:D:323:PRO:HD2	1:D:324[A]:GLN:HE22	1.57	0.70
1:C:299:GLU:OE1	1:C:365:MSE:HG3	1.92	0.70
1:D:59:MSE:HE1	1:D:67:PHE:HB3	1.75	0.68
1:A:216:VAL:HG12	1:A:252:MSE:HE3	1.76	0.68
1:B:296:ALA:CA	1:B:365:MSE:HE1	2.24	0.67
1:D:1:MSE:HE1	1:D:217:ILE:HD13	1.76	0.67
1:C:159[B]:CYS:O	1:C:162:GLU:HG3	1.95	0.66
1:D:260:ASP:HB3	1:D:283:ALA:HB2	1.78	0.64
1:C:265[A]:THR:HG23	2:C:543:HOH:O	2.00	0.62
1:A:127:MSE:H	1:A:127:MSE:SE	2.32	0.61
1:D:300:GLN:HG2	2:D:597:HOH:O	2.00	0.60
1:B:223:PRO:HB3	1:B:275:PHE:CZ	2.37	0.59
1:B:49:GLN:HG3	1:B:56:TYR:OH	2.01	0.59
1:B:223:PRO:HB3	1:B:275:PHE:CE1	2.38	0.59
1:B:41:VAL:HG12	1:B:43:ILE:HD11	1.83	0.59
1:D:419:ALA:HA	1:D:420:GLU:C	2.22	0.59
1:C:3[A]:THR:HG22	1:C:7[A]:ARG:NH1	2.18	0.58
1:C:260:ASP:HB3	1:C:283:ALA:HB2	1.84	0.58
1:C:125:ALA:HA	1:C:127:MSE:CE	2.31	0.58
1:C:91:PRO:CG	1:C:127:MSE:HE3	2.28	0.58
1:B:289:ARG:HD3	2:B:451:HOH:O	2.03	0.57
1:D:324[A]:GLN:CD	1:D:324[A]:GLN:H	2.08	0.56
1:B:111:LYS:O	1:B:115:ARG:HG3	2.06	0.56
1:C:91:PRO:HG2	1:C:127:MSE:CE	2.28	0.56
1:A:218:ALA:C	1:A:252:MSE:HE2	2.25	0.55
1:C:1:MSE:HG2	1:C:83:ILE:CD1	2.36	0.55
1:B:330:TYR:CG	1:B:340:ASP:HB3	2.41	0.55
1:B:5:ILE:HD11	1:B:217:ILE:HD12	1.89	0.55
1:A:299:GLU:OE1	1:A:365:MSE:HG3	2.07	0.55
1:D:96:GLN:OE1	1:D:96:GLN:HA	2.07	0.54
1:A:164:LEU:O	1:A:215:ARG:HD2	2.08	0.54
1:B:215:ARG:HH11	1:B:215:ARG:CG	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:VAL:HG22	1:D:113:TYR:OH	2.08	0.53
1:D:264:ARG:NH2	2:D:568:HOH:O	2.42	0.53
1:C:46:THR:HG22	1:C:87:ASP:OD2	2.08	0.53
1:B:379:ILE:HG22	1:B:387:PHE:HB2	1.92	0.52
1:B:260:ASP:HB3	1:B:283:ALA:HB2	1.92	0.52
1:B:5:ILE:CD1	1:B:217:ILE:HD12	2.40	0.51
1:A:48:ASN:HD21	1:A:92:ASN:HD22	1.59	0.51
1:A:34:ASP:OD1	1:A:39:ARG:HD3	2.10	0.51
1:D:230:SER:HB2	2:D:584:HOH:O	2.09	0.51
1:C:3[A]:THR:O	1:C:7[A]:ARG:HG3	2.11	0.51
1:C:91:PRO:CD	1:C:127:MSE:CE	2.87	0.50
1:B:41:VAL:HG12	1:B:43:ILE:CD1	2.41	0.50
1:C:384:PRO:HG2	1:D:384:PRO:HG2	1.92	0.50
1:B:265[B]:THR:HG22	2:B:497:HOH:O	2.12	0.49
1:C:311:CYS:O	1:C:315:ILE:HG13	2.13	0.49
1:A:260:ASP:HB3	1:A:283:ALA:HB2	1.94	0.49
1:B:103:MSE:O	1:B:107:VAL:HG13	2.14	0.48
1:D:59:MSE:CE	1:D:67:PHE:HB2	2.34	0.48
1:D:1:MSE:HG2	1:D:83:ILE:HD13	1.96	0.48
1:A:291:ALA:HB2	1:A:406:LYS:HG3	1.96	0.47
