



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:30 AM GMT

PDB ID : 3AYY
Title : Membrane-bound respiratory [NiFe] hydrogenase from *Hydrogenovibrio marinus* in a ferricyanide-oxidized condition
Authors : Shomura, Y.; Yoon, K.S.; Nishihara, H.; Higuchi, Y.
Deposited on : 2011-05-20
Resolution : 1.32 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
<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

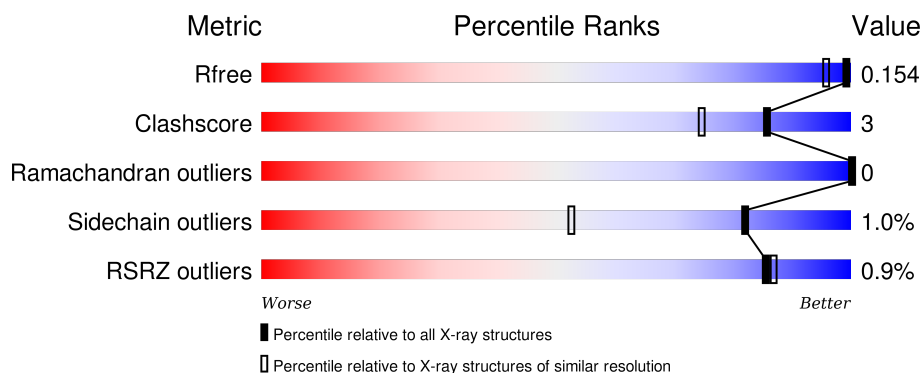
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.32 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}	91344	1004 (1.34-1.30)
Clashscore	102246	1059 (1.34-1.30)
Ramachandran outliers	100387	1015 (1.34-1.30)
Sidechain outliers	100360	1015 (1.34-1.30)
RSRZ outliers	91569	1002 (1.34-1.30)

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 ≥ 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	596	<div> <div>89%</div> <div>10% •</div> </div>
1	C	596	<div> <div>%</div> <div>87%</div> <div>12% •</div> </div>
2	B	283	<div> <div>2%</div> <div>82%</div> <div>12% • •</div> </div>
2	D	283	<div> <div>%</div> <div>80%</div> <div>13% • 6%</div> </div>

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
6	CYN	A	605	-	-	-	X
7	O	A	607	-	-	X	X
7	O	A	608	-	-	-	X
7	O	A	609	-	-	-	X
7	O	A	610	-	-	-	X
7	O	C	607	-	-	X	X
7	O	C	609	-	-	-	X
7	O	C	610	-	-	-	X
8	GOL	A	702	-	-	-	X
8	GOL	A	703	-	-	-	X
8	GOL	C	702	-	-	-	X
8	GOL	C	703	-	-	-	X

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 15488 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 Membrane-bound hydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	17	0
			4755	3017	828	885	25			
1	C	595	Total	C	N	O	S	0	12	0
			4734	3001	828	880	25			

- Molecule 2 is a protein called Membrane-bound hydrogenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	273	Total	C	N	O	S	0	7	0
			2148	1363	366	398	21			
2	D	267	Total	C	N	O	S	0	8	0
			2108	1340	359	389	20			

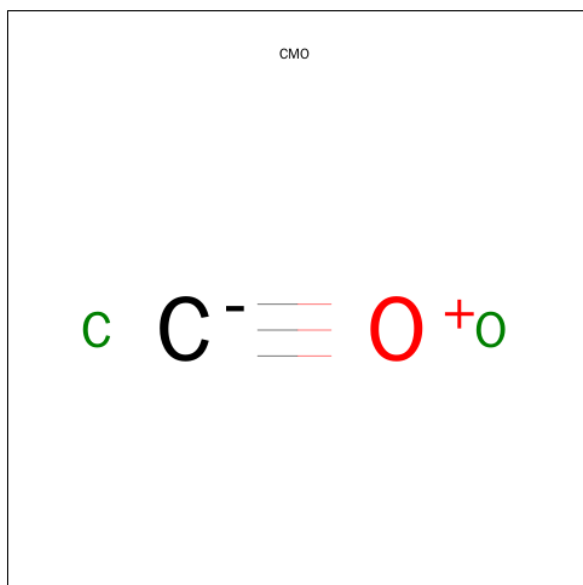
- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 4 is NICKEL (III) ION (three-letter code: 3NI) (formula: Ni).

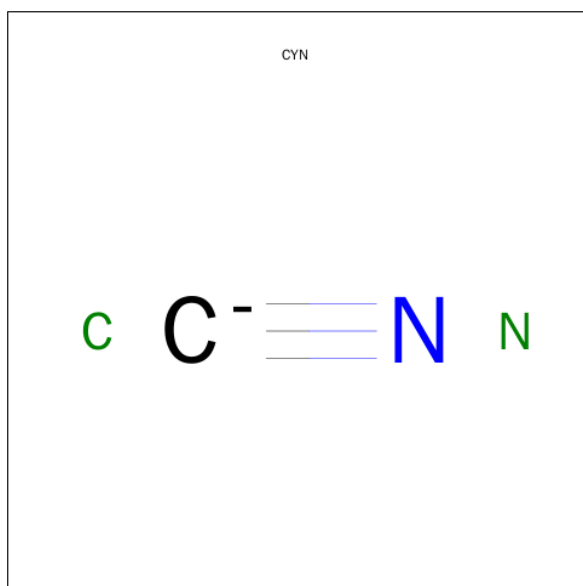
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	C	1	Total	Ni	0	0
			1	1		

- Molecule 5 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			2	1	1		
5	C	1	Total	C	O	0	0
			2	1	1		

- Molecule 6 is CYANIDE ION (three-letter code: CYN) (formula: CN).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			2	1	1		
6	A	1	Total	C	N	0	0
			2	1	1		

