Full wwPDB X-ray Structure Validation Report (i)

Mar 6, 2026 – 07:16 AM UTC

PDB ID	:	5YFN / pdb_00005yfn
Title	:	Human isocitrate dehydrogenase 1 bound with isocitrate
Authors	:	Nordlund, P.; Chen, D.; Jansson, A.; Larsson, A.
Deposited on	:	2017-09-21
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

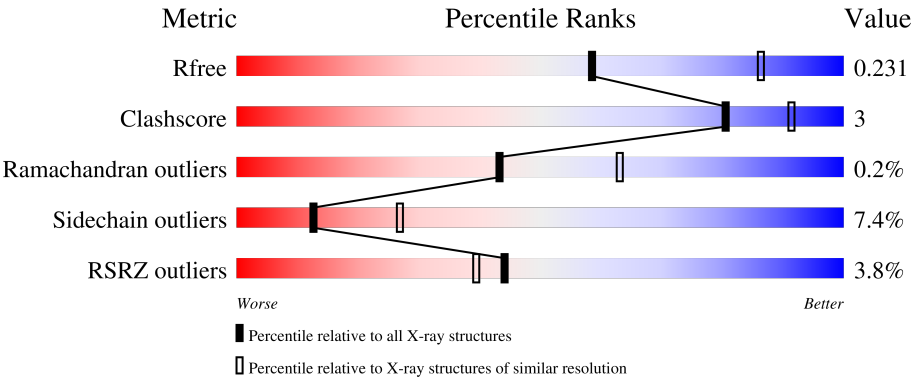
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 <=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	421	3% 81% 16%
1	B	421	4% 81% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ICT	A	502	-	X	-	-
3	ICT	A	505	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6734 atoms, of which 10 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3292	2093	555	625	19			
1	B	406	Total	C	N	O	S	0	0	0
			3197	2035	536	608	18			

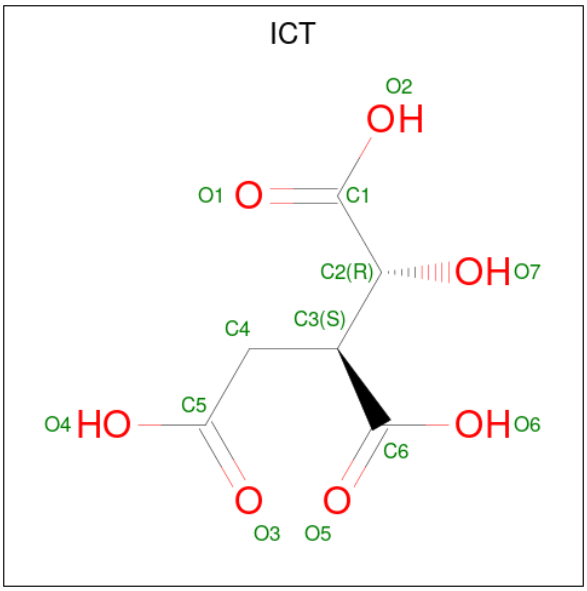
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASN	-	expression tag	UNP O75874
A	-5	LEU	-	expression tag	UNP O75874
A	-4	TYR	-	expression tag	UNP O75874
A	-3	PHE	-	expression tag	UNP O75874
A	-2	GLN	-	expression tag	UNP O75874
A	-1	SER	-	expression tag	UNP O75874
A	0	MET	-	expression tag	UNP O75874
B	-6	ASN	-	expression tag	UNP O75874
B	-5	LEU	-	expression tag	UNP O75874
B	-4	TYR	-	expression tag	UNP O75874
B	-3	PHE	-	expression tag	UNP O75874
B	-2	GLN	-	expression tag	UNP O75874
B	-1	SER	-	expression tag	UNP O75874
B	0	MET	-	expression tag	UNP O75874

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is ISOCITRIC ACID (CCD ID: ICT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 18 6 5 7	0	0
3	A	1	Total C H O 18 6 5 7	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0

- Molecule 5 is water.

