



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:47 PM GMT

PDB ID : 1CHU  
Title : STRUCTURE OF L-ASPARTATE OXIDASE: IMPLICATIONS FOR THE  
SUCCINATE DEHYDROGENASE/ FUMARATE REDUCATSE FAMILY  
Authors : Mattevi, A.  
Deposited on : 1999-03-29  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

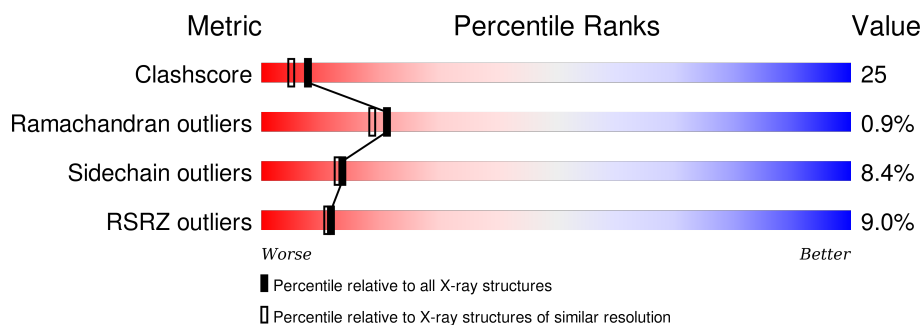
# 1 Overall quality at a glance

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))
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  $\geq 3$ , 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  $\leq 5\%$ . 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	540	<div> <div>8%</div> <div>52%</div> <div>25%</div> <div>9%</div> <div>•</div> <div>11%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3957 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 PROTEIN (L-ASPARTATE OXIDASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	88	0	0
			3761	2365	677	698	21			

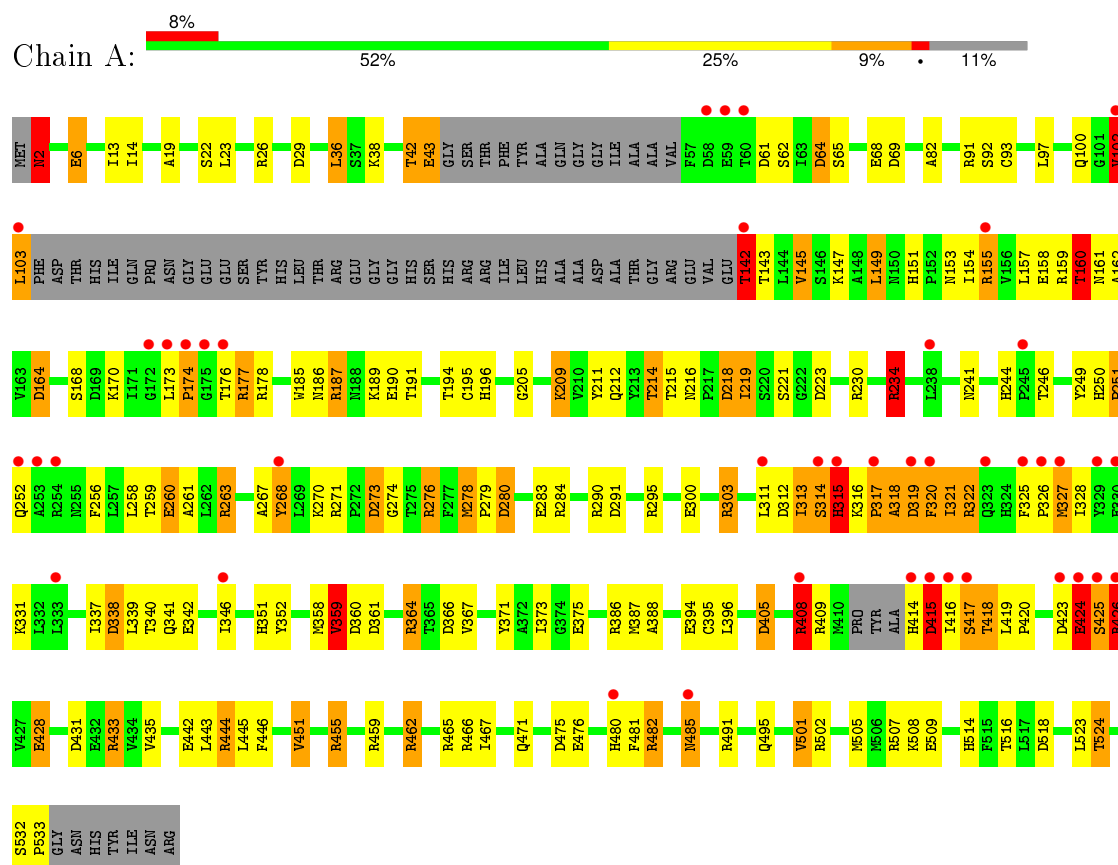
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	196	Total	O	2	0
			196	196		

