Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:45 PM GMT

PDB ID	:	1UZR
Title	:	CRYSTAL STRUCTURE OF THE CLASS IB RIBONUCLEOTIDE REDUCTASE R2F-2 SUBUNIT FROM MYCOBACTERIUM TUBERCULOSIS
Authors	:	Uppsten, M.; Davis, J.; Rubin, H.; Uhlin, U.
Deposited on	:	2004-03-15
Resolution	:	2.20 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:

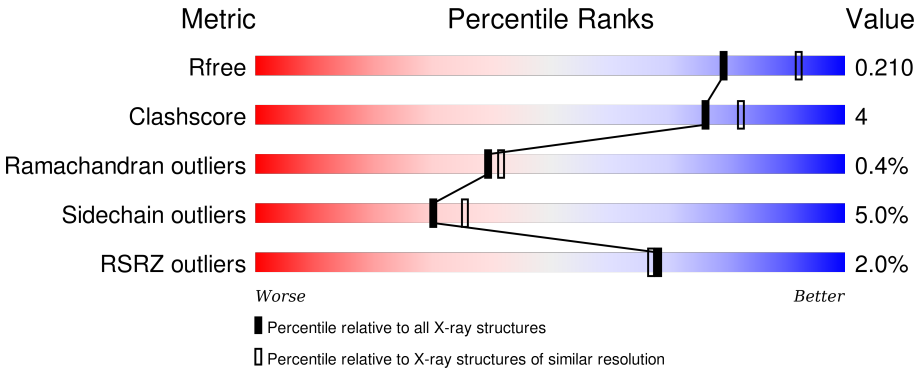
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	296	81% 11% • • 5%
1	B	296	3% 81% 14% • • •
1	C	296	2% 83% 10% • • •

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	CIT	A	1294	-	-	-	X
3	CIT	B	1299	-	-	-	X
3	CIT	C	1294	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7359 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 RIBONUCLEOTIDE REDUCTASE R2-2 SMALL SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2285	1461	376	441	7			
1	B	288	Total	C	N	O	S	0	0	0
			2327	1484	383	453	7			
1	C	283	Total	C	N	O	S	0	0	0
			2293	1465	377	444	7			

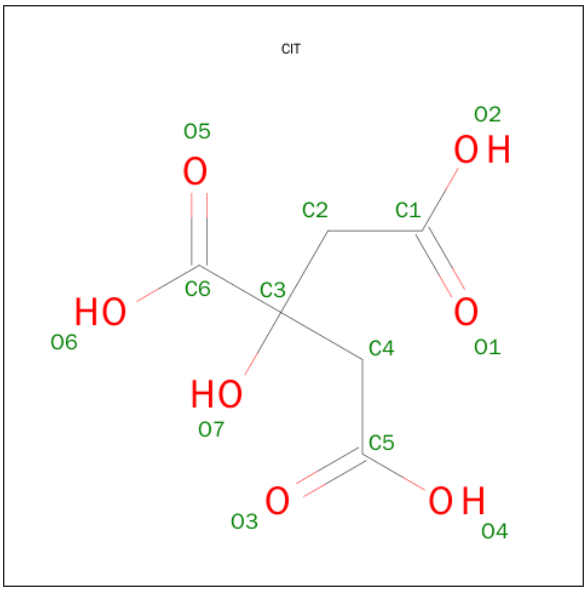
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	SER	TYR	CONFLICT	UNP Q50549
B	146	SER	TYR	CONFLICT	UNP Q50549
C	146	SER	TYR	CONFLICT	UNP Q50549

