



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:44 AM UTC

PDB ID : 1OVT / pdb_00001ovt
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 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

<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>.

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

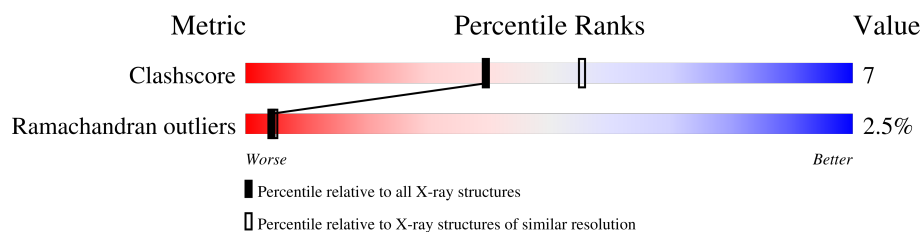
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	686	 67% 28% . .

2 Entry composition [i](#)

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

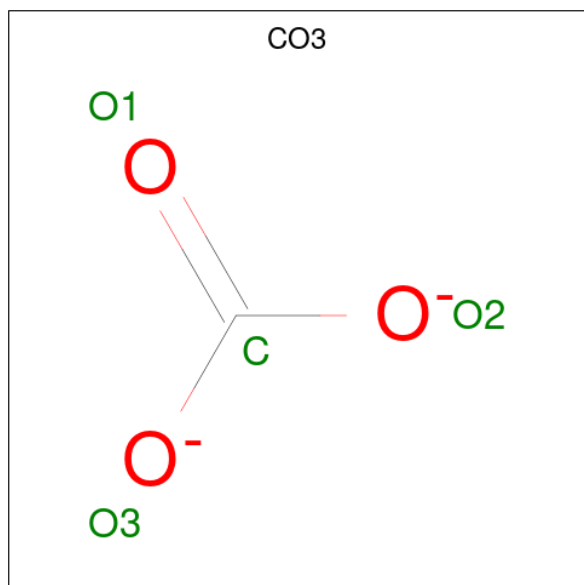
- Molecule 1 is a protein called OVOTRANSFERRIN.

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 (CCD ID: FE) (formula: Fe).

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

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



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.

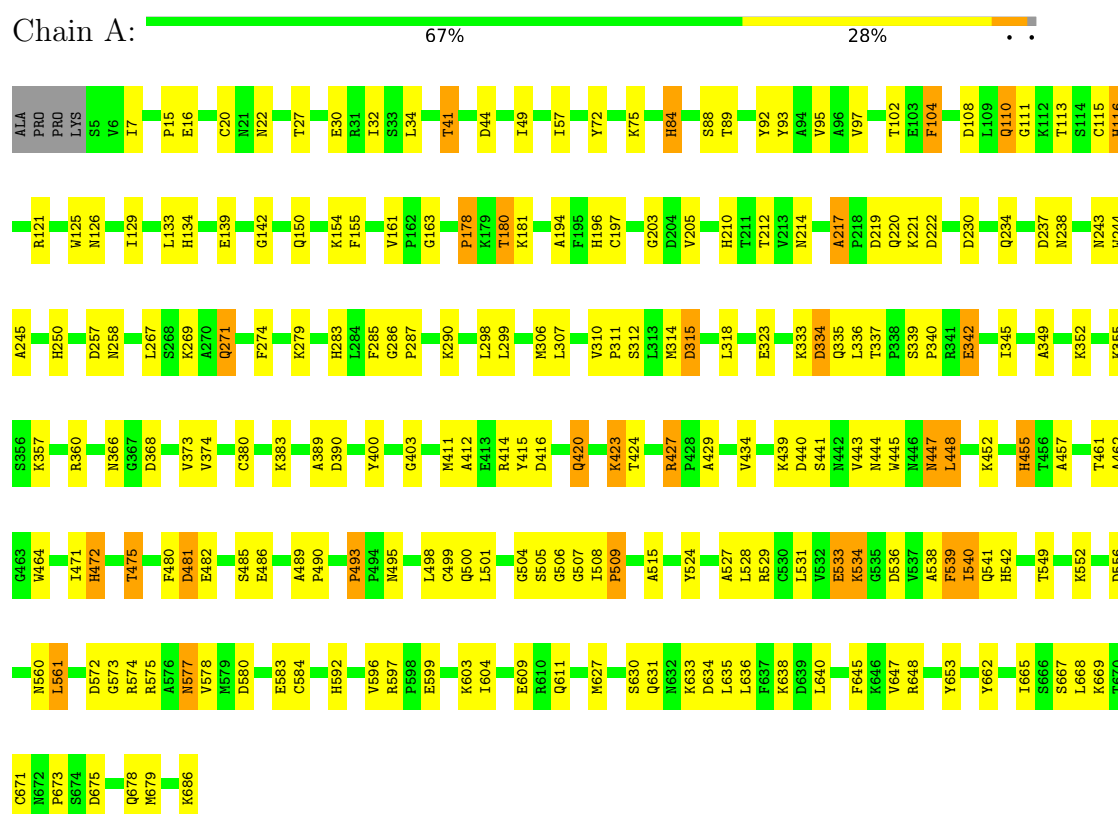
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total 132	O 132	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, 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. 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. 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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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: FE, CO3

