



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 07:50 PM UTC

PDB ID : 3KBC / pdb\_00003kbc  
Title : Crystal structure of GltPh K55C-A364C mutant crosslinked with divalent mercury  
Authors : Reyes, N.; Ginter, C.; Boudker, O.  
Deposited on : 2009-10-20  
Resolution : 3.51 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) 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

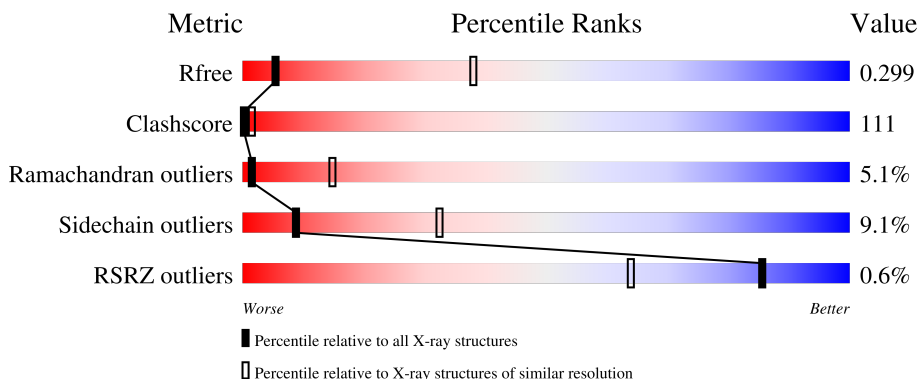
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

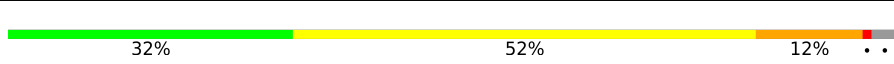
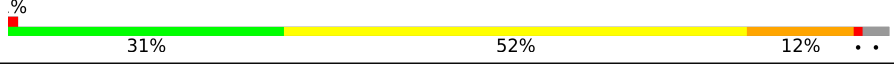
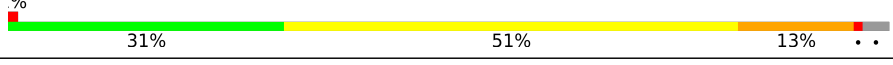
The reported resolution of this entry is 3.51 Å.

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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	425	
1	B	425	
1	C	425	

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
2	ASP	A	500	-	-	X	-
2	ASP	B	500	-	-	X	-
2	ASP	C	500	-	-	X	-
3	HG	B	501	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9096 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 425aa long hypothetical proton glutamate symport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	411	3020	1989	483	530	18	0	0	0
1	B	411	3020	1989	483	530	18	0	0	0
1	C	411	3020	1989	483	530	18	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

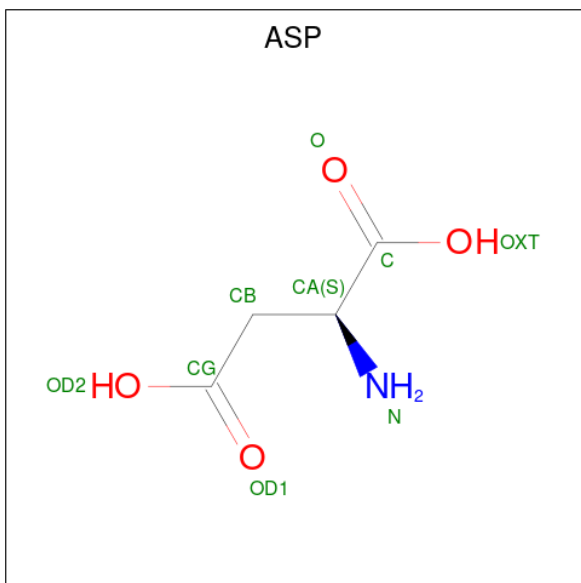
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	55	CYS	LYS	engineered mutation	UNP O59010
A	125	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010
A	321	ALA	CYS	engineered mutation	UNP O59010
A	364	CYS	ALA	engineered mutation	UNP O59010
A	368	HIS	GLU	engineered mutation	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010
B	55	CYS	LYS	engineered mutation	UNP O59010
B	125	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	321	ALA	CYS	engineered mutation	UNP O59010
B	364	CYS	ALA	engineered mutation	UNP O59010
B	368	HIS	GLU	engineered mutation	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	55	CYS	LYS	engineered mutation	UNP O59010