### 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: PROTEIN (L-ASPARTATE OXIDASE)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.75Å 84.75Å 159.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.73 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.00-2.20) 96.7 (19.73-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.224 , 0.281 0.208 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.3	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 33258 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3957	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	1.00	7/3840 (0.2%)	2.26	128/5214 (2.5%)

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	A	0	15

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	428	GLU	CG-CD	-9.92	1.37	1.51
1	A	414	HIS	CB-CG	8.29	1.65	1.50
1	A	320	PHE	CB-CG	-7.93	1.37	1.51
1	A	61	ASP	CB-CG	-7.22	1.36	1.51
1	A	2	ASN	CB-CG	6.42	1.65	1.51
1	A	322	ARG	CB-CG	5.26	1.66	1.52
1	A	68	GLU	CD-OE2	5.24	1.31	1.25

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	ARG	CD-NE-CZ	35.08	172.72	123.60
1	A	187	ARG	CD-NE-CZ	25.93	159.91	123.60
1	A	320	PHE	CB-CG-CD2	-21.86	105.50	120.80
1	A	61	ASP	CB-CG-OD1	-20.97	99.43	118.30
1	A	428	GLU	CG-CD-OE1	-20.81	76.68	118.30
1	A	61	ASP	CB-CG-OD2	19.84	136.16	118.30
1	A	428	GLU	CG-CD-OE2	19.38	157.07	118.30
1	A	320	PHE	CB-CG-CD1	18.73	133.91	120.80
1	A	502	ARG	NE-CZ-NH1	17.90	129.25	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ARG	NE-CZ-NH1	16.57	128.59	120.30
1	A	466	ARG	NE-CZ-NH2	16.09	128.35	120.30
1	A	431	ASP	CB-CG-OD2	15.00	131.80	118.30
1	A	187	ARG	NE-CZ-NH1	-14.88	112.86	120.30
1	A	178	ARG	NE-CZ-NH2	-14.73	112.93	120.30
1	A	465	ARG	NE-CZ-NH2	-14.69	112.96	120.30
1	A	187	ARG	NE-CZ-NH2	14.27	127.44	120.30
1	A	319	ASP	N-CA-CB	-13.99	85.41	110.60
1	A	91	ARG	NE-CZ-NH2	-13.96	113.32	120.30
1	A	360	ASP	CB-CG-OD1	13.92	130.83	118.30
1	A	455	ARG	NE-CZ-NH2	-13.57	113.52	120.30
1	A	386	ARG	CD-NE-CZ	13.54	142.55	123.60
1	A	462	ARG	NE-CZ-NH2	13.41	127.01	120.30
1	A	280	ASP	CB-CG-OD1	12.40	129.46	118.30
1	A	405	ASP	CB-CG-OD2	12.10	129.19	118.30
1	A	502	ARG	CD-NE-CZ	12.07	140.51	123.60
1	A	273	ASP	CB-CG-OD1	-11.92	107.57	118.30
1	A	43	GLU	OE1-CD-OE2	-11.79	109.15	123.30
1	A	428	GLU	CB-CG-CD	11.67	145.71	114.20
1	A	462	ARG	NE-CZ-NH1	11.67	126.14	120.30
1	A	291	ASP	CB-CG-OD1	11.55	128.70	118.30
1	A	462	ARG	NH1-CZ-NH2	-11.50	106.75	119.40
1	A	364	ARG	NE-CZ-NH2	-11.07	114.76	120.30
1	A	465	ARG	NE-CZ-NH1	10.91	125.76	120.30
1	A	507	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	A	462	ARG	CD-NE-CZ	10.34	138.07	123.60
1	A	371	TYR	CB-CG-CD1	10.26	127.16	121.00
1	A	341	GLN	CA-CB-CG	10.16	135.76	113.40
1	A	273	ASP	CB-CA-C	-10.09	90.23	110.40
1	A	317	PRO	O-C-N	10.03	138.75	122.70
1	A	371	TYR	CB-CG-CD2	-9.99	115.00	121.00
1	A	276	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	A	459	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	A	290	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	A	223	ASP	CB-CG-OD1	9.46	126.82	118.30
1	A	317	PRO	CA-C-N	-9.44	96.44	117.20
1	A	352	TYR	CB-CG-CD2	-9.40	115.36	121.00
1	A	502	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	A	164	ASP	CB-CG-OD1	9.22	126.60	118.30
1	A	295	ARG	NE-CZ-NH1	-9.18	115.71	120.30
1	A	218	ASP	CB-CG-OD1	9.02	126.42	118.30
1	A	482	ARG	CB-CG-CD	8.38	133.40	111.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	ASP	CB-CG-OD2	8.27	125.74	118.30
1	A	466	ARG	NH1-CZ-NH2	-8.16	110.42	119.40
