



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:44 AM UTC

PDB ID : 3B3L / pdb_00003b3l
Title : Crystal structures of alternatively-spliced isoforms of human ketohexokinase
Authors : Trinh, C.H.; Asipu, A.; Bonthron, D.T.; Phillips, S.E.V.
Deposited on : 2007-10-22
Resolution : 2.90 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

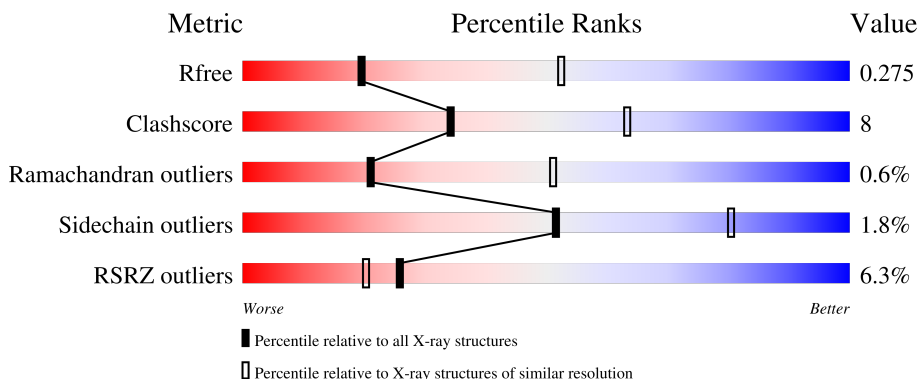
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	298	0% 83% 15% ..
1	B	298	5% 86% 12% ..
1	C	298	16% 80% 19% .
1	D	298	3% 77% 21% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8916 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 Ketohexokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2232	1399	399	422	12			
1	B	296	Total	C	N	O	S	0	0	0
			2201	1382	392	415	12			
1	C	296	Total	C	N	O	S	0	0	0
			2230	1399	399	420	12			
1	D	296	Total	C	N	O	S	0	0	0
			2235	1401	398	424	12			

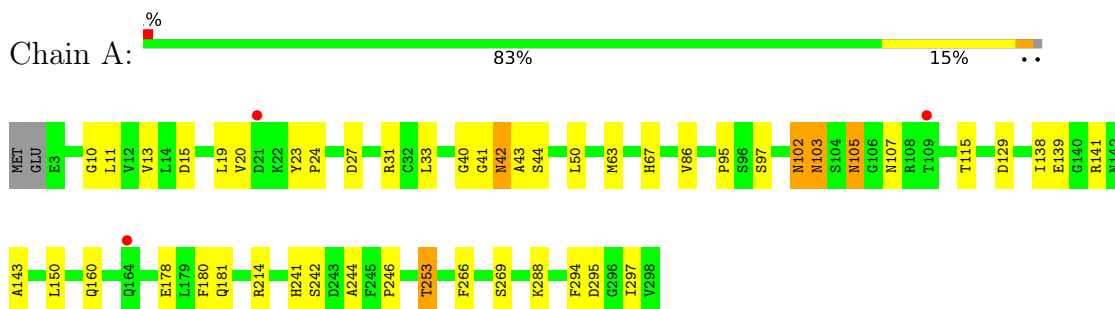
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	O	0	0
			7	7		
2	B	2	Total	O	0	0
			2	2		
2	C	6	Total	O	0	0
			6	6		
2	D	3	Total	O	0	0
			3	3		

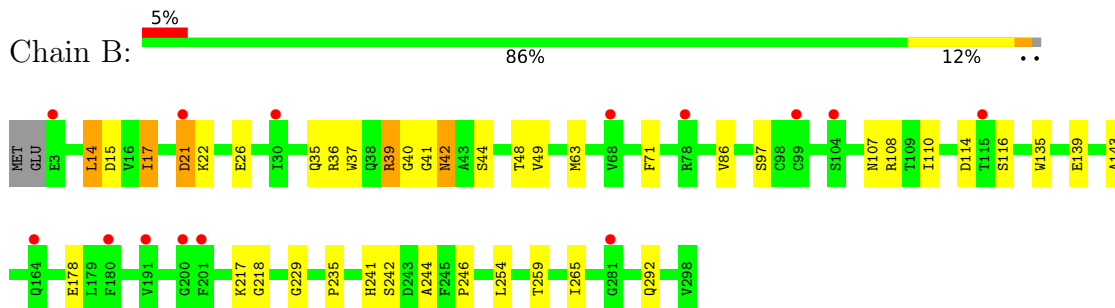
3 Residue-property plots [i](#)

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.