1:D:3:THR:HG22	2:D:513:HOH:O	2.13	0.47
1:B:2:LYS:NZ	1:B:215:ARG:HG3	2.28	0.47
1:D:49:GLN:HG3	1:D:56:TYR:OH	2.14	0.47
1:C:198[B]:ARG:HE	1:C:202:LYS:HE2	1.79	0.47
1:D:125:ALA:HB3	1:D:144:ARG:HB3	1.97	0.46
1:C:35:ARG:HD2	2:C:568:HOH:O	2.16	0.46
1:A:65:ARG:HH21	1:A:116:ALA:HA	1.81	0.46
1:B:1:MSE:HE2	1:B:3:THR:H	1.80	0.46
1:B:56:TYR:CZ	1:B:351:TYR:HE1	2.33	0.46
1:B:226:GLU:HG2	1:B:227:PHE:N	2.30	0.46
1:C:159[A]:CYS:O	1:C:162:GLU:HG3	2.14	0.46
1:A:366:MSE:O	1:A:370:GLN:HG3	2.15	0.46
1:A:365:MSE:HE3	1:A:369:LEU:HD12	1.98	0.46
1:D:299:GLU:OE1	1:D:365:MSE:HG3	2.16	0.46
1:D:223:PRO:HB3	1:D:275:PHE:CZ	2.51	0.46
1:D:201:GLN:HG2	1:D:213:LEU:HD21	1.98	0.46
1:C:291:ALA:HB2	1:C:406:LYS:HG3	1.98	0.46
1:B:241:GLN:O	1:B:245:GLN:HG2	2.15	0.45
1:D:1:MSE:CG	1:D:83:ILE:HD13	2.46	0.45
1:A:127:MSE:HE1	2:A:614:HOH:O	2.16	0.45
1:A:365:MSE:HE3	1:A:369:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:PHE:CE1	1:D:81:ARG:HB2	2.52	0.45
1:D:134:ILE:HA	1:D:135:PRO:HA	1.80	0.44
1:D:365:MSE:HE3	1:D:369:LEU:HD12	1.99	0.44
1:D:135:PRO:HG3	1:D:174:VAL:HG13	1.99	0.44
1:D:50:VAL:HB	1:D:59:MSE:O	2.18	0.44
1:C:50:VAL:HG22	1:C:113:TYR:OH	2.17	0.44
1:A:330:TYR:CD1	1:A:340:ASP:HB3	2.53	0.44
1:A:48:ASN:HD21	1:A:92:ASN:ND2	2.15	0.43
1:B:50:VAL:HG22	1:B:113:TYR:OH	2.18	0.43
1:B:134:ILE:HA	1:B:135:PRO:HA	1.74	0.43
1:C:330:TYR:CD1	1:C:340:ASP:HB3	2.53	0.43
1:C:280:VAL:HB	1:C:414:TYR:CZ	2.53	0.43
1:D:47:SER:HB3	1:D:109:LEU:HD21	2.01	0.43
1:D:172:VAL:HA	1:D:173:PRO:HD3	1.93	0.43
1:D:29:ALA:HA	1:D:404:MSE:HE1	2.01	0.43
1:B:164:LEU:O	1:B:215:ARG:CG	2.62	0.43
1:C:1:MSE:C	1:C:1:MSE:SE	3.07	0.43
1:D:140:THR:HA	1:D:143:GLU:HG3	2.00	0.43
1:B:291:ALA:HB2	1:B:406:LYS:HG3	2.01	0.42
1:A:290:GLU:OE2	1:B:380:SER:OG	2.26	0.42
1:A:228:ASP:O	1:A:345:LEU:HB2	2.19	0.42
1:C:190:VAL:HG13	2:C:501:HOH:O	2.18	0.42
1:A:129:CYS:O	1:A:132:ASP:HB2	2.20	0.42
1:C:198[B]:ARG:HE	1:C:202:LYS:CE	2.33	0.42
1:B:153:GLU:OE1	1:B:161:ARG:HD3	2.19	0.42
1:D:228:ASP:O	1:D:345:LEU:HD12	2.20	0.42
1:A:218:ALA:C	1:A:252:MSE:CE	2.88	0.42
1:A:344:SER:OG	1:A:346:SER:HB3	2.20	0.42
1:A:50:VAL:HB	1:A:59:MSE:O	2.19	0.41
1:D:247:ILE:HB	1:D:254:TYR:CE2	2.55	0.41
1:B:18:SER:HB2	1:B:42:LEU:HD13	2.02	0.41
1:D:202:LYS:NZ	1:D:202:LYS:HB3	2.35	0.41
