Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:54 AM GMT

PDB ID	:	3QAN
Title	:	Crystal structure of 1-pyrroline-5-carboxylate dehydrogenase from bacillus halodurans
Authors	:	Patskovsky, Y.; Toro, R.; Foti, R.; Seidel, R.D.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2011-01-11
Resolution	:	1.95 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:

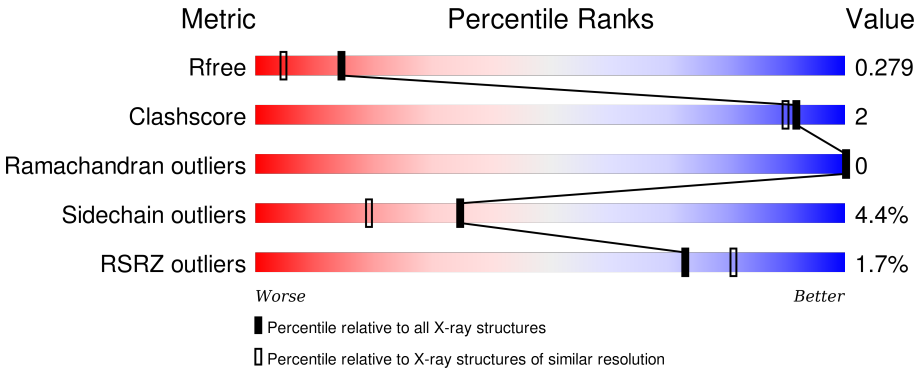
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	538	2% 89% 7%
1	B	538	2% 87% 7%
1	C	538	% 89% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12781 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 1-pyrroline-5-carboxylate dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	5	0
			4021	2549	685	772	15			
1	B	516	Total	C	N	O	S	0	6	0
			4034	2557	689	774	14			
1	C	515	Total	C	N	O	S	0	2	0
			3993	2531	684	765	13			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	VAL	-	EXPRESSION TAG	UNP Q9K9B2
A	516	ALA	-	EXPRESSION TAG	UNP Q9K9B2
A	517	GLU	-	EXPRESSION TAG	UNP Q9K9B2
A	518	ASN	-	EXPRESSION TAG	UNP Q9K9B2
A	519	LEU	-	EXPRESSION TAG	UNP Q9K9B2
A	520	TYR	-	EXPRESSION TAG	UNP Q9K9B2
A	521	PHE	-	EXPRESSION TAG	UNP Q9K9B2
A	522	GLN	-	EXPRESSION TAG	UNP Q9K9B2
A	523	SER	-	EXPRESSION TAG	UNP Q9K9B2
A	524	HIS	-	EXPRESSION TAG	UNP Q9K9B2
A	525	HIS	-	EXPRESSION TAG	UNP Q9K9B2
A	526	HIS	-	EXPRESSION TAG	UNP Q9K9B2
A	527	HIS	-	EXPRESSION TAG	UNP Q9K9B2
A	528	HIS	-	EXPRESSION TAG	UNP Q9K9B2
A	529	HIS	-	EXPRESSION TAG	UNP Q9K9B2
A	530	TRP	-	EXPRESSION TAG	UNP Q9K9B2
A	531	SER	-	EXPRESSION TAG	UNP Q9K9B2
A	532	HIS	-	EXPRESSION TAG	UNP Q9K9B2
A	533	PRO	-	EXPRESSION TAG	UNP Q9K9B2
A	534	GLN	-	EXPRESSION TAG	UNP Q9K9B2
A	535	PHE	-	EXPRESSION TAG	UNP Q9K9B2
A	536	GLU	-	EXPRESSION TAG	UNP Q9K9B2
A	537	LYS	-	EXPRESSION TAG	UNP Q9K9B2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	VAL	-	EXPRESSION TAG	UNP Q9K9B2
B	516	ALA	-	EXPRESSION TAG	UNP Q9K9B2
B	517	GLU	-	EXPRESSION TAG	UNP Q9K9B2
B	518	ASN	-	EXPRESSION TAG	UNP Q9K9B2
B	519	LEU	-	EXPRESSION TAG	UNP Q9K9B2
B	520	TYR	-	EXPRESSION TAG	UNP Q9K9B2
B	521	PHE	-	EXPRESSION TAG	UNP Q9K9B2
B	522	GLN	-	EXPRESSION TAG	UNP Q9K9B2
B	523	SER	-	EXPRESSION TAG	UNP Q9K9B2
B	524	HIS	-	EXPRESSION TAG	UNP Q9K9B2
B	525	HIS	-	EXPRESSION TAG	UNP Q9K9B2
B	526	HIS	-	EXPRESSION TAG	UNP Q9K9B2
B	527	HIS	-	EXPRESSION TAG	UNP Q9K9B2
B	528	HIS	-	EXPRESSION TAG	UNP Q9K9B2
B	529	HIS	-	EXPRESSION TAG	UNP Q9K9B2
B	530	TRP	-	EXPRESSION TAG	UNP Q9K9B2
B	531	SER	-	EXPRESSION TAG	UNP Q9K9B2
B	532	HIS	-	EXPRESSION TAG	UNP Q9K9B2
B	533	PRO	-	EXPRESSION TAG	UNP Q9K9B2
B	534	GLN	-	EXPRESSION TAG	UNP Q9K9B2
B	535	PHE	-	EXPRESSION TAG	UNP Q9K9B2
B	536	GLU	-	EXPRESSION TAG	UNP Q9K9B2
B	537	LYS	-	EXPRESSION TAG	UNP Q9K9B2
C	0	VAL	-	EXPRESSION TAG	UNP Q9K9B2
C	516	ALA	-	EXPRESSION TAG	UNP Q9K9B2
C	517	GLU	-	EXPRESSION TAG	UNP Q9K9B2
C	518	ASN	-	EXPRESSION TAG	UNP Q9K9B2
C	519	LEU	-	EXPRESSION TAG	UNP Q9K9B2
C	520	TYR	-	EXPRESSION TAG	UNP Q9K9B2
C	521	PHE	-	EXPRESSION TAG	UNP Q9K9B2
C	522	GLN	-	EXPRESSION TAG	UNP Q9K9B2
C	523	SER	-	EXPRESSION TAG	UNP Q9K9B2
C	524	HIS	-	EXPRESSION TAG	UNP Q9K9B2
C	525	HIS	-	EXPRESSION TAG	UNP Q9K9B2
C	526	HIS	-	EXPRESSION TAG	UNP Q9K9B2
C	527	HIS	-	EXPRESSION TAG	UNP Q9K9B2
C	528	HIS	-	EXPRESSION TAG	UNP Q9K9B2
C	529	HIS	-	EXPRESSION TAG	UNP Q9K9B2
C	530	TRP	-	EXPRESSION TAG	UNP Q9K9B2
C	531	SER	-	EXPRESSION TAG	UNP Q9K9B2
C	532	HIS	-	EXPRESSION TAG	UNP Q9K9B2
C	533	PRO	-	EXPRESSION TAG	UNP Q9K9B2