1	A	2	ASN	CA-CB-CG	8.10	131.22	113.40
1	A	455	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	273	ASP	CB-CG-OD2	8.04	125.53	118.30
1	A	426	ARG	NE-CZ-NH2	8.03	124.31	120.30
1	A	394	GLU	OE1-CD-OE2	-7.85	113.88	123.30
1	A	178	ARG	NH1-CZ-NH2	7.84	128.02	119.40
1	A	291	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	A	322	ARG	NE-CZ-NH2	7.55	124.08	120.30
1	A	303	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	A	276	ARG	CD-NE-CZ	7.04	133.46	123.60
1	A	360	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	A	338	ASP	CB-CG-OD1	6.93	124.54	118.30
1	A	415	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	A	64	ASP	CB-CG-OD2	6.73	124.36	118.30
1	A	482	ARG	CG-CD-NE	6.71	125.89	111.80
1	A	361	ASP	CB-CG-OD1	-6.52	112.43	118.30
1	A	518	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	321	ILE	CA-CB-CG2	6.49	123.88	110.90
1	A	341	GLN	CB-CG-CD	6.46	128.41	111.60
1	A	290	ARG	CD-NE-CZ	-6.46	114.55	123.60
1	A	177	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	263	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	A	162	ALA	N-CA-CB	6.23	118.82	110.10
1	A	280	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	214	THR	CA-CB-CG2	5.93	120.71	112.40
1	A	273	ASP	N-CA-CB	5.87	121.16	110.60
1	A	219	ILE	CA-CB-CG2	5.86	122.62	110.90
1	A	418	THR	CA-CB-CG2	-5.86	104.20	112.40
1	A	417	SER	N-CA-C	5.83	126.75	111.00
1	A	359	VAL	CG1-CB-CG2	5.82	120.21	110.90
1	A	417	SER	CA-C-O	5.78	132.24	120.10
1	A	43	GLU	CG-CD-OE1	5.73	129.76	118.30
1	A	249	TYR	CB-CG-CD1	-5.73	117.56	121.00
1	A	424	GLU	N-CA-CB	5.72	120.90	110.60
1	A	442	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	A	405	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	A	209	LYS	CA-CB-CG	5.70	125.94	113.40
1	A	388	ALA	C-N-CA	5.61	135.73	121.70
1	A	145	VAL	CG1-CB-CG2	-5.58	101.98	110.90
1	A	501	VAL	CG1-CB-CG2	-5.54	102.03	110.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ARG	CD-NE-CZ	5.54	131.35	123.60
1	A	364	ARG	NH1-CZ-NH2	5.54	125.49	119.40
1	A	317	PRO	N-CA-C	5.50	126.41	112.10
1	A	533	PRO	CA-C-O	-5.44	107.14	120.20
1	A	93	CYS	CA-CB-SG	-5.44	104.21	114.00
1	A	444	ARG	CD-NE-CZ	5.38	131.13	123.60
1	A	219	ILE	CB-CG1-CD1	-5.38	98.84	113.90
1	A	322	ARG	CA-CB-CG	-5.37	101.59	113.40
1	A	64	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	A	268	TYR	CA-CB-CG	5.34	123.55	113.40
1	A	142	THR	N-CA-CB	5.33	120.42	110.30
1	A	186	ASN	N-CA-CB	-5.31	101.04	110.60
1	A	26	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	A	43	GLU	CB-CA-C	5.30	121.01	110.40
1	A	475	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	284	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	A	43	GLU	CB-CG-CD	5.29	128.47	114.20
1	A	359	VAL	N-CA-CB	-5.27	99.90	111.50
1	A	65	SER	CA-CB-OG	-5.25	97.04	111.20
1	A	317	PRO	C-N-CA	5.24	134.81	121.70
1	A	425	SER	N-CA-C	-5.24	96.86	111.00
1	A	234	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	408	ARG	CA-CB-CG	5.20	124.84	113.40
1	A	230	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	451	VAL	CB-CA-C	-5.16	101.59	111.40
1	A	102	VAL	CB-CA-C	5.15	121.19	111.40
1	A	431	ASP	OD1-CG-OD2	-5.15	113.52	123.30
1	A	278	MET	CA-CB-CG	5.14	122.04	113.30
1	A	6	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	A	476	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	A	443	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	A	42	THR	CA-C-N	5.07	128.36	117.20
1	A	92	SER	N-CA-CB	5.05	118.08	110.50
1	A	319	ASP	CA-CB-CG	-5.02	102.35	113.40
1	A	160	THR	OG1-CB-CG2	-5.01	98.47	110.00