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Chain	Residue	Modelled	Actual	Comment	Reference
C	125	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	321	ALA	CYS	engineered mutation	UNP O59010
C	364	CYS	ALA	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010

- Molecule 2 is ASPARTIC ACID (CCD ID: ASP) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	9	4	1	4	0	0
2	B	1	9	4	1	4	0	0
2	C	1	9	4	1	4	0	0

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Hg 1 1	0	0

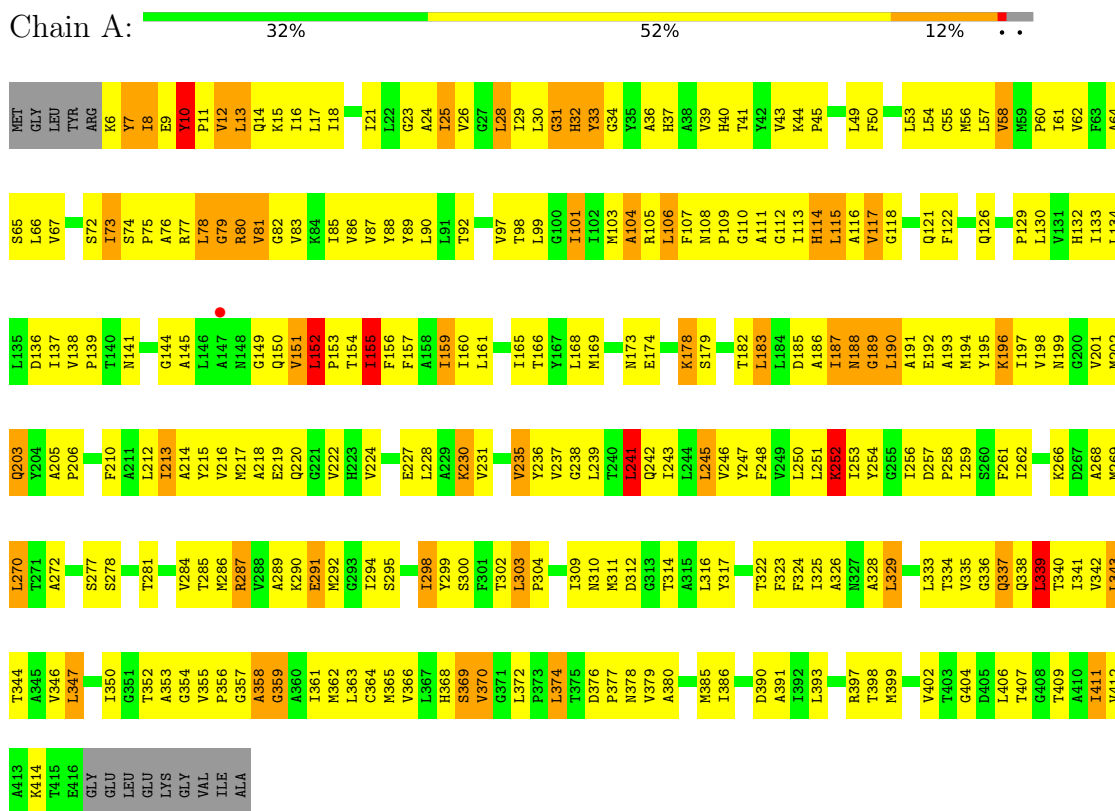
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