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

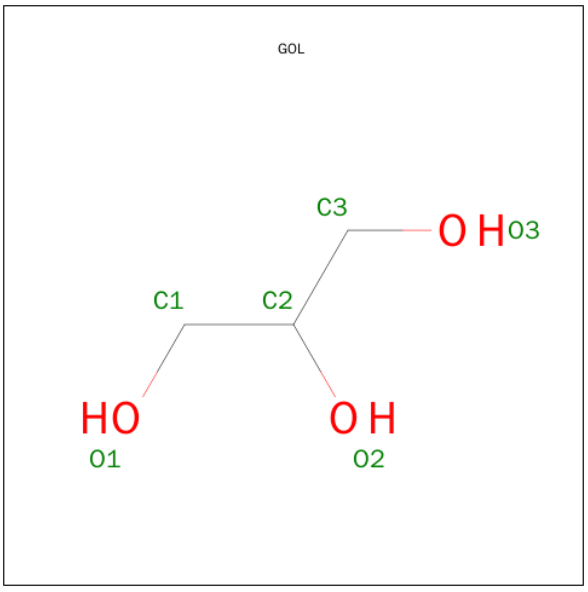
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Fe	0	0
			2	2		
2	A	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

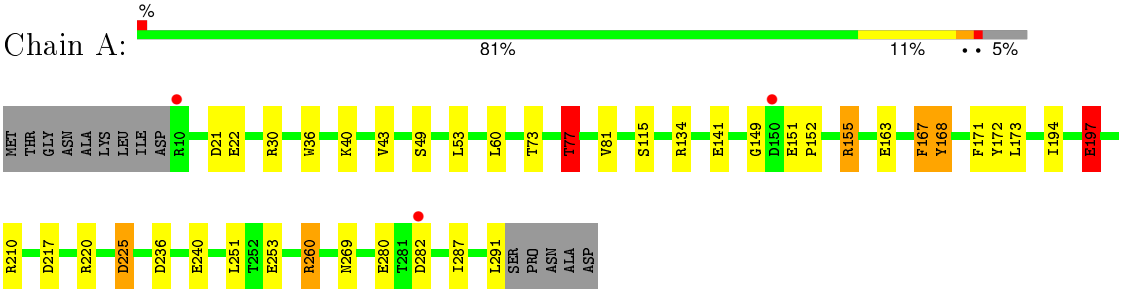
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	152	Total O 152 152	0	0
5	B	128	Total O 128 128	0	0
5	C	111	Total O 111 111	0	0

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.

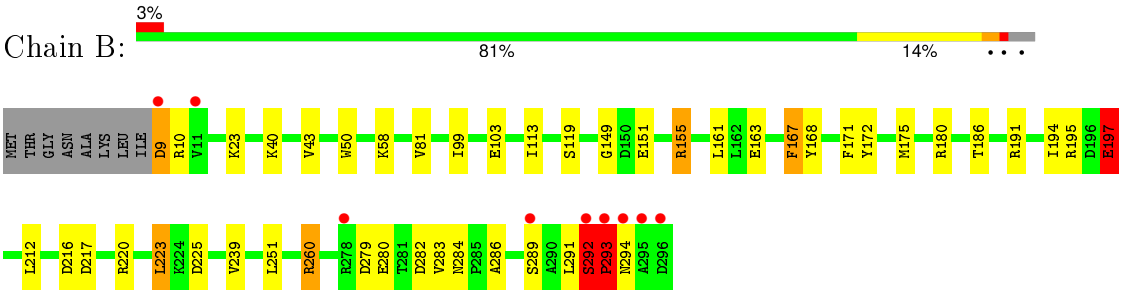
• Molecule 1: RIBONUCLEOTIDE REDUCTASE R2-2 SMALL SUBUNIT

Chain A:



