



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:30 AM GMT

PDB ID : 3AYX
Title : Membrane-bound respiratory [NiFe] hydrogenase from *Hydrogenovibrio marinus* in an H₂-reduced condition
Authors : Shomura, Y.; Yoon, K.S.; Nishihara, H.; Higuchi, Y.
Deposited on : 2011-05-20
Resolution : 1.18 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

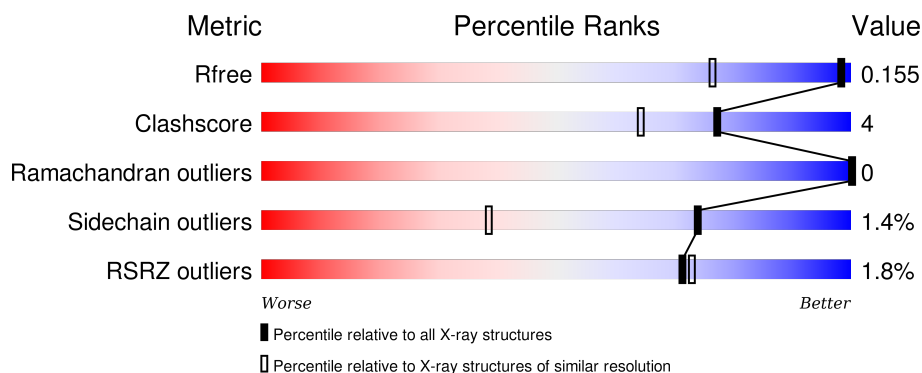
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 1.18 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	1018 (1.22-1.14)
Clashscore	102246	1094 (1.22-1.14)
Ramachandran outliers	100387	1047 (1.22-1.14)
Sidechain outliers	100360	1046 (1.22-1.14)
RSRZ outliers	91569	1020 (1.22-1.14)

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	 86% 12% •
1	C	596	 84% 13% •
2	B	283	 85% 9% • •
2	D	283	 83% 9% • 6%

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
4	NI	A	602	-	-	-	X
4	NI	C	602	-	-	-	X
7	O	A	606	-	-	-	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	606	-	-	X	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 15472 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	14	0
			4739	3008	825	880	26			
1	C	595	Total	C	N	O	S	0	14	0
			4739	3010	827	877	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
			2151	1366	366	398	21			
2	D	267	Total	C	N	O	S	0	5	0
			2092	1328	356	387	21			

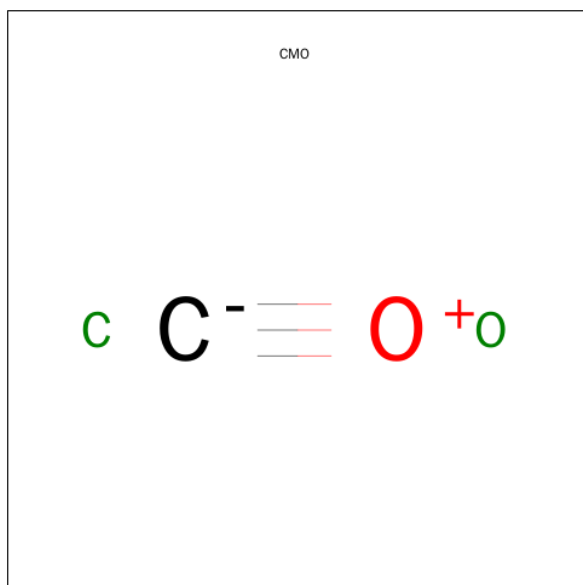
- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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 (II) ION (three-letter code: NI) (formula: Ni).

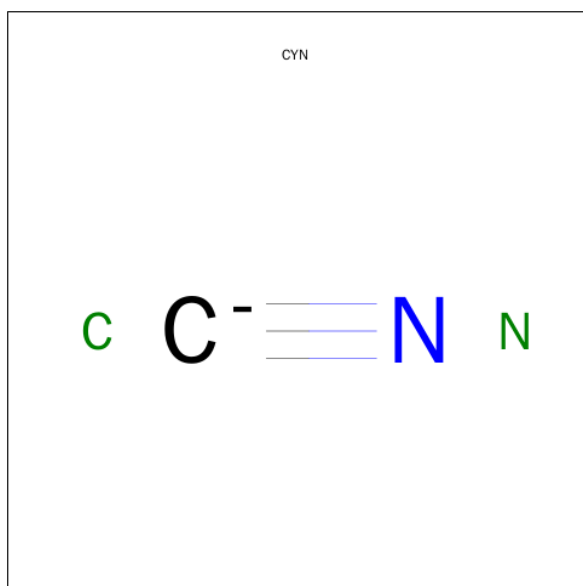
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	C	1	Total	Ni	0	0
			1	1		

