



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 08:58 PM EDT

PDB ID : 1FWX / pdb_00001fwx
Title : CRYSTAL STRUCTURE OF NITROUS OXIDE REDUCTASE FROM P. DENITRIFICANS
Authors : Brown, K.; Djinovic-Carugo, K.; Haltia, T.; Cabrito, I.; Saraste, M.; Moura, J.J.; Moura, I.; Tegoni, M.; Cambillau, C.
Deposited on : 2000-09-25
Resolution : 1.60 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

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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

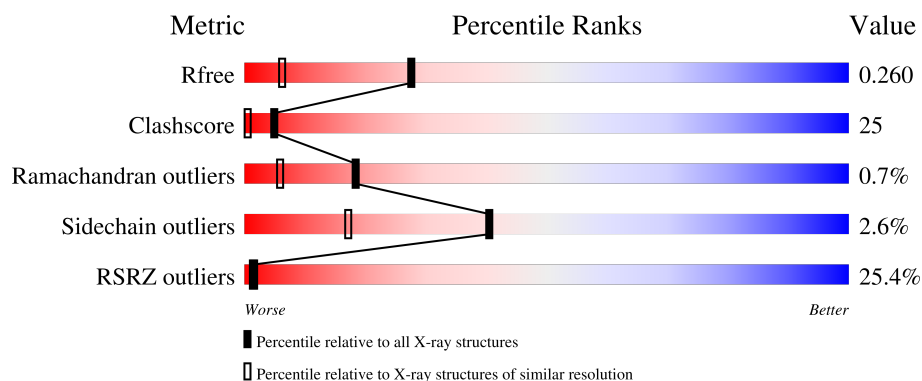
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 $\leq 5\%$. 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	595	
1	B	595	
1	C	595	
1	D	595	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 21176 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 NITROUS OXIDE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4633	2913	796	892	32			
1	B	589	Total	C	N	O	S	0	0	0
			4619	2904	793	890	32			
1	C	590	Total	C	N	O	S	0	0	0
			4628	2910	795	891	32			
1	D	588	Total	C	N	O	S	0	0	0
			4611	2900	792	887	32			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	VAL	ALA	see remark 999	UNP Q51705
A	8	ALA	GLY	see remark 999	UNP Q51705
B	291	VAL	ALA	see remark 999	UNP Q51705
B	8	ALA	GLY	see remark 999	UNP Q51705
C	291	VAL	ALA	see remark 999	UNP Q51705
C	8	ALA	GLY	see remark 999	UNP Q51705
D	291	VAL	ALA	see remark 999	UNP Q51705
D	8	ALA	GLY	see remark 999	UNP Q51705

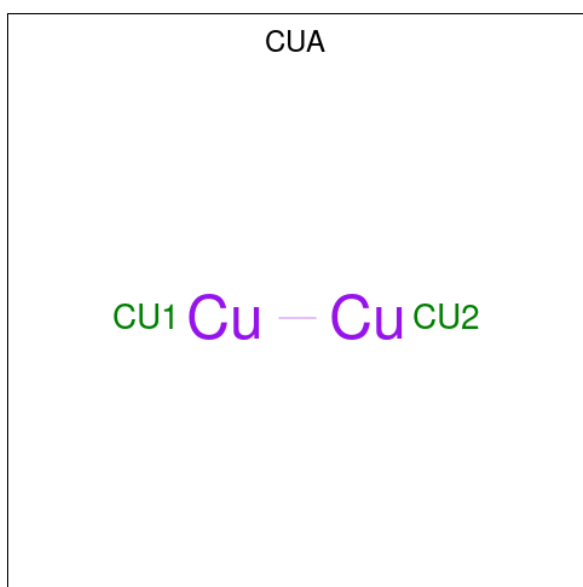
- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

