



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:27 AM GMT

PDB ID : 1OVT  
Title : REFINED CRYSTALLOGRAPHIC STRUCTURE OF HEN OVOTRANS-  
FERRIN AT 2.4 ANGSTROMS RESOLUTION  
Authors : Kurokawa, H.; Mikami, B.; Hirose, M.  
Deposited on : 1995-04-28  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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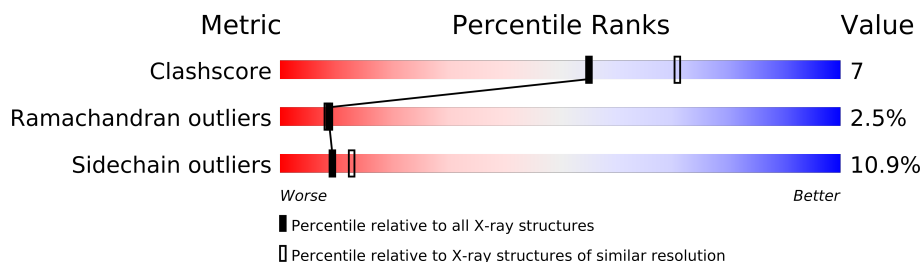
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
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 2.40 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	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	686	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5426 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.

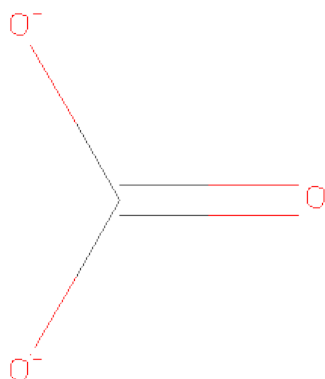
- Molecule 1 is a protein called OVOTRANSFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	682	Total	C	N	O	S	0	0	0
			5284	3302	917	1024	41			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total 132	O 132	0	0

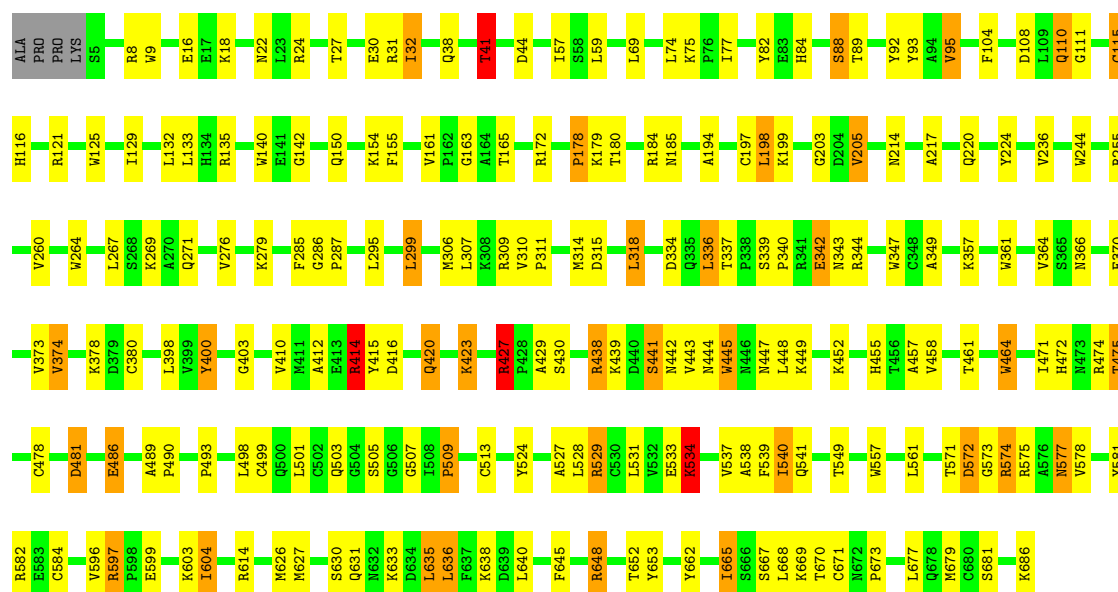
### 3 Residue-property plots

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.

Note EDS was not executed.

#### • Molecule 1: OVOTRANSFERRIN

Chain A: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.19Å 60.94Å 90.24Å 90.00° 83.95° 90.00°	Depositor
Resolution (Å)	11.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (11.00-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, FE

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	0.82	0/5388	1.61	89/7273 (1.2%)

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	5

There are no bond length outliers.