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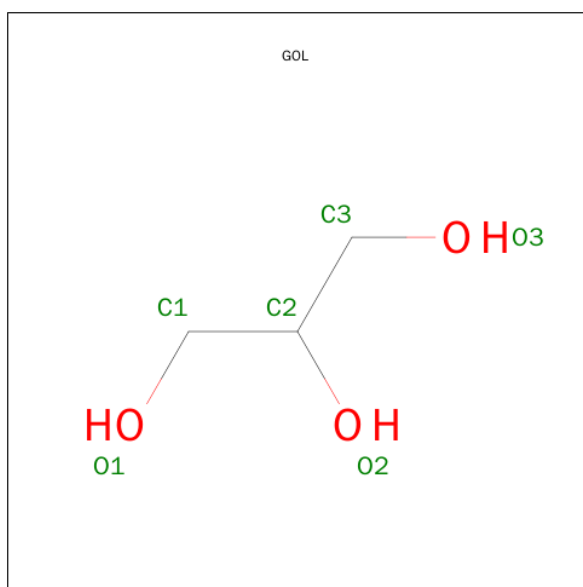
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	N	0	0
			2	1	1		
6	C	1	Total	C	N	0	0
			2	1	1		

- 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).

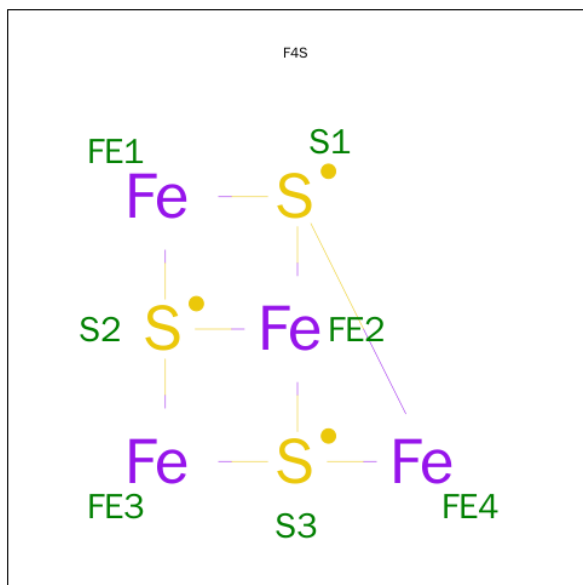


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

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

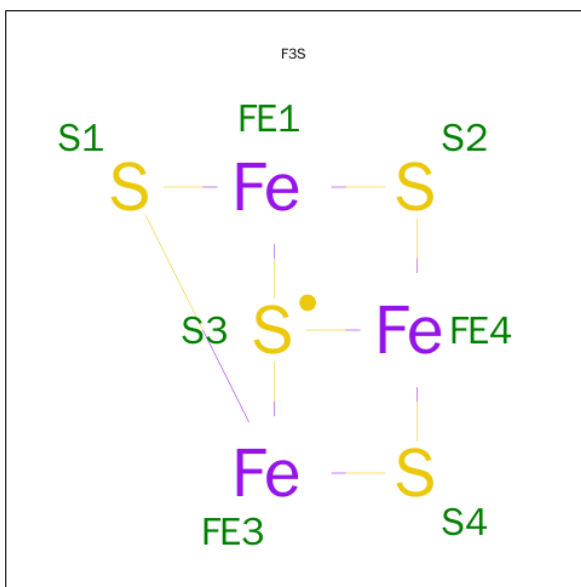
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Mg	0	0
			1	1		
9	C	1	Total	Mg	0	0
			1	1		

- Molecule 10 is FE4-S3 CLUSTER (three-letter code: F4S) (formula: Fe_4S_3).



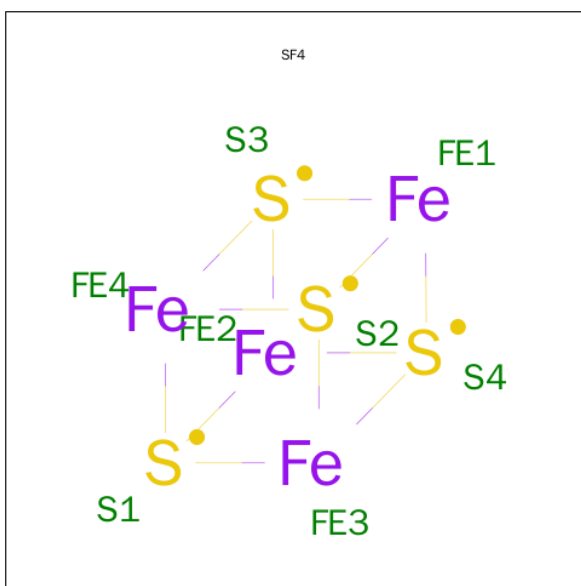
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			7	4	3		
10	D	1	Total	Fe	S	0	0
			7	4	3		