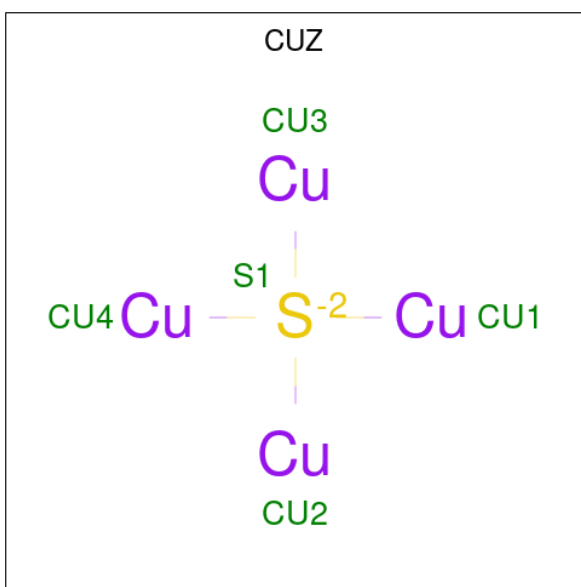
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Ca 3	0	0
3	B	3	Total 3	Ca 3	0	0
3	C	3	Total 3	Ca 3	0	0
3	D	2	Total 2	Ca 2	0	0

- Molecule 4 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 2	Cu 2	0	0
4	B	1	Total 2	Cu 2	0	0
4	C	1	Total 2	Cu 2	0	0
4	D	1	Total 2	Cu 2	0	0

- Molecule 5 is (MU-4-SULFIDO)-TETRA-NUCLEAR COPPER ION (CCD ID: CUZ) (formula: Cu₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Cu	S	0	0
			5	4	1		
5	B	1	Total	Cu	S	0	0
			5	4	1		
5	C	1	Total	Cu	S	0	0
			5	4	1		
5	D	1	Total	Cu	S	0	0
			5	4	1		

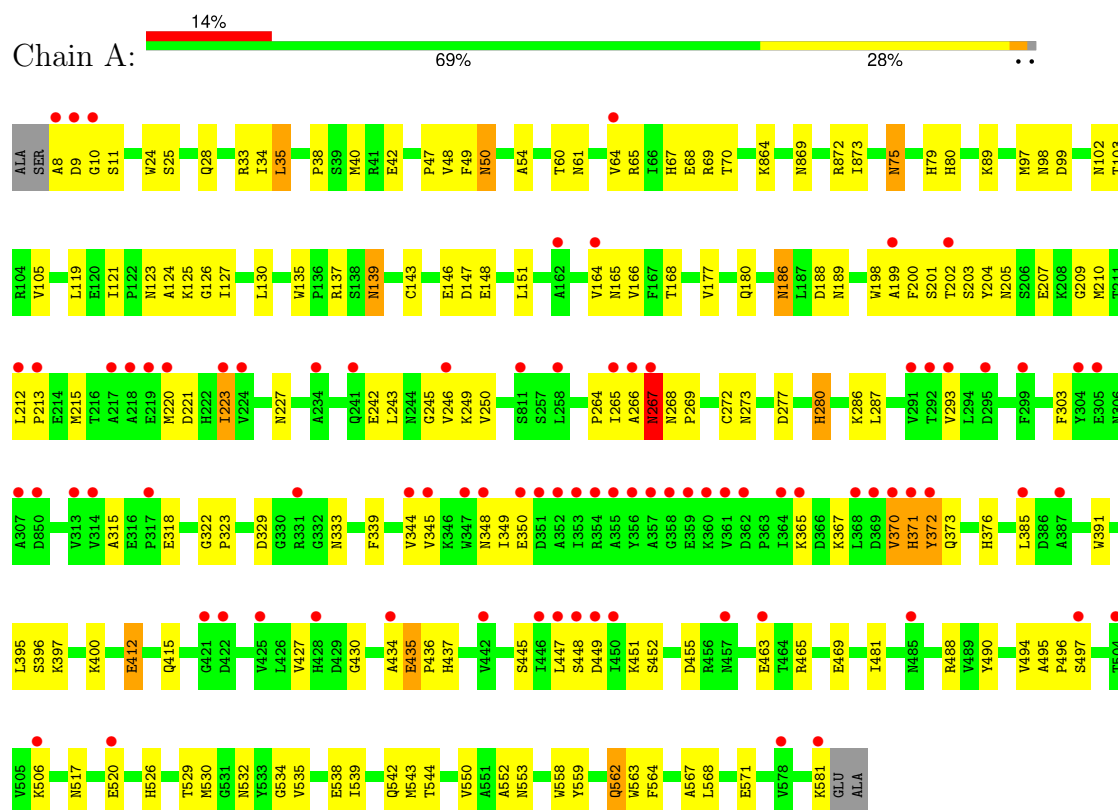
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	724	Total	O	0	0
			724	724		
6	B	750	Total	O	0	0
			750	750		
6	C	657	Total	O	0	0
			657	657		
6	D	511	Total	O	0	0
			511	511		