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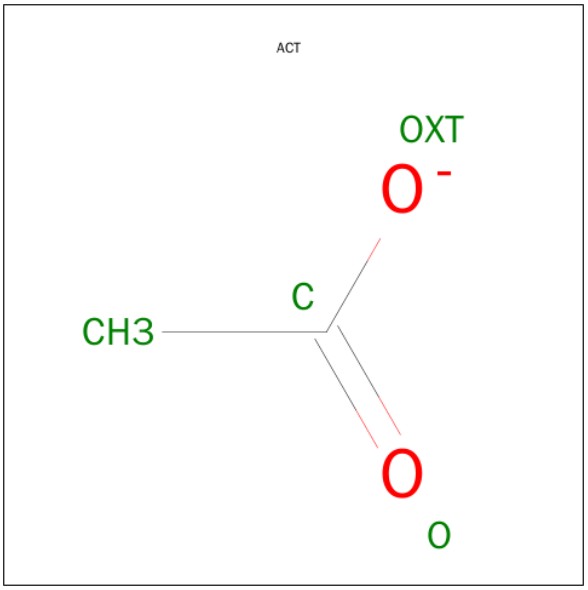
Chain	Residue	Modelled	Actual	Comment	Reference
C	534	GLN	-	EXPRESSION TAG	UNP Q9K9B2
C	535	PHE	-	EXPRESSION TAG	UNP Q9K9B2
C	536	GLU	-	EXPRESSION TAG	UNP Q9K9B2
C	537	LYS	-	EXPRESSION TAG	UNP Q9K9B2