- 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		

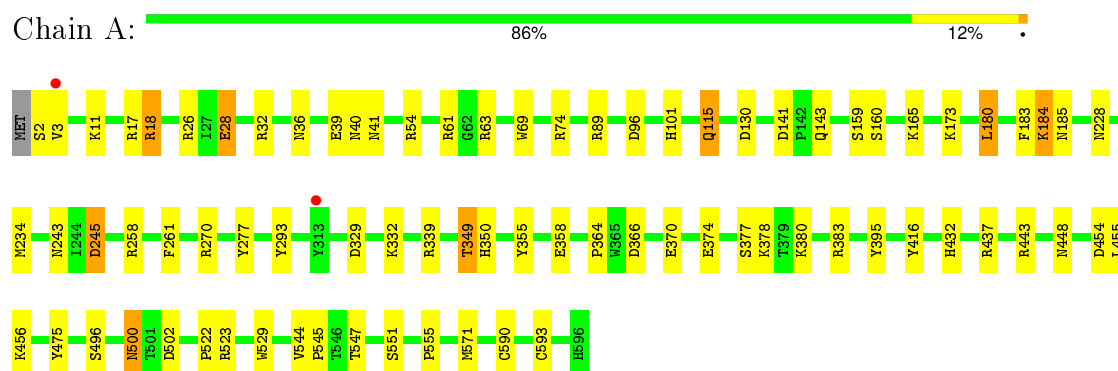
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	638	Total 638	O 638	0	0
13	B	271	Total 271	O 271	0	0
13	C	529	Total 529	O 529	0	0
13	D	217	Total 217	O 217	0	0

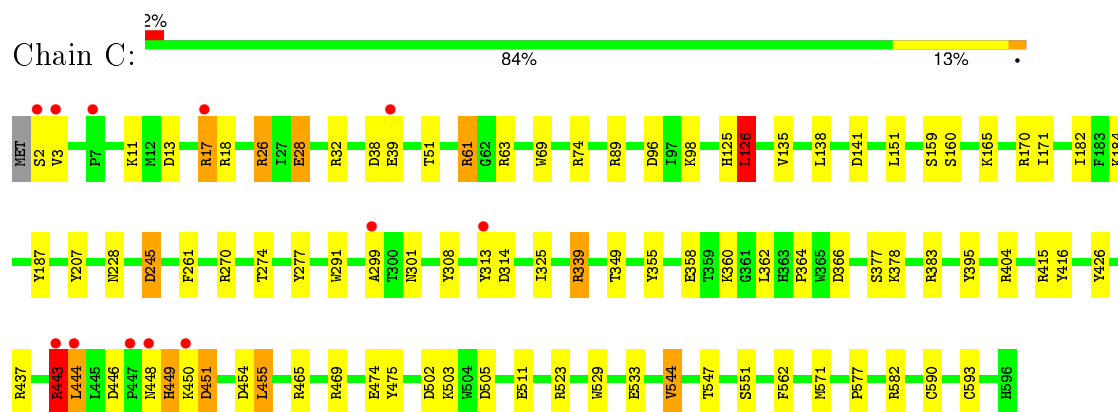
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

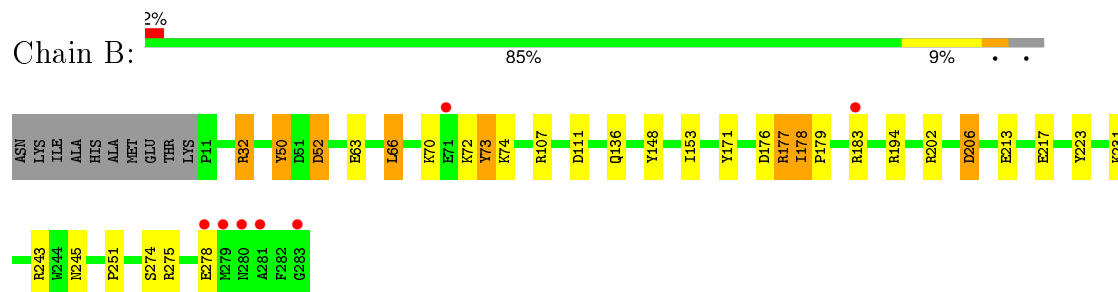
- Molecule 1: Membrane-bound hydrogenase large subunit



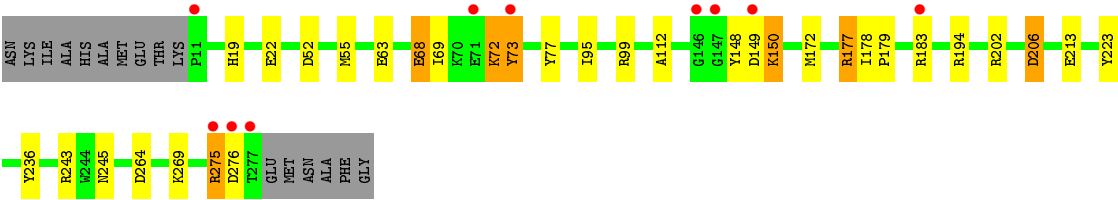
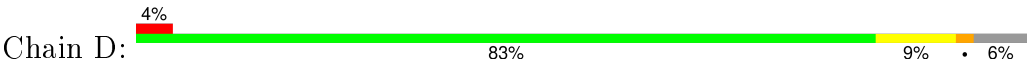
- Molecule 1: Membrane-bound hydrogenase large subunit