1:A:1:MSE:HG2	2:A:466:HOH:O	2.20	0.41
1:C:48:ASN:H	1:C:48:ASN:HD22	1.68	0.41
1:C:330:TYR:CG	1:C:340:ASP:HB3	2.55	0.41
1:A:46:THR:HG22	1:A:87:ASP:OD2	2.20	0.41
1:D:125:ALA:CB	1:D:144:ARG:HB3	2.50	0.41
1:A:353:TRP:N	1:A:354:PRO:CD	2.84	0.41
1:D:328:LYS:HE2	1:D:328:LYS:HB2	1.82	0.41
1:A:218:ALA:HA	1:A:253:VAL:O	2.21	0.41
1:A:223:PRO:HB3	1:A:275:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ARG:HA	1:A:164:LEU:HD12	2.03	0.41
1:A:48:ASN:H	1:A:48:ASN:ND2	2.19	0.41
1:D:3:THR:CG2	2:D:513:HOH:O	2.68	0.41
1:B:91:PRO:HD2	1:B:125:ALA:HA	2.02	0.41
1:B:136:LEU:HD22	1:B:140:THR:HG21	2.03	0.41
1:C:389:ARG:NH2	1:C:409:ASP:OD2	2.50	0.41
1:C:265[A]:THR:HG22	2:C:586:HOH:O	2.21	0.41
1:A:134:ILE:HA	1:A:135:PRO:HA	1.82	0.41
1:A:211:GLU:OE2	1:A:215:ARG:NH1	2.54	0.40
1:B:286:PHE:CE2	1:B:345:LEU:HD23	2.56	0.40
1:D:49:GLN:HG3	1:D:56:TYR:CZ	2.56	0.40
1:B:215:ARG:NH1	1:B:215:ARG:CG	2.82	0.40
1:D:223:PRO:HB3	1:D:275:PHE:CE1	2.56	0.40
1:C:172:VAL:HA	1:C:173:PRO:HD3	1.91	0.40
1:C:45:ALA:HB1	1:C:50:VAL:HG13	2.03	0.40
1:D:330:TYR:CD1	1:D:340:ASP:HB3	2.56	0.40
1:A:384:PRO:HG2	1:B:384:PRO:HG2	2.04	0.40
1:A:139:GLU:H	1:A:139:GLU:CD	2.25	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	409/420 (97%)	399 (98%)	9 (2%)	1 (0%)	52	61
1	B	406/420 (97%)	394 (97%)	11 (3%)	1 (0%)	52	61
1	C	411/420 (98%)	399 (97%)	11 (3%)	1 (0%)	52	61
1	D	409/420 (97%)	403 (98%)	5 (1%)	1 (0%)	52	61
All	All	1635/1680 (97%)	1595 (98%)	36 (2%)	4 (0%)	52	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	281	GLY
1	A	281	GLY
1	B	281	GLY
1	C	281	GLY

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	346/339 (102%)	334 (96%)	12 (4%)	43	53
1	B	343/339 (101%)	323 (94%)	20 (6%)	25	25
1	C	348/339 (103%)	333 (96%)	15 (4%)	35	41
1	D	346/339 (102%)	333 (96%)	13 (4%)	40	49
All	All	1383/1356 (102%)	1323 (96%)	60 (4%)	36	41

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	40	LYS
1	A	127	MSE
1	A	136	LEU
1	A	186	HIS
1	A	211	GLU
1	A	229	HIS
1	A	288	LEU
1	A	311	CYS
1	A	324[A]	GLN
1	A	324[B]	GLN
1	A	345	LEU
1	B	1	MSE
1	B	42	LEU
1	B	47	SER
1	B	50	VAL
1	B	96	GLN
1	B	100	ASP

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Mol	Chain	Res	Type
1	B	104	GLU
1	B	127	MSE
1	B	143	GLU
1	B	164	LEU
1	B	171	GLU
1	B	202	LYS
1	B	213	LEU
