



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 04:08 PM GMT

PDB ID : 1JSW
Title : NATIVE L-ASPARTATE AMMONIA LYASE
Authors : Shi, W.; Dunbar, J.; Farber, G.K.
Deposited on : 1997-02-19
Resolution : 2.70 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

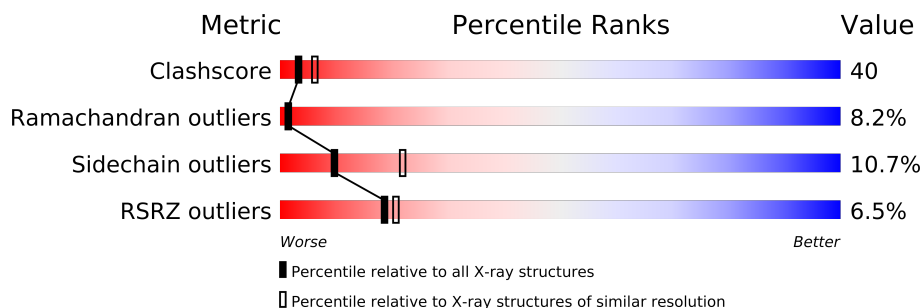
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	478	
1	B	478	
1	C	478	
1	D	478	

2 Entry composition i

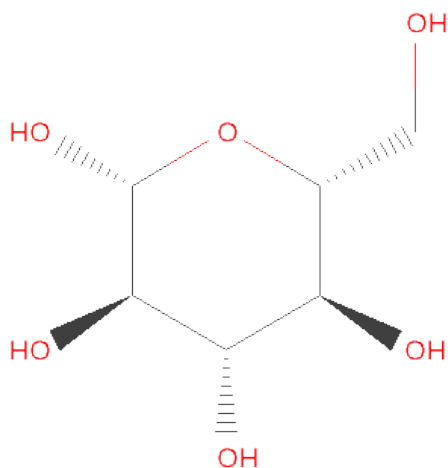
There are 4 unique types of molecules in this entry. The entry contains 13764 atoms, of which 0 are hydrogen and 0 are deuterium.

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 L-ASPARTATE AMMONIA-LYASE.

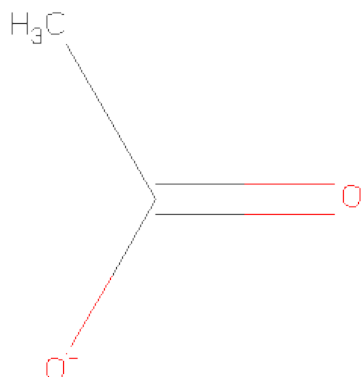
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3502	2205	595	676	26			
1	B	460	Total	C	N	O	S	0	0	0
			3511	2210	597	678	26			
1	C	413	Total	C	N	O	S	0	0	0
			3152	1988	534	606	24			
1	D	459	Total	C	N	O	S	0	0	0
			3502	2205	595	676	26			