- 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	75.73 Å 116.33 Å 113.63 Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	20.00 – 1.18 19.96 – 1.18	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.18) 93.1 (19.96-1.18)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.18 Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.139 , 0.169 0.134 , 0.155	Depositor DCC
R_{free} test set	31752 reflections (5.81%)	DCC
Wilson B-factor (Å ²)	11.7	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.5	EDS
Estimated twinning fraction	0.007 for -h,-l,-k 0.002 for -h,l,k 0.105 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 1166292 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	15472	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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, NI, SF4, F4S, O, 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	0.97	6/4905 (0.1%)	1.45	76/6679 (1.1%)
1	C	0.95	4/4909 (0.1%)	1.56	87/6685 (1.3%)
2	B	0.94	1/2230 (0.0%)	1.49	31/3019 (1.0%)
2	D	0.93	0/2164	1.51	29/2931 (1.0%)
All	All	0.95	11/14208 (0.1%)	1.50	223/19314 (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
2	B	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	377[A]	SER	CB-OG	9.08	1.54	1.42
1	C	377[B]	SER	CB-OG	9.08	1.54	1.42
1	A	377[A]	SER	CB-OG	8.44	1.53	1.42
1	A	377[B]	SER	CB-OG	8.44	1.53	1.42
1	A	101	HIS	CB-CG	6.85	1.62	1.50
1	A	28	GLU	CD-OE1	6.49	1.32	1.25
1	C	28	GLU	CD-OE2	6.33	1.32	1.25
2	B	177	ARG	CZ-NH2	5.49	1.40	1.33
1	A	374	GLU	CD-OE1	-5.40	1.19	1.25
1	A	18	ARG	CZ-NH2	-5.13	1.26	1.33
1	C	26	ARG	CZ-NH1	5.03	1.39	1.33