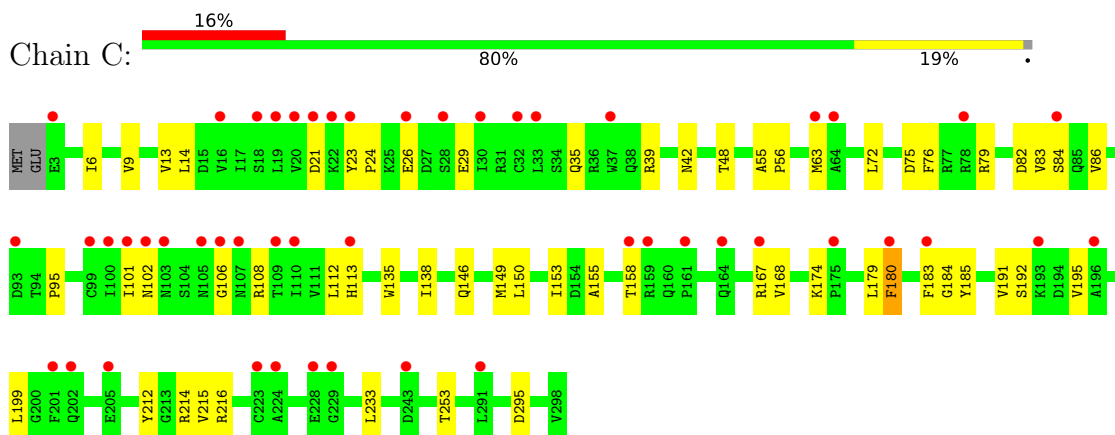
• Molecule 1: Ketohexokinase



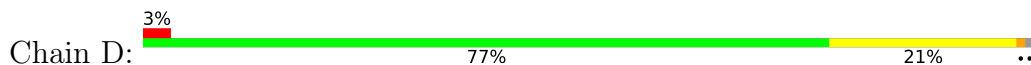
• Molecule 1: Ketohexokinase

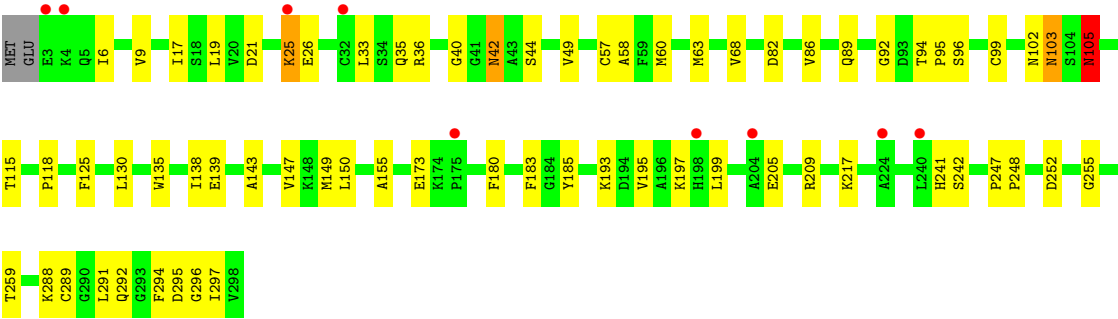


• Molecule 1: Ketohexokinase



• Molecule 1: Ketohexokinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.56Å 140.70Å 179.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.38 – 2.90 25.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.38-2.90) 99.6 (25.38-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.281 0.230 , 0.275	Depositor DCC
R_{free} test set	2608 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8916	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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	0.86	0/2274	0.95	7/3080 (0.2%)
1	B	0.69	0/2243	0.91	6/3043 (0.2%)
1	C	0.74	0/2272	0.88	2/3077 (0.1%)
1	D	0.72	0/2277	0.89	4/3083 (0.1%)
All	All	0.75	0/9066	0.91	19/12283 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	ASP	N-CA-C	8.25	119.97	110.97
1	B	41	GLY	N-CA-C	-6.89	104.15	112.48
1	C	26	GLU	N-CA-C	6.34	118.48	110.24
1	D	295	ASP	N-CA-C	6.31	118.96	111.33
1	A	33	LEU	N-CA-C	-6.27	103.15	111.24
1	B	143	ALA	N-CA-C	6.00	118.34	111.02
1	A	143	ALA	N-CA-C	5.92	118.21	111.11
1	A	41	GLY	N-CA-C	-5.91	104.26	112.18
1	B	116	SER	N-CA-C	5.83	118.13	111.02
1	B	39	ARG	N-CA-C	-5.78	101.73	110.28
1	A	160	GLN	CA-C-N	5.75	123.86	119.66
1	A	160	GLN	C-N-CA	5.75	123.86	119.66
1	D	130	LEU	N-CA-C	5.75	119.39	112.38
1	A	103	ASN	N-CA-C	5.62	117.49	111.36
1	C	42	ASN	N-CA-C	5.56	120.50	111.37
1	B	42	ASN	N-CA-C	5.35	116.80	110.97
1	D	138	ILE	N-CA-C	5.21	115.35	107.75
1	B	110	ILE	N-CA-C	5.13	115.30	108.11
1	D	155	ALA	N-CA-C	-5.00	105.10	111.11