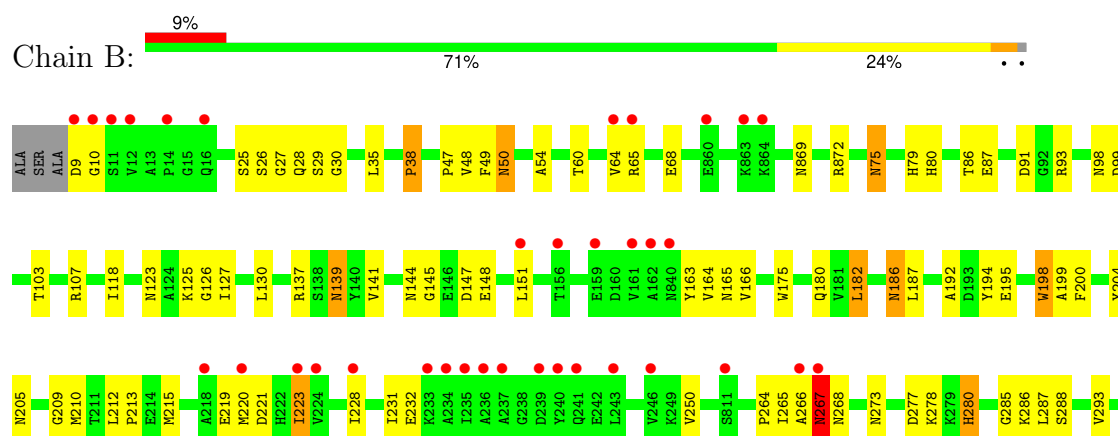
3 Residue-property plots

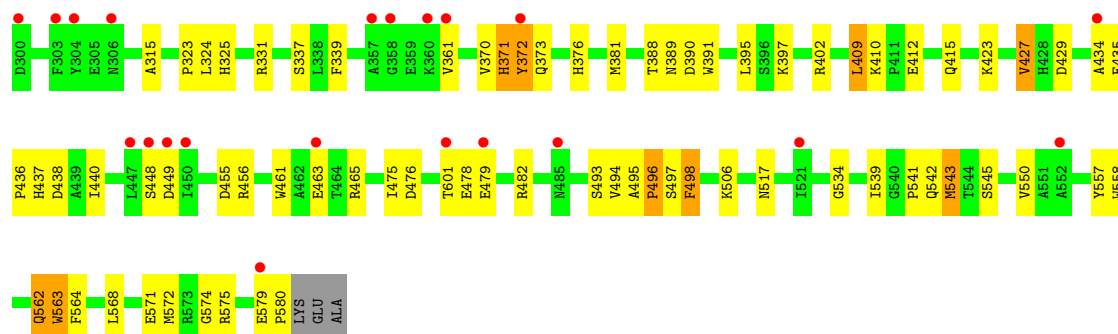
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