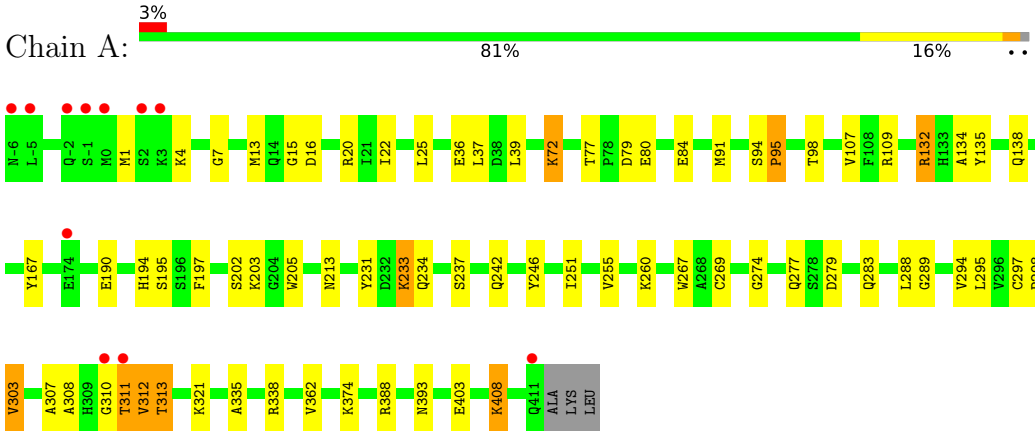
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	111	Total O 111 111	0	0
5	B	94	Total O 94 94	0	0

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.

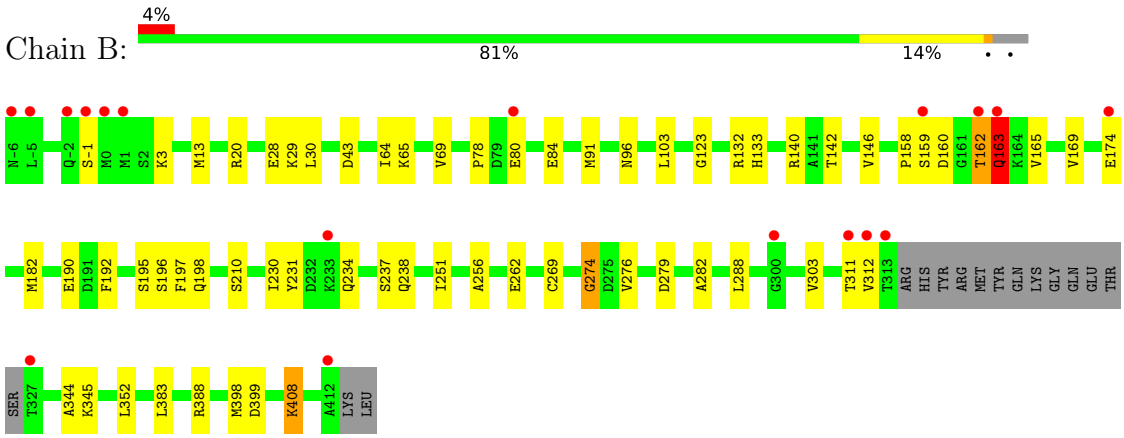
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain A:



• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	111.56Å 92.00Å 138.84Å 90.00° 109.94° 90.00°	Depositor
Resolution (Å)	41.80 – 2.50 41.80 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.80-2.50) 99.4 (41.80-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.173 , 0.226 0.187 , 0.231	Depositor DCC
R_{free} test set	2300 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6734	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, ICT, MG