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	574	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	A	572	ASP	CA-C-N	-10.82	94.55	116.20
1	A	309	ARG	NE-CZ-NH1	10.45	125.53	120.30
1	A	597	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	A	309	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	A	574	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	A	264	TRP	CD1-CG-CD2	8.96	113.47	106.30
1	A	573	GLY	CA-C-N	-8.53	98.43	117.20
1	A	140	TRP	CD1-CG-CD2	8.48	113.08	106.30
1	A	24	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	464	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	A	557	TRP	CD1-CG-CD2	7.87	112.60	106.30
1	A	310	VAL	CG1-CB-CG2	-7.77	98.46	110.90
1	A	41	THR	CA-CB-CG2	7.77	123.27	112.40
1	A	614	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	414	ARG	NE-CZ-NH2	-7.67	116.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	TRP	CE2-CD2-CG	-7.61	101.22	107.30
1	A	9	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	A	140	TRP	CE2-CD2-CG	-7.53	101.28	107.30
1	A	581	TYR	CB-CG-CD2	-7.46	116.53	121.00
1	A	597	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	A	125	TRP	CD1-CG-CD2	7.37	112.20	106.30
1	A	361	TRP	CD1-CG-CD2	7.36	112.19	106.30
1	A	125	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	A	24	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	575	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	529	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	31	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	A	574	ARG	CA-C-N	-7.03	101.73	117.20
1	A	336	LEU	CA-CB-CG	7.01	131.44	115.30
1	A	464	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	A	423	LYS	CA-C-N	-7.00	101.80	117.20
1	A	255	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	445	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	A	125	TRP	CG-CD2-CE3	6.92	140.13	133.90
1	A	557	TRP	CE2-CD2-CG	-6.92	101.77	107.30
1	A	575	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	184	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	361	TRP	CE2-CD2-CG	-6.71	101.93	107.30
1	A	445	TRP	CD1-CG-CD2	6.71	111.67	106.30
1	A	9	TRP	CE2-CD2-CG	-6.69	101.95	107.30
1	A	244	TRP	CG-CD2-CE3	6.67	139.90	133.90
1	A	347	TRP	CE2-CD2-CG	-6.58	102.03	107.30
1	A	244	TRP	CE2-CD2-CG	-6.57	102.05	107.30
1	A	400	TYR	CB-CG-CD1	-6.48	117.11	121.00
1	A	224	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	A	438	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	614	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	347	TRP	CD1-CG-CD2	6.18	111.24	106.30
1	A	255	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	244	TRP	CD1-CG-CD2	6.10	111.18	106.30
1	A	41	THR	CA-CB-OG1	-6.08	96.24	109.00
1	A	125	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	A	264	TRP	CG-CD1-NE1	-5.93	104.17	110.10
1	A	8	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	260	VAL	CA-CB-CG2	-5.78	102.23	110.90
1	A	318	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	110	GLN	CA-CB-CG	-5.67	100.91	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	140	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	A	95	VAL	N-CA-CB	-5.64	99.10	111.50
1	A	648	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	75	LYS	CA-CB-CG	5.59	125.69	113.40
1	A	236	VAL	CA-CB-CG2	-5.57	102.55	110.90
1	A	69	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	205	VAL	CB-CA-C	-5.47	101.01	111.40
1	A	198	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	464	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	A	347	TRP	CG-CD2-CE3	5.46	138.81	133.90
1	A	627	MET	CA-CB-CG	5.43	122.53	113.30
1	A	445	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	A	264	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	A	121	ARG	CA-CB-CG	-5.33	101.68	113.40
1	A	115	CYS	CA-CB-SG	5.33	123.58	114.00
1	A	374	VAL	CG1-CB-CG2	-5.31	102.41	110.90
1	A	534	LYS	CA-C-N	5.24	126.69	116.20
1	A	414	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	478	CYS	CA-C-N	-5.17	105.82	117.20
1	A	582	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	336	LEU	CB-CA-C	-5.15	100.42	110.20
1	A	557	TRP	CG-CD1-NE1	-5.15	104.95	110.10
1	A	573	GLY	CA-C-O	5.14	129.86	120.60
1	A	314	MET	CG-SD-CE	-5.12	92.00	100.20
1	A	135	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	475	THR	CA-CB-CG2	5.09	119.52	112.40
1	A	458	VAL	CG1-CB-CG2	-5.08	102.77	110.90
1	A	121	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	336	LEU	CA-C-N	-5.04	106.12	117.20
1	A	82	TYR	CB-CG-CD2	-5.03	117.98	121.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	339	SER	Peptide
1	A	427	ARG	Peptide
1	A	509	PRO	Peptide
1	A	662	TYR	Sidechain
1	A	92	TYR	Sidechain

## 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	5284	0	5151	70	0
2	A	2	0	0	0	0
3	A	8	0	0	0	0
4	A	132	0	0	1	0
All	All	5426	0	5151	70	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 7.