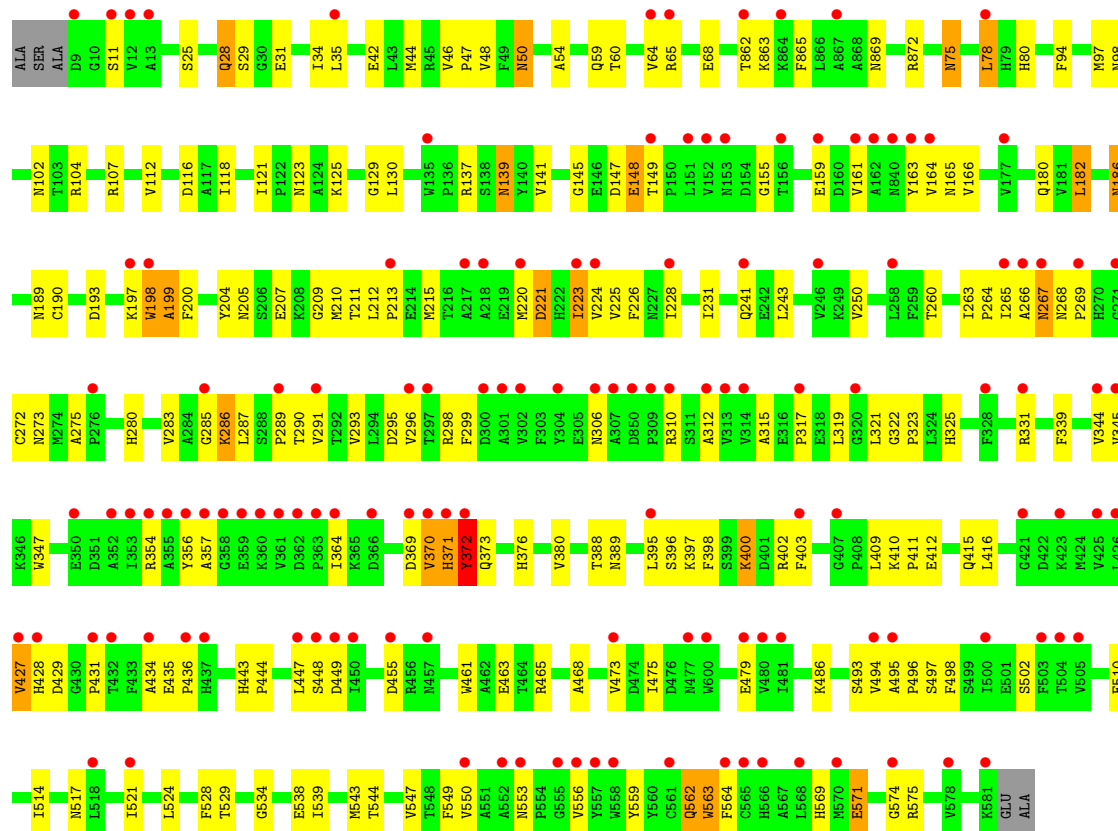


• Molecule 1: NITROUS OXIDE REDUCTASE

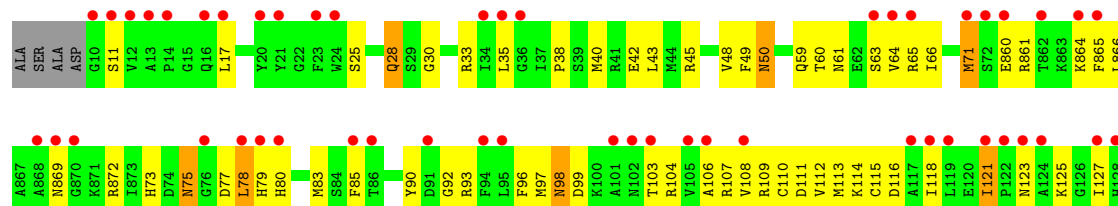




● Molecule 1: NITROUS OXIDE REDUCTASE



● Molecule 1: NITROUS OXIDE REDUCTASE



N517	D438	D369	P309	V251	D188	G129
L518	A439	V370	R310	D252	N189	L130
D519	I440	H371	S311	G253	C190	R131
E520	A441	Y372	A312	R254		P132
I521	V442	Q373	V313	K255	N193	Q133
D522	H443	P374	V314	E256	Y194	K134
D523	P444	G375	A315	E256	E195	W135
L524	S445	H376	E316	S811	G196	F136
T525	I446	L377	P317	K197	L137	T526
H526	L447D	K378	E318	L258	W198	S138
G527	S448	T379	L319	F259	A199	N139
F528	D449	V380	G320	T260	F200	M39
T529	I450	M381	L321	R261	F200	Y140
M530	K451	G382	G322	T262	S201	V141
	S452	E383	P323	L263	T202	F142
G534	V453	T384	L324	P264	G203	C143
V535	W454	L385	H325	T265	Y204	N144
	D455	D386	T326	A266	N205	G145
E538	R456	A387	A327	N267	S206	E146
I539	N457	T388	F328	R268	E207	D147
G540	D458	R389	D329	P269	K208	E148
P541	P459	D390	G330	H270	G209	T149
Q542	M460	W391	R331	G271	N210	P150
M543	W461	L392	G332	C272	T211	L151
T544	A462	V393	N333	T273	L212	V152
	E463	C394	A334	M274	M153	M153
V547	T464	L395	Y335	A275	G154	D154
	R465	S396	T336	P276	N215	G155
V550	A466	K397	S337	D277	T216	T156
A551	Q467	F398	L338	K278	A217	M157
A552	A468	S399	F339	K279	A218	M158
P554	E469	K400	L340	E220	E219	M159
G555		D401	D341	L281	N220	D160
V556	V473	R402	S342	H222	V161	D221
Y557	D474		Q343	I223	A162	A162
	I475	P408	V344	A284	N840	N840
W558	T601	L409	V345	G285	V224	Y163
Y559	E478	K410	K346	K286	V225	V164
	E479	P411	W347	L287	N227	V164
C561	W480	E412	N348	S288	N227	V166
Q562	V480	M413	I349	P289	I228	F167
W563		D414	E350	T290	A229	T168
F564	W485	Q415	D351	V291	E230	A169
		L416	A352	T292	L231	V170
		I417	R353	V293	E232	D171
		D418	I354	L294	K233	A172
M569	S492	I419	K354	D295	A234	D173
M570	S493	S420	A355	V296	L235	K174
E571	V494	G421	Y356	T297	A236	W175
M572	A495	D421	A357	T297	A237	E176
R573	P496	D422	G358	R298	G238	V177
G574	S497	K423	E359	F299	D239	A178