- Molecule 2 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

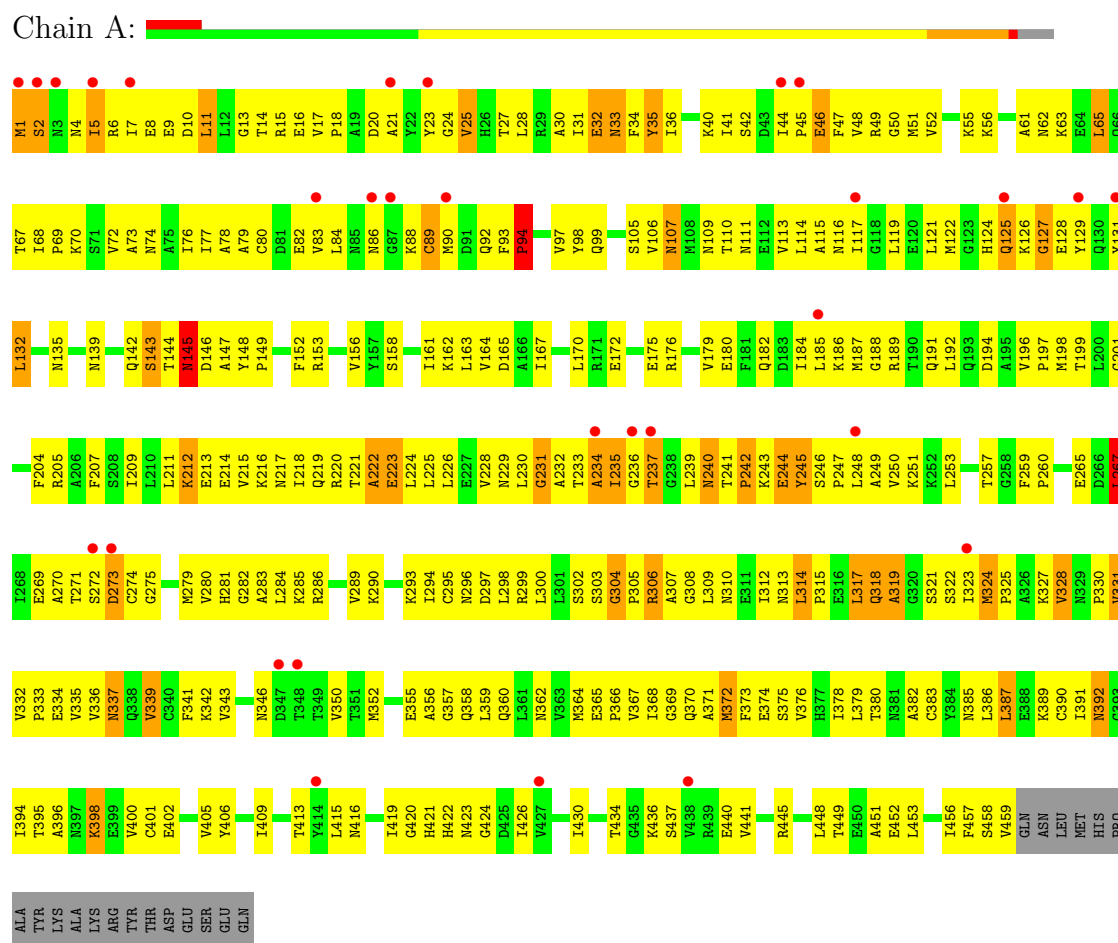
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	16	Total	O	0	0
			16	16		
4	C	11	Total	O	0	0
			11	11		
4	D	23	Total	O	0	0
			23	23		

