WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:22 PM GMT

PDB ID	:	5CTE
Title	:	Humanized yeast ACC carboxyltransferase domain bound to 2,2-dimethylpropyl (1S)-1-methyl-8-[(7-methyl-1H-indazol-5-yl)carbonyl]-2,8-diazaspiro[4.5]decane-2-carboxylate
Authors	:	Vajdos, F.F.
Deposited on	:	2015-07-23
Resolution	:	2.34 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 (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
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)	:	rb-20026982

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 2.34 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	Percentile Ranks	Value
Rfree		0.221
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		8.5%
RSRZ outliers		11.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
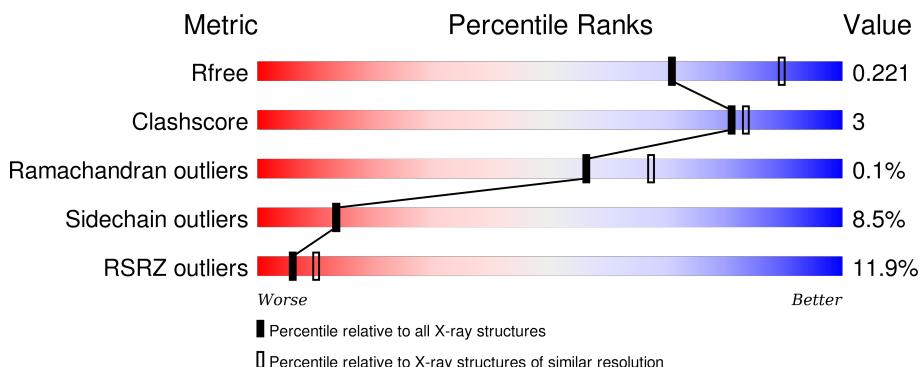
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	B	769	14% / 80% / 14% / • 5%
1	C	769	9% / 81% / 12% / • 6%
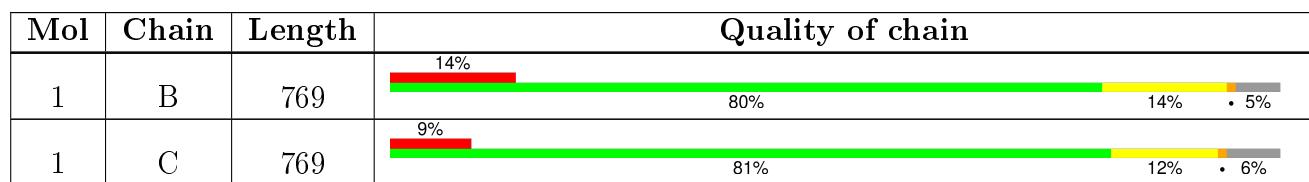
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12599 atoms, of which 68 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 Acetyl-CoA carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	728	Total 5796	C 3687	N 1000	O 1092	S 17	0	1	0
1	C	721	Total 5731	C 3638	N 990	O 1085	S 18	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1473	MET	-	expression tag	UNP Q00955
B	1474	ALA	-	expression tag	UNP Q00955
B	1475	SER	-	expression tag	UNP Q00955
B	1760	SER	PRO	engineered mutation	UNP Q00955
B	1762	LEU	ILE	engineered mutation	UNP Q00955
B	1765	VAL	MET	engineered mutation	UNP Q00955
B	1919	GLN	GLU	engineered mutation	UNP Q00955
B	1920	ALA	PRO	engineered mutation	UNP Q00955
B	1925	PHE	HIS	engineered mutation	UNP Q00955
B	2028	GLU	GLN	engineered mutation	UNP Q00955
B	2030	THR	MET	engineered mutation	UNP Q00955
B	2032	GLU	GLY	engineered mutation	UNP Q00955
B	2234	LEU	-	expression tag	UNP Q00955
B	2235	GLU	-	expression tag	UNP Q00955
B	2236	HIS	-	expression tag	UNP Q00955
B	2237	HIS	-	expression tag	UNP Q00955
B	2238	HIS	-	expression tag	UNP Q00955
B	2239	HIS	-	expression tag	UNP Q00955
B	2240	HIS	-	expression tag	UNP Q00955
B	2241	HIS	-	expression tag	UNP Q00955
C	1473	MET	-	expression tag	UNP Q00955
C	1474	ALA	-	expression tag	UNP Q00955
C	1475	SER	-	expression tag	UNP Q00955
C	1760	SER	PRO	engineered mutation	UNP Q00955
C	1762	LEU	ILE	engineered mutation	UNP Q00955