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	ARG	Mainchain
1	A	195	CYS	Mainchain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	205	GLY	Mainchain
1	A	22	SER	Mainchain
1	A	234	ARG	Mainchain
1	A	251	PRO	Mainchain
1	A	273	ASP	Mainchain
1	A	29	ASP	Mainchain
1	A	303	ARG	Mainchain
1	A	375	GLU	Sidechain
1	A	395	CYS	Mainchain
1	A	396	LEU	Mainchain
1	A	408	ARG	Mainchain
1	A	415	ASP	Sidechain
1	A	82	ALA	Mainchain

## 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	3761	0	3709	181	2
2	A	196	0	0	22	1
All	All	3957	0	3709	181	3

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 25.

All (181) 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:A:187:ARG:NH1	2:A:633:HOH:O	1.60	1.32
1:A:234:ARG:HB3	1:A:358:MET:CE	1.60	1.28
1:A:317:PRO:O	1:A:320:PHE:HB2	1.18	1.27
1:A:69:ASP:HB3	1:A:387:MET:CE	1.72	1.20
1:A:69:ASP:C	1:A:387:MET:HE1	1.62	1.20
1:A:317:PRO:O	1:A:320:PHE:CB	1.91	1.18
1:A:462:ARG:CZ	2:A:735:HOH:O	1.91	1.17
1:A:234:ARG:CB	1:A:358:MET:CE	2.23	1.16