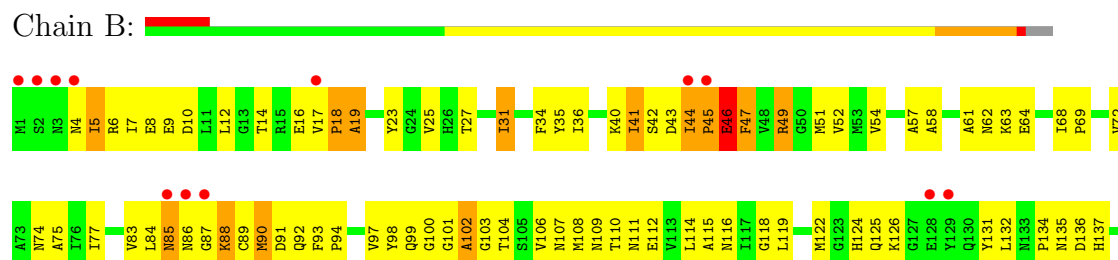
3 Residue-property plots

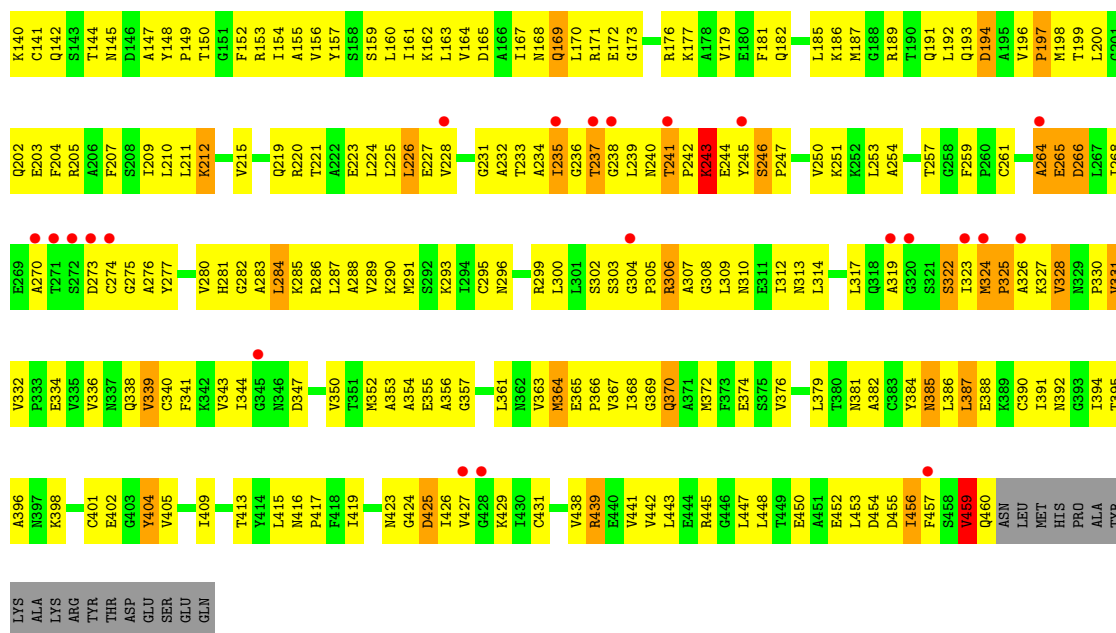
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: L-ASPARTATE AMMONIA-LYASE