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	383	ARG	NE-CZ-NH1	25.76	133.18	120.30
1	A	383	ARG	NE-CZ-NH1	-19.22	110.69	120.30
1	C	17	ARG	CD-NE-CZ	17.45	148.03	123.60
2	D	177	ARG	NE-CZ-NH1	17.22	128.91	120.30
1	A	339	ARG	NE-CZ-NH2	-16.34	112.13	120.30
1	A	245[A]	ASP	CB-CG-OD1	16.06	132.75	118.30
1	A	245[B]	ASP	CB-CG-OD1	16.06	132.75	118.30
1	A	18	ARG	NE-CZ-NH2	15.58	128.09	120.30
2	D	177	ARG	NE-CZ-NH2	-15.54	112.53	120.30
1	A	96	ASP	CB-CG-OD1	14.37	131.23	118.30
1	C	451	ASP	CB-CG-OD2	-14.14	105.58	118.30
2	B	194	ARG	NE-CZ-NH2	-13.93	113.34	120.30
1	C	505	ASP	CB-CG-OD1	13.59	130.53	118.30
2	D	275	ARG	NE-CZ-NH2	13.41	127.00	120.30
2	B	107	ARG	NE-CZ-NH2	-12.84	113.88	120.30
1	A	17	ARG	NE-CZ-NH2	-12.60	114.00	120.30
1	C	443	ARG	CD-NE-CZ	12.56	141.19	123.60
1	C	465	ARG	NE-CZ-NH1	12.56	126.58	120.30
2	B	177	ARG	CD-NE-CZ	11.99	140.39	123.60
2	D	202	ARG	NE-CZ-NH2	11.77	126.19	120.30
1	C	61[A]	ARG	NE-CZ-NH1	-11.66	114.47	120.30
1	C	61[B]	ARG	NE-CZ-NH1	-11.66	114.47	120.30
1	C	443	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	A	437	ARG	NE-CZ-NH1	-11.53	114.53	120.30
1	C	69	TRP	CZ3-CH2-CZ2	10.75	134.50	121.60
1	C	383	ARG	NE-CZ-NH2	-10.73	114.94	120.30
1	C	451	ASP	CB-CG-OD1	10.57	127.81	118.30
1	A	355	TYR	CB-CG-CD1	10.50	127.30	121.00
1	C	339	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	C	313	TYR	CB-CG-CD2	10.33	127.20	121.00
1	C	170	ARG	NE-CZ-NH2	-10.27	115.16	120.30
1	C	141	ASP	CB-CG-OD2	10.21	127.49	118.30
1	A	17	ARG	NE-CZ-NH1	9.91	125.26	120.30
2	D	206	ASP	CB-CG-OD2	-9.83	109.46	118.30
1	C	449	HIS	ND1-CE1-NE2	9.78	131.41	109.90
1	C	17	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	C	544[A]	VAL	CA-CB-CG1	9.26	124.78	110.90
1	C	544[B]	VAL	CA-CB-CG1	9.26	124.78	110.90
1	C	32	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	C	38	ASP	CB-CG-OD2	-8.99	110.21	118.30
1	C	69	TRP	CE3-CZ3-CH2	-8.97	111.33	121.20
1	A	270	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	C	270	ARG	NE-CZ-NH1	8.88	124.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASP	CB-CG-OD2	8.83	126.25	118.30
1	A	28	GLU	CG-CD-OE2	8.70	135.70	118.30
1	C	562	PHE	CB-CG-CD1	8.63	126.84	120.80
1	A	443	ARG	NE-CZ-NH1	-8.57	116.01	120.30
2	B	202	ARG	NE-CZ-NH2	-8.46	116.07	120.30
2	D	68	GLU	CA-CB-CG	8.46	132.01	113.40
1	A	366	ASP	CB-CG-OD1	-8.43	110.71	118.30
1	A	437	ARG	NH1-CZ-NH2	8.42	128.66	119.40
1	C	449	HIS	CG-ND1-CE1	-8.34	94.85	105.70
1	C	141	ASP	CB-CG-OD1	-8.34	110.80	118.30
1	C	582	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	C	358	GLU	OE1-CD-OE2	8.23	133.17	123.30
1	C	426	TYR	CB-CG-CD2	8.19	125.92	121.00
1	C	18	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	C	28	GLU	CG-CD-OE1	8.08	134.46	118.30
1	C	314	ASP	CB-CG-OD2	8.07	125.56	118.30
1	A	28	GLU	OE1-CD-OE2	-8.04	113.66	123.30
1	C	469	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	C	26	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	A	358	GLU	OE1-CD-OE2	7.80	132.66	123.30
2	B	73	TYR	CG-CD2-CE2	7.75	127.50	121.30
1	C	404	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	C	358	GLU	CG-CD-OE2	-7.67	102.95	118.30
1	C	465	ARG	NE-CZ-NH2	-7.65	116.47	120.30
2	D	194	ARG	NE-CZ-NH2	-7.61	116.50	120.30
2	B	183[A]	ARG	NE-CZ-NH2	7.59	124.10	120.30
2	B	183[B]	ARG	NE-CZ-NH2	7.59	124.10	120.30
1	A	69	TRP	CZ3-CH2-CZ2	7.58	130.69	121.60
1	C	582	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	245[A]	ASP	CA-CB-CG	-7.37	97.18	113.40
1	A	245[B]	ASP	CA-CB-CG	-7.37	97.18	113.40
1	C	426	TYR	CB-CG-CD1	-7.34	116.60	121.00