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1765	VAL	MET	engineered mutation	UNP Q00955
C	1919	GLN	GLU	engineered mutation	UNP Q00955
C	1920	ALA	PRO	engineered mutation	UNP Q00955
C	1925	PHE	HIS	engineered mutation	UNP Q00955
C	2028	GLU	GLN	engineered mutation	UNP Q00955
C	2030	THR	MET	engineered mutation	UNP Q00955
C	2032	GLU	GLY	engineered mutation	UNP Q00955
C	2234	LEU	-	expression tag	UNP Q00955
C	2235	GLU	-	expression tag	UNP Q00955
C	2236	HIS	-	expression tag	UNP Q00955
C	2237	HIS	-	expression tag	UNP Q00955
C	2238	HIS	-	expression tag	UNP Q00955
C	2239	HIS	-	expression tag	UNP Q00955
C	2240	HIS	-	expression tag	UNP Q00955
C	2241	HIS	-	expression tag	UNP Q00955

- Molecule 2 is 2,2-dimethylpropyl (1S)-1-methyl-8-[(7-methyl-1H-indazol-5-yl)carbonyl]-2,8-diazaspiro[4.5]decane-2-carboxylate (three-letter code: 57L) (formula: $C_{24}H_{34}N_4O_3$).
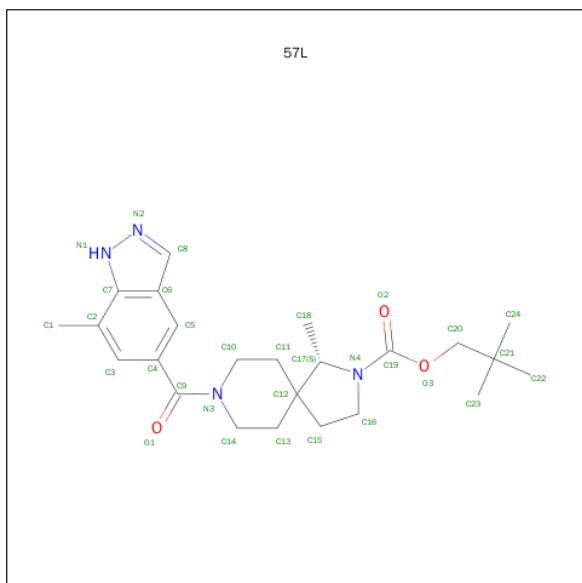
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			65	24	34	4	3		
2	C	1	Total	C	H	N	O	0	0