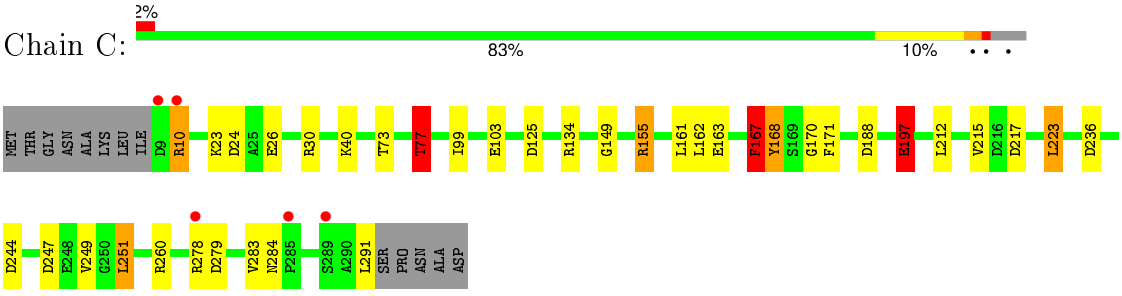
• Molecule 1: RIBONUCLEOTIDE REDUCTASE R2-2 SMALL SUBUNIT

Chain B:



• Molecule 1: RIBONUCLEOTIDE REDUCTASE R2-2 SMALL SUBUNIT

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	161.49Å 161.49Å 115.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.80 – 2.20 39.17 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (111.80-2.20) 99.0 (39.17-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.175 , 0.202 0.183 , 0.210	Depositor DCC
R_{free} test set	3868 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 32.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 77074 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7359	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FE, CIT

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	1.17	10/2335 (0.4%)	1.26	16/3172 (0.5%)
1	B	1.17	5/2378 (0.2%)	1.15	17/3232 (0.5%)
1	C	1.04	3/2343 (0.1%)	0.99	13/3183 (0.4%)
All	All	1.13	18/7056 (0.3%)	1.14	46/9587 (0.5%)

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	B	0	2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	167	PHE	CB-CG	-7.77	1.38	1.51
1	B	167	PHE	CB-CG	-7.33	1.38	1.51
1	A	36	TRP	CB-CG	6.08	1.61	1.50
1	B	81	VAL	CB-CG2	-6.08	1.40	1.52
1	A	167	PHE	CB-CG	-6.02	1.41	1.51
1	A	141	GLU	CD-OE1	5.87	1.32	1.25
1	A	49	SER	CB-OG	-5.84	1.34	1.42
1	A	260	ARG	CD-NE	-5.70	1.36	1.46
1	C	26	GLU	CD-OE1	5.65	1.31	1.25
1	B	260	ARG	CD-NE	-5.62	1.36	1.46
1	A	253	GLU	CD-OE2	5.62	1.31	1.25
1	B	172	TYR	CD2-CE2	5.49	1.47	1.39
1	A	197	GLU	CD-OE1	5.47	1.31	1.25
1	B	197	GLU	CD-OE2	5.37	1.31	1.25
1	C	197	GLU	CD-OE2	5.27	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	ARG	CD-NE	-5.15	1.37	1.46
1	A	260	ARG	CG-CD	5.15	1.64	1.51
1	A	81	VAL	CB-CG2	-5.07	1.42	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	260	ARG	NE-CZ-NH2	-24.44	108.08	120.30
1	B	260	ARG	NE-CZ-NH2	-20.48	110.06	120.30
1	A	220	ARG	NE-CZ-NH2	-19.33	110.64	120.30
1	A	260	ARG	NE-CZ-NH1	17.57	129.09	120.30
1	A	220	ARG	NE-CZ-NH1	14.98	127.79	120.30
1	B	260	ARG	NE-CZ-NH1	14.29	127.44	120.30
1	A	155	ARG	NE-CZ-NH2	-9.55	115.53	120.30
1	A	155	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	B	279	ASP	CB-CG-OD2	8.73	126.16	118.30
1	B	191	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	C	155	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	A	260	ARG	CD-NE-CZ	7.64	134.29	123.60
1	B	216	ASP	CB-CG-OD2	7.62	125.16	118.30
1	A	225	ASP	CB-CG-OD2	7.61	125.15	118.30
1	B	225	ASP	CB-CG-OD2	7.54	125.08	118.30
1	B	180	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	A	236	ASP	CB-CG-OD2	7.36	124.92	118.30
1	C	125	ASP	CB-CG-OD2	7.23	124.81	118.30
1	B	155	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	B	223	LEU	CA-CB-CG	-7.02	99.15	115.30
1	C	155	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	C	77	THR	N-CA-CB	-6.90	97.19	110.30
1	A	260	ARG	CG-CD-NE	-6.79	97.55	111.80
1	B	260	ARG	CG-CD-NE	-6.70	97.73	111.80
1	A	220	ARG	CD-NE-CZ	6.45	132.63	123.60
1	C	244	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	217	ASP	CB-CG-OD2	6.14	123.83	118.30
1	C	236	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	220	ARG	CG-CD-NE	-5.99	99.21	111.80
1	B	220	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	260	ARG	CD-NE-CZ	5.91	131.88	123.60
1	A	217	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	77	THR	N-CA-CB	-5.86	99.17	110.30
1	B	155	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	C	247	ASP	CB-CG-OD2	5.66	123.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	21	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	279	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	9	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	22	GLU	CB-CA-C	-5.46	99.47	110.40
1	B	217	ASP	CB-CG-OD1	5.44	123.20	118.30
1	C	223	LEU	CA-CB-CG	-5.41	102.85	115.30
1	B	180	ARG	CG-CD-NE	-5.32	100.63	111.80
1	C	260	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	195	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	C	24	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	188	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	292	SER	Peptide
1	B	293	PRO	Peptide