1	C	469	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	329	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	18	ARG	NH1-CZ-NH2	-7.29	111.38	119.40
1	A	380	LYS	CA-CB-CG	7.25	129.34	113.40
2	B	52	ASP	CB-CG-OD2	7.15	124.74	118.30
1	A	500	ASN	CA-CB-CG	7.11	129.05	113.40
2	B	275	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	26	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	C	355	TYR	CB-CG-CD1	7.07	125.24	121.00
1	A	339	ARG	NE-CZ-NH1	7.02	123.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	C	415	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	370	GLU	OE1-CD-OE2	6.95	131.64	123.30
1	C	28	GLU	OE1-CD-OE2	-6.95	114.96	123.30
1	C	533	GLU	OE1-CD-OE2	6.94	131.62	123.30
1	C	69	TRP	CH2-CZ2-CE2	-6.93	110.47	117.40
2	D	236	TYR	CB-CG-CD2	6.91	125.15	121.00
2	B	243	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	383	ARG	NH1-CZ-NH2	6.89	126.98	119.40
1	C	383	ARG	NH1-CZ-NH2	-6.84	111.87	119.40
1	A	258	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	A	454	ASP	CB-CG-OD1	6.83	124.45	118.30
1	C	562	PHE	CB-CG-CD2	-6.83	116.02	120.80
2	B	243	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	293	TYR	CB-CG-CD2	6.73	125.04	121.00
2	B	213	GLU	OE1-CD-OE2	6.73	131.37	123.30
2	B	206	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	C	32	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	C	502	ASP	CB-CG-OD2	6.68	124.31	118.30
2	B	194	ARG	NH1-CZ-NH2	6.67	126.73	119.40
2	D	194	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	A	184	LYS	CA-CB-CG	6.60	127.91	113.40
1	C	454	ASP	CB-CG-OD2	-6.59	112.37	118.30
2	D	202	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	C	313	TYR	CB-CG-CD1	-6.59	117.05	121.00
1	C	245[A]	ASP	CB-CG-OD1	6.58	124.22	118.30
1	C	245[B]	ASP	CB-CG-OD1	6.58	124.22	118.30
1	C	13	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	96	ASP	CB-CG-OD2	-6.58	112.38	118.30
2	B	176	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	332	LYS	CB-CG-CD	6.57	128.67	111.60
1	A	475	TYR	CB-CG-CD1	6.56	124.94	121.00
2	D	52	ASP	CB-CG-OD1	-6.54	112.41	118.30
1	A	245[A]	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	245[B]	ASP	CB-CG-OD2	-6.53	112.42	118.30
2	B	223	TYR	CB-CG-CD1	6.51	124.90	121.00
1	C	475	TYR	CB-CG-CD1	6.48	124.89	121.00
2	D	194	ARG	NH1-CZ-NH2	6.46	126.50	119.40
1	A	277	TYR	CB-CG-CD1	6.44	124.87	121.00
2	D	223	TYR	CB-CG-CD1	6.43	124.86	121.00
1	C	61[A]	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	C	61[B]	ARG	NE-CZ-NH2	6.42	123.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	223	TYR	CB-CG-CD2	-6.39	117.17	121.00
2	B	217	GLU	OE1-CD-OE2	-6.38	115.64	123.30
1	C	395	TYR	CA-CB-CG	6.38	125.53	113.40
2	D	236	TYR	CB-CG-CD1	-6.38	117.17	121.00
2	D	264	ASP	CB-CG-OD1	6.34	124.00	118.30
1	A	416	TYR	CD1-CE1-CZ	6.31	125.48	119.80
2	B	171	TYR	CB-CG-CD2	6.28	124.77	121.00
1	C	455	LEU	CA-CB-CG	6.26	129.71	115.30
2	D	275	ARG	O-C-N	6.26	132.72	122.70
1	A	383	ARG	CD-NE-CZ	6.24	132.34	123.60
1	A	63	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	C	74	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	C	443	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	63	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	355	TYR	CB-CG-CD2	-6.14	117.31	121.00
2	D	63	GLU	OE1-CD-OE2	6.13	130.66	123.30
1	C	26	ARG	NH1-CZ-NH2	-6.10	112.69	119.40
1	C	13	ASP	CB-CG-OD1	6.05	123.74	118.30
1	A	502	ASP	CB-CG-OD1	6.01	123.71	118.30
1	C	416	TYR	CA-CB-CG	-5.95	102.10	113.40
2	D	148	TYR	CB-CG-CD2	5.94	124.56	121.00