All (70) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:633:LYS:HB3	1:A:635:LEU:HD13	1.64	0.80
1:A:527:ALA:HB3	1:A:540:ILE:HD11	1.69	0.75
1:A:414:ARG:NH1	1:A:429:ALA:HB2	2.02	0.74
1:A:116:HIS:CD2	1:A:161:VAL:HG22	2.34	0.63
1:A:524:TYR:CE2	1:A:638:LYS:HE2	2.35	0.62
1:A:549:THR:HG22	1:A:561:LEU:HB3	1.82	0.61
1:A:457:ALA:HA	1:A:490:PRO:HD2	1.82	0.61
1:A:444:ASN:ND2	1:A:447:ASN:HB2	2.16	0.61
1:A:486:GLU:HG3	1:A:501:LEU:HD21	1.82	0.61
1:A:115:CYS:SG	1:A:203:GLY:HA3	2.40	0.60
1:A:374:VAL:HG21	1:A:380:CYS:SG	2.45	0.57
1:A:452:LYS:HA	1:A:486:GLU:O	2.05	0.56
1:A:441:SER:HB3	1:A:443:VAL:HG12	1.89	0.54
1:A:471:ILE:O	1:A:475:THR:HB	2.07	0.53
1:A:445:TRP:O	1:A:448:LEU:HB2	2.10	0.52
1:A:357:LYS:HD3	1:A:636:LEU:HD23	1.90	0.52
1:A:311:PRO:HG3	1:A:679:MET:HA	1.92	0.51
1:A:16:GLU:CG	1:A:299:LEU:HD13	2.41	0.51
1:A:527:ALA:HB3	1:A:540:ILE:CD1	2.39	0.51
1:A:41:THR:HG22	1:A:44:ASP:H	1.77	0.50
1:A:32:ILE:HD12	1:A:32:ILE:H	1.76	0.50
1:A:630:SER:HB2	1:A:635:LEU:HB2	1.94	0.49
1:A:420:GLN:O	1:A:423:LYS:HD3	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:455:HIS:CD2	1:A:489:ALA:HB2	2.48	0.49
1:A:110:GLN:HG2	1:A:111:GLY:N	2.26	0.49
1:A:400:TYR:CD1	1:A:665:ILE:HD13	2.48	0.48
1:A:150:GLN:HE21	1:A:154:LYS:NZ	2.11	0.48
1:A:315:ASP:OD1	1:A:318:LEU:HB2	2.14	0.48
1:A:539:PHE:O	1:A:540:ILE:HD12	2.14	0.48
1:A:455:HIS:HB2	1:A:489:ALA:HA	1.96	0.48
1:A:285:PHE:CE2	1:A:306:MET:HA	2.49	0.47
1:A:84:HIS:HE1	1:A:93:TYR:CE2	2.32	0.47
1:A:481:ASP:HA	1:A:498:LEU:HD21	1.96	0.47
1:A:584:CYS:SG	1:A:584:CYS:O	2.73	0.47
1:A:84:HIS:HE1	1:A:93:TYR:HE2	1.63	0.46
1:A:541:GLN:OE1	1:A:640:LEU:HD12	2.16	0.46
1:A:472:HIS:CE1	1:A:671:CYS:SG	3.09	0.46
1:A:531:LEU:HB2	1:A:538:ALA:HB2	1.98	0.46
1:A:129:ILE:O	1:A:133:LEU:HD13	2.16	0.46
1:A:142:GLY:HA3	1:A:334:ASP:HA	1.97	0.46
1:A:403:GLY:HA3	1:A:653:TYR:CG	2.51	0.46
1:A:110:GLN:HG3	1:A:155:PHE:CD1	2.51	0.45
1:A:524:TYR:CE1	1:A:541:GLN:HB2	2.52	0.45
1:A:89:THR:HB	1:A:686:LYS:C	2.38	0.44
1:A:104:PHE:HB2	1:A:108:ASP:HB2	1.99	0.44
1:A:493:PRO:O	1:A:499:CYS:SG	2.76	0.44
1:A:217:ALA:HB1	1:A:220:GLN:HB2	2.00	0.44
1:A:529:ARG:O	1:A:533:GLU:HG2	2.17	0.43
1:A:412:ALA:HB3	1:A:645:PHE:CZ	2.53	0.43
1:A:271:GLN:OE1	1:A:306:MET:HB2	2.17	0.43
1:A:349:ALA:O	1:A:373:VAL:HA	2.19	0.43
1:A:194:ALA:O	1:A:197:CYS:HB3	2.19	0.43
1:A:455:HIS:HD2	1:A:489:ALA:HB2	1.84	0.43
1:A:630:SER:O	1:A:631:GLN:HB2	2.19	0.42
1:A:279:LYS:HD3	1:A:279:LYS:HA	1.87	0.42
1:A:150:GLN:HE21	1:A:154:LYS:HZ2	1.66	0.42
1:A:414:ARG:HH11	1:A:423:LYS:NZ	2.18	0.42
1:A:286:GLY:HA3	1:A:287:PRO:HA	1.93	0.42
1:A:596:VAL:HG11	1:A:604:ILE:HG12	2.02	0.41
1:A:597:ARG:HD3	1:A:599:GLU:OE2	2.20	0.41
1:A:577:ASN:HD22	1:A:578:VAL:N	2.17	0.41
1:A:267:LEU:HD13	1:A:307:LEU:HD13	2.03	0.41
1:A:342:GLU:HA	1:A:603:LYS:HD2	2.03	0.41
1:A:445:TRP:HA	1:A:448:LEU:HD13	2.03	0.41
1:A:214:ASN:HB2	4:A:744:HOH:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:669:LYS:O	1:A:673:PRO:HG3	2.21	0.41
1:A:668:LEU:O	1:A:671:CYS:HB2	2.21	0.40
1:A:27:THR:O	1:A:30:GLU:HB2	2.22	0.40
1:A:415:TYR:CE1	1:A:638:LYS:HD2	2.56	0.40
1:A:342:GLU:HG3	1:A:603:LYS:HD2	2.03	0.40