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ARG:NH1	1:A:409:ARG:NH2	1.97	1.13
1:A:425:SER:HB2	1:A:480:HIS:O	1.46	1.12
1:A:256:PHE:CD1	1:A:331:LYS:HE3	1.83	1.12
1:A:259:THR:HG22	1:A:261:ALA:H	1.01	1.10
1:A:256:PHE:CD1	1:A:331:LYS:CE	2.34	1.09
1:A:69:ASP:CB	1:A:387:MET:HE1	1.83	1.09
1:A:256:PHE:CE1	1:A:331:LYS:CE	2.36	1.07
1:A:425:SER:CB	1:A:480:HIS:HB3	1.85	1.05
1:A:256:PHE:CD1	1:A:331:LYS:NZ	2.25	1.04
1:A:433:ARG:HH22	1:A:482:ARG:HG2	1.24	1.01
1:A:234:ARG:HD2	1:A:358:MET:HE1	1.40	0.99
1:A:455:ARG:HH11	1:A:514:HIS:HD2	1.07	0.99
1:A:234:ARG:HB3	1:A:358:MET:HE2	1.01	0.97
1:A:462:ARG:NE	2:A:735:HOH:O	1.93	0.97
1:A:258:LEU:HD13	1:A:311:LEU:HD23	1.47	0.96
1:A:317:PRO:C	1:A:320:PHE:HB2	1.85	0.96
1:A:69:ASP:HB3	1:A:387:MET:HE1	1.39	0.95
1:A:258:LEU:CD1	1:A:311:LEU:HD23	1.96	0.95
1:A:69:ASP:HB3	1:A:387:MET:HE2	1.45	0.95
1:A:234:ARG:CB	1:A:358:MET:HE3	1.95	0.95
1:A:524:THR:HG22	2:A:556:HOH:O	1.65	0.95
1:A:268:TYR:CD1	1:A:276:ARG:NE	2.38	0.92
1:A:259:THR:HG22	1:A:261:ALA:N	1.85	0.92
1:A:234:ARG:HB2	1:A:358:MET:HE3	1.51	0.92
1:A:424:GLU:HG3	2:A:575:HOH:O	1.69	0.91
1:A:69:ASP:CA	1:A:387:MET:HE1	2.00	0.91
1:A:250:HIS:HD2	1:A:252:GLN:H	1.19	0.90
1:A:313:ILE:HD11	1:A:339:LEU:HG	1.54	0.89
1:A:319:ASP:HA	1:A:322:ARG:HB2	1.52	0.88
1:A:69:ASP:C	1:A:387:MET:CE	2.43	0.86
1:A:364:ARG:NH1	1:A:409:ARG:HH22	1.70	0.85
1:A:312:ASP:OD1	1:A:314:SER:HB2	1.77	0.83
1:A:234:ARG:CB	1:A:358:MET:HE2	1.91	0.83
1:A:364:ARG:HH11	1:A:409:ARG:NH2	1.75	0.82
1:A:256:PHE:CE1	1:A:331:LYS:HE2	2.14	0.82
1:A:425:SER:CB	1:A:480:HIS:CB	2.51	0.81
1:A:256:PHE:CE1	1:A:331:LYS:HE3	2.08	0.81
1:A:250:HIS:CD2	1:A:251:PRO:HD2	2.14	0.81
1:A:185:TRP:CZ2	2:A:658:HOH:O	2.33	0.80
1:A:433:ARG:NH2	1:A:482:ARG:HG2	1.97	0.80
1:A:256:PHE:HD1	1:A:331:LYS:NZ	1.78	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ILE:HD11	1:A:339:LEU:CG	2.11	0.80
1:A:451:VAL:HG21	1:A:501:VAL:HG22	1.66	0.77
1:A:234:ARG:CD	1:A:358:MET:HE1	2.14	0.77
1:A:161:ASN:ND2	1:A:485:ASN:OD1	2.17	0.77
1:A:268:TYR:CD1	1:A:276:ARG:HD2	2.21	0.76
1:A:209:LYS:HA	1:A:214:THR:HG21	1.67	0.76
1:A:337:ILE:HA	1:A:342:GLU:OE2	1.85	0.75
1:A:6:GLU:OE1	1:A:194:THR:N	2.19	0.75
1:A:69:ASP:CB	1:A:387:MET:CE	2.50	0.73
1:A:417:SER:O	1:A:418:THR:HG23	1.89	0.72
1:A:212:GLN:NE2	1:A:445:LEU:HD23	2.04	0.72
1:A:267:ALA:HB2	1:A:313:ILE:HG23	1.71	0.71
1:A:268:TYR:CD1	1:A:276:ARG:CD	2.73	0.71
1:A:215:THR:OG1	1:A:351:HIS:HD2	1.74	0.71
1:A:250:HIS:CD2	1:A:252:GLN:H	2.07	0.71
1:A:256:PHE:CG	1:A:331:LYS:HE3	2.25	0.70