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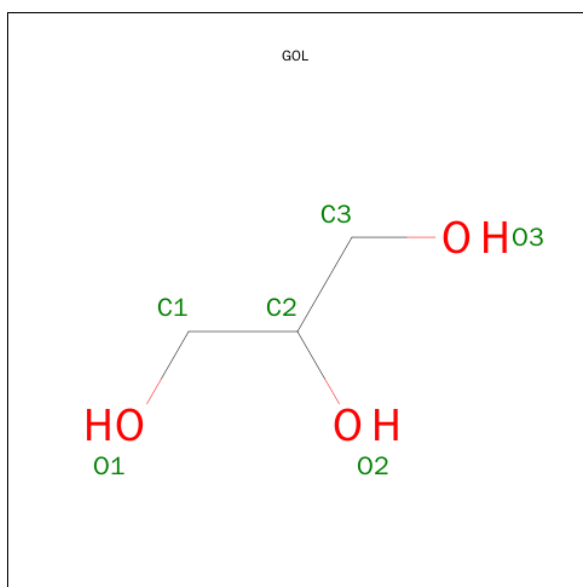
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	N	0	0
			2	1	1		
6	C	1	Total	C	N	0	0
			2	1	1		

- Molecule 7 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total	O	0	0
			5	5		
7	C	5	Total	O	0	0
			5	5		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

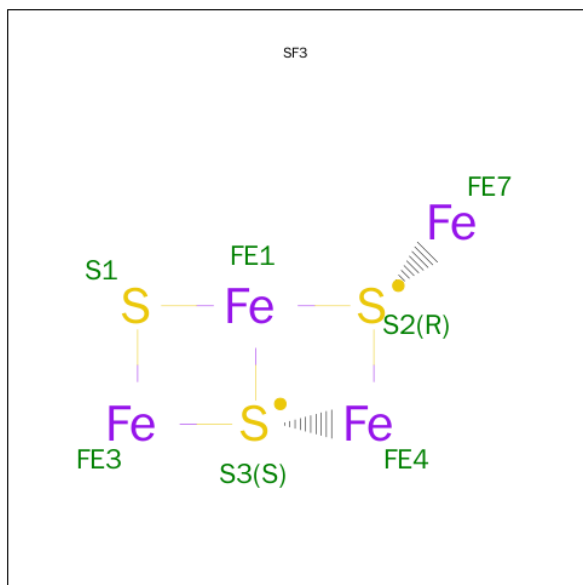


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

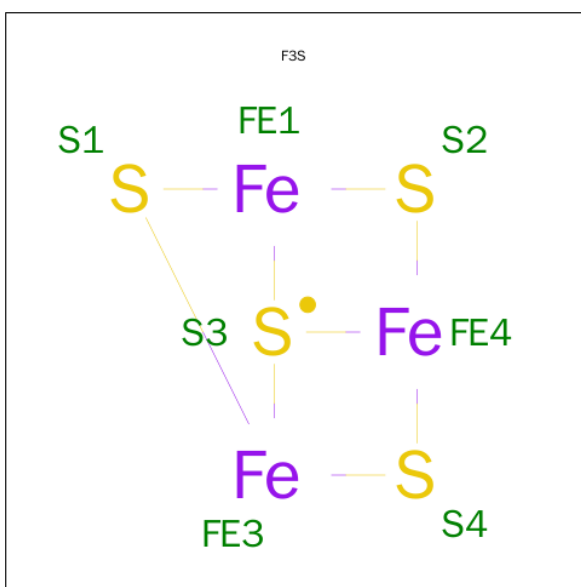
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Mg 1 1	0	0
9	C	1	Total Mg 1 1	0	0

- Molecule 10 is FE4-S3 CLUSTER (three-letter code: SF3) (formula: Fe_4S_3).



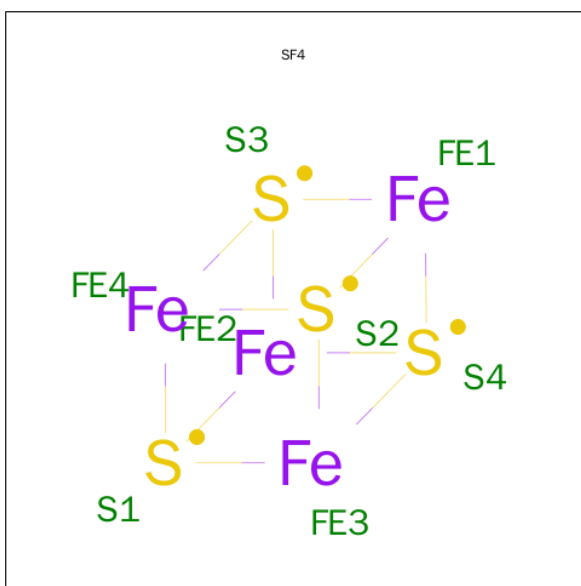
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Fe S 7 4 3	0	0
10	D	1	Total Fe S 7 4 3	0	0

- Molecule 11 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			7	3	4		
11	D	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 12 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	Fe	S	0	0
			8	4	4		
12	D	1	Total	Fe	S	0	0
			8	4	4		

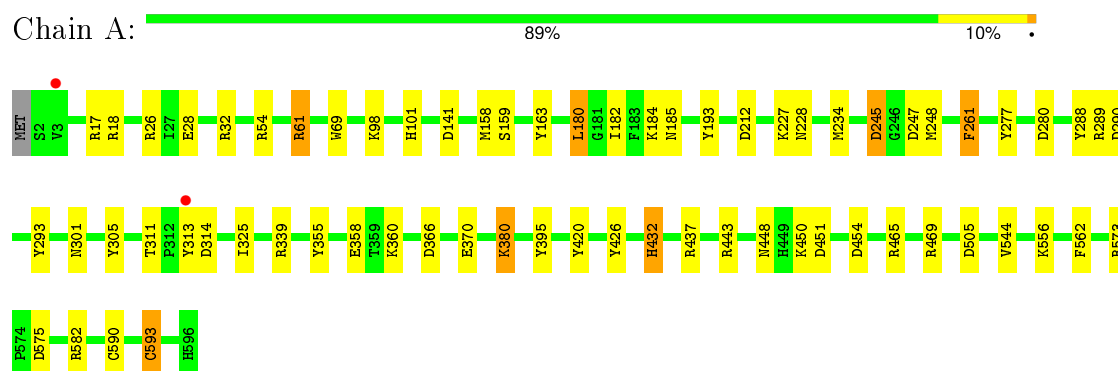
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	626	Total 626	O 626	0	0
13	B	258	Total 258	O 258	0	0
13	C	532	Total 532	O 532	0	0
13	D	231	Total 231	O 231	0	0