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	1.51	20/3362 (0.6%)	1.21	15/4538 (0.3%)
1	B	1.40	8/3263 (0.2%)	1.20	10/4404 (0.2%)
All	All	1.45	28/6625 (0.4%)	1.20	25/8942 (0.3%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	VAL	C-O	-6.71	1.15	1.24
1	A	95	PRO	C-O	-6.27	1.16	1.24
1	A	279	ASP	C-O	-6.22	1.16	1.24
1	A	205	TRP	CA-C	-5.97	1.46	1.52
1	B	96	ASN	C-O	-5.89	1.17	1.24
1	A	98	THR	C-O	-5.88	1.17	1.24
1	A	107	VAL	C-O	-5.73	1.17	1.24
1	B	282	ALA	C-O	-5.64	1.17	1.24
1	B	190	GLU	C-O	-5.58	1.17	1.24
1	B	279	ASP	C-O	-5.57	1.17	1.24
1	A	190	GLU	C-O	-5.52	1.17	1.24
1	A	289	GLY	C-O	-5.41	1.17	1.24
1	B	3	LYS	CA-C	5.41	1.60	1.52
1	A	246	TYR	C-O	-5.39	1.17	1.24
1	A	132	ARG	C-O	-5.34	1.17	1.24
1	A	213	ASN	C-O	-5.34	1.17	1.24
1	A	109	ARG	C-O	-5.33	1.17	1.24
1	A	251	ILE	C-O	-5.27	1.18	1.24
1	A	295	LEU	C-O	-5.23	1.17	1.24
1	A	294	VAL	C-O	-5.17	1.18	1.24
1	A	303	VAL	C-O	-5.16	1.18	1.24
1	B	165	VAL	C-O	-5.14	1.18	1.24
1	A	195	SER	C-O	-5.12	1.18	1.24
1	B	269	CYS	CA-C	-5.06	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	HIS	C-O	-5.05	1.18	1.24
1	A	313	THR	C-O	-5.04	1.18	1.24
1	B	274	GLY	C-O	-5.04	1.17	1.23
1	A	277	GLN	C-O	-5.01	1.17	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	310	GLY	N-CA-C	9.93	125.59	111.19
1	B	312	VAL	N-CA-C	9.06	123.58	111.44
1	B	251	ILE	N-CA-C	7.78	119.49	110.62
1	B	276	VAL	N-CA-C	7.24	117.34	110.53
1	A	313	THR	N-CA-C	7.05	118.97	111.28
1	B	169	VAL	N-CA-C	-6.87	105.14	111.67
1	A	251	ILE	N-CA-C	6.86	118.44	110.62
1	A	307	ALA	N-CA-C	-6.35	98.86	108.96
1	B	174	GLU	N-CA-C	-6.34	101.22	111.04
1	A	233	LYS	N-CA-C	6.24	118.16	111.36
1	B	146	VAL	N-CA-C	-6.18	100.99	107.60
1	B	78	PRO	N-CA-C	6.08	120.74	111.19
1	A	374	LYS	N-CA-C	6.07	117.56	111.07
1	A	335	ALA	N-CA-C	-5.96	104.86	111.36
1	B	163	GLN	N-CA-C	5.84	117.60	110.41
1	A	135	TYR	N-CA-C	5.72	118.72	109.40
1	A	4	LYS	N-CA-C	5.71	118.07	110.53
1	B	234	GLN	N-CA-C	5.69	121.25	113.97
1	B	230	ILE	N-CA-C	5.57	116.30	110.62
1	A	72	LYS	N-CA-C	5.42	117.74	108.90
1	A	134	ALA	N-CA-C	5.34	119.66	113.20
1	A	138	GLN	N-CA-C	5.23	118.45	111.75
1	A	311	THR	N-CA-CB	5.21	119.29	110.49
1	A	16	ASP	N-CA-C	5.19	118.04	109.85
1	A	308	ALA	N-CA-C	5.14	119.56	113.28

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	3292	0	3225	18	0
1	B	3197	0	3149	17	0
2	A	2	0	0	0	0
3	A	26	10	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	111	0	0	0	0
5	B	94	0	0	1	0
All	All	6724	10	6382	33	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 3.