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	680/686 (99%)	604 (89%)	59 (9%)	17 (2%)	9 8

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	427	ARG
1	A	461	THR
1	A	505	SER
1	A	509	PRO
1	A	180	THR
1	A	534	LYS
1	A	648	ARG
1	A	88	SER
1	A	366	ASN
1	A	667	SER
1	A	342	GLU
1	A	178	PRO
1	A	464	TRP
1	A	57	ILE
1	A	163	GLY
1	A	507	GLY
1	A	340	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	577/580 (100%)	514 (89%)	63 (11%)	9 13

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	22	ASN
1	A	32	ILE
1	A	38	GLN
1	A	41	THR
1	A	59	LEU
1	A	74	LEU
1	A	77	ILE
1	A	88	SER
1	A	95	VAL
1	A	132	LEU
1	A	165	THR
1	A	172	ARG
1	A	178	PRO
1	A	179	LYS
1	A	185	ASN
1	A	198	LEU
1	A	199	LYS
1	A	205	VAL
1	A	269	LYS
1	A	276	VAL
1	A	295	LEU
1	A	299	LEU
1	A	336	LEU
1	A	337	THR
1	A	343	ASN
1	A	344	ARG
1	A	364	VAL
1	A	370	GLU
1	A	378	LYS
1	A	398	LEU

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Mol	Chain	Res	Type
1	A	410	VAL
1	A	414	ARG
1	A	416	ASP
1	A	420	GLN
1	A	430	SER
1	A	438	ARG
1	A	439	LYS
1	A	441	SER
1	A	442	ASN
1	A	449	LYS
1	A	474	ARG
1	A	481	ASP
1	A	486	GLU
1	A	503	GLN
1	A	513	CYS
1	A	528	LEU
1	A	534	LYS
1	A	537	VAL
1	A	540	ILE
1	A	571	THR
1	A	572	ASP
1	A	574	ARG
1	A	577	ASN
1	A	604	ILE
1	A	626	MET
1	A	635	LEU
1	A	636	LEU
1	A	652	THR
1	A	665	ILE
1	A	670	THR
1	A	677	LEU
1	A	681	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	38	GLN
1	A	63	GLN
1	A	84	HIS
1	A	150	GLN
1	A	185	ASN

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Mol	Chain	Res	Type
1	A	196	HIS
1	A	283	HIS
1	A	442	ASN
1	A	444	ASN
1	A	455	HIS
1	A	479	ASN
1	A	500	GLN
1	A	503	GLN
1	A	560	ASN
1	A	577	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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
3	CO3	A	688	2	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	A	690	2	0,3,3	0.00	-	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
3	CO3	A	688	2	-	0/0/0/0	0/0/0/0
3	CO3	A	690	2	-	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.

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.