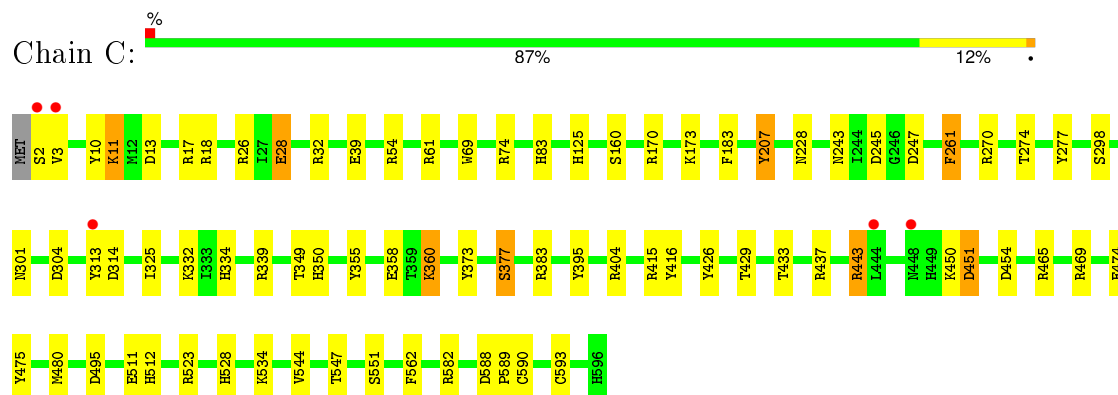
3 Residue-property plots

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.

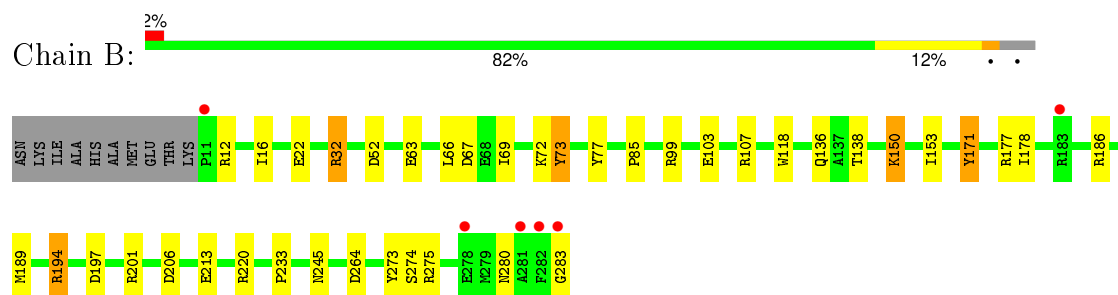
- Molecule 1: Membrane-bound hydrogenase large subunit



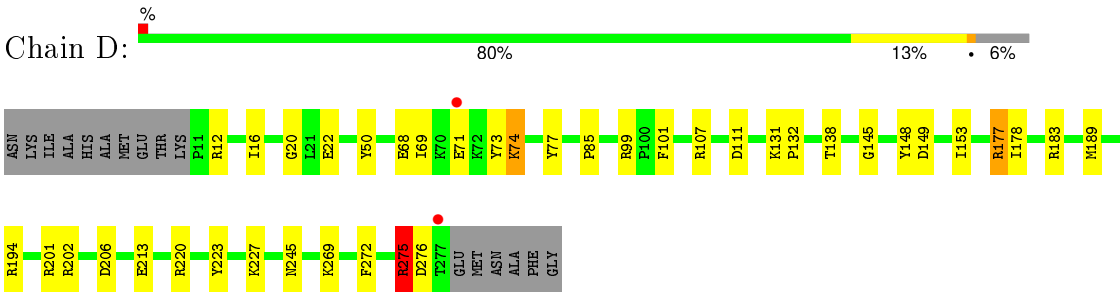
- Molecule 1: Membrane-bound hydrogenase large subunit



- Molecule 2: Membrane-bound hydrogenase small subunit



- Molecule 2: Membrane-bound hydrogenase small subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.63Å 116.94Å 113.34Å 90.00° 91.42° 90.00°	Depositor
Resolution (Å)	20.00 – 1.32 19.89 – 1.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.32) 94.5 (19.89-1.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.32Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.136 , 0.173 0.127 , 0.154	Depositor DCC
R_{free} test set	23288 reflections (5.84%)	DCC
Wilson B-factor (Å ²)	11.5	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 64.3	EDS
Estimated twinning fraction	0.005 for -h,-l,-k 0.000 for -h,l,k 0.087 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 895659 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	15488	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CMO, GOL, MG, SF4, SF3, O, 3NI, F3S, FE2, CYN

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	0.89	3/4934 (0.1%)	1.42	72/6717 (1.1%)
1	C	0.85	2/4895 (0.0%)	1.45	63/6666 (0.9%)
2	B	0.91	1/2227 (0.0%)	1.51	33/3014 (1.1%)
2	D	0.87	0/2189	1.52	37/2964 (1.2%)
All	All	0.88	6/14245 (0.0%)	1.46	205/19361 (1.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	377	SER	CB-OG	7.88	1.52	1.42
1	C	28	GLU	CD-OE2	5.71	1.31	1.25
2	B	22	GLU	CD-OE2	-5.65	1.19	1.25
1	A	101[A]	HIS	ND1-CE1	-5.57	1.20	1.34
1	A	101[B]	HIS	ND1-CE1	-5.57	1.20	1.34
1	A	593	CYS	CB-SG	-5.06	1.73	1.81