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

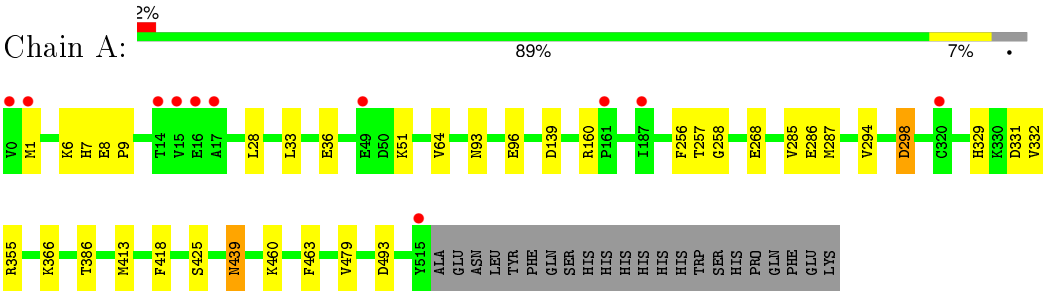
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	238	Total O 238 238	0	0
3	B	205	Total O 205 205	0	0
3	C	286	Total O 286 286	0	0

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.

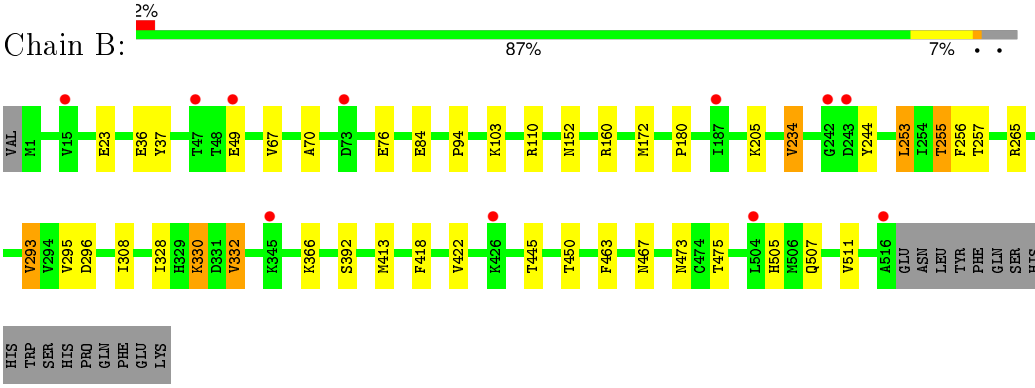
- Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase 1

Chain A:



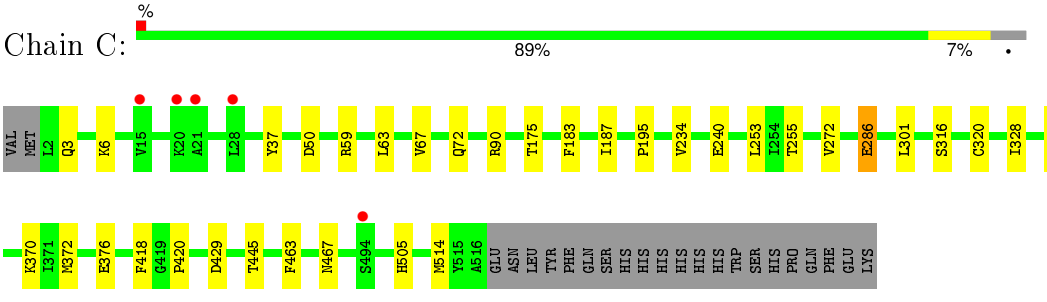
- Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase 1

Chain B:



- Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase 1

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	101.90Å 75.56Å 217.39Å 90.00° 98.48° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 44.42 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-1.95) 99.4 (44.42-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.216 , 0.280 0.217 , 0.279	Depositor DCC
R_{free} test set	3567 reflections (3.10%)	DCC
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 119738 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12781	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.20% 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: ACT

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	0.50	0/4118	0.62	0/5580
1	B	0.49	0/4134	0.60	0/5600
1	C	0.54	0/4081	0.64	0/5531
All	All	0.51	0/12333	0.62	0/16711

There are no bond length outliers.

There are no bond angle outliers.