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	2232	0	2175	35	0
1	B	2201	0	2131	24	0
1	C	2230	0	2180	39	0
1	D	2235	0	2183	45	0
2	A	7	0	0	0	0
2	B	2	0	0	0	0
2	C	6	0	0	0	0
2	D	3	0	0	0	0
All	All	8916	0	8669	134	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 8.

All (134) 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:21:ASP:HA	1:D:103:ASN:HB2	1.52	0.88
1:C:146:GLN:HA	1:C:149:MET:HE3	1.60	0.82
1:C:138:ILE:HD12	1:C:150:LEU:HD21	1.62	0.81
1:D:36:ARG:NH1	1:D:292:GLN:HE21	1.80	0.78
1:D:19:LEU:HD22	1:D:33:LEU:HD12	1.72	0.70
1:A:31:ARG:HD3	1:B:114:ASP:OD1	1.92	0.70
1:D:63:MET:HE2	1:D:86:VAL:HG21	1.75	0.68
1:D:42:ASN:HB2	1:D:139:GLU:CD	2.18	0.68
1:A:42:ASN:H	1:A:42:ASN:HD22	1.44	0.66
1:D:17:ILE:O	1:D:35:GLN:HA	1.98	0.63
1:A:13:VAL:HG22	1:A:95:PRO:HB2	1.80	0.63
1:D:195:VAL:O	1:D:199:LEU:HG	1.99	0.63
1:A:42:ASN:H	1:A:42:ASN:ND2	1.97	0.62
1:C:106:GLY:O	1:C:253:THR:HG23	1.99	0.62
1:B:244:ALA:O	1:B:246:PRO:HD3	1.99	0.62
1:A:107:ASN:ND2	1:B:26:GLU:OE2	2.33	0.61
1:C:35:GLN:NE2	1:D:96:SER:OG	2.34	0.60
1:A:107:ASN:HD22	1:B:26:GLU:CD	2.10	0.59
1:C:63:MET:HE3	1:C:86:VAL:HG11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:GLY:HA2	1:D:115:THR:HG21	1.85	0.58
1:A:102:ASN:HD22	1:A:103:ASN:N	2.01	0.58
1:A:105:ASN:N	1:A:105:ASN:OD1	2.32	0.58
1:D:288:LYS:HD2	1:D:288:LYS:O	2.04	0.57
1:A:115:THR:HG22	1:A:115:THR:O	2.05	0.57
1:C:29:GLU:N	1:C:29:GLU:OE2	2.36	0.57
1:B:229:GLY:HA3	1:B:242:SER:O	2.05	0.56
1:D:241:HIS:CG	1:D:242:SER:N	2.74	0.55
1:D:17:ILE:HG13	1:D:99:CYS:HB3	1.89	0.55
1:B:42:ASN:HB2	1:B:139:GLU:CD	2.32	0.55
1:D:40:GLY:O	1:D:44:SER:HB3	2.05	0.55
1:A:11:LEU:HD21	1:A:141:ARG:CD	2.37	0.54
1:D:25:LYS:O	1:D:25:LYS:HD3	2.07	0.54
1:C:214:ARG:HB3	1:C:214:ARG:HH11	1.73	0.54
1:A:20:VAL:O	1:A:103:ASN:HB2	2.07	0.54
1:D:6:ILE:HG23	1:D:135:TRP:HB3	1.89	0.54
1:A:138:ILE:HD12	1:A:150:LEU:HD21	1.90	0.53
1:C:135:TRP:HA	1:C:167:ARG:O	2.08	0.53
1:B:15:ASP:OD1	1:B:97:SER:OG	2.24	0.53
1:D:63:MET:HE3	1:D:86:VAL:HG11	1.91	0.53
1:A:178:GLU:O	1:A:181:GLN:HG2	2.09	0.52
1:B:63:MET:CE	1:B:86:VAL:HG21	2.40	0.52
1:C:138:ILE:HD12	1:C:150:LEU:CD2	2.36	0.52