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	32	ARG	NE-CZ-NH2	18.56	129.58	120.30
1	A	141	ASP	CB-CG-OD2	16.77	133.40	118.30
2	D	177	ARG	NE-CZ-NH1	16.39	128.50	120.30
1	C	465	ARG	NE-CZ-NH1	15.28	127.94	120.30
2	D	194	ARG	NE-CZ-NH2	-14.79	112.90	120.30
2	D	275	ARG	CD-NE-CZ	14.50	143.90	123.60
1	A	465	ARG	NE-CZ-NH1	14.07	127.33	120.30
1	C	170	ARG	NE-CZ-NH2	-13.86	113.37	120.30
2	D	177	ARG	NE-CZ-NH2	-13.74	113.43	120.30
1	C	437	ARG	NE-CZ-NH1	-13.49	113.56	120.30
1	C	69	TRP	CZ3-CH2-CZ2	13.42	137.70	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	ARG	NE-CZ-NH2	-13.27	113.67	120.30
1	C	17	ARG	NE-CZ-NH1	-12.37	114.11	120.30
1	A	339	ARG	NE-CZ-NH1	12.26	126.43	120.30
1	C	32	ARG	NE-CZ-NH2	-11.73	114.44	120.30
1	A	437	ARG	NE-CZ-NH1	-11.56	114.52	120.30
2	B	107	ARG	NE-CZ-NH2	-11.36	114.62	120.30
1	A	465	ARG	NE-CZ-NH2	-11.09	114.75	120.30
1	A	26	ARG	NE-CZ-NH1	11.07	125.83	120.30
1	A	69	TRP	CZ3-CH2-CZ2	11.01	134.81	121.60
1	A	61	ARG	NE-CZ-NH1	10.97	125.79	120.30
2	B	194	ARG	CD-NE-CZ	10.68	138.55	123.60
1	C	454	ASP	CB-CG-OD2	-10.66	108.71	118.30
1	C	69	TRP	CH2-CZ2-CE2	-10.47	106.93	117.40
1	A	18	ARG	NE-CZ-NH1	10.45	125.53	120.30
2	B	194	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	A	61	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	C	69	TRP	CE3-CZ3-CH2	-9.56	110.68	121.20
2	B	52	ASP	CB-CG-OD2	9.26	126.63	118.30
1	A	69	TRP	CH2-CZ2-CE2	-8.84	108.56	117.40
2	B	220	ARG	NE-CZ-NH1	-8.63	115.99	120.30
2	D	12	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	C	426	TYR	CB-CG-CD2	8.42	126.05	121.00
1	C	26	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	C	523	ARG	NE-CZ-NH2	-8.36	116.12	120.30
2	D	202	ARG	NE-CZ-NH2	8.26	124.43	120.30
2	D	194	ARG	NH1-CZ-NH2	8.24	128.46	119.40
2	B	171	TYR	CZ-CE2-CD2	-8.11	112.50	119.80
1	C	277	TYR	CB-CG-CD2	-8.07	116.16	121.00
1	C	277	TYR	CB-CG-CD1	8.06	125.83	121.00
1	C	313	TYR	CB-CG-CD2	7.85	125.71	121.00
1	C	454	ASP	CB-CG-OD1	7.84	125.36	118.30
2	D	50	TYR	CD1-CE1-CZ	7.81	126.83	119.80
1	A	69	TRP	CE3-CZ3-CH2	-7.68	112.75	121.20
2	B	197	ASP	CB-CG-OD1	-7.68	111.39	118.30
1	C	28	GLU	CG-CD-OE2	-7.68	102.94	118.30
2	D	99	ARG	CD-NE-CZ	7.66	134.33	123.60
1	A	290	ASP	CB-CG-OD2	7.58	125.12	118.30
1	A	18	ARG	NH1-CZ-NH2	-7.57	111.07	119.40
1	A	54	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	C	582	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	355	TYR	CB-CG-CD1	7.50	125.50	121.00
1	A	426	TYR	CG-CD2-CE2	7.42	127.24	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	77	TYR	CB-CG-CD1	7.37	125.42	121.00
2	B	171	TYR	CG-CD2-CE2	7.37	127.19	121.30
2	B	273	TYR	CB-CG-CD1	-7.36	116.58	121.00
1	C	28	GLU	CG-CD-OE1	7.30	132.90	118.30
1	C	13	ASP	CB-CG-OD1	7.22	124.80	118.30
2	D	202	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	C	383	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	A	193	TYR	CB-CG-CD2	7.11	125.27	121.00
2	B	99	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	C	465	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	C	437	ARG	NH1-CZ-NH2	7.04	127.14	119.40
1	A	141	ASP	CB-CG-OD1	-7.03	111.97	118.30
1	C	443	ARG	CD-NE-CZ	6.98	133.37	123.60
1	C	183	PHE	CB-CG-CD1	-6.96	115.92	120.80
2	D	107	ARG	CG-CD-NE	6.96	126.41	111.80
1	A	573	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	426	TYR	CB-CG-CD2	6.91	125.15	121.00
2	B	99	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	C	358	GLU	CG-CD-OE2	-6.84	104.61	118.30
2	B	275	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	212	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	248	MET	CG-SD-CE	-6.76	89.38	100.20
2	D	275	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	C	270	ARG	CD-NE-CZ	6.72	133.00	123.60
1	C	469	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	C	261	PHE	CB-CG-CD2	-6.59	116.19	120.80
2	B	275	ARG	NE-CZ-NH1	6.55	123.58	120.30
2	B	32	ARG	NH1-CZ-NH2	-6.54	112.21	119.40
1	C	358	GLU	OE1-CD-OE2	6.50	131.10	123.30
1	C	395	TYR	CA-CB-CG	6.50	125.74	113.40
1	A	380	LYS	CA-CB-CG	6.48	127.66	113.40
1	A	448	ASN	CB-CG-ND2	-6.48	101.16	116.70
1	C	314	ASP	CB-CG-OD1	6.45	124.11	118.30
2	D	223	TYR	CB-CG-CD1	6.45	124.87	121.00
1	A	245[A]	ASP	CB-CG-OD1	6.44	124.10	118.30
1	A	245[B]	ASP	CB-CG-OD1	6.44	124.10	118.30
2	D	149	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	313	TYR	CB-CG-CD2	6.40	124.84	121.00
2	B	189	MET	CB-CA-C	-6.40	97.59	110.40
1	A	305	TYR	CB-CG-CD1	6.40	124.84	121.00
1	C	170	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	D	272	PHE	CB-CG-CD1	-6.37	116.34	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	355	TYR	CB-CG-CD1	6.35	124.81	121.00
2	D	148	TYR	CD1-CE1-CZ	-6.34	114.09	119.80
1	A	505	ASP	CB-CG-OD2	6.32	123.98	118.30
1	C	32	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	A	61	ARG	CD-NE-CZ	-6.29	114.79	123.60
1	A	17	ARG	CD-NE-CZ	6.28	132.38	123.60
1	A	582	ARG	NE-CZ-NH2	-6.26	117.17	120.30