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	4021	0	3987	14	0
1	B	4034	0	4002	23	0
1	C	3993	0	3952	17	0
2	C	4	0	3	1	0
3	A	238	0	0	0	0
3	B	205	0	0	1	0
3	C	286	0	0	2	0
All	All	12781	0	11944	51	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 2.

All (51) 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:257:THR:HG23	1:B:286:GLU:HG3	1.73	0.69
1:A:329:HIS:HD2	1:A:331:ASP:H	1.45	0.64
1:A:298:ASP:N	1:A:298:ASP:OD1	2.33	0.60
1:B:255:THR:HG21	3:B:543:HOH:O	2.01	0.60
1:C:59:ARG:HH11	1:C:59:ARG:HG2	1.68	0.59
1:A:268[A]:GLU:HG2	1:B:272:VAL:HA	1.87	0.57
1:B:257:THR:HG23	1:B:286:GLU:CG	2.36	0.56
1:C:183:PHE:HB2	1:C:187:ILE:HD12	1.86	0.56
1:B:234:VAL:O	1:B:234:VAL:HG13	2.06	0.56
1:A:93:ASN:HB2	1:A:96[A]:GLU:HG2	1.88	0.56
1:B:332:VAL:HG13	1:B:332:VAL:O	2.05	0.55
1:C:316:SER:HB3	1:C:420:PRO:HG3	1.89	0.54
1:C:301:LEU:CD2	1:C:332:VAL:HG21	2.38	0.53
1:B:172:MET:HG2	1:B:507:GLN:HG2	1.91	0.52
1:C:320:CYS:HB2	2:C:538:ACT:O	2.09	0.52
1:C:37:TYR:HB2	1:C:67:VAL:HG12	1.93	0.51
1:C:301:LEU:HD21	1:C:332:VAL:HG21	1.92	0.50
1:B:256:PHE:HB3	1:B:285:VAL:HG12	1.94	0.49
1:A:493:ASP:OD1	1:B:507:GLN:HB2	2.13	0.49
1:B:293:VAL:HG11	1:B:308:ILE:HG12	1.94	0.49
1:A:329:HIS:CD2	1:A:331:ASP:H	2.29	0.48
1:B:253:LEU:HD11	1:B:505:HIS:HA	1.96	0.48
1:C:372:MET:O	1:C:376:GLU:HG2	2.13	0.48
1:B:295:VAL:HB	1:B:328:ILE:HG23	1.95	0.48
1:B:180:PRO:HD3	1:B:257:THR:HB	1.96	0.47
1:C:286:GLU:HG3	3:C:868:HOH:O	2.13	0.47
1:B:330:LYS:HE3	1:B:330:LYS:HB2	1.53	0.46
1:B:94:PRO:HG2	1:B:152:ASN:ND2	2.31	0.46
1:C:175:THR:HG21	1:C:195:PRO:HG3	1.98	0.46
1:B:76:GLU:OE2	1:B:244:TYR:OH	2.21	0.46
1:C:72:GLN:HG2	1:C:240:GLU:O	2.16	0.45
1:C:370:LYS:HE2	1:C:370:LYS:HB3	1.76	0.45
1:B:70:ALA:HB2	1:B:234:VAL:HG22	2.00	0.44
1:C:234:VAL:HG13	1:C:234:VAL:O	2.17	0.44
1:B:332:VAL:O	1:B:332:VAL:CG1	2.67	0.43
1:C:255:THR:HG21	3:C:546:HOH:O	2.18	0.43
1:A:33:LEU:HD22	1:A:64:VAL:HA	2.00	0.43
1:B:296:ASP:HB2	1:B:450:THR:HB	2.01	0.43
1:B:37:TYR:HB2	1:B:67:VAL:HG12	2.02	0.42
1:A:439:ASN:ND2	1:A:439:ASN:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:PHE:HB3	1:A:285:VAL:HG12	2.01	0.42
1:A:139:ASP:HB3	1:A:479:VAL:HB	2.02	0.42
1:C:445:THR:HG22	1:C:467:ASN:HB2	2.02	0.41
1:B:473:ASN:HD22	1:B:475:THR:H	1.69	0.41
1:C:253:LEU:HD21	1:C:505:HIS:CD2	2.55	0.41
1:A:8:GLU:HA	1:A:9:PRO:HD3	1.95	0.41
1:B:445:THR:HG22	1:B:467:ASN:HB2	2.02	0.41
1:A:257:THR:HG23	1:A:286:GLU:HB3	2.03	0.41
1:A:460:LYS:HE2	1:B:511:VAL:HG11	2.01	0.41
1:C:328:ILE:HB	1:C:333:TYR:HD1	1.86	0.41
1:A:258:GLY:O	1:A:287:MET:HA	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	519/538 (96%)	506 (98%)	13 (2%)	0	100	100
1	B	520/538 (97%)	507 (98%)	13 (2%)	0	100	100
1	C	515/538 (96%)	504 (98%)	11 (2%)	0	100	100
All	All	1554/1614 (96%)	1517 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	426/442 (96%)	406 (95%)	20 (5%)	32 16
1	B	426/442 (96%)	403 (95%)	23 (5%)	27 12
1	C	420/442 (95%)	408 (97%)	12 (3%)	50 38
All	All	1272/1326 (96%)	1217 (96%)	55 (4%)	35 20