R575	F498	M424	K360	D300	Y240	W179
W576		W425	V361	A301	Q241	Q180
		L426	D362	V302	E242	V181
L577	S502	V427	P363	F303	L243	L182
V578			I364	Y304	N244	V183
E579	K506		K365	F304	G245	S184
P580	E507	A434	D366	N306	V246	G185
LYS	G508	E435	R367	A307	K249	N186
GLU		P436	K367	R850	V250	L197
ALA	T516	H437	L369			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.59Å 105.09Å 116.70Å 90.00° 110.69° 90.00°	Depositor
Resolution (Å)	29.83 – 1.60 29.83 – 1.60	Depositor EDS
% Data completeness (in resolution range)	89.4 (29.83-1.60) 89.5 (29.83-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 1.60Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.241 , 0.264 0.236 , 0.260	Depositor DCC
R_{free} test set	1331 reflections (0.49%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21176	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 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CUZ, CL, CUA

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	0.40	0/4744	1.03	27/6443 (0.4%)
1	B	0.42	1/4730 (0.0%)	1.04	29/6425 (0.5%)
1	C	0.39	0/4739	1.02	29/6436 (0.5%)
1	D	0.37	1/4722 (0.0%)	0.97	24/6414 (0.4%)
All	All	0.39	2/18935 (0.0%)	1.01	109/25718 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	543	MET	SD-CE	-6.17	1.64	1.79
1	D	71	MET	SD-CE	-5.91	1.64	1.79

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	435	GLU	N-CA-C	13.88	140.48	109.81
1	C	435	GLU	N-CA-C	13.07	138.70	109.81
1	A	435	GLU	N-CA-C	12.50	137.44	109.81
1	B	267	ASN	N-CA-C	9.90	131.88	110.80
1	C	267	ASN	N-CA-C	9.66	131.37	110.80

There are no chirality outliers.

There are no planarity outliers.

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	4633	0	4443	185	0
1	B	4619	0	4425	164	0
1	C	4628	0	4438	244	0
1	D	4611	0	4421	359	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	724	0	0	82	0
6	B	750	0	0	69	0
6	C	657	0	0	132	0
6	D	511	0	0	208	0
All	All	21176	0	17727	914	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 25.