2	B	12	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	234	MET	CA-CB-CG	-6.25	102.68	113.30
1	A	451	ASP	C-N-CA	6.24	137.29	121.70
1	A	193	TYR	CB-CG-CD1	-6.23	117.26	121.00
1	C	54	ARG	NE-CZ-NH1	-6.22	117.19	120.30
2	D	276	ASP	CB-CG-OD1	6.21	123.89	118.30
2	B	186	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	C	304	ASP	CB-CG-OD1	6.20	123.88	118.30
1	C	404	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	A	313	TYR	CG-CD2-CE2	6.14	126.22	121.30
1	C	10	TYR	CG-CD1-CE1	-6.14	116.39	121.30
1	A	582	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	18	ARG	NE-CZ-NH2	6.09	123.35	120.30
1	C	207	TYR	CA-CB-CG	6.09	124.97	113.40
2	B	103	GLU	OE1-CD-OE2	6.09	130.60	123.30
1	C	562	PHE	CB-CG-CD2	-6.06	116.56	120.80
2	D	50	TYR	CG-CD2-CE2	6.06	126.15	121.30
1	C	582	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	A	289	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	C	443	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	C	451	ASP	C-N-CA	5.96	136.60	121.70
1	A	288	TYR	CB-CG-CD1	5.96	124.57	121.00
1	A	443	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	18	ARG	NE-CZ-NH2	-5.93	117.34	120.30
2	D	50	TYR	CG-CD1-CE1	-5.91	116.57	121.30
1	C	523	ARG	NE-CZ-NH1	5.91	123.25	120.30
2	D	68	GLU	CA-CB-CG	5.89	126.37	113.40
1	A	28	GLU	CG-CD-OE2	5.89	130.07	118.30
2	B	73	TYR	CG-CD2-CE2	5.82	125.95	121.30
1	C	426	TYR	CG-CD2-CE2	5.81	125.95	121.30
2	D	77	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	A	247[A]	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	247[B]	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	451	ASP	O-C-N	-5.78	113.45	122.70
2	D	189	MET	CA-CB-CG	5.76	123.09	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	PHE	CB-CG-CD2	5.75	124.83	120.80
2	D	101	PHE	CB-CG-CD1	5.74	124.82	120.80
2	B	32	ARG	CD-NE-CZ	5.70	131.57	123.60
2	B	12	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	293	TYR	CB-CG-CD2	5.65	124.39	121.00
2	D	220	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	311	THR	O-C-N	5.64	131.82	121.10
1	C	74	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	298	SER	C-N-CA	-5.63	107.61	121.70
1	C	480	MET	CG-SD-CE	-5.62	91.21	100.20
1	C	183	PHE	CB-CG-CD2	5.60	124.72	120.80
1	C	17	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	C	247	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	B	213	GLU	OE1-CD-OE2	5.58	129.99	123.30
1	A	32	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	B	52	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	A	101[A]	HIS	CG-ND1-CE1	5.52	115.93	108.20
1	A	101[B]	HIS	CG-ND1-CE1	5.52	115.93	108.20
2	B	77	TYR	CB-CG-CD1	5.51	124.31	121.00
1	A	469	ARG	CD-NE-CZ	5.50	131.30	123.60
1	A	280	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	562	PHE	CB-CG-CD2	-5.50	116.95	120.80
1	A	277	TYR	CB-CG-CD1	5.49	124.29	121.00
1	A	437	ARG	CD-NE-CZ	5.46	131.25	123.60
1	A	432	HIS	CA-CB-CG	-5.44	104.35	113.60
2	B	171	TYR	CB-CG-CD2	5.44	124.26	121.00
2	B	274	SER	C-N-CA	5.43	135.27	121.70
1	A	437	ARG	NH1-CZ-NH2	5.42	125.37	119.40
1	C	373	TYR	CG-CD1-CE1	-5.40	116.98	121.30
1	C	415	ARG	NE-CZ-NH1	5.35	122.98	120.30
2	D	275	ARG	NH1-CZ-NH2	-5.35	113.52	119.40
2	B	264	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	314	ASP	CB-CG-OD1	5.34	123.10	118.30
1	C	475	TYR	CB-CG-CD1	5.33	124.20	121.00
1	A	366	ASP	CB-CG-OD1	-5.32	113.51	118.30
2	D	213	GLU	OE1-CD-OE2	5.32	129.68	123.30
1	C	355	TYR	CB-CG-CD2	-5.30	117.82	121.00
2	D	177	ARG	CA-CB-CG	5.30	125.06	113.40
2	B	201	ARG	NE-CZ-NH2	5.29	122.94	120.30
2	D	275	ARG	CG-CD-NE	5.28	122.88	111.80
1	A	448	ASN	CB-CG-OD1	5.27	132.14	121.60
2	D	145	GLY	CA-C-O	5.26	130.08	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	GLU	OE1-CD-OE2	-5.26	116.98	123.30
1	A	355	TYR	CB-CG-CD2	-5.26	117.84	121.00
2	D	101	PHE	CB-CG-CD2	-5.26	117.12	120.80
2	B	118	TRP	CA-CB-CG	5.24	123.66	113.70
1	C	416	TYR	CA-CB-CG	-5.24	103.44	113.40
1	A	370	GLU	OE1-CD-OE2	5.24	129.58	123.30
1	C	10	TYR	CD1-CE1-CZ	5.23	124.50	119.80
2	B	274	SER	O-C-N	-5.21	114.37	122.70
1	A	395	TYR	CA-CB-CG	5.16	123.20	113.40
2	D	269	LYS	CA-C-N	5.14	126.49	116.20
1	C	495	ASP	CB-CG-OD2	-5.14	113.67	118.30
2	D	111	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	A	227	LYS	C-N-CA	5.12	134.50	121.70
1	A	180	LEU	CA-CB-CG	5.08	126.98	115.30
2	D	183	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	395	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	A	454	ASP	CB-CG-OD1	5.06	122.86	118.30
2	D	73	TYR	CB-CG-CD2	5.05	124.03	121.00
1	A	261	PHE	CB-CG-CD1	-5.05	117.27	120.80
1	A	358	GLU	CG-CD-OE2	-5.04	108.23	118.30
1	C	339	ARG	NE-CZ-NH2	-5.03	117.79	120.30
2	D	275	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	C	469	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	D	201	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	B	63[A]	GLU	CB-CG-CD	5.00	127.71	114.20
2	B	63[B]	GLU	CB-CG-CD	5.00	127.71	114.20