All (33) 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:20:ARG:NH2	1:B:43:ASP:OD1	2.21	0.74
1:B:132:ARG:HG3	1:B:274:GLY:HA3	1.71	0.71
1:A:13:MET:HE3	1:A:72:LYS:HB2	1.79	0.62
1:A:362:VAL:HG23	1:A:408:LYS:HD2	1.84	0.60
1:B:158:PRO:HG2	1:B:162:THR:HB	1.84	0.60
1:A:167:TYR:HB3	1:B:142:THR:HG21	1.83	0.59
1:A:132:ARG:HG3	1:A:274:GLY:HA3	1.89	0.54
1:A:297:CYS:HB3	1:A:298:PRO:HD2	1.92	0.52
1:B:20:ARG:HH22	1:B:43:ASP:CG	2.17	0.51
1:B:13:MET:HE1	1:B:64:ILE:HD11	1.92	0.51
1:A:267:TRP:CD1	1:A:269:CYS:HG	2.29	0.50
1:B:30:LEU:CD1	1:B:398:MET:HE1	2.43	0.49
1:A:160:ASP:OD1	1:A:162:THR:HG23	2.13	0.48
1:B:123:GLY:O	1:B:262:GLU:HA	2.14	0.48
1:B:13:MET:CE	1:B:64:ILE:HD11	2.44	0.47
1:A:197:PHE:CZ	1:A:231:TYR:HB2	2.49	0.47
1:A:80:GLU:N	1:A:91:MET:HE2	2.30	0.46
1:A:13:MET:CE	1:A:72:LYS:HB2	2.45	0.46
1:A:94:SER:HA	1:A:95:PRO:HD2	1.80	0.46
1:A:297:CYS:HB3	1:A:298:PRO:CD	2.47	0.45
1:A:283:GLN:HG2	1:B:256:ALA:O	2.16	0.45
1:B:163:GLN:N	1:B:163:GLN:OE1	2.50	0.45
1:B:344:ALA:HB2	1:B:352:LEU:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:HIS:HB2	1:B:192:PHE:CE2	2.52	0.44
1:B:197:PHE:CZ	1:B:231:TYR:HB2	2.53	0.44
1:B:408:LYS:HE2	1:B:408:LYS:HB2	1.89	0.44
1:B:29:LYS:HE2	1:B:399:ASP:OD1	2.19	0.43
1:B:182:MET:CE	5:B:610:HOH:O	2.68	0.42
1:A:79:ASP:C	1:A:91:MET:HE2	2.45	0.42
1:A:80:GLU:OE2	1:A:84:GLU:OE1	2.36	0.42
1:A:15:GLY:O	1:A:20:ARG:HD2	2.19	0.41
1:A:160:ASP:CG	1:A:162:THR:HG23	2.46	0.40
1:A:7:GLY:HA3	1:A:37:LEU:HD23	2.03	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	416/421 (99%)	398 (96%)	17 (4%)	1 (0%)	43	63
1	B	402/421 (96%)	381 (95%)	20 (5%)	1 (0%)	43	63
All	All	818/842 (97%)	779 (95%)	37 (4%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	160	ASP
1	A	312	VAL

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	348/357 (98%)	322 (92%)	26 (8%)	12	26
1	B	340/357 (95%)	315 (93%)	25 (7%)	13	27
All	All	688/714 (96%)	637 (93%)	51 (7%)	13	27

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	22	ILE
1	A	25	LEU
1	A	36	GLU
1	A	39	LEU
1	A	77	THR
1	A	163	GLN
1	A	202	SER
1	A	203	LYS
1	A	233	LYS
1	A	234	GLN
1	A	237	SER
1	A	242	GLN
1	A	260	LYS
1	A	288	LEU
1	A	301	LYS
1	A	303	VAL
1	A	311	THR
1	A	312	VAL
1	A	313	THR
1	A	321	LYS
1	A	338	ARG
1	A	388	ARG
1	A	393	ASN
1	A	403	GLU
1	A	408	LYS
1	B	-1	SER
1	B	28	GLU
1	B	65	LYS
1	B	69	VAL
1	B	80	GLU
1	B	84	GLU
1	B	91	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	103	LEU
1	B	140	ARG
1	B	159	SER
1	B	162	THR
1	B	163	GLN
1	B	195	SER
1	B	196	SER
1	B	198	GLN
1	B	210	SER
1	B	237	SER
1	B	238	GLN
1	B	288	LEU
1	B	303	VAL
1	B	311	THR
1	B	345	LYS
1	B	383	LEU
1	B	388	ARG
1	B	408	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-6	ASN
1	A	14	GLN
1	A	67	HIS
1	A	96	ASN
1	A	198	GLN
1	A	213	ASN
1	A	228	GLN
1	B	101	ASN
1	B	228	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)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ICT	A	505	2	12,12,12	2.65	7 (58%)	13,16,16	2.64	9 (69%)
3	ICT	A	502	2	12,12,12	2.11	6 (50%)	13,16,16	3.69	9 (69%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ICT	A	505	2	-	2/16/16/16	-
3	ICT	A	502	2	-	8/16/16/16	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	505	ICT	C3-C2	-4.41	1.48	1.54
3	A	505	ICT	O7-C2	-3.73	1.34	1.42
3	A	505	ICT	O4-C5	-3.59	1.19	1.30
3	A	502	ICT	O2-C1	-3.31	1.20	1.30
3	A	502	ICT	O6-C6	-3.27	1.20	1.30
3	A	505	ICT	C3-C6	-3.06	1.46	1.51
3	A	505	ICT	O6-C6	-3.01	1.21	1.30
3	A	502	ICT	O4-C5	-3.00	1.20	1.30
3	A	505	ICT	O2-C1	-2.97	1.21	1.30
3	A	502	ICT	C3-C2	-2.78	1.50	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	ICT	C2-C1	-2.42	1.49	1.52
3	A	505	ICT	C2-C1	-2.09	1.49	1.52
3	A	502	ICT	O7-C2	-2.02	1.38	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	ICT	O7-C2-C3	6.23	124.69	110.63
3	A	502	ICT	C3-C4-C5	5.53	124.29	113.95
3	A	502	ICT	C4-C3-C6	4.98	119.16	111.25
3	A	502	ICT	O2-C1-O1	-4.62	113.60	124.08
3	A	502	ICT	O6-C6-C3	4.18	124.78	113.93
3	A	505	ICT	O2-C1-O1	-4.03	114.93	124.08
3	A	505	ICT	C4-C3-C6	3.92	117.48	111.25
3	A	502	ICT	O4-C5-O3	-3.75	113.67	123.33
3	A	505	ICT	O2-C1-C2	3.54	123.15	113.31
3	A	502	ICT	O2-C1-C2	3.30	122.48	113.31
3	A	505	ICT	C3-C4-C5	3.06	119.67	113.95
3	A	505	ICT	O6-C6-O5	-2.89	117.53	124.08
3	A	505	ICT	O4-C5-O3	-2.71	116.37	123.33
3	A	502	ICT	O6-C6-O5	-2.65	118.07	124.08
3	A	505	ICT	O6-C6-C3	2.57	120.60	113.93
3	A	505	ICT	O4-C5-C4	2.50	121.78	114.00
3	A	502	ICT	O5-C6-C3	-2.49	117.13	123.01
3	A	505	ICT	O7-C2-C3	2.45	116.16	110.63