1:B:14:LEU:C	1:B:14:LEU:HD12	2.35	0.52
1:D:42:ASN:HD21	1:D:173:GLU:HG3	1.74	0.52
1:D:294:PHE:O	1:D:297:ILE:HG12	2.11	0.51
1:D:25:LYS:HD3	1:D:25:LYS:C	2.36	0.51
1:A:42:ASN:HB2	1:A:139:GLU:OE1	2.10	0.51
1:C:180:PHE:CE2	1:C:199:LEU:HD21	2.46	0.51
1:A:10:GLY:HA3	1:A:43:ALA:HB2	1.93	0.50
1:C:192:SER:OG	1:C:195:VAL:HG23	2.11	0.50
1:A:266:PHE:O	1:A:269:SER:HB3	2.11	0.50
1:C:112:LEU:HD12	1:C:113:HIS:H	1.77	0.50
1:A:67:HIS:HB3	1:B:37:TRP:CZ3	2.47	0.50
1:B:63:MET:HE3	1:B:86:VAL:HG11	1.93	0.50
1:C:48:THR:HG23	1:C:79:ARG:HD2	1.93	0.49
1:C:6:ILE:HG23	1:C:135:TRP:HB3	1.93	0.49
1:D:58:ALA:HB2	1:D:82:ASP:HB3	1.93	0.49
1:A:23:TYR:HB2	1:B:26:GLU:OE1	2.13	0.49
1:C:13:VAL:HG22	1:C:95:PRO:HB2	1.93	0.49
1:C:180:PHE:HD1	1:C:180:PHE:N	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ILE:HG21	1:C:168:VAL:HG21	1.94	0.48
1:C:83:VAL:O	1:C:86:VAL:HG23	2.13	0.48
1:A:27:ASP:HB2	1:B:107:ASN:HD22	1.79	0.48
1:B:135:TRP:CE2	1:B:265:ILE:HG23	2.49	0.47
1:C:180:PHE:N	1:C:180:PHE:CD1	2.80	0.47
1:B:17:ILE:HG21	1:B:36:ARG:NH1	2.29	0.47
1:C:150:LEU:HD13	1:C:185:TYR:HB2	1.96	0.47
1:D:63:MET:CE	1:D:86:VAL:HG21	2.44	0.47
1:C:9:VAL:HB	1:C:138:ILE:HG12	1.97	0.47
1:A:244:ALA:C	1:A:246:PRO:HD3	2.39	0.47
1:A:15:ASP:OD1	1:A:97:SER:OG	2.33	0.47
1:B:218:GLY:HA2	1:B:235:PRO:HB3	1.96	0.46
1:D:247:PRO:O	1:D:248:PRO:C	2.58	0.46
1:A:129:ASP:OD1	1:A:129:ASP:C	2.58	0.46
1:C:23:TYR:HA	1:C:24:PRO:HD3	1.74	0.46
1:D:49:VAL:HG21	1:D:259:THR:HA	1.97	0.46
1:D:150:LEU:HD13	1:D:185:TYR:CB	2.46	0.46
1:C:39:ARG:HG3	1:C:72:LEU:HD22	1.98	0.46
1:A:102:ASN:HD22	1:A:103:ASN:H	1.64	0.46
1:C:48:THR:HG23	1:C:79:ARG:CD	2.46	0.45
1:C:184:GLY:O	1:C:216:ARG:HB3	2.17	0.45
1:A:294:PHE:O	1:A:297:ILE:HG23	2.16	0.45
1:B:36:ARG:HH12	1:B:292:GLN:HE21	1.65	0.45
1:A:253:THR:O	1:A:253:THR:CG2	2.64	0.45
1:D:252:ASP:O	1:D:289:CYS:HA	2.17	0.45
1:B:21:ASP:CG	1:B:22:LYS:H	2.25	0.45
1:D:125:PHE:CB	1:D:149:MET:HG2	2.48	0.44
1:B:241:HIS:CG	1:B:242:SER:N	2.85	0.44
1:D:42:ASN:ND2	1:D:173:GLU:HG3	2.32	0.44
1:B:40:GLY:O	1:B:44:SER:HB3	2.18	0.43
1:C:23:TYR:HB2	1:D:26:GLU:OE1	2.19	0.43