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	4755	0	4671	19	0
1	C	4734	0	4638	36	0
2	B	2148	0	2088	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2108	0	2061	11	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
6	A	4	0	0	0	0
6	C	4	0	0	0	0
7	A	5	0	0	5	0
7	C	5	0	0	6	0
8	A	12	0	16	1	0
8	C	12	0	16	2	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	B	7	0	0	0	0
10	D	7	0	0	0	0
11	B	7	0	0	0	0
11	D	7	0	0	0	0
12	B	8	0	0	0	0
12	D	8	0	0	0	0
13	A	626	0	0	4	0
13	B	258	0	0	4	0
13	C	532	0	0	7	0
13	D	231	0	0	2	0
All	All	15488	0	13490	77	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 3.

All (77) 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:593:CYS:CB	7:C:607:O:O	2.06	1.03
1:A:593:CYS:CB	7:A:607:O:O	2.10	1.00
1:A:593:CYS:SG	7:A:607:O:O	2.23	0.95
1:A:593:CYS:HB2	7:A:607:O:O	1.72	0.90
1:C:593:CYS:HB2	7:C:607:O:O	1.77	0.85
1:C:349[A]:THR:HB	13:C:1447:HOH:O	1.82	0.79
1:C:349[B]:THR:HG22	13:C:1447:HOH:O	1.83	0.79
2:B:283:GLY:HA3	13:B:1335:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131[B]:LYS:HE3	13:D:1477:HOH:O	1.91	0.70
1:C:593:CYS:N	7:C:607:O:O	2.26	0.67
1:A:593:CYS:N	7:A:607:O:O	2.30	0.64
2:B:16[B]:ILE:HD11	2:B:69:ILE:HG21	1.79	0.63
1:C:590:CYS:CB	7:C:606:O:O	2.47	0.62
1:A:182:ILE:HG22	13:B:1058:HOH:O	1.99	0.61
1:C:83:HIS:HD2	1:C:528:HIS:NE2	1.99	0.61
2:B:153:ILE:HD11	2:B:178[A]:ILE:HD12	1.83	0.60
1:A:556[A]:LYS:HD2	13:A:1029:HOH:O	2.01	0.60
1:C:274[A]:THR:HG22	1:C:474:GLU:OE2	2.01	0.59
2:B:72:LYS:HG2	2:B:73:TYR:CD2	2.36	0.59
1:C:511:GLU:HG2	1:C:512:HIS:CD2	2.38	0.59
1:A:590:CYS:CB	7:A:606:O:O	2.50	0.59
1:C:332:LYS:HE3	1:C:334:HIS:ND1	2.20	0.56
2:B:16[B]:ILE:HD11	2:B:69:ILE:CG2	2.35	0.56
1:C:377:SER:HB2	13:C:1378:HOH:O	2.06	0.56
1:C:593:CYS:CA	7:C:607:O:O	2.54	0.54
2:D:16:ILE:HD11	2:D:69:ILE:HG21	1.91	0.53
1:A:184:LYS:O	1:A:185:ASN:HB2	2.09	0.52
1:C:245[B]:ASP:OD1	8:C:703:GOL:O3	2.28	0.50
2:D:131[B]:LYS:HG3	13:D:1477:HOH:O	2.10	0.50
1:A:61:ARG:NH2	13:A:1538:HOH:O	2.44	0.50
1:C:243:ASN:OD1	8:C:703:GOL:H31	2.13	0.49
1:A:228:ASN:HD21	2:B:32:ARG:HH21	1.60	0.49
1:A:159:SER:HG	1:C:160[B]:SER:HB3	1.78	0.48
1:C:83:HIS:HE1	1:C:593:CYS:SG	2.37	0.47
2:B:177:ARG:NH2	13:B:1590:HOH:O	2.46	0.47
1:C:443:ARG:NH1	1:C:451:ASP:OD1	2.48	0.47