1:A:69:ASP:O	1:A:387:MET:CE	2.40	0.69
1:A:185:TRP:CZ3	1:A:187:ARG:HG2	2.26	0.69
1:A:417:SER:O	1:A:418:THR:CG2	2.40	0.69
1:A:185:TRP:HZ2	2:A:658:HOH:O	1.74	0.69
1:A:338:ASP:OD1	1:A:340:THR:HB	1.92	0.68
1:A:234:ARG:CD	1:A:358:MET:CE	2.72	0.68
1:A:268:TYR:HD1	1:A:276:ARG:HE	1.40	0.68
1:A:268:TYR:CG	1:A:276:ARG:HD2	2.29	0.67
1:A:158:GLU:OE1	2:A:674:HOH:O	2.14	0.65
1:A:185:TRP:CE3	1:A:187:ARG:HG2	2.31	0.65
1:A:258:LEU:HD12	1:A:311:LEU:HD23	1.75	0.65
1:A:212:GLN:NE2	1:A:445:LEU:CD2	2.60	0.65
1:A:250:HIS:CD2	1:A:251:PRO:CD	2.80	0.64
1:A:455:ARG:HH11	1:A:514:HIS:CD2	2.00	0.63
1:A:13:ILE:CD1	1:A:23:LEU:HD23	2.31	0.61
1:A:69:ASP:O	1:A:387:MET:HE3	2.01	0.61
1:A:313:ILE:CD1	1:A:339:LEU:HG	2.30	0.60
1:A:185:TRP:HZ2	1:A:190:GLU:OE1	1.85	0.59
1:A:13:ILE:HD13	1:A:23:LEU:HD23	1.84	0.59
1:A:154:ILE:O	2:A:628:HOH:O	2.17	0.59
1:A:270:LYS:HD3	1:A:274:GLY:O	2.03	0.58
1:A:364:ARG:HH12	1:A:409:ARG:NH2	1.96	0.58
1:A:259:THR:CG2	1:A:261:ALA:H	1.94	0.58
1:A:19:ALA:HB1	1:A:373:ILE:HD12	1.85	0.58
1:A:501:VAL:O	1:A:505:MET:HG3	2.03	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:PHE:CE1	1:A:331:LYS:NZ	2.64	0.57
1:A:102:VAL:HG21	1:A:143:THR:O	2.05	0.57
1:A:100:GLN:O	1:A:147:LYS:HE3	2.04	0.57
1:A:185:TRP:NE1	2:A:658:HOH:O	2.37	0.57
1:A:313:ILE:HD11	1:A:339:LEU:CD1	2.35	0.57
1:A:256:PHE:HD1	1:A:331:LYS:HZ1	1.42	0.56
1:A:314:SER:O	1:A:316:LYS:N	2.38	0.56
1:A:451:VAL:CG2	1:A:501:VAL:HG22	2.35	0.56
1:A:455:ARG:NH1	1:A:514:HIS:HD2	1.90	0.55
1:A:234:ARG:HD2	1:A:358:MET:CE	2.22	0.55
1:A:322:ARG:O	1:A:326:PRO:HG3	2.07	0.55
1:A:315:HIS:CD2	1:A:315:HIS:H	2.24	0.54
1:A:405:ASP:OD1	1:A:408:ARG:NH2	2.40	0.54
1:A:102:VAL:O	1:A:103:LEU:C	2.47	0.54
1:A:270:LYS:NZ	1:A:312:ASP:OD2	2.41	0.54
1:A:185:TRP:CZ2	1:A:190:GLU:OE1	2.60	0.53
1:A:417:SER:C	1:A:418:THR:HG23	2.28	0.53
1:A:491:ARG:HG2	2:A:705:HOH:O	2.08	0.53
1:A:151:HIS:CE1	1:A:153:ASN:HB2	2.44	0.52
1:A:387:MET:CE	2:A:719:HOH:O	2.58	0.52
1:A:462:ARG:NH2	2:A:735:HOH:O	2.24	0.52
1:A:425:SER:CB	1:A:480:HIS:HB2	2.36	0.52
1:A:524:THR:CG2	2:A:556:HOH:O	2.37	0.52
1:A:38:LYS:NZ	1:A:218:ASP:HA	2.25	0.51
1:A:185:TRP:CE2	2:A:658:HOH:O	2.57	0.51
1:A:177:ARG:NH2	1:A:366:ASP:O	2.44	0.51
1:A:509:GLU:HB3	1:A:523:LEU:HG	1.93	0.51
1:A:267:ALA:CB	1:A:313:ILE:HG23	2.40	0.50
1:A:425:SER:HB2	1:A:480:HIS:CB	2.40	0.50
1:A:426:ARG:O	1:A:428:GLU:HG2	2.12	0.50
1:A:212:GLN:HE22	1:A:445:LEU:CD2	2.25	0.49
1:A:250:HIS:HD2	1:A:252:GLN:N	1.99	0.48
1:A:271:ARG:NE	1:A:300:GLU:OE2	2.47	0.48