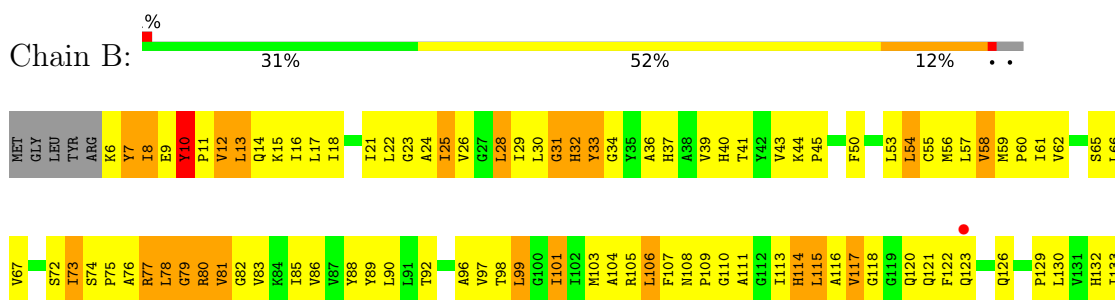
### 3 Residue-property plots i

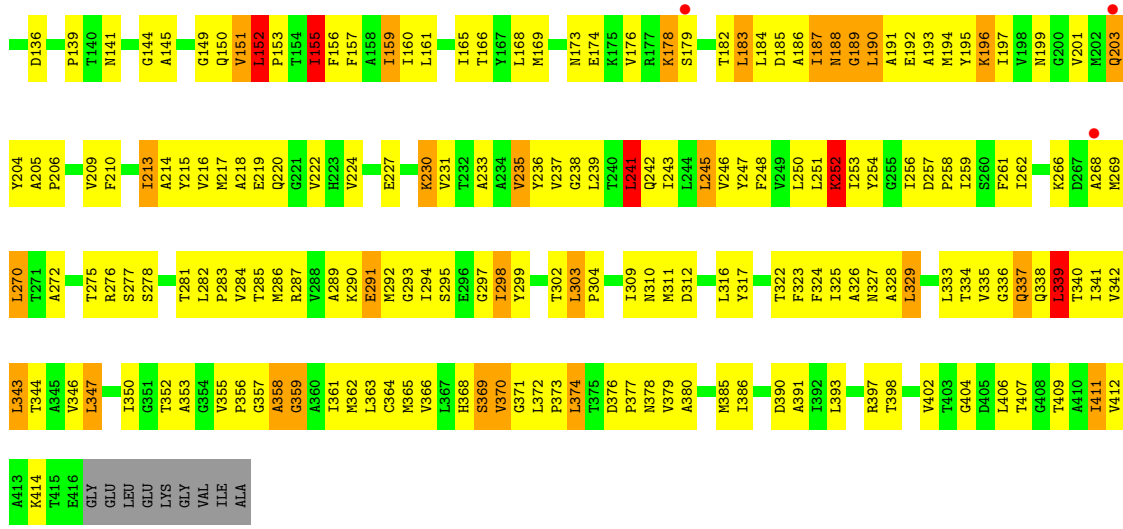
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 425aa long hypothetical proton glutamate symport protein