1:A:42:ASN:ND2	1:A:42:ASN:N	2.66	0.43
1:B:39:ARG:NH2	1:B:48:THR:OG1	2.50	0.43
1:C:75:ASP:O	1:C:76:PHE:C	2.60	0.43
1:D:89:GLN:OE1	1:D:118:PRO:HG2	2.18	0.43
1:A:10:GLY:HA3	1:A:43:ALA:CB	2.48	0.43
1:A:67:HIS:CE1	1:B:71:PHE:HE1	2.35	0.43
1:D:205:GLU:HB3	1:D:209:ARG:HH12	1.84	0.43
1:B:49:VAL:HG21	1:B:259:THR:HA	2.00	0.43
1:D:9:VAL:HA	1:D:60:MET:O	2.19	0.43
1:C:174:LYS:HB2	1:C:179:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ILE:O	1:D:57:CYS:HB2	2.19	0.43
1:D:150:LEU:HD13	1:D:185:TYR:HB2	2.00	0.43
1:A:63:MET:HE3	1:A:86:VAL:HG21	2.01	0.43
1:D:193:LYS:HE2	1:D:197:LYS:HD2	1.99	0.43
1:A:23:TYR:HA	1:A:24:PRO:HD3	1.91	0.42
1:A:50:LEU:HD23	1:A:50:LEU:HA	1.84	0.42
1:D:94:THR:HG22	1:D:95:PRO:HD2	2.01	0.42
1:C:183:PHE:O	1:C:215:VAL:HA	2.19	0.42
1:C:55:ALA:HA	1:C:56:PRO:HD2	1.94	0.42
1:D:291:LEU:HD13	1:D:296:GLY:C	2.44	0.42
1:D:115:THR:HG22	1:D:115:THR:O	2.20	0.42
1:C:82:ASP:OD1	1:C:84:SER:HB3	2.19	0.42
1:C:155:ALA:O	1:C:158:THR:HB	2.19	0.42
1:C:214:ARG:HB3	1:C:214:ARG:NH1	2.33	0.42
1:D:217:LYS:HE2	1:D:217:LYS:HB3	1.83	0.42
1:A:40:GLY:O	1:A:44:SER:HB3	2.19	0.42
1:D:102:ASN:HD22	1:D:103:ASN:H	1.68	0.42
1:A:180:PHE:CD2	1:A:214:ARG:NH1	2.88	0.42
1:C:212:TYR:HB2	1:C:233:LEU:HD23	2.01	0.42
1:C:82:ASP:OD1	1:C:84:SER:CB	2.68	0.41
1:D:143:ALA:O	1:D:147:VAL:HG23	2.20	0.41
1:C:21:ASP:C	1:C:102:ASN:ND2	2.79	0.41
1:C:191:VAL:O	1:C:191:VAL:HG13	2.21	0.41
1:D:255:GLY:O	1:D:259:THR:OG1	2.34	0.41
1:D:102:ASN:HB3	1:D:105:ASN:HB2	2.03	0.41
1:B:217:LYS:HE2	1:B:217:LYS:HB3	1.87	0.40
1:D:180:PHE:HD1	1:D:183:PHE:HE1	1.69	0.40
1:C:146:GLN:O	1:C:149:MET:HB2	2.21	0.40
1:D:63:MET:HE2	1:D:86:VAL:CG2	2.49	0.40
1:D:105:ASN:OD1	1:D:105:ASN:N	2.52	0.40
1:C:153:ILE:HG21	1:C:168:VAL:CG2	2.51	0.40
1:A:11:LEU:HD21	1:A:141:ARG:NE	2.36	0.40
1:A:241:HIS:CG	1:A:242:SER:N	2.90	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	294/298 (99%)	283 (96%)	11 (4%)	0	100	100
1	B	294/298 (99%)	276 (94%)	15 (5%)	3 (1%)	12	39
1	C	294/298 (99%)	274 (93%)	19 (6%)	1 (0%)	36	65
1	D	294/298 (99%)	276 (94%)	15 (5%)	3 (1%)	12	39
All	All	1176/1192 (99%)	1109 (94%)	60 (5%)	7 (1%)	21	51