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	1.04	22/5388 (0.4%)	1.92	134/7273 (1.8%)

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

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	455	HIS	CD2-NE2	-6.52	1.30	1.37
1	A	283	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	84	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	345	ILE	CA-CB	6.07	1.61	1.53
1	A	472	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	210	HIS	CG-ND1	-5.95	1.31	1.38
1	A	210	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	116	HIS	CD2-NE2	-5.82	1.31	1.37
1	A	250	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	116	HIS	CG-ND1	-5.81	1.31	1.38
1	A	542	HIS	CD2-NE2	-5.77	1.31	1.37
1	A	542	HIS	CG-ND1	-5.69	1.31	1.38
1	A	134	HIS	CD2-NE2	-5.50	1.31	1.37
1	A	592	HIS	CG-ND1	-5.39	1.32	1.38
1	A	472	HIS	CG-ND1	-5.31	1.32	1.38
1	A	647	VAL	CA-CB	5.26	1.59	1.53
1	A	180	THR	CA-CB	5.20	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	GLU	CA-CB	-5.18	1.46	1.53
1	A	283	HIS	CG-ND1	-5.17	1.32	1.38
1	A	196	HIS	CG-ND1	-5.17	1.32	1.38
1	A	337	THR	CA-CB	5.09	1.60	1.53