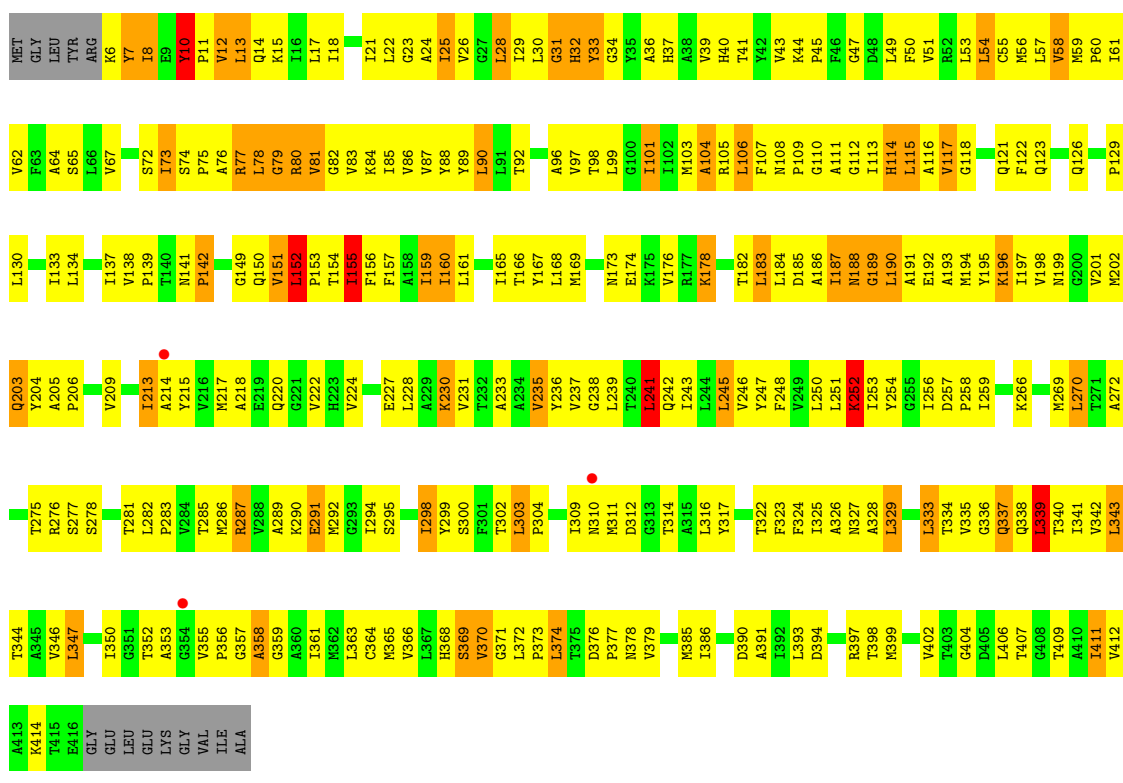


- Molecule 1: 425aa long hypothetical proton glutamate symport protein





• Molecule 1: 425aa long hypothetical proton glutamate symport protein



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.14Å 206.78Å 205.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.51 12.00 – 3.51	Depositor EDS
% Data completeness (in resolution range)	97.2 (12.00-3.51) 80.7 (12.00-3.51)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 3.48Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.267 , 0.270 (Not available) , 0.299	Depositor DCC
$R_{free}$ test set	1507 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	139.8	Xtrriage
Anisotropy	0.412	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 117.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.073 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.088 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9096	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: HG, NA

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	0.71	0/3078	1.07	20/4202 (0.5%)
1	B	0.70	0/3078	1.07	20/4202 (0.5%)
1	C	0.67	0/3078	1.06	22/4202 (0.5%)
All	All	0.70	0/9234	1.07	62/12606 (0.5%)

There are no bond length outliers.

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	337	GLN	N-CA-C	-12.22	98.47	113.50
1	A	337	GLN	N-CA-C	-12.15	98.56	113.50
1	B	337	GLN	N-CA-C	-12.09	98.63	113.50
1	A	31	GLY	N-CA-C	-10.08	100.81	112.50
1	B	31	GLY	N-CA-C	-9.98	100.92	112.50

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	3020	0	3181	527	2
1	B	3020	0	3181	547	2
1	C	3020	0	3181	535	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	9	0	3	5	0
2	B	9	0	3	4	0
2	C	9	0	3	5	0
3	A	1	0	0	1	0
3	B	1	0	0	2	0
3	C	1	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
All	All	9096	0	9552	1581	4

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 111.

The worst 5 of 1581 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:106:LEU:HD11	1:C:107:PHE:CD1	1.33	1.64
1:A:106:LEU:HD11	1:A:107:PHE:CD1	1.33	1.61
1:B:106:LEU:HD11	1:B:107:PHE:CD1	1.33	1.59
1:B:195:TYR:CE1	1:B:353:ALA:HB2	1.38	1.57
1:C:195:TYR:CE1	1:C:353:ALA:HB2	1.39	1.54

All (4) 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)
1:A:126:GLN:OE1	1:C:121:GLN:O[3_454]	1.82	0.38
1:B:121:GLN:O	1:B:126:GLN:OE1[3_454]	1.85	0.35
1:A:121:GLN:O	1:C:126:GLN:OE1[3_454]	1.89	0.31
1:B:120:GLN:NE2	1:B:129:PRO:CD[3_454]	2.16	0.04