			65	24	34	4	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
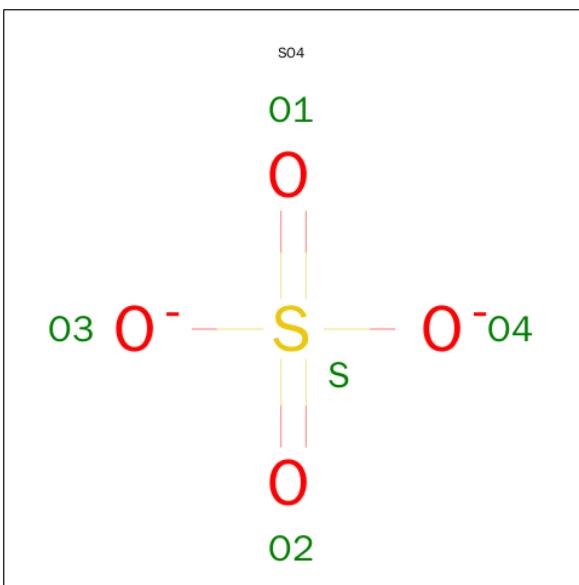
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	462	Total 462	O 462	0	0
4	C	475	Total 475	O 475	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: Acetyl-CoA carboxylase
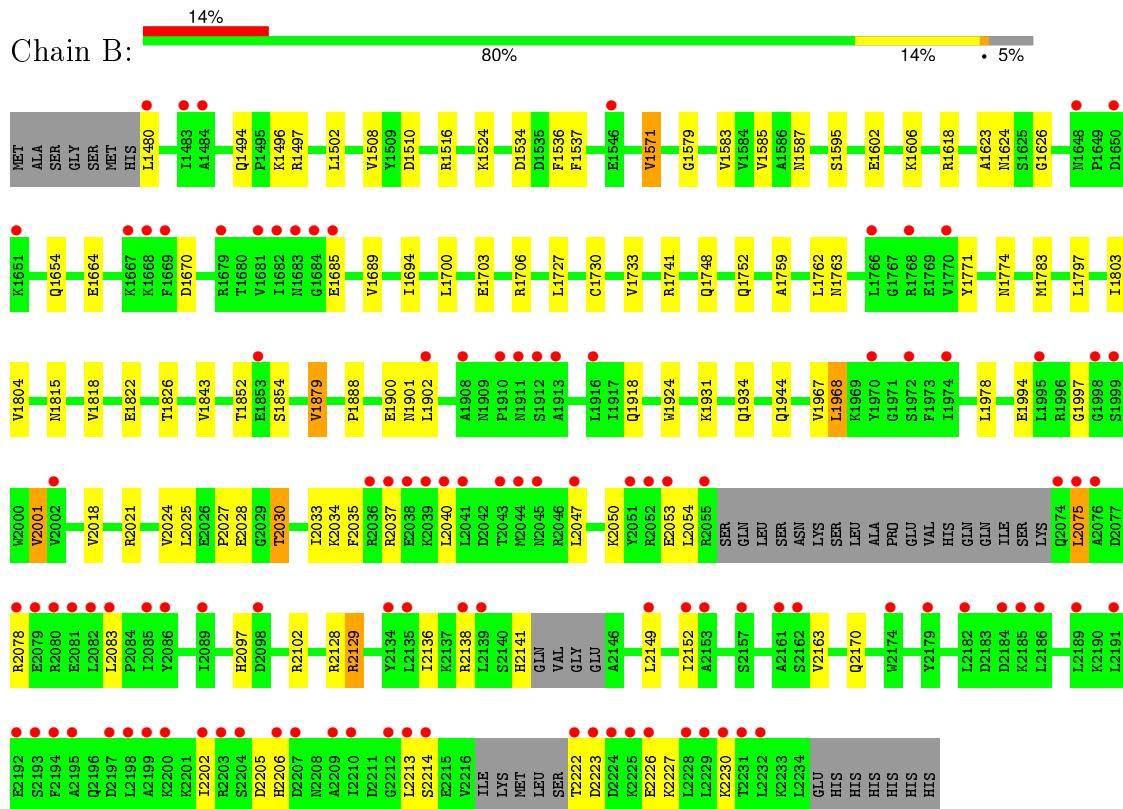
- Molecule 1: Acetyl-CoA carboxylase
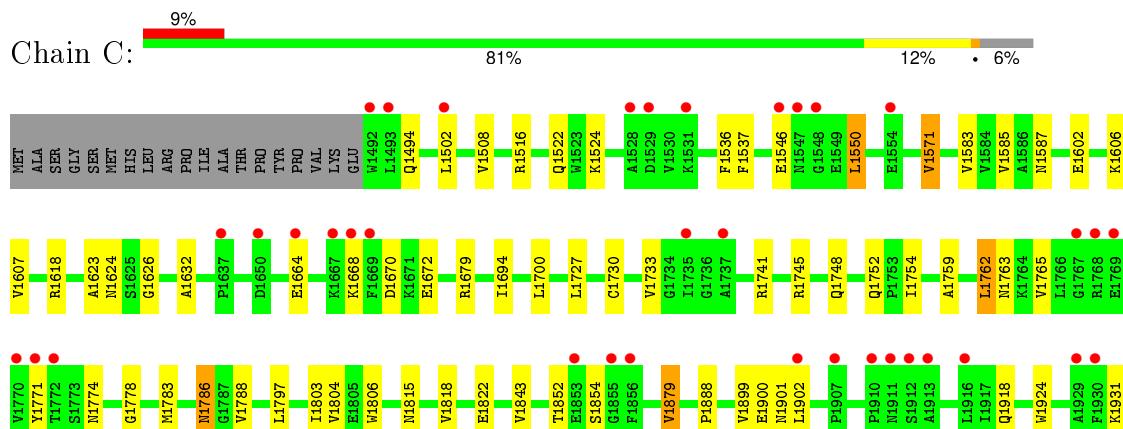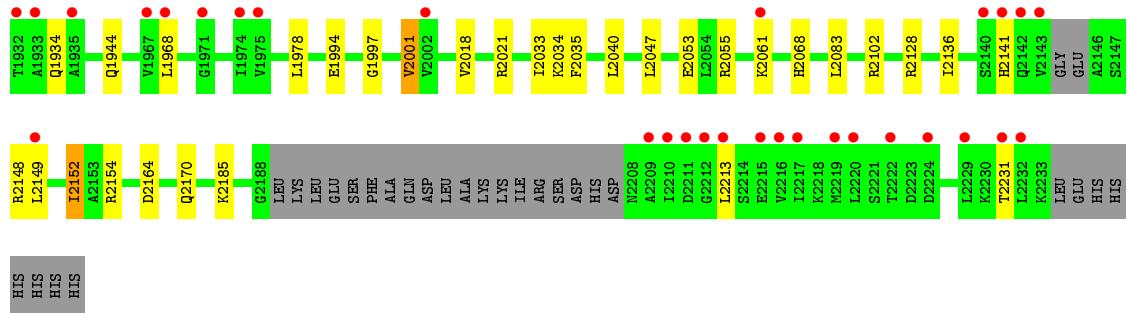
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.34Å 138.12Å 185.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.05 – 2.34 42.05 – 2.34	Depositor EDS
% Data completeness (in resolution range)	92.4 (42.05-2.34) 92.5 (42.05-2.34)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.34Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.185 , 0.217 0.186 , 0.221	Depositor DCC
R_{free} test set	4686 reflections (5.19%)	DCC
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 94915 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12599	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 57L