The worst 5 of 914 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:D:326:THR:HG22	1:D:336:THR:HG22	1.19	1.14
1:B:456:ARG:HA	6:B:6235:HOH:O	1.54	1.04
1:D:547:VAL:HA	6:D:8122:HOH:O	1.58	1.04
1:D:71:MET:SD	6:D:8077:HOH:O	2.18	1.02
1:C:215:MET:HG2	6:C:7335:HOH:O	1.59	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	589/595 (99%)	557 (95%)	29 (5%)	3 (0%)	24	10
1	B	587/595 (99%)	561 (96%)	23 (4%)	3 (0%)	24	10
1	C	588/595 (99%)	553 (94%)	31 (5%)	4 (1%)	18	6
1	D	586/595 (98%)	545 (93%)	35 (6%)	6 (1%)	12	3
All	All	2350/2380 (99%)	2216 (94%)	118 (5%)	16 (1%)	18	6

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	B	434	ALA
1	D	267	ASN
1	A	434	ALA
1	B	267	ASN

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	501/503 (100%)	492 (98%)	9 (2%)	51	28
1	B	500/503 (99%)	487 (97%)	13 (3%)	40	17
1	C	501/503 (100%)	486 (97%)	15 (3%)	36	13
1	D	499/503 (99%)	483 (97%)	16 (3%)	34	12
All	All	2001/2012 (100%)	1948 (97%)	53 (3%)	40	17

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	182	LEU
1	C	563	TRP
1	D	402	ARG
1	C	186	ASN
1	C	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	562	GLN
1	D	267	ASN
1	D	50	ASN
1	D	144	ASN
1	D	415	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 15 are monoatomic - leaving 8 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
4	CUA	C	4701	1	0,1,1	-	-	-		
5	CUZ	D	7801	6,1	0,4,4	-	-	-		
4	CUA	D	4701	6,1	0,1,1	-	-	-		
5	CUZ	B	5801	6,1	0,4,4	-	-	-		
4	CUA	B	4701	1	0,1,1	-	-	-		
4	CUA	A	4701	1	0,1,1	-	-	-		
5	CUZ	C	6801	1	0,4,4	-	-	-		
5	CUZ	A	4801	6,1	0,4,4	-	-	-		

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 [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, 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	591/595 (99%)	0.98	83 (14%) 6 6	10, 18, 28, 39	0
1	B	589/595 (98%)	0.58	56 (9%) 14 14	10, 16, 25, 32	0
1	C	590/595 (99%)	1.37	134 (22%) 2 2	15, 23, 31, 42	0
1	D	588/595 (98%)	2.28	325 (55%) 0 0	17, 28, 38, 46	156 (26%)
All	All	2358/2380 (99%)	1.30	598 (25%) 1 1	10, 21, 33, 46	156 (6%)

The worst 5 of 598 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	ALA	7.4
1	C	357	ALA	6.8
1	D	449	ASP	6.5
1	B	434	ALA	6.4
1	A	434	ALA	6.2

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, 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	C	4910	1/1	0.73	0.18	66,66,66,66	0
3	CA	A	4904	1/1	0.74	0.24	74,74,74,74	0
3	CA	D	4903	1/1	0.82	0.17	36,36,36,36	0
3	CA	B	4909	1/1	0.85	0.12	67,67,67,67	0
5	CUZ	D	7801	5/5	0.92	0.15	31,31,32,32	0
2	CL	D	4908	1/1	0.93	0.15	32,32,32,32	0
4	CUA	C	4701	2/2	0.95	0.09	24,24,24,25	0
3	CA	D	4904	1/1	0.97	0.10	25,25,25,25	0
2	CL	A	4901	1/1	0.97	0.05	17,17,17,17	0
5	CUZ	A	4801	5/5	0.97	0.09	18,19,19,20	0
5	CUZ	C	6801	5/5	0.97	0.12	21,21,21,22	0
3	CA	A	4903	1/1	0.97	0.05	21,21,21,21	0
4	CUA	D	4701	2/2	0.98	0.10	17,17,17,18	0
3	CA	A	4905	1/1	0.98	0.04	17,17,17,17	0
4	CUA	B	4701	2/2	0.98	0.05	17,17,17,17	0
2	CL	C	4907	1/1	0.98	0.06	18,18,18,18	0
3	CA	C	4905	1/1	0.99	0.12	22,22,22,22	0
3	CA	B	4905	1/1	0.99	0.04	14,14,14,14	0
3	CA	C	4903	1/1	0.99	0.10	17,17,17,17	0
5	CUZ	B	5801	5/5	0.99	0.07	14,15,15,15	0
4	CUA	A	4701	2/2	0.99	0.04	10,10,10,10	0
2	CL	B	4906	1/1	0.99	0.03	12,12,12,12	0
3	CA	B	4903	1/1	1.00	0.06	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.