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	GLN	N-CA-C	11.93	124.28	111.28
1	A	540	ILE	N-CA-CB	-11.11	99.54	112.32
1	A	580	ASP	CA-CB-CG	10.45	123.05	112.60
1	A	352	LYS	N-CA-C	9.34	121.55	111.36
1	A	49	ILE	N-CA-C	-8.97	102.07	111.58
1	A	41	THR	CA-CB-OG1	-8.91	96.24	109.60
1	A	181	LYS	N-CA-C	8.85	123.18	112.38
1	A	423	LYS	N-CA-C	8.81	123.05	107.80
1	A	572	ASP	CA-C-O	8.76	130.56	120.75
1	A	222	ASP	CA-CB-CG	8.76	121.36	112.60
1	A	212	THR	N-CA-C	8.69	120.75	111.28
1	A	290	LYS	N-CA-C	-8.51	97.69	110.28
1	A	506	GLY	N-CA-C	-8.44	102.27	112.49
1	A	230	ASP	CA-CB-CG	8.42	121.02	112.60
1	A	675	ASP	CA-CB-CG	8.35	120.95	112.60
1	A	424	THR	N-CA-C	-8.07	102.39	112.72
1	A	312	SER	N-CA-C	8.01	122.62	113.01
1	A	72	TYR	N-CA-C	7.93	119.70	111.14
1	A	556	ASP	CA-CB-CG	7.87	120.47	112.60
1	A	481	ASP	CA-CB-CG	7.64	120.24	112.60
1	A	41	THR	CA-CB-CG2	7.51	123.27	110.50
1	A	7	ILE	N-CA-CB	-7.42	102.64	110.95
1	A	84	HIS	CA-CB-CG	-7.37	106.43	113.80
1	A	274	PHE	N-CA-C	7.23	121.42	112.59
1	A	333	LYS	N-CA-C	7.21	120.14	108.32
1	A	439	LYS	N-CA-C	7.14	121.09	112.38
1	A	448	LEU	N-CA-C	7.13	121.61	112.34
1	A	572	ASP	N-CA-C	7.12	119.34	108.52
1	A	420	GLN	N-CA-C	7.10	121.79	113.20
1	A	134	HIS	CA-CB-CG	-6.94	106.86	113.80
1	A	533	GLU	N-CA-C	6.92	120.68	112.93
1	A	416	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	485	SER	N-CA-C	-6.89	102.12	112.04
1	A	360	ARG	N-CA-C	-6.88	103.23	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	315	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	95	VAL	N-CA-CB	-6.86	99.10	111.92
1	A	540	ILE	N-CA-C	6.83	116.86	108.53
1	A	104	PHE	N-CA-C	6.76	120.03	110.50
1	A	536	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	336	LEU	O-C-N	6.67	129.19	122.12
1	A	34	LEU	N-CA-C	6.63	120.09	108.75
1	A	423	LYS	CA-C-O	6.62	128.59	120.25
1	A	110	GLN	CA-CB-CG	-6.59	100.91	114.10
1	A	611	GLN	N-CA-C	6.58	118.53	111.36
1	A	577	ASN	CA-CB-CG	6.50	119.10	112.60
1	A	257	ASP	N-CA-C	6.41	116.70	108.24
1	A	634	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	310	VAL	CA-C-N	6.36	126.39	119.90
1	A	310	VAL	C-N-CA	6.36	126.39	119.90
1	A	334	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	627	MET	N-CA-C	6.35	119.02	111.71
1	A	560	ASN	N-CA-C	6.34	121.09	113.23
1	A	243	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	A	500	GLN	N-CA-C	6.34	119.17	111.82
1	A	495	ASN	CA-CB-CG	6.30	118.90	112.60
1	A	472	HIS	CB-CG-CD2	-6.28	123.04	131.20
1	A	368	ASP	N-CA-C	6.26	120.47	112.34
1	A	336	LEU	CB-CA-C	-6.25	100.42	110.79
1	A	125	TRP	CG-CD2-CE3	6.23	140.13	133.90
1	A	121	ARG	CA-CB-CG	-6.21	101.68	114.10
1	A	237	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	205	VAL	CB-CA-C	-6.17	101.01	110.50
1	A	283	HIS	CB-CG-CD2	-6.17	123.19	131.20
1	A	434	VAL	N-CA-C	6.13	117.19	108.42
1	A	572	ASP	O-C-N	6.12	130.04	123.56
1	A	575	ARG	N-CA-C	-6.01	99.90	109.76
1	A	244	TRP	CG-CD2-CE3	6.00	139.90	133.90
1	A	258	ASN	N-CA-C	5.98	118.58	111.71
1	A	245	ALA	O-C-N	-5.97	117.55	123.46
1	A	97	VAL	N-CA-C	5.93	117.12	108.58
1	A	678	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	A	257	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	390	ASP	CA-CB-CG	5.88	118.48	112.60
1	A	389	ALA	O-C-N	-5.82	117.19	123.42
1	A	462	ALA	N-CA-C	5.80	119.18	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	LYS	CA-CB-CG	5.79	125.69	114.10
1	A	508	ILE	N-CA-CB	-5.73	103.19	111.21
1	A	574	ARG	O-C-N	5.71	130.19	122.59
1	A	126	ASN	N-CA-C	5.71	117.96	111.11
1	A	528	LEU	N-CA-C	-5.70	105.14	111.36
1	A	234	GLN	CA-C-N	5.70	125.65	119.78
1	A	234	GLN	C-N-CA	5.70	125.65	119.78
1	A	243	ASN	CB-CG-ND2	5.68	124.92	116.40
1	A	7	ILE	CB-CA-C	5.65	117.69	111.08
1	A	244	TRP	N-CA-C	-5.64	106.53	113.41
1	A	577	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	310	VAL	CG1-CB-CG2	-5.61	98.46	110.80
1	A	455	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	A	139	GLU	CB-CG-CD	-5.58	103.11	112.60
1	A	20	CYS	O-C-N	5.57	127.81	122.07
1	A	577	ASN	CB-CG-ND2	5.57	124.75	116.40
1	A	552	LYS	N-CA-C	5.57	119.79	112.89
1	A	573	GLY	O-C-N	5.56	129.93	122.70
1	A	22	ASN	CA-CB-CG	5.48	118.08	112.60
1	A	238	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	561	LEU	N-CA-C	5.45	118.26	110.24
1	A	219	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	583	GLU	CB-CG-CD	5.39	121.77	112.60
1	A	573	GLY	CA-C-O	5.34	129.86	120.57
1	A	314	MET	N-CA-C	5.31	117.57	110.35
1	A	475	THR	CA-CB-CG2	5.31	119.52	110.50
1	A	269	LYS	N-CA-C	-5.29	105.16	111.03
1	A	515	ALA	N-CA-C	5.28	119.42	111.81
1	A	434	VAL	N-CA-CB	-5.28	101.59	111.62
1	A	323	GLU	CB-CG-CD	5.28	121.57	112.60
1	A	178	PRO	N-CA-C	5.25	123.29	112.47
1	A	221	LYS	N-CA-C	5.25	118.47	111.75
1	A	504	GLY	CA-C-N	5.25	131.57	121.54
1	A	504	GLY	C-N-CA	5.25	131.57	121.54
1	A	102	THR	O-C-N	-5.25	116.82	123.01
1	A	355	LYS	CA-C-N	5.19	127.19	120.44
1	A	355	LYS	C-N-CA	5.19	127.19	120.44
1	A	217	ALA	CA-C-N	5.19	124.81	119.05
1	A	217	ALA	C-N-CA	5.19	124.81	119.05
1	A	539	PHE	CA-CB-CG	-5.18	108.62	113.80
1	A	528	LEU	CA-C-N	5.18	127.64	120.29
1	A	528	LEU	C-N-CA	5.18	127.64	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	THR	N-CA-C	5.17	121.82	110.80
1	A	298	LEU	CA-C-N	5.15	131.38	121.54
1	A	298	LEU	C-N-CA	5.15	131.38	121.54
1	A	575	ARG	O-C-N	-5.12	117.20	123.19
1	A	447	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	113	THR	O-C-N	-5.10	116.73	123.21
1	A	534	LYS	O-C-N	-5.10	115.81	122.59
1	A	493	PRO	CA-C-N	5.09	124.89	119.28
1	A	493	PRO	C-N-CA	5.09	124.89	119.28
1	A	125	TRP	CB-CG-CD1	-5.09	119.27	126.90
1	A	15	PRO	N-CA-C	5.08	120.51	113.65
1	A	480	PHE	N-CA-C	-5.07	107.09	113.28
1	A	482	GLU	CB-CG-CD	5.06	121.20	112.60
1	A	383	LYS	CA-CB-CG	-5.03	104.03	114.10
1	A	41	THR	N-CA-CB	-5.02	103.63	111.56
1	A	271	GLN	CB-CG-CD	-5.01	104.09	112.60