2	D	149	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	349[A]	THR	OG1-CB-CG2	5.93	123.63	110.00
1	A	349[B]	THR	OG1-CB-CG2	5.93	123.63	110.00
1	C	308	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	A	61	ARG	NE-CZ-NH2	5.88	123.24	120.30
2	D	99	ARG	CD-NE-CZ	5.86	131.80	123.60
1	C	38	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	234[A]	MET	CA-CB-CG	-5.82	103.40	113.30
1	A	234[B]	MET	CA-CB-CG	-5.82	103.40	113.30
2	B	111	ASP	CB-CG-OD2	-5.81	113.07	118.30
2	B	278	GLU	CA-C-O	5.79	132.25	120.10
2	B	50	TYR	CD1-CE1-CZ	5.77	124.99	119.80
1	C	291	TRP	CD1-CG-CD2	-5.75	101.70	106.30
1	A	89	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	180	LEU	CB-CG-CD2	5.73	120.75	111.00
2	B	107	ARG	CA-CB-CG	5.70	125.94	113.40
2	D	177	ARG	CA-CB-CG	-5.65	100.96	113.40
2	D	275	ARG	NE-CZ-NH1	-5.65	117.48	120.30
1	C	377[A]	SER	CB-CA-C	5.64	120.81	110.10
1	C	377[B]	SER	CB-CA-C	5.64	120.81	110.10
1	A	173	LYS	CA-CB-CG	5.63	125.78	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	50	TYR	CG-CD1-CE1	-5.58	116.83	121.30
1	C	299	ALA	N-CA-CB	-5.55	102.33	110.10
1	A	358	GLU	CG-CD-OE2	-5.53	107.25	118.30
1	C	126[A]	LEU	CB-CG-CD2	5.49	120.34	111.00
1	C	126[B]	LEU	CB-CG-CD2	5.49	120.34	111.00
1	A	500	ASN	CB-CG-OD1	5.49	132.57	121.60
1	C	26	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	A	130	ASP	CB-CG-OD1	5.44	123.19	118.30
2	B	148	TYR	CG-CD2-CE2	-5.44	116.95	121.30
1	A	32	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	475	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	A	69	TRP	CE3-CZ3-CH2	-5.36	115.31	121.20
1	A	141	ASP	CB-CG-OD1	-5.35	113.49	118.30
1	A	448	ASN	CB-CG-ND2	-5.34	103.88	116.70
2	D	276	ASP	C-N-CA	-5.33	108.37	121.70
2	D	243	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	377[A]	SER	CB-CA-C	5.31	120.19	110.10
1	A	377[B]	SER	CB-CA-C	5.31	120.19	110.10
1	A	432	HIS	CA-CB-CG	-5.29	104.60	113.60
2	D	183	ARG	CD-NE-CZ	5.29	131.01	123.60
1	A	183	PHE	CG-CD2-CE2	5.29	126.62	120.80
1	A	183	PHE	CZ-CE2-CD2	-5.28	113.76	120.10
1	A	571	MET	CG-SD-CE	-5.27	91.77	100.20
2	B	206	ASP	CB-CG-OD1	5.27	123.04	118.30
2	D	213	GLU	OE1-CD-OE2	5.27	129.62	123.30
2	B	274	SER	O-C-N	-5.26	114.28	122.70
1	C	245[A]	ASP	OD1-CG-OD2	-5.22	113.37	123.30
1	C	245[B]	ASP	OD1-CG-OD2	-5.22	113.37	123.30
1	C	511	GLU	OE1-CD-OE2	5.22	129.57	123.30
1	A	443	ARG	NE-CZ-NH2	5.22	122.91	120.30
2	B	176	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	366	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	39	GLU	CG-CD-OE1	5.21	128.72	118.30
1	A	54	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	B	178[A]	ILE	CA-CB-CG1	5.20	120.87	111.00
2	B	178[B]	ILE	CA-CB-CG1	5.20	120.87	111.00
1	C	89	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	245[A]	ASP	OD1-CG-OD2	-5.16	113.51	123.30
1	A	245[B]	ASP	OD1-CG-OD2	-5.16	113.51	123.30
1	A	395	TYR	CA-CB-CG	5.14	123.17	113.40
1	C	135	VAL	CA-C-O	5.13	130.88	120.10
1	A	74	ARG	NE-CZ-NH2	-5.13	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	277	TYR	CB-CG-CD1	5.12	124.08	121.00
2	B	202	ARG	NH1-CZ-NH2	5.12	125.03	119.40
1	C	135	VAL	O-C-N	-5.09	114.55	122.70
1	C	454	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	571	MET	CG-SD-CE	-5.08	92.08	100.20
1	C	437	ARG	CD-NE-CZ	5.07	130.70	123.60
2	D	269	LYS	CA-C-N	5.07	126.34	116.20
1	C	170	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	D	77	TYR	CB-CG-CD2	5.06	124.03	121.00
1	A	378	LYS	CD-CE-NZ	-5.03	100.14	111.70
1	A	28	GLU	CG-CD-OE1	-5.03	108.25	118.30
2	D	73	TYR	CB-CG-CD2	5.02	124.01	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	32	ARG	Sidechain