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	2285	0	2235	21	0
1	B	2327	0	2266	18	0
1	C	2293	0	2239	14	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	13	0	5	2	0
3	B	13	0	5	1	0
3	C	13	0	5	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
5	A	152	0	0	5	1
5	B	128	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	111	0	0	5	0
All	All	7359	0	6779	52	1

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 4.

All (52) 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:C:167:PHE:HE1	5:C:2043:HOH:O	1.55	0.89
1:B:284:ASN:HB3	5:B:2127:HOH:O	1.79	0.81
1:B:286:ALA:HB3	5:B:2127:HOH:O	1.90	0.71
1:C:167:PHE:CE1	5:C:2043:HOH:O	2.38	0.66
1:A:172:TYR:CZ	1:A:287:ILE:HD13	2.34	0.63
1:B:175:MET:HG3	1:B:291:LEU:HD13	1.83	0.60
1:B:282:ASP:HB3	5:B:2125:HOH:O	2.01	0.60
1:A:152:PRO:HD2	3:A:1294:CIT:O1	2.02	0.60
1:A:73:THR:O	1:A:77:THR:HB	2.03	0.59
1:A:172:TYR:CE1	1:A:287:ILE:HD13	2.39	0.58
1:A:260:ARG:HD2	1:A:280:GLU:O	2.03	0.58
1:C:73:THR:O	1:C:77:THR:HB	2.04	0.56
1:B:260:ARG:HD2	1:B:280:GLU:O	2.07	0.55
1:A:151:GLU:OE2	3:A:1294:CIT:O6	2.25	0.54
1:C:163:GLU:OE1	1:C:197:GLU:HG3	2.08	0.53
1:C:99:ILE:O	1:C:103:GLU:HG2	2.09	0.53
1:B:151:GLU:HG2	3:B:1299:CIT:O5	2.10	0.52
1:A:134:ARG:NH2	1:A:240:GLU:OE1	2.44	0.51
1:B:280:GLU:HB3	5:B:2126:HOH:O	2.12	0.50
1:B:171:PHE:CD2	1:B:194:ILE:HG12	2.49	0.48
1:C:168:TYR:HA	1:C:171:PHE:CD2	2.48	0.48
1:B:167:PHE:HE2	5:B:2037:HOH:O	1.96	0.47
1:A:77:THR:CG2	5:C:2039:HOH:O	2.62	0.47
1:A:149:GLY:O	1:A:155:ARG:NH2	2.47	0.47
1:A:171:PHE:CD2	1:A:194:ILE:HG12	2.49	0.47
1:A:225:ASP:OD1	1:B:260:ARG:NH2	2.49	0.45
1:C:249:VAL:HG23	1:C:251:LEU:HD22	1.96	0.45
1:C:149:GLY:O	1:C:155:ARG:NH2	2.49	0.45
5:A:2059:HOH:O	1:C:77:THR:CG2	2.64	0.45
1:B:163:GLU:OE1	1:B:197:GLU:HG3	2.17	0.45
1:A:282:ASP:CB	5:A:2150:HOH:O	2.65	0.45
1:B:113:ILE:HD13	1:B:186:THR:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:GLY:HA2	5:C:2068:HOH:O	2.17	0.44
1:A:163:GLU:OE1	1:A:197:GLU:HG3	2.17	0.44
1:A:77:THR:HG21	5:C:2039:HOH:O	2.18	0.43
1:A:269:ASN:HA	1:A:269:ASN:HD22	1.63	0.43
1:B:283:VAL:O	1:B:284:ASN:C	2.57	0.43
1:C:283:VAL:O	1:C:284:ASN:C	2.58	0.42
1:A:168:TYR:HA	1:A:171:PHE:CD2	2.54	0.42
1:A:282:ASP:HB3	5:A:2150:HOH:O	2.19	0.42
1:A:291:LEU:C	5:A:2152:HOH:O	2.57	0.42
1:C:212:LEU:O	1:C:215:VAL:HG22	2.20	0.41
1:B:50:TRP:CZ2	1:B:58:LYS:HG2	2.55	0.41
1:A:53:LEU:HD23	1:A:53:LEU:N	2.36	0.41
1:B:99:ILE:O	1:B:103:GLU:HG2	2.20	0.41
1:A:60:LEU:HG	1:A:173:LEU:HD21	2.02	0.41
1:B:292:SER:CB	1:B:293:PRO:HD3	2.51	0.40
1:B:149:GLY:O	1:B:155:ARG:NH2	2.55	0.40
1:B:171:PHE:CE2	1:B:194:ILE:HG12	2.57	0.40
1:A:43:VAL:HB	5:A:2066:HOH:O	2.21	0.40
1:C:162:LEU:HD23	1:C:162:LEU:C	2.42	0.40
1:C:10:ARG:HH11	1:C:10:ARG:HB3	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2018:HOH:O	5:A:2048:HOH:O[7_555]	2.12	0.08