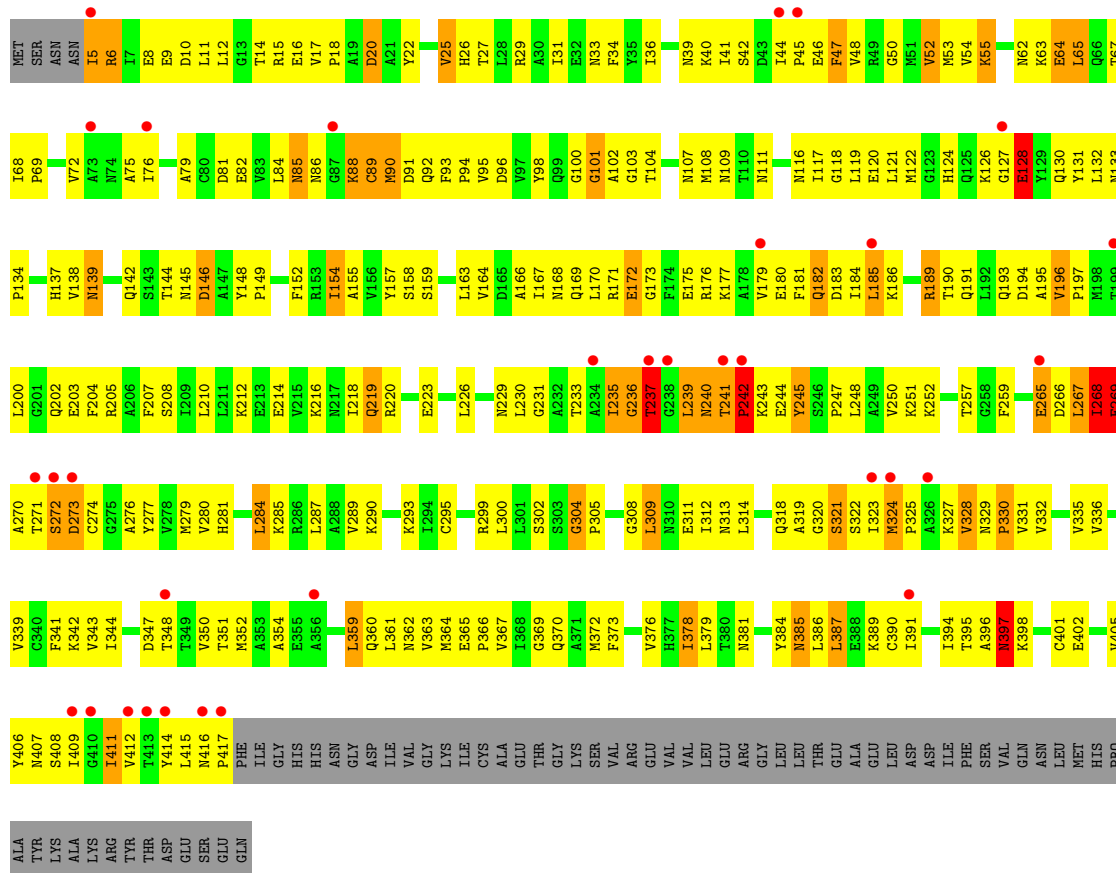
• Molecule 1: L-ASPARTATE AMMONIA-LYASE





• Molecule 1: L-ASPARTATE AMMONIA-LYASE

Chain C:



• Molecule 1: L-ASPARTATE AMMONIA-LYASE

Chain D:

ALA	Y406	V335	A270	E203	L132	L65	M1
LYS	N407	V336	T271	F204	M133	Q66	S2
ARG	S408		S272	R205	P134	T67	M3
TYR	I409	V339	D273	A206	M135	I68	N4
THR	G410	C340	C274	F207	D136	P69	I5
ASP	I411	F341	G275	S208	H137	K70	R6
GLU	V412	K342	A276	I209	V138	S71	I7
SER	T413	G345	V278	L210	Q142	A72	E8
GLN	Y414	N346	M279	L211	N145	V73	E9
	L415	D347	V280	K212		I76	D10
	N416		H281	E213	Y148	I77	L11
	P417	V350		E214	A78	A79	L12
	F418		L284	K216	P149	C80	G13
	I419	A353	K285	N217	T150		T14
		A356	R286	I218	G151		R15
	H422		L287	Q219	F152		E16
	G424	L359	A288	R220	R153		E17
	D425	V289	K290	T221	I154		G18
	I426	Q360	K291	A222	A155		P18
	G428	L361	S292	E223	V156		
	K429	N362	K293	L226	Y157		A21
	I430	M364	I294	E227	S158		Y22
	C431	E365	C295	V228	C89		Y23
	A432	P366	N296		N90		G24
	E433	V367		T233	I160		V25
		I368	R299	A234	I161		H26
	K436	G369	L300	L163	A162		T27
	S437	Q370		V164	V97		L28
	V438	A371	S303	T237	N168		A30
	R439	M372	G304	C238	Q169		I31
	E440	F373	P305	L239	L170		E32
	V441		R306	N240	R171		N33
	V442	V376	A307	T241	E172		F34
	L443		G308	P242	G173		Y35
	E444	L379	L309	K243			I36
	R445	T380		E244	R176		
	G446	N381	T312	Y245			N39
	L447		N313	S246	M107		K40
	L448	N385	L314	P247	M108		I41
		L386	P315	L248	N109		S42
	A451	L387	E316	A249	T110		D43
	E452	E388		V250	L114		I44
	L453	K389	A319	L253	A115		P45
	D454	C390	G320		M116		E46
	D455	I391	S321	V256	I117		F47
	I456		S322	T257	G118		V48
	F457	I394	I323		G119		G50
	S458	T395	M324		L119		M51
	V459	A396	P325		Q120		V52
	GLN	N397	A326	P260	L121		M53
ASN	ASN	K398	K327	C261	Q193		V54
LEU	LEU	E399	V262	V262	D194		K55
MET	MET	V400	A195	P263	A196		K56
HIS	HIS	C401	A264	A264	V196		A57
PRO	PRO	E402	E265	E265	P197		A58
ALA	ALA	G403	V331	D266	M198		
TYR	TYR	V404	V332	L267	L200		N62
LYS	LYS	V405	E334	E269	Y129		K63