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	B	0.50	0/5919	0.69	0/8013
1	C	0.51	0/5848	0.70	0/7916
All	All	0.51	0/11767	0.70	0/15929

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 (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	B	5796	0	5716	45	0
1	C	5731	0	5653	36	0
2	B	31	34	34	0	0
2	C	31	34	34	0	0
3	C	5	0	0	0	0
4	B	462	0	0	7	0
4	C	475	0	0	3	0
All	All	12531	68	11437	76	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 (76) 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:1595:SER:HB3	4:B:2406:HOH:O	1.64	0.94
1:B:2129:ARG:HH11	1:B:2129:ARG:HG2	1.39	0.86
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.27	0.79
1:C:1763:ASN:HD21	1:C:1771:TYR:H	1.29	0.78
1:C:1730:CYS:HA	1:C:1752:GLN:HE21	1.48	0.77
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.49	0.76
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.34	0.74
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.48	0.62
1:C:1672:GLU:HG3	4:C:2590:HOH:O	1.99	0.62
1:C:1899:VAL:HB	4:C:2576:HOH:O	2.00	0.60
1:B:2163:VAL:HA	1:B:2170:GLN:NE2	2.16	0.60
1:B:1759:ALA:H	1:B:1774:ASN:ND2	2.00	0.60
1:C:1759:ALA:H	1:C:1774:ASN:ND2	2.01	0.59
1:B:2129:ARG:HH11	1:B:2129:ARG:CG	2.13	0.59
1:C:1900:GLU:HB3	1:C:1918:GLN:HE21	1.68	0.58
1:B:1900:GLU:HB3	1:B:1918:GLN:HE21	1.67	0.58
1:B:2163:VAL:HG12	4:B:2475:HOH:O	2.02	0.58
1:B:2040:LEU:HD21	4:B:2415:HOH:O	2.02	0.58
1:C:1754:ILE:O	1:C:1778:GLY:HA3	2.05	0.57
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.50	0.57
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	2.02	0.57
1:B:1497:ARG:HD3	1:B:1510:ASP:OD2	2.06	0.56
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.72	0.55
1:B:2136:ILE:HD11	1:B:2152:ILE:HG22	1.88	0.54
1:B:1815:ASN:ND2	1:B:1944:GLN:HE22	2.05	0.53
1:C:1624:ASN:HD21	1:C:1733:VAL:H	1.57	0.53
1:C:1745:ARG:HG2	1:C:1806:TRP:CZ2	2.44	0.52
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.74	0.52
1:B:1968:LEU:HD13	4:B:2526:HOH:O	2.10	0.52
1:B:1741:ARG:HH22	1:B:1934:GLN:NE2	2.07	0.52
1:C:1537:PHE:HD2	1:C:1571:VAL:HG13	1.75	0.51
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.75	0.50
1:C:1624:ASN:ND2	1:C:1733:VAL:H	2.10	0.50
1:B:2054:LEU:HB3	1:B:2075:LEU:HG	1.94	0.49
1:C:1762:LEU:HA	1:C:1765:VAL:HG22	1.94	0.49
1:B:2027:PRO:HA	1:B:2030:THR:HG23	1.94	0.49
1:C:2033:ILE:HG22	1:C:2034:LYS:HG2	1.95	0.49
1:C:2136:ILE:HD11	1:C:2152:ILE:HG23	1.94	0.49
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.60	0.48
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1550:LEU:HD21	1:C:1607:VAL:HG22	1.96	0.47
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.33	0.47
1:B:1703:GLU:OE1	1:C:2102:ARG:NH2	2.47	0.47
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.61	0.47
1:C:1741:ARG:HH22	1:C:1934:GLN:NE2	2.13	0.47
1:B:2050:LYS:HB3	4:B:2746:HOH:O	2.16	0.46
1:C:1537:PHE:CD2	1:C:1571:VAL:HG13	2.51	0.45
1:C:1727:LEU:HB2	1:C:1803:ILE:HD11	1.99	0.44
1:B:2033:ILE:HG22	1:B:2034:LYS:HG2	1.98	0.44
1:C:1624:ASN:HD22	1:C:1626:GLY:H	1.66	0.44
1:C:1879:VAL:HG13	1:C:1931:LYS:HE2	2.00	0.44
1:B:1727:LEU:HB2	1:B:1803:ILE:HD11	2.00	0.44
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.65	0.44
1:C:1997:GLY:O	1:C:2001:VAL:HG12	2.18	0.44
1:C:1786:ASN:HD22	1:C:1786:ASN:C	2.20	0.43
1:B:1537:PHE:CD2	1:B:1571:VAL:HG13	2.52	0.43
1:B:2214:SER:CB	1:C:2231:THR:HG21	2.48	0.43
1:B:1967:VAL:CG1	4:B:2526:HOH:O	2.67	0.43
1:B:1826:THR:HA	4:B:2447:HOH:O	2.19	0.43
1:C:2068:HIS:HE1	4:C:2429:HOH:O	2.00	0.43
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	2.01	0.42
1:B:2102:ARG:HD2	1:C:1694:ILE:HA	1.99	0.42
1:B:2222:THR:HG23	1:B:2223:ASP:H	1.84	0.42
1:B:1879:VAL:HG13	1:B:1931:LYS:HE2	2.00	0.42
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.18	0.42
1:C:1786:ASN:ND2	1:C:1788:VAL:H	2.17	0.42
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	2.01	0.42
1:B:1571:VAL:O	1:B:1579:GLY:HA2	2.20	0.41
1:B:1997:GLY:O	1:B:2001:VAL:HG12	2.20	0.41
1:B:2024:VAL:HG12	1:B:2025:LEU:HD13	2.01	0.41
1:B:1694:ILE:HA	1:C:2102:ARG:HD2	2.03	0.41
1:B:2227:LYS:HA	1:B:2230:LYS:HE3	2.01	0.41
1:C:1994:GLU:HA	1:C:2021:ARG:O	2.21	0.41
1:B:1994:GLU:HA	1:B:2021:ARG:O	2.20	0.40
1:B:1494:GLN:NE2	1:B:1496:LYS:HB2	2.37	0.40
1:B:2129:ARG:CG	1:B:2129:ARG:NH1	2.80	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	B	721/769 (94%)	703 (98%)	17 (2%)	1 (0%)	56	67
1	C	715/769 (93%)	696 (97%)	19 (3%)	0	100	100
All	All	1436/1538 (93%)	1399 (97%)	36 (2%)	1 (0%)	56	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2206	HIS