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	ICT	C1-C2-C3-C4
3	A	502	ICT	O7-C2-C3-C4
3	A	502	ICT	C6-C3-C4-C5
3	A	505	ICT	C1-C2-C3-C4
3	A	502	ICT	O1-C1-C2-C3
3	A	502	ICT	O2-C1-C2-C3
3	A	505	ICT	O7-C2-C3-C4
3	A	502	ICT	C3-C4-C5-O3
3	A	502	ICT	C1-C2-C3-C6
3	A	502	ICT	C3-C4-C5-O4

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	418/421 (99%)	-0.12	13 (3%)	51	47	19, 35, 62, 119	0
1	B	406/421 (96%)	0.03	18 (4%)	39	34	19, 37, 70, 104	0
All	All	824/842 (97%)	-0.04	31 (3%)	44	39	19, 36, 66, 119	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	THR	5.1
1	A	-2	GLN	5.0
1	B	412	ALA	4.5
1	B	312	VAL	4.1
1	B	0	MET	3.8
1	A	300	GLY	3.6
1	A	0	MET	3.5
1	B	300	GLY	3.5
1	A	2	SER	3.3
1	A	174	GLU	3.3
1	B	-6	ASN	3.2
1	A	-6	ASN	3.2
1	B	-1	SER	3.1
1	A	310	GLY	3.1
1	A	162	THR	3.0
1	B	311	THR	2.9
1	A	-5	LEU	2.7
1	A	-1	SER	2.7
1	A	311	THR	2.6
1	B	174	GLU	2.6
1	B	-5	LEU	2.5
1	B	233	LYS	2.4
1	B	159	SER	2.3
1	A	3	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	-2	GLN	2.2
1	B	313	THR	2.2
1	B	163	GLN	2.1
1	B	162	THR	2.1
1	B	1	MET	2.1
1	A	411	GLN	2.0
1	B	80	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 oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	A	503	1/1	0.79	0.20	36,36,36,36	0
2	MG	A	501	1/1	0.88	0.20	34,34,34,34	0
3	ICT	A	502	13/13	0.93	0.11	20,20,20,20	0
3	ICT	A	505	13/13	0.95	0.10	20,20,20,20	0
4	K	A	504	1/1	0.98	0.14	30,30,30,30	0
4	K	B	501	1/1	0.98	0.14	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.