1:C:2:SER:N	13:C:654:HOH:O	2.48	0.46
2:B:136[A]:GLN:NE2	13:B:313:HOH:O	2.49	0.46
1:C:511:GLU:OE1	1:C:534:LYS:HE3	2.15	0.46
2:D:227:LYS:O	2:D:275:ARG:NH1	2.49	0.45
1:C:360:LYS:NZ	13:C:967:HOH:O	2.49	0.45
1:A:158[A]:MET:HE2	1:A:163:TYR:CZ	2.51	0.45
2:B:206:ASP:OD2	2:D:206:ASP:OD2	2.34	0.45
1:C:61[B]:ARG:NH2	13:C:1645:HOH:O	2.50	0.45
2:B:72:LYS:HG2	2:B:73:TYR:CE2	2.52	0.45
1:C:332:LYS:HE3	1:C:334:HIS:CE1	2.52	0.45
1:C:228:ASN:H	2:D:245:ASN:HD21	1.65	0.45
1:A:98:LYS:NZ	13:A:685:HOH:O	2.48	0.45
1:A:228:ASN:H	2:B:245:ASN:HD21	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:LYS:NZ	13:C:1498:HOH:O	2.50	0.45
2:D:71:GLU:OE1	2:D:74:LYS:NZ	2.50	0.44
2:B:85:PRO:HD2	2:B:138:THR:O	2.17	0.44
1:A:301:ASN:HA	1:A:325:ILE:O	2.17	0.44
2:B:171:TYR:OH	1:C:245[B]:ASP:OD2	2.28	0.44
2:B:16[A]:ILE:HD11	2:B:69:ILE:HG21	2.00	0.44
1:C:301:ASN:HA	1:C:325:ILE:O	2.17	0.44
1:C:125:HIS:HE1	1:C:207:TYR:O	1.99	0.44
1:C:349[A]:THR:HG22	1:C:350:HIS:CD2	2.52	0.44
1:A:420:TYR:OH	1:A:432:HIS:HE1	2.02	0.43
1:C:28:GLU:OE2	7:C:608:O:O	2.37	0.43
2:B:150:LYS:N	2:B:150:LYS:HD3	2.34	0.42
2:B:67:ASP:OD1	2:B:67:ASP:N	2.50	0.42
2:D:153:ILE:HD11	2:D:178[A]:ILE:HD12	2.01	0.42
1:C:3:VAL:CG1	1:C:11:LYS:HG3	2.49	0.42
1:A:245[A]:ASP:OD1	2:D:177:ARG:NH1	2.49	0.42
1:C:544[B]:VAL:HG21	1:C:593:CYS:HB3	2.01	0.41
1:A:544[A]:VAL:HG21	1:A:593:CYS:HB3	2.02	0.41
1:C:39:GLU:H	1:C:39:GLU:CD	2.23	0.41
1:C:588:ASP:N	1:C:589:PRO:HD3	2.36	0.41
2:B:194:ARG:HD2	2:B:233:PRO:O	2.21	0.41
1:C:429:THR:O	1:C:433:THR:HG23	2.21	0.41
2:D:85:PRO:HD2	2:D:138:THR:O	2.21	0.41
2:D:20:GLY:O	2:D:22[A]:GLU:HG2	2.21	0.41
1:C:547:THR:O	1:C:551[B]:SER:HB3	2.21	0.41
8:A:703:GOL:H12	13:A:1139:HOH:O	2.21	0.41
2:B:177:ARG:NH2	1:C:245[A]:ASP:OD1	2.54	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	610/596 (102%)	596 (98%)	14 (2%)	0	100	100
1	C	605/596 (102%)	594 (98%)	11 (2%)	0	100	100
2	B	278/283 (98%)	269 (97%)	9 (3%)	0	100	100
2	D	273/283 (96%)	263 (96%)	10 (4%)	0	100	100
All	All	1766/1758 (100%)	1722 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	521/505 (103%)	516 (99%)	5 (1%)	82	52
1	C	516/505 (102%)	512 (99%)	4 (1%)	86	62
2	B	232/233 (100%)	229 (99%)	3 (1%)	76	39
2	D	229/233 (98%)	226 (99%)	3 (1%)	76	39
All	All	1498/1476 (102%)	1483 (99%)	15 (1%)	82	52