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	B	612/658 (93%)	558 (91%)	54 (9%)	12	11
1	C	609/658 (93%)	558 (92%)	51 (8%)	14	14
All	All	1221/1316 (93%)	1116 (91%)	105 (9%)	13	13

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1480	LEU
1	B	1502	LEU
1	B	1508	VAL
1	B	1516	ARG
1	B	1524	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1534	ASP
1	B	1536	PHE
1	B	1571	VAL
1	B	1583	VAL
1	B	1585	VAL
1	B	1602	GLU
1	B	1606	LYS
1	B	1618	ARG
1	B	1654	GLN
1	B	1664	GLU
1	B	1670	ASP
1	B	1685	GLU
1	B	1689	VAL
1	B	1700	LEU
1	B	1706	ARG
1	B	1762	LEU
1	B	1797	LEU
1	B	1804	VAL
1	B	1822	GLU
1	B	1843	VAL
1	B	1852	THR
1	B	1854	SER
1	B	1879	VAL
1	B	1901	ASN
1	B	1902	LEU
1	B	1924	TRP
1	B	1968	LEU
1	B	1978	LEU
1	B	2001	VAL
1	B	2018	VAL
1	B	2028[A]	GLU
1	B	2028[B]	GLU
1	B	2030	THR
1	B	2035	PHE
1	B	2037	ARG
1	B	2047	LEU
1	B	2053	GLU
1	B	2075	LEU
1	B	2078	ARG
1	B	2083	LEU
1	B	2128	ARG
1	B	2129	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2138	ARG
1	B	2141	HIS
1	B	2149	LEU
1	B	2202	ILE
1	B	2205	ASP
1	B	2213	LEU
1	B	2226	GLU
1	C	1494	GLN
1	C	1502	LEU
1	C	1508	VAL
1	C	1516	ARG
1	C	1522	GLN
1	C	1524	LYS
1	C	1536	PHE
1	C	1546	GLU
1	C	1550	LEU
1	C	1571	VAL
1	C	1583	VAL
1	C	1585	VAL
1	C	1602	GLU
1	C	1606	LYS
1	C	1618	ARG
1	C	1664	GLU
1	C	1668	LYS
1	C	1670	ASP
1	C	1679	ARG
1	C	1700	LEU
1	C	1762	LEU
1	C	1786	ASN
1	C	1797	LEU
1	C	1804	VAL
1	C	1822	GLU
1	C	1843	VAL
1	C	1852	THR
1	C	1854	SER
1	C	1879	VAL
1	C	1901	ASN
1	C	1902	LEU
1	C	1924	TRP
1	C	1968	LEU
1	C	1978	LEU
1	C	2001	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2018	VAL
1	C	2035	PHE
1	C	2040	LEU
1	C	2047	LEU
1	C	2053	GLU
1	C	2055	ARG
1	C	2061	LYS
1	C	2083	LEU
1	C	2128	ARG
1	C	2141	HIS
1	C	2148	ARG
1	C	2149	LEU
1	C	2152	ILE
1	C	2154	ARG
1	C	2185	LYS
1	C	2213	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1494	GLN
1	B	1517	GLN
1	B	1587	ASN
1	B	1605	ASN
1	B	1624	ASN
1	B	1654	GLN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1774	ASN
1	B	1815	ASN
1	B	1837	ASN
1	B	1918	GLN
1	B	1934	GLN
1	B	1941	ASN
1	B	2011	GLN
1	B	2092	GLN
1	B	2097	HIS
1	B	2170	GLN
1	C	1517	GLN
1	C	1587	ASN
1	C	1605	ASN

Continued from previous page...