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	280/296 (95%)	277 (99%)	3 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	286/296 (97%)	277 (97%)	6 (2%)	3 (1%)	19 16
1	C	281/296 (95%)	278 (99%)	3 (1%)	0	100 100
All	All	847/888 (95%)	832 (98%)	12 (1%)	3 (0%)	39 42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	292	SER
1	B	293	PRO
1	B	294	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	247/258 (96%)	238 (96%)	9 (4%)	42 52
1	B	252/258 (98%)	238 (94%)	14 (6%)	26 29
1	C	248/258 (96%)	234 (94%)	14 (6%)	26 29
All	All	747/774 (96%)	710 (95%)	37 (5%)	30 35

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	40	LYS
1	A	77	THR
1	A	115	SER
1	A	167	PHE
1	A	168	TYR
1	A	197	GLU
1	A	210	ARG
1	A	251	LEU
1	B	9	ASP
1	B	10	ARG

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Mol	Chain	Res	Type
1	B	23	LYS
1	B	40	LYS
1	B	43	VAL
1	B	119	SER
1	B	161	LEU
1	B	168	TYR
1	B	197	GLU
1	B	212	LEU
1	B	223	LEU
1	B	239	VAL
1	B	251	LEU
1	B	289	SER
1	C	10	ARG
1	C	23	LYS
1	C	30	ARG
1	C	40	LYS
1	C	77	THR
1	C	134	ARG
1	C	161	LEU
1	C	167	PHE
1	C	168	TYR
1	C	197	GLU
1	C	223	LEU
1	C	251	LEU
1	C	278	ARG
1	C	291	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	45	ASN
1	A	269	ASN
1	B	34	ASN
1	B	45	ASN
1	B	284	ASN
1	C	20	GLN
1	C	34	ASN
1	C	45	ASN
1	C	137	GLN