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 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	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

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 7.

All (70) 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: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:H	1:A:32:ILE:HD12	1.76	0.50
1:A:89:THR:HB	1:A:686:LYS:C	2.38	0.49
1:A:420:GLN:O	1:A:423:LYS:HD3	2.12	0.49
1:A:630:SER:HB2	1:A:635:LEU:HB2	1.94	0.49
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:472:HIS:CE1	1:A:671:CYS:SG	3.09	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:GLN:OE1	1:A:640:LEU:HD12	2.16	0.46
1:A:129:ILE:O	1:A:133:LEU:HD13	2.16	0.46
1:A:531:LEU:HB2	1:A:538:ALA:HB2	1.98	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: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:286:GLY:HA3	1:A:287:PRO:HA	1.93	0.42
1:A:414:ARG:HH11	1:A:423:LYS:NZ	2.18	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
1:A:669:LYS:O	1:A:673:PRO:HG3	2.21	0.41
1:A:27:THR:O	1:A:30:GLU:HB2	2.22	0.40
1:A:668:LEU:O	1:A:671:CYS:HB2	2.21	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
1:A:411:MET:HE1	1:A:609:GLU:HG3	2.04	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	A	680/686 (99%)	604 (89%)	59 (9%)	17 (2%)	4 5

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 [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 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	3,3,3	1.25	0	2,3,3	0.72	0
3	CO3	A	690	2	3,3,3	1.18	0	2,3,3	1.18	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.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.