1:A:196:HIS:HD2	1:A:419:LEU:HD11	1.79	0.48
1:A:359:VAL:HA	1:A:364:ARG:O	2.14	0.48
1:A:142:THR:HB	1:A:143:THR:H	1.65	0.48
1:A:417:SER:OG	1:A:418:THR:N	2.46	0.47
1:A:495:GLN:NE2	2:A:608:HOH:O	2.38	0.47
1:A:173:LEU:HD23	1:A:174:PRO:HD3	1.96	0.47
1:A:168:SER:C	1:A:170:LYS:H	2.17	0.47
1:A:433:ARG:HH22	1:A:482:ARG:CG	2.13	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ALA:O	1:A:321:ILE:N	2.46	0.47
1:A:338:ASP:OD1	1:A:340:THR:CB	2.63	0.47
1:A:313:ILE:HD12	1:A:321:ILE:HG12	1.97	0.47
1:A:318:ALA:O	1:A:321:ILE:HB	2.14	0.47
1:A:480:HIS:O	1:A:481:PHE:C	2.50	0.46
1:A:433:ARG:NE	2:A:606:HOH:O	2.21	0.46
1:A:268:TYR:CE1	1:A:276:ARG:NE	2.81	0.46
1:A:417:SER:O	1:A:418:THR:HG22	2.16	0.46
1:A:508:LYS:NZ	2:A:732:HOH:O	2.46	0.46
1:A:244:HIS:HE1	2:A:629:HOH:O	2.00	0.45
1:A:157:LEU:O	1:A:160:THR:OG1	2.34	0.45
1:A:419:LEU:HB3	1:A:420:PRO:HD2	1.98	0.45
1:A:467:ILE:O	1:A:471:GLN:HG3	2.17	0.45
1:A:14:ILE:HG12	1:A:36:LEU:HD22	1.99	0.45
1:A:250:HIS:CG	1:A:251:PRO:CD	2.99	0.45
1:A:338:ASP:N	1:A:342:GLU:OE2	2.46	0.45
1:A:408:ARG:NH2	2:A:626:HOH:O	2.50	0.45
1:A:185:TRP:CZ3	1:A:187:ARG:CD	3.00	0.44
1:A:244:HIS:CD2	1:A:246:THR:H	2.34	0.44
1:A:314:SER:C	1:A:316:LYS:N	2.71	0.44
1:A:215:THR:OG1	1:A:216:ASN:ND2	2.48	0.44
1:A:325:PHE:N	1:A:326:PRO:HD3	2.32	0.44
1:A:234:ARG:NE	1:A:358:MET:HE3	2.33	0.44
1:A:364:ARG:NH1	1:A:409:ARG:HH21	2.06	0.44
1:A:314:SER:C	1:A:316:LYS:H	2.21	0.44
1:A:256:PHE:CZ	1:A:328:ILE:HG12	2.52	0.43
1:A:211:TYR:O	1:A:214:THR:HG22	2.18	0.43
1:A:244:HIS:HD2	1:A:246:THR:H	1.66	0.43
1:A:338:ASP:C	1:A:340:THR:H	2.22	0.43
1:A:338:ASP:C	1:A:340:THR:N	2.70	0.43
1:A:278:MET:N	1:A:279:PRO:CD	2.81	0.43
1:A:185:TRP:CZ3	1:A:187:ARG:CG	2.99	0.43
1:A:313:ILE:HD11	1:A:339:LEU:HD11	2.00	0.43
1:A:327:MET:H	1:A:327:MET:HG2	1.60	0.42
1:A:145:VAL:HG22	1:A:149:LEU:HD22	2.01	0.42
1:A:451:VAL:HG21	1:A:501:VAL:CG2	2.44	0.42
1:A:176:THR:HG22	1:A:177:ARG:O	2.19	0.42
1:A:214:THR:HG23	1:A:444:ARG:NH2	2.35	0.42
1:A:189:LYS:O	1:A:191:THR:HG23	2.19	0.42
1:A:250:HIS:CG	1:A:251:PRO:HD2	2.54	0.42
1:A:42:THR:OG1	1:A:43:GLU:OE1	2.34	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LYS:O	1:A:190:GLU:HB2	2.19	0.41
1:A:194:THR:HG21	1:A:419:LEU:HB2	2.01	0.41
1:A:241:ASN:HB3	2:A:612:HOH:O	2.21	0.41
1:A:142:THR:N	2:A:709:HOH:O	2.53	0.41
1:A:260:GLU:HG3	1:A:263:ARG:NH2	2.35	0.41
1:A:267:ALA:CA	1:A:313:ILE:HG23	2.51	0.40
1:A:177:ARG:CZ	1:A:367:VAL:HG22	2.51	0.40
1:A:313:ILE:H	1:A:313:ILE:HG13	1.68	0.40
1:A:158:GLU:O	1:A:159:ARG:C	2.60	0.40