Mol	Chain	Res	Type
1	C	1624	ASN
1	C	1654	GLN
1	C	1748	GLN
1	C	1752	GLN
1	C	1763	ASN
1	C	1774	ASN
1	C	1786	ASN
1	C	1815	ASN
1	C	1918	GLN
1	C	1934	GLN
1	C	2068	HIS
1	C	2070	GLN
1	C	2170	GLN
1	C	2178	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

3 ligands are 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	57L	B	2301	-	31,34,34	0.98	2 (6%)	32,52,52	0.98	1 (3%)
2	57L	C	2301	-	31,34,34	0.95	1 (3%)	32,52,52	1.04	2 (6%)
3	SO4	C	2302	-	4,4,4	0.28	0	6,6,6	0.25	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
2	57L	B	2301	-	-	0/18/46/46	0/4/4/4
2	57L	C	2301	-	-	0/18/46/46	0/4/4/4
3	SO4	C	2302	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2301	57L	C19-N4	2.02	1.38	1.35
2	C	2301	57L	C9-N3	2.17	1.39	1.34
2	B	2301	57L	C9-N3	2.35	1.40	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2301	57L	C5-C4-C3	2.09	122.63	119.96
2	B	2301	57L	C5-C4-C3	2.13	122.69	119.96
2	C	2301	57L	O3-C19-N4	2.19	113.36	111.11

There are no chirality outliers.