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	LYS
1	A	7	HIS
1	A	28	LEU
1	A	36	GLU
1	A	51	LYS
1	A	160	ARG
1	A	294	VAL
1	A	298	ASP
1	A	332	VAL
1	A	335	GLU
1	A	354	ASN
1	A	355	ARG
1	A	366	LYS
1	A	386	THR
1	A	413	MET
1	A	418	PHE
1	A	425	SER
1	A	439	ASN
1	A	463	PHE
1	B	23	GLU
1	B	36	GLU
1	B	49	GLU
1	B	84	GLU
1	B	103	LYS
1	B	110	ARG
1	B	160	ARG
1	B	205	LYS
1	B	234	VAL
1	B	253	LEU
1	B	255	THR
1	B	265	ARG

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Mol	Chain	Res	Type
1	B	272	VAL
1	B	286	GLU
1	B	293	VAL
1	B	330	LYS
1	B	332	VAL
1	B	366	LYS
1	B	392	SER
1	B	413	MET
1	B	418	PHE
1	B	422	VAL
1	B	463	PHE
1	C	3	GLN
1	C	6	LYS
1	C	50	ASP
1	C	63	LEU
1	C	90	ARG
1	C	272	VAL
1	C	286	GLU
1	C	366	LYS
1	C	418	PHE
1	C	429	ASP
1	C	463	PHE
1	C	514	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	113	HIS
1	A	147	GLN
1	A	152	ASN
1	A	329	HIS
1	A	354	ASN
1	B	80	GLN
1	B	91	ASN
1	B	473	ASN
1	C	152	ASN
1	C	507	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

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
2	ACT	C	538	-	1,3,3	0.87	0	0,3,3	0.00	-

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
2	ACT	C	538	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	538	ACT	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	516/538 (95%)	0.12	11 (2%) 67 75	20, 33, 48, 76	0
1	B	516/538 (95%)	0.22	11 (2%) 67 75	23, 35, 51, 66	0
1	C	515/538 (95%)	0.03	5 (0%) 84 89	20, 30, 46, 56	0
All	All	1547/1614 (95%)	0.12	27 (1%) 73 81	20, 33, 50, 76	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	VAL	6.4
1	B	516	ALA	3.8
1	A	515	TYR	3.6
1	A	14	THR	3.5
1	C	28	LEU	3.3
1	A	1	MET	3.0
1	A	15	VAL	3.0
1	B	15	VAL	2.9
1	B	187	ILE	2.9
1	A	16	GLU	2.9
1	B	49	GLU	2.9
1	C	15	VAL	2.9
1	B	504	LEU	2.7
1	B	73	ASP	2.6
1	A	320[A]	CYS	2.4
1	A	17	ALA	2.4
1	C	494	SER	2.4
1	A	49	GLU	2.3
1	C	21	ALA	2.2
1	A	187	ILE	2.2
1	B	426	LYS	2.2
1	B	47	THR	2.1
1	B	243	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	242	GLY	2.0
1	C	20	LYS	2.0
1	A	161	PRO	2.0
1	B	345	LYS	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)

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
2	ACT	C	538	4/4	0.91	0.14	1.13	43,44,47,48	0

6.5 Other polymers (i)

There are no such residues in this entry.