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	4739	0	4657	34	0
1	C	4739	0	4663	51	0
2	B	2151	0	2091	11	0
2	D	2092	0	2032	12	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	1	0
6	C	4	0	0	0	0
7	A	5	0	0	4	0
7	C	5	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	12	0	15	4	0
8	C	12	0	15	1	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	638	0	0	8	0
13	B	271	0	0	2	0
13	C	529	0	0	13	0
13	D	217	0	0	2	0
All	All	15472	0	13473	100	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 4.

All (100) 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:590:CYS:CB	7:A:606:O:O	2.09	0.99
1:C:590:CYS:CB	7:C:606:O:O	2.08	0.97
1:C:151[A]:LEU:HD11	1:C:444:LEU:HD23	1.64	0.78
1:C:274[A]:THR:HG22	1:C:474:GLU:OE2	1.86	0.75
8:A:703:GOL:H32	13:A:1420:HOH:O	1.88	0.74
2:B:136:GLN:HG2	13:B:1448:HOH:O	1.88	0.73
1:A:544[B]:VAL:HG11	1:A:593:CYS:HB3	1.77	0.67
1:A:349[A]:THR:HB	13:A:1347:HOH:O	1.95	0.66
1:A:544[A]:VAL:HG21	1:A:593:CYS:HB3	1.78	0.66
1:A:547:THR:O	1:A:551[B]:SER:HB3	1.96	0.64
1:C:593:CYS:N	7:C:607:O:O	2.29	0.64
1:A:593:CYS:N	7:A:607:O:O	2.29	0.63
1:C:138:LEU:HD21	1:C:171[A]:ILE:HG22	1.81	0.63
1:C:593:CYS:CB	7:C:607:O:O	2.49	0.61
1:C:544[A]:VAL:HG11	1:C:593:CYS:HB3	1.83	0.61
1:A:593:CYS:CB	7:A:607:O:O	2.48	0.61
1:C:349:THR:HB	13:C:1385:HOH:O	2.00	0.61
1:A:228:ASN:HD21	2:B:32:ARG:HH21	1.49	0.61
2:B:72:LYS:HG2	2:B:73:TYR:CE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544[B]:VAL:HG11	1:C:593:CYS:HB3	1.86	0.58
1:A:3:VAL:HG11	1:A:11:LYS:HE2	1.85	0.58
1:C:444:LEU:HD13	13:C:1576:HOH:O	2.04	0.57
1:A:184:LYS:HE2	13:A:1043:HOH:O	2.05	0.56
1:C:544[A]:VAL:CG1	1:C:593:CYS:HB3	2.36	0.55
2:B:63[A]:GLU:HG2	13:B:350:HOH:O	2.07	0.55
2:B:206:ASP:OD2	2:D:206:ASP:OD2	2.24	0.55
1:C:449:HIS:HD2	13:C:1327:HOH:O	1.90	0.55
1:A:544[B]:VAL:CG1	1:A:593:CYS:HB3	2.37	0.54
1:C:228:ASN:H	2:D:245:ASN:HD21	1.56	0.54
2:D:68:GLU:O	2:D:72:LYS:HB2	2.07	0.54
1:A:228:ASN:H	2:B:245:ASN:HD21	1.57	0.53
1:C:26:ARG:O	1:C:126[B]:LEU:HD13	2.07	0.53
1:C:184:LYS:HZ3	2:D:69:ILE:HD11	1.74	0.53
1:C:28:GLU:OE2	7:C:608:O:O	2.27	0.53
2:D:72:LYS:HE2	2:D:73:TYR:CZ	2.45	0.52
2:D:172[B]:MET:HG2	2:D:177:ARG:O	2.09	0.52
1:C:182:ILE:HG22	13:D:1323:HOH:O	2.11	0.51
1:A:243:ASN:OD1	8:A:703:GOL:H12	2.11	0.50
1:C:590:CYS:HB2	7:C:606:O:O	1.96	0.50
1:A:245[A]:ASP:OD1	8:A:703:GOL:O1	2.31	0.48
1:C:138:LEU:HD21	1:C:171[A]:ILE:CG2	2.42	0.48
2:D:72:LYS:HE2	2:D:73:TYR:CE2	2.49	0.48
1:C:182:ILE:HG23	13:C:920:HOH:O	2.12	0.48
1:A:523:ARG:CD	1:A:590:CYS:HB2	2.43	0.48
1:A:159:SER:HG	1:C:160[B]:SER:HB3	1.79	0.47
1:C:61[B]:ARG:NH2	13:C:1247:HOH:O	2.47	0.47
2:B:177:ARG:NH1	1:C:245[B]:ASP:OD2	2.47	0.47
1:C:378:LYS:HE2	13:C:928:HOH:O	2.12	0.47
1:A:143[B]:GLN:HG2	13:A:1437:HOH:O	2.14	0.47
1:C:523:ARG:CD	1:C:590:CYS:HB2	2.45	0.46
1:C:61[A]:ARG:NH1	13:C:1633:HOH:O	2.49	0.46
1:C:125:HIS:HE1	1:C:207:TYR:O	1.97	0.46
1:A:160[B]:SER:HB3	1:C:159:SER:HG	1.79	0.46
1:C:503:LYS:NZ	13:C:1582:HOH:O	2.49	0.45
1:A:456:LYS:HD3	13:A:1487:HOH:O	2.16	0.45
1:C:61[B]:ARG:NH2	13:C:780:HOH:O	2.46	0.45
1:C:360:LYS:HE2	1:C:362:LEU:HD23	1.97	0.45
1:A:40:ASN:O	1:A:41:ASN:HB2	2.16	0.45
1:A:28:GLU:OE1	7:A:608:O:O	2.35	0.45
1:A:2:SER:N	13:A:1548:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:LYS:HG2	2:B:73:TYR:CD2	2.51	0.45
1:A:165:LYS:HE3	13:A:888:HOH:O	2.17	0.45
2:B:50:TYR:CD1	2:B:66[A]:LEU:HD13	2.52	0.44
1:C:544[B]:VAL:HG12	1:C:547:THR:H	1.82	0.44
1:C:339:ARG:HD3	13:C:689:HOH:O	2.17	0.44
1:A:349[B]:THR:OG1	1:A:555:PRO:HG3	2.18	0.44
1:A:544[B]:VAL:HG12	1:A:545:PRO:HD2	2.00	0.44
1:C:593:CYS:HB2	7:C:607:O:O	2.16	0.44
2:D:55:MET:HB2	13:D:1199:HOH:O	2.18	0.44
2:D:112:ALA:O	2:D:150:LYS:HE3	2.17	0.43
1:C:151[A]:LEU:HD21	1:C:444:LEU:HD21	2.00	0.43
1:C:2:SER:N	13:C:1026:HOH:O	2.50	0.43
1:C:26:ARG:HA	1:C:126[B]:LEU:HD22	2.00	0.43
1:C:443:ARG:NH2	1:C:451:ASP:OD1	2.48	0.43
1:C:51:THR:HB	2:D:95:ILE:HB	1.99	0.43
1:A:115:GLN:NE2	1:A:522:PRO:HA	2.33	0.43
1:C:245[A]:ASP:OD1	8:C:703:GOL:O1	2.34	0.43
1:A:364:PRO:HB2	1:A:529:TRP:CD2	2.53	0.43
1:C:26:ARG:CA	1:C:126[B]:LEU:HD22	2.49	0.42
1:A:455:LEU:HA	1:A:455:LEU:HD23	1.83	0.42
2:D:19:HIS:HD1	2:D:22[B]:GLU:CD	2.21	0.42
1:C:446:ASP:OD1	1:C:448:ASN:HB2	2.19	0.42
1:C:96:ASP:OD1	1:C:98:LYS:NZ	2.48	0.42
1:C:39:GLU:H	1:C:39:GLU:CD	2.22	0.42
1:C:547:THR:O	1:C:551[B]:SER:HB3	2.20	0.42
1:A:496:SER:CB	8:A:703:GOL:H31	2.50	0.42
1:C:3:VAL:HG13	1:C:11:LYS:HG3	2.02	0.42
1:A:593:CYS:CB	6:A:605:CYN:C	2.98	0.42
1:A:349[A]:THR:HG22	1:A:350:HIS:CD2	2.55	0.41
1:C:184:LYS:NZ	13:C:1322:HOH:O	2.53	0.41
1:C:165:LYS:HD3	13:C:1196:HOH:O	2.20	0.41
2:B:153:ILE:HD11	2:B:178[B]:ILE:HG23	2.02	0.41
1:A:544[A]:VAL:HG22	1:A:547:THR:OG1	2.20	0.41
1:C:364:PRO:HB2	1:C:529:TRP:CD2	2.56	0.41
1:C:301:ASN:HA	1:C:325:ILE:O	2.21	0.41
1:A:185:ASN:ND2	13:A:1090