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

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	CIT	A	1294	-	3,12,12	2.12	1 (33%)	3,17,17	2.48	2 (66%)
4	GOL	A	1295	-	5,5,5	0.47	0	5,5,5	0.59	0
3	CIT	B	1299	-	3,12,12	2.13	2 (66%)	3,17,17	3.03	2 (66%)
4	GOL	B	1300	-	5,5,5	0.35	0	5,5,5	0.45	0
3	CIT	C	1294	-	3,12,12	1.30	0	3,17,17	1.66	1 (33%)
4	GOL	C	1295	-	5,5,5	0.44	0	5,5,5	0.85	0

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	CIT	A	1294	-	-	0/6/16/16	0/0/0/0
4	GOL	A	1295	-	-	0/4/4/4	0/0/0/0
3	CIT	B	1299	-	-	0/6/16/16	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	1300	-	-	0/4/4/4	0/0/0/0
3	CIT	C	1294	-	-	0/6/16/16	0/0/0/0
4	GOL	C	1295	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1299	CIT	C2-C3	2.04	1.57	1.54
3	B	1299	CIT	O7-C3	2.84	1.47	1.43
3	A	1294	CIT	O7-C3	2.85	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1294	CIT	C3-C2-C1	-3.14	109.94	114.96
3	A	1294	CIT	C4-C3-C2	-2.63	103.51	109.81
3	C	1294	CIT	C3-C4-C5	-2.37	111.17	114.96
3	B	1299	CIT	C3-C4-C5	2.38	118.76	114.96
3	B	1299	CIT	C3-C2-C1	4.69	122.45	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1294	CIT	2	0
3	B	1299	CIT	1	0

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	282/296 (95%)	-0.48	3 (1%)	82	82	20, 26, 43, 61	0
1	B	288/296 (97%)	-0.28	9 (3%)	52	51	18, 27, 54, 80	0
1	C	283/296 (95%)	-0.28	5 (1%)	71	70	19, 31, 52, 62	0
All	All	853/888 (96%)	-0.35	17 (1%)	68	67	18, 28, 48, 80	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	PRO	7.3
1	B	294	ASN	5.8
1	B	296	ASP	4.2
1	C	289	SER	3.9
1	B	295	ALA	3.5
1	B	292	SER	3.2
1	B	9	ASP	3.2
1	C	278	ARG	3.1
1	A	282	ASP	3.0
1	B	289	SER	2.7
1	A	10	ARG	2.5
1	B	278	ARG	2.4
1	A	150	ASP	2.4
1	C	285	PRO	2.3
1	C	9	ASP	2.2
1	B	11	VAL	2.1
1	C	10	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	CIT	B	1299	13/13	0.67	0.41	5.64	47,69,75,76	0
3	CIT	C	1294	13/13	0.78	0.36	5.01	80,88,90,90	0
3	CIT	A	1294	13/13	0.84	0.40	4.07	42,62,68,69	0
2	FE	B	1298	1/1	1.00	0.06	-3.16	27,27,27,27	0
2	FE	A	1293	1/1	1.00	0.05	-3.18	29,29,29,29	0
2	FE	C	1293	1/1	1.00	0.06	-3.22	30,30,30,30	0
2	FE	A	1292	1/1	0.99	0.04	-3.94	37,37,37,37	0
2	FE	B	1297	1/1	0.99	0.06	-4.44	37,37,37,37	0
2	FE	C	1292	1/1	0.99	0.05	-6.65	41,41,41,41	0
4	GOL	C	1295	6/6	0.83	0.22	-	59,63,64,64	0
4	GOL	A	1295	6/6	0.84	0.20	-	58,62,63,64	0
4	GOL	B	1300	6/6	0.83	0.18	-	59,61,61,62	0

6.5 Other polymers (i)

There are no such residues in this entry.