There are no torsion outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	B	728/769 (94%)	0.69	107 (14%)	3	6	32, 53, 125, 152	0
1	C	721/769 (93%)	0.36	66 (9%)	11	17	30, 55, 97, 126	0
All	All	1449/1538 (94%)	0.53	173 (11%)	6	10	30, 54, 110, 152	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2202	ILE	10.2
1	B	2076	ALA	8.6
1	B	2213	LEU	8.5
1	B	2075	LEU	7.9
1	B	2189	LEU	7.9
1	B	2161	ALA	7.7
1	B	2186	LEU	7.3
1	B	2082	LEU	7.0
1	C	2232	LEU	6.4
1	B	2079	GLU	6.3
1	B	1911	ASN	6.2
1	B	2153	ALA	6.1
1	B	2074	GLN	6.0
1	B	2209	ALA	6.0
1	B	2224	ASP	5.7
1	C	2213	LEU	5.7
1	B	2193	SER	5.7
1	B	2152	ILE	5.5
1	B	2195	ALA	5.5
1	B	2228	LEU	5.5
1	B	2182	LEU	5.3
1	B	2139	LEU	5.2
1	C	2217	ILE	5.2
1	B	2179	TYR	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	2210	ILE	4.9
1	B	1684	GLY	4.9
1	B	1683	ASN	4.9
1	C	1911	ASN	4.8
1	C	2209	ALA	4.8
1	B	2086	TYR	4.6
1	C	2219	MET	4.5
1	C	1913	ALA	4.5
1	C	2220	LEU	4.5
1	B	2053	GLU	4.4
1	B	2055	ARG	4.4
1	B	2199	ALA	4.4
1	C	2143	VAL	4.4
1	C	1493	LEU	4.3
1	B	2198	LEU	4.3
1	B	2191	LEU	4.2
1	B	2149	LEU	4.2
1	B	1913	ALA	4.2
1	B	2052	ARG	4.2
1	B	1916	LEU	4.0
1	B	2207	ASP	4.0
1	C	1912	SER	4.0
1	B	1682	ILE	3.9
1	B	2210	ILE	3.9
1	B	2041	LEU	3.9
1	B	2229	LEU	3.9
1	C	2216	VAL	3.9
1	B	2214	SER	3.9
1	C	1547	ASN	3.8
1	B	2157	SER	3.8
1	B	2222	THR	3.8
1	B	2225	LYS	3.8
1	B	2230	LYS	3.8
1	C	2229	LEU	3.8
1	B	1685	GLU	3.7
1	B	2162	SER	3.6
1	B	2223	ASP	3.6
1	B	2081	GLU	3.6
1	C	2231	THR	3.6
1	C	1668	LYS	3.6
1	C	2212	GLY	3.6
1	C	1853	GLU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1910	PRO	3.4
1	B	1480	LEU	3.4
1	B	2206	HIS	3.4
1	C	1492	TRP	3.4
1	B	1853	GLU	3.4
1	B	1669	PHE	3.4
1	B	1912	SER	3.3
1	B	2039	LYS	3.3
1	C	1529	ASP	3.2
1	C	1855	GLY	3.2
1	B	2226	GLU	3.2
1	B	2200	LYS	3.2
1	B	2174	TRP	3.2
1	B	1902	LEU	3.2
1	B	2080	ARG	3.2
1	B	1766	LEU	3.2
1	B	1998	GLY	3.1
1	B	2036	ARG	3.1
1	C	2211	ASP	3.1
1	B	2085	ILE	3.1
1	B	2232	LEU	3.0
1	B	2078	ARG	3.0