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	ASP
1	C	295	ASP
1	D	42	ASN
1	D	103	ASN
1	B	178	GLU
1	B	254	LEU
1	D	105	ASN

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	236/248 (95%)	230 (98%)	6 (2%)	42	74
1	B	230/248 (93%)	226 (98%)	4 (2%)	53	82
1	C	236/248 (95%)	232 (98%)	4 (2%)	53	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	238/248 (96%)	235 (99%)	3 (1%)	61	86
All	All	940/992 (95%)	923 (98%)	17 (2%)	51	80

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	42	ASN
1	A	102	ASN
1	A	105	ASN
1	A	253	THR
1	A	288	LYS
1	B	14	LEU
1	B	17	ILE
1	B	35	GLN
1	B	108	ARG
1	C	14	LEU
1	C	101	ILE
1	C	108	ARG
1	C	180	PHE
1	D	25	LYS
1	D	68	VAL
1	D	105	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	102	ASN
1	A	107	ASN
1	A	113	HIS
1	A	156	HIS
1	B	102	ASN
1	B	103	ASN
1	B	107	ASN
1	B	156	HIS
1	B	283	GLN
1	B	292	GLN
1	C	5	GLN
1	C	35	GLN
1	C	67	HIS

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Mol	Chain	Res	Type
1	C	113	HIS
1	C	181	GLN
1	C	275	GLN
1	D	35	GLN
1	D	160	GLN
1	D	292	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

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	296/298 (99%)	0.09	3 (1%) 79 73	39, 54, 77, 97	0
1	B	296/298 (99%)	0.66	14 (4%) 36 28	48, 66, 84, 94	0
1	C	296/298 (99%)	1.07	49 (16%) 4 3	44, 63, 104, 130	0
1	D	296/298 (99%)	0.52	9 (3%) 52 43	37, 59, 82, 97	0
All	All	1184/1192 (99%)	0.59	75 (6%) 26 20	37, 61, 86, 130	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	109	THR	5.7
1	B	200	GLY	5.0
1	D	3	GLU	4.9
1	C	33	LEU	4.3
1	C	99	CYS	4.0
1	C	105	ASN	4.0
1	C	107	ASN	4.0
1	C	20	VAL	3.8
1	C	100	ILE	3.7
1	D	224	ALA	3.7
1	B	281	GLY	3.7
1	B	30	ILE	3.5
1	A	109	THR	3.3
1	D	175	PRO	3.3
1	C	28	SER	3.3
1	C	159	ARG	3.3
1	C	3	GLU	3.3
1	C	23	TYR	3.2
1	B	180	PHE	3.2
1	C	19	LEU	3.1
1	C	101	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	103	ASN	3.0
1	D	32	CYS	2.9
1	C	224	ALA	2.9
1	B	201	PHE	2.8
1	C	196	ALA	2.8
1	C	193	LYS	2.7
1	C	30	ILE	2.7
1	A	21	ASP	2.7
1	C	32	CYS	2.7
1	C	229	GLY	2.6
1	C	164	GLN	2.6
1	D	198	HIS	2.5
1	D	240	LEU	2.5
1	B	164	GLN	2.5
1	C	102	ASN	2.5
1	C	21	ASP	2.5
1	C	113	HIS	2.5
1	C	291	LEU	2.5
1	C	18	SER	2.5
1	C	110	ILE	2.4
1	C	180	PHE	2.4
1	B	115	THR	2.4
1	C	223	CYS	2.4
1	B	3	GLU	2.4
1	C	106	GLY	2.4
1	C	228	GLU	2.4
1	C	84	SER	2.4
1	C	161	PRO	2.4
1	C	22	LYS	2.3
1	B	99	CYS	2.3
1	C	202	GLN	2.3
1	C	93	ASP	2.3
1	D	25	LYS	2.3
1	C	175	PRO	2.3
1	C	167	ARG	2.2
1	C	78	ARG	2.2
1	C	26	GLU	2.2
1	B	78	ARG	2.2
1	A	164	GLN	2.2
1	C	243	ASP	2.2
1	D	204	ALA	2.2
1	B	104	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	64	ALA	2.1
1	C	205	GLU	2.1
1	C	201	PHE	2.1
1	B	21	ASP	2.1
1	C	16	VAL	2.1
1	C	37	TRP	2.1
1	C	63	MET	2.0
1	D	4	LYS	2.0
1	B	68	VAL	2.0
1	B	191	VAL	2.0
1	C	183	PHE	2.0
1	C	158	THR	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 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.