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	153.50Å 146.20Å 103.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 46.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 75.6 (46.38-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.81Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.216 , 0.371 0.256 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 79.2	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 43803 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13764	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, 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	0.48	0/3553	0.76	1/4815 (0.0%)
1	B	0.47	0/3562	0.73	0/4827
1	C	0.47	0/3199	0.75	2/4338 (0.0%)
1	D	0.47	0/3553	0.74	0/4815
All	All	0.47	0/13867	0.74	3/18795 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	GLU	N-CA-C	5.93	127.02	111.00
1	C	240	ASN	N-CA-C	5.63	126.21	111.00
1	A	132	LEU	N-CA-C	-5.43	96.33	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3502	0	3539	338	0
1	B	3511	0	3547	299	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3152	0	3191	268	0
1	D	3502	0	3539	318	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	4	0	3	0	0
4	A	19	0	0	1	0
4	B	16	0	0	0	0
4	C	11	0	0	0	0
4	D	23	0	0	1	0
All	All	13764	0	13843	1112	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 40.

The worst 5 of 1112 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:269:GLU:HG3	1:A:270:ALA:H	1.20	1.05
1:D:273:ASP:HB2	1:D:362:ASN:HD22	1.22	1.04
1:B:319:ALA:HB2	1:D:26:HIS:CE1	1.94	1.02
1:B:119:LEU:HG	1:B:132:LEU:HB3	1.42	1.01
1:A:83:VAL:HG13	1:A:90:MET:HB3	1.43	1.01

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	457/478 (96%)	341 (75%)	82 (18%)	34 (7%)	2	1
1	B	458/478 (96%)	352 (77%)	70 (15%)	36 (8%)	1	1
1	C	411/478 (86%)	295 (72%)	77 (19%)	39 (10%)	1	1
1	D	457/478 (96%)	356 (78%)	63 (14%)	38 (8%)	1	1
All	All	1783/1912 (93%)	1344 (75%)	292 (16%)	147 (8%)	1	1

5 of 147 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	A	25	VAL
1	A	84	LEU
1	A	88	LYS
1	A	232	ALA

5.3.2 Protein sidechains ⓘ

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	385/402 (96%)	345 (90%)	40 (10%)	10	23
1	B	386/402 (96%)	347 (90%)	39 (10%)	11	24
1	C	346/402 (86%)	306 (88%)	40 (12%)	8	18
1	D	385/402 (96%)	343 (89%)	42 (11%)	9	21
All	All	1502/1608 (93%)	1341 (89%)	161 (11%)	10	22

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	361	LEU
1	C	95	VAL
1	D	334	GLU
1	B	385	ASN
1	C	15	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	168	ASN
1	C	62	ASN
1	D	338	GLN
1	B	191	GLN
1	B	346	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	BGC	A	601	-	12,12,12	0.51	0	17,17,17	0.80	1 (5%)
3	ACT	A	701	-	1,3,3	2.93	1 (100%)	0,3,3	0.00	-
2	BGC	B	701	-	12,12,12	0.21	0	17,17,17	0.45	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	BGC	A	601	-	-	0/2/22/22	0/1/1/1
3	ACT	A	701	-	-	0/0/0/0	0/0/0/0
2	BGC	B	701	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ACT	CH3-C	2.93	1.53	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	601	BGC	C1-C2-C3	-2.52	106.54	110.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	459/478 (96%)	0.34	30 (6%) 18 21	2, 23, 50, 79	0
1	B	460/478 (96%)	0.33	34 (7%) 14 15	4, 22, 50, 69	0
1	C	413/478 (86%)	0.41	32 (7%) 13 14	3, 23, 46, 81	0
1	D	459/478 (96%)	0.25	21 (4%) 31 35	4, 21, 49, 100	0
All	All	1791/1912 (93%)	0.33	117 (6%) 18 21	2, 22, 49, 100	0

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	87	GLY	11.7
1	A	87	GLY	7.6
1	C	413	THR	7.4
1	C	412	VAL	6.7
1	B	323	ILE	5.9

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

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BGC	B	701	12/12	0.24	1.46	43,43,43,43	0
2	BGC	A	601	12/12	0.19	0.51	43,43,43,43	0
3	ACT	A	701	4/4	0.15	-0.48	31,31,31,31	0

6.5 Other polymers

There are no such residues in this entry.