1	B	215	ARG
1	B	239	GLU
1	B	265[A]	THR
1	B	265[B]	THR
1	B	285	THR
1	B	396[A]	SER
1	B	396[B]	SER
1	C	1	MSE
1	C	48	ASN
1	C	96	GLN
1	C	127	MSE
1	C	136	LEU
1	C	155	VAL
1	C	161	ARG
1	C	162	GLU
1	C	189	HIS
1	C	260	ASP
1	C	288	LEU
1	C	345	LEU
1	C	392	SER
1	C	404	MSE
1	C	415	ARG
1	D	3	THR
1	D	50	VAL
1	D	92	ASN
1	D	104	GLU
1	D	127	MSE
1	D	140	THR
1	D	143	GLU
1	D	144	ARG
1	D	189	HIS
1	D	285	THR
1	D	359	LYS
1	D	376	LEU
1	D	406	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	B	98	ASN
1	B	297	GLN
1	C	48	ASN
1	C	92	ASN
1	D	400	HIS

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	400/420 (95%)	0.21	14 (3%)	48	52	30, 37, 47, 54	0
1	B	398/420 (94%)	0.68	35 (8%)	12	14	30, 37, 47, 54	0
1	C	400/420 (95%)	0.39	17 (4%)	39	43	29, 37, 47, 56	0
1	D	399/420 (95%)	0.36	7 (1%)	71	75	29, 37, 46, 58	1 (0%)
All	All	1597/1680 (95%)	0.41	73 (4%)	36	40	29, 37, 47, 58	1 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131	GLY	6.8
1	A	131	GLY	6.3
1	C	96	GLN	6.2
1	B	99	VAL	6.1
1	C	98	ASN	5.6
1	C	131	GLY	5.2
1	C	130	ALA	5.1
1	A	130	ALA	4.9
1	B	98	ASN	4.6
1	C	174	VAL	4.6
1	B	100	ASP	4.5
1	B	94	TRP	4.3
1	B	146	ALA	4.2
1	B	102	ALA	4.1
1	B	130	ALA	4.0
1	A	96	GLN	3.8
1	B	101	ALA	3.7
1	A	132	ASP	3.5
1	B	145	ALA	3.5
1	D	129	CYS	3.5
1	B	136	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	159	CYS	3.5
1	B	129	CYS	3.4
1	A	98	ASN	3.3
1	B	91	PRO	3.3
1	B	128	SER	3.2
1	B	132	ASP	3.2
1	A	173	PRO	3.1
1	B	135	PRO	3.1
1	B	174	VAL	3.1
1	C	173	PRO	3.1
1	C	134	ILE	3.1
1	B	93	CYS	3.0
1	C	95	GLN	3.0
1	B	50	VAL	3.0
1	B	53	PHE	3.0
1	B	148	LEU	3.0
1	B	104	GLU	2.9
1	A	129	CYS	2.9
1	B	142	ALA	2.8
1	A	134	ILE	2.8
1	B	186	HIS	2.8
1	A	420	GLU	2.8
1	C	186	HIS	2.8
1	B	134	ILE	2.8
1	D	420	GLU	2.7
1	B	96	GLN	2.7
1	A	133	PRO	2.7
1	B	95	GLN	2.6
1	B	147	VAL	2.6
1	C	100	ASP	2.6
1	A	99	VAL	2.5
1	C	94	TRP	2.5
1	D	419	ALA	2.4
1	C	101	ALA	2.4
1	A	328	LYS	2.4
1	D	229	HIS	2.4
1	B	133	PRO	2.4
1	A	136	LEU	2.3
1	C	10	ALA	2.3
1	D	230	SER	2.3
1	B	144	ARG	2.3
1	C	102	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	152	ALA	2.2
1	D	107	VAL	2.2
1	B	47	SER	2.2
1	B	162	GLU	2.2
1	C	93	CYS	2.1
1	D	136	LEU	2.1
1	B	139	GLU	2.0
1	C	99	VAL	2.0
1	C	104	GLU	2.0
1	A	135	PRO	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.