1	C	1770	VAL	3.0
1	C	1910	PRO	2.9
1	B	2194	PHE	2.9
1	B	1681	VAL	2.9
1	B	1650	ASP	2.9
1	C	1664	GLU	2.9
1	B	1908	ALA	2.9
1	B	2185	LYS	2.9
1	B	1667	LYS	2.8
1	B	1651	LYS	2.8
1	C	1546	GLU	2.8
1	C	1502	LEU	2.8
1	B	2038	GLU	2.8
1	C	1769	GLU	2.8
1	B	1768	ARG	2.8
1	B	1770	VAL	2.8
1	C	1767	GLY	2.7
1	C	2141	HIS	2.7
1	B	2083	LEU	2.7
1	B	2197	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2212	GLY	2.7
1	B	2231	THR	2.7
1	C	1902	LEU	2.7
1	B	1999	SER	2.6
1	B	1483	ILE	2.6
1	C	1772	THR	2.6
1	C	1737	ALA	2.6
1	C	1650	ASP	2.6
1	C	1967	VAL	2.6
1	C	1975	VAL	2.6
1	C	2215	GLU	2.6
1	B	2045	ASN	2.5
1	B	1648	ASN	2.5
1	B	2037	ARG	2.5
1	C	1974	ILE	2.5
1	B	1995	LEU	2.5
1	B	2047	LEU	2.5
1	C	1916	LEU	2.5
1	C	1768	ARG	2.5
1	B	2002	VAL	2.5
1	C	1856	PHE	2.5
1	B	2051	TYR	2.5
1	C	1669	PHE	2.4
1	C	2224	ASP	2.4
1	B	2204	SER	2.4
1	C	1554	GLU	2.4
1	B	1974	ILE	2.4
1	C	1933	ALA	2.4
1	C	2142	GLN	2.4
1	B	2135	LEU	2.3
1	C	1968	LEU	2.3
1	C	2061	LYS	2.3
1	B	1546	GLU	2.3
1	C	1771	TYR	2.3
1	B	2089	ILE	2.3
1	B	1970	TYR	2.3
1	C	1637	PRO	2.2
1	B	2192	GLU	2.2
1	C	1929	ALA	2.2
1	C	2222	THR	2.2
1	C	1528	ALA	2.2
1	C	1531	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2040	LEU	2.2
1	C	1971	GLY	2.2
1	C	1735	ILE	2.2
1	B	2043	THR	2.2
1	B	2203	ARG	2.2
1	B	1972	SER	2.2
1	B	2184	ASP	2.2
1	B	1668	LYS	2.2
1	C	1667	LYS	2.2
1	B	2138	ARG	2.2
1	C	2002	VAL	2.1
1	C	1930	PHE	2.1
1	B	2098	ASP	2.1
1	B	1679	ARG	2.1
1	C	1935	ALA	2.1
1	B	1484	ALA	2.1
1	C	1548	GLY	2.1
1	C	2140	SER	2.1
1	C	1907	PRO	2.1
1	B	2044	MET	2.0
1	C	2149	LEU	2.0
1	B	2134	TYR	2.0
1	C	1932	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 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, 95th 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	57L	C	2301	31/31	0.95	0.14	-0.26	39,48,54,60	0
2	57L	B	2301	31/31	0.94	0.15	-1.14	46,57,76,79	0
3	SO4	C	2302	5/5	0.98	0.14	-	83,85,86,87	0

6.5 Other polymers (i)

There are no such residues in this entry.