All (3) 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)
2:A:650:HOH:O	2:A:650:HOH:O[4_555]	1.20	1.00
1:A:2:ASN:ND2	1:A:480:HIS:NE2[5_675]	1.60	0.60
1:A:435:VAL:CG1	1:A:462:ARG:NH1[4_555]	1.98	0.22

## 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	470/540 (87%)	446 (95%)	20 (4%)	4 (1%)	21 19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	HIS
1	A	416	ILE
1	A	318	ALA
1	A	174	PRO

### 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	405/452 (90%)	371 (92%)	34 (8%)	14	13

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	36	LEU
1	A	62	SER
1	A	64	ASP
1	A	97	LEU
1	A	102	VAL
1	A	103	LEU
1	A	142	THR
1	A	149	LEU
1	A	155	ARG
1	A	160	THR
1	A	164	ASP
1	A	219	ILE
1	A	221	SER
1	A	260	GLU
1	A	280	ASP
1	A	283	GLU
1	A	313	ILE
1	A	314	SER
1	A	315	HIS
1	A	327	MET
1	A	346	ILE
1	A	359	VAL
1	A	408	ARG
1	A	415	ASP
1	A	423	ASP
1	A	424	GLU
1	A	426	ARG
1	A	433	ARG
1	A	446	PHE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	485	ASN
1	A	516	THR
1	A	524	THR
1	A	532	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	66	HIS
1	A	196	HIS
1	A	212	GLN
1	A	216	ASN
1	A	242	GLN
1	A	244	HIS
1	A	250	HIS
1	A	351	HIS
1	A	362	HIS
1	A	439	ASN
1	A	514	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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<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	478/540 (88%)	0.33	43 (8%) <b>12</b> <b>11</b>	23, 37, 73, 86	23 (4%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	HIS	7.0
1	A	425	SER	5.9
1	A	414	HIS	5.5
1	A	415	ASP	5.3
1	A	317	PRO	5.3
1	A	172	GLY	4.6
1	A	416	ILE	4.5
1	A	102	VAL	3.9
1	A	323	GLN	3.9
1	A	326	PRO	3.8
1	A	333	LEU	3.8
1	A	327	MET	3.8
1	A	480	HIS	3.7
1	A	252	GLN	3.7
1	A	424	GLU	3.6
1	A	142	THR	3.5
1	A	176	THR	3.5
1	A	60	THR	3.5
1	A	320	PHE	3.3
1	A	417	SER	3.0
1	A	103	LEU	2.9
1	A	314	SER	2.8
1	A	319	ASP	2.8
1	A	329	TYR	2.8
1	A	175	GLY	2.7
1	A	253	ALA	2.7
1	A	59	GLU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	174	PRO	2.6
1	A	426	ARG	2.4
1	A	423	ASP	2.4
1	A	325	PHE	2.3
1	A	245	PRO	2.3
1	A	346	ILE	2.2
1	A	485	ASN	2.2
1	A	155	ARG	2.1
1	A	238	LEU	2.1
1	A	311	LEU	2.1
1	A	254	ARG	2.1
1	A	330	GLU	2.1
1	A	408	ARG	2.1
1	A	173	LEU	2.1
1	A	58	ASP	2.0
1	A	268	TYR	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.