## 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	409/425 (96%)	341 (83%)	47 (12%)	21 (5%)	1	15
1	B	409/425 (96%)	342 (84%)	47 (12%)	20 (5%)	1	16
1	C	409/425 (96%)	341 (83%)	47 (12%)	21 (5%)	1	15
All	All	1227/1275 (96%)	1024 (84%)	141 (12%)	62 (5%)	1	15

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	12	VAL
1	A	73	ILE
1	A	151	VAL
1	A	291	GLU

### 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	316/331 (96%)	289 (92%)	27 (8%)	10	34
1	B	316/331 (96%)	287 (91%)	29 (9%)	8	32
1	C	316/331 (96%)	285 (90%)	31 (10%)	7	30
All	All	948/993 (96%)	861 (91%)	87 (9%)	9	32

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	25	ILE
1	C	196	LYS
1	C	54	LEU
1	C	152	LEU
1	C	245	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	108	ASN
1	C	368	HIS
1	C	338	GLN
1	B	125	HIS
1	C	40	HIS

### 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 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\# Z  > 2$
2	ASP	C	500	-	7,8,8	1.17	1 (14%)	6,10,10	1.39	1 (16%)
2	ASP	A	500	-	7,8,8	1.12	1 (14%)	6,10,10	1.39	1 (16%)
2	ASP	B	500	-	7,8,8	1.18	1 (14%)	6,10,10	1.34	1 (16%)

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	ASP	C	500	-	-	4/8/8/8	-
2	ASP	A	500	-	-	4/8/8/8	-
2	ASP	B	500	-	-	4/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	ASP	OXT-C	-2.20	1.23	1.30
2	C	500	ASP	OXT-C	-2.17	1.23	1.30
2	A	500	ASP	OXT-C	-2.06	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	ASP	OXT-C-O	-2.81	117.70	124.08
2	A	500	ASP	OXT-C-O	-2.77	117.80	124.08
2	B	500	ASP	OXT-C-O	-2.66	118.05	124.08

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	ASP	OXT-C-CA-CB
2	C	500	ASP	OXT-C-CA-CB
2	B	500	ASP	OXT-C-CA-CB
2	A	500	ASP	OXT-C-CA-N
2	B	500	ASP	OXT-C-CA-N

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	ASP	5	0
2	A	500	ASP	5	0
2	B	500	ASP	4	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	411/425 (96%)	-0.42	1 (0%) 91 81	94, 101, 104, 109	0
1	B	411/425 (96%)	0.02	4 (0%) 79 54	94, 101, 104, 109	0
1	C	411/425 (96%)	-0.19	3 (0%) 84 61	95, 101, 104, 108	0
All	All	1233/1275 (96%)	-0.20	8 (0%) 85 64	94, 101, 104, 109	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	354	GLY	3.1
1	B	123	GLN	2.8
1	C	214	ALA	2.6
1	C	310	ASN	2.5
1	B	268	ALA	2.3

### 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	NA	C	454	1/1	0.82	0.23	86,86,86,86	0
2	ASP	B	500	9/9	0.86	0.23	107,107,107,107	0
2	ASP	C	500	9/9	0.87	0.26	107,108,108,108	0
2	ASP	A	500	9/9	0.90	0.27	107,107,108,108	0
4	NA	A	453	1/1	0.91	0.09	97,97,97,97	0
4	NA	C	453	1/1	0.93	0.06	98,98,98,98	0
4	NA	B	454	1/1	0.95	0.07	85,85,85,85	0
3	HG	C	501	1/1	0.97	0.09	94,94,94,94	1
3	HG	A	501	1/1	0.98	0.04	95,95,95,95	1
4	NA	B	453	1/1	0.98	0.03	98,98,98,98	0
4	NA	A	454	1/1	0.98	0.04	86,86,86,86	0
3	HG	B	501	1/1	0.98	0.04	92,92,92,92	1

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.