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	LEU
1	A	261	PHE
1	A	360	LYS
1	A	380	LYS
1	A	450	LYS
2	B	66	LEU
2	B	150	LYS
2	B	280	ASN
1	C	11	LYS
1	C	261	PHE
1	C	360	LYS
1	C	450	LYS
2	D	74	LYS

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Mol	Chain	Res	Type
2	D	132	PRO
2	D	275	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	36	ASN
1	A	41	ASN
1	A	168	GLN
1	A	228	ASN
1	A	232	ASN
1	A	273	ASN
1	A	432	HIS
1	A	439	ASN
1	A	493	ASN
2	B	245	ASN
1	C	41	ASN
1	C	83	HIS
1	C	125	HIS
1	C	168	GLN
1	C	232	ASN
1	C	273	ASN
1	C	432	HIS
1	C	439	ASN
1	C	558	ASN
2	D	245	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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
5	CMO	A	603	-	0,1,1	0.00	-	0,0,0	0.00	-
6	CYN	A	604	-	0,1,1	0.00	-	0,0,0	0.00	-
6	CYN	A	605	-	0,1,1	0.00	-	0,0,0	0.00	-
8	GOL	A	702	-	5,5,5	0.78	0	5,5,5	4.75	4 (80%)
8	GOL	A	703	-	5,5,5	0.88	0	5,5,5	3.43	4 (80%)
10	SF3	B	301	2	0,8,8	0.00	-	0,12,12	0.00	-
11	F3S	B	308	2	0,9,9	0.00	-	0,15,15	0.00	-
12	SF4	B	309	2	0,12,12	0.00	-	0,24,24	0.00	-
5	CMO	C	603	-	0,1,1	0.00	-	0,0,0	0.00	-
6	CYN	C	604	-	0,1,1	0.00	-	0,0,0	0.00	-
6	CYN	C	605	-	0,1,1	0.00	-	0,0,0	0.00	-
8	GOL	C	702	-	5,5,5	0.54	0	5,5,5	0.89	0
8	GOL	C	703	-	5,5,5	1.23	0	5,5,5	1.99	1 (20%)
10	SF3	D	301	2	0,8,8	0.00	-	0,12,12	0.00	-
11	F3S	D	308	2	0,9,9	0.00	-	0,15,15	0.00	-
12	SF4	D	309	2	0,12,12	0.00	-	0,24,24	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
5	CMO	A	603	-	-	0/0/0/0	0/0/0/0
6	CYN	A	604	-	-	0/0/0/0	0/0/0/0
6	CYN	A	605	-	-	0/0/0/0	0/0/0/0
8	GOL	A	702	-	-	0/4/4/4	0/0/0/0
8	GOL	A	703	-	-	0/4/4/4	0/0/0/0
10	SF3	B	301	2	-	0/0/17/17	0/2/2/2
11	F3S	B	308	2	-	0/0/24/24	0/0/3/3
12	SF4	B	309	2	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CMO	C	603	-	-	0/0/0/0	0/0/0/0
6	CYN	C	604	-	-	0/0/0/0	0/0/0/0
6	CYN	C	605	-	-	0/0/0/0	0/0/0/0
8	GOL	C	702	-	-	0/4/4/4	0/0/0/0
8	GOL	C	703	-	-	0/4/4/4	0/0/0/0
10	SF3	D	301	2	-	0/0/17/17	0/2/2/2
11	F3S	D	308	2	-	0/0/24/24	0/0/3/3
12	SF4	D	309	2	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	702	GOL	C3-C2-C1	-7.18	82.96	111.12
8	A	703	GOL	C3-C2-C1	-4.88	92.00	111.12
8	A	702	GOL	O3-C3-C2	-4.60	87.87	110.18
8	A	703	GOL	O3-C3-C2	-2.90	96.13	110.18
8	A	702	GOL	O1-C1-C2	2.82	123.86	110.18
8	A	703	GOL	O2-C2-C1	3.45	124.45	108.65
8	C	703	GOL	O2-C2-C1	3.70	125.64	108.65
8	A	703	GOL	O2-C2-C3	3.71	125.67	108.65
8	A	702	GOL	O2-C2-C1	5.42	133.51	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	703	GOL	1	0
8	C	703	GOL	2	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 ⓘ

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, 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	595/596 (99%)	-0.69	2 (0%) 94 93	8, 13, 29, 48	0
1	C	595/596 (99%)	-0.59	5 (0%) 87 88	8, 16, 35, 64	0
2	B	273/283 (96%)	-0.60	6 (2%) 65 65	8, 12, 38, 66	0
2	D	267/283 (94%)	-0.58	2 (0%) 89 89	8, 14, 39, 75	0
All	All	1730/1758 (98%)	-0.63	15 (0%) 85 87	8, 14, 34, 75	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	277	THR	4.8
1	A	313	TYR	4.3
2	B	278	GLU	3.1
2	B	281	ALA	3.0
1	C	313	TYR	2.9
1	C	3	VAL	2.7
2	D	71	GLU	2.5
1	A	3	VAL	2.5
2	B	282	PHE	2.4
1	C	2	SER	2.2
2	B	183	ARG	2.2
1	C	444	LEU	2.1
1	C	448	ASN	2.1
2	B	11	PRO	2.1
2	B	283	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
7	O	A	609	1/1	0.95	0.20	17.06	9,9,9,9	1
7	O	A	610	1/1	0.99	0.21	12.74	5,5,5,5	1
8	GOL	C	702	6/6	0.85	0.16	7.45	25,27,39,44	0
8	GOL	A	702	6/6	0.92	0.14	6.25	23,25,31,35	0
7	O	C	609	1/1	0.98	0.13	6.12	8,8,8,8	1
7	O	A	607	1/1	0.86	0.13	5.86	6,6,6,6	1
7	O	C	607	1/1	0.94	0.11	3.76	9,9,9,9	1
8	GOL	C	703	6/6	0.91	0.15	3.75	22,22,28,34	0
7	O	A	608	1/1	0.97	0.10	3.66	10,10,10,10	1
7	O	C	610	1/1	0.99	0.12	3.50	8,8,8,8	1
8	GOL	A	703	6/6	0.96	0.11	3.28	20,29,34,36	0
6	CYN	A	605	2/2	0.99	0.06	2.14	8,8,8,9	0
5	CMO	C	603	2/2	0.99	0.06	1.80	10,10,10,13	0
4	3NI	A	602	1/1	0.99	0.06	1.46	15,15,15,15	0
5	CMO	A	603	2/2	0.98	0.05	1.24	8,8,8,10	0
6	CYN	C	605	2/2	0.99	0.05	0.77	10,10,10,11	0
7	O	C	608	1/1	0.98	0.07	0.51	14,14,14,14	1
4	3NI	C	602	1/1	1.00	0.06	0.47	17,17,17,17	0
7	O	C	606	1/1	0.98	0.05	0.23	14,14,14,14	0
6	CYN	C	604	2/2	0.99	0.03	-1.08	12,12,12,13	0
6	CYN	A	604	2/2	0.99	0.03	-1.47	9,9,9,9	0
12	SF4	D	309	8/8	1.00	0.03	-1.90	9,10,10,10	0
12	SF4	B	309	8/8	1.00	0.03	-1.96	9,9,9,10	0
11	F3S	D	308	7/7	1.00	0.02	-2.40	9,9,10,10	0
10	SF3	B	301	7/7	1.00	0.02	-2.72	9,9,10,16	0
10	SF3	D	301	7/7	1.00	0.02	-2.80	10,11,11,17	0
9	MG	A	701	1/1	1.00	0.02	-2.98	8,8,8,8	0
3	FE2	A	601	1/1	1.00	0.01	-3.01	9,9,9,9	0
11	F3S	B	308	7/7	1.00	0.02	-3.11	8,8,8,9	0
3	FE2	C	601	1/1	1.00	0.01	-3.35	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	MG	C	701	1/1	1.00	0.02	-3.91	11,11,11,11	0
7	O	A	606	1/1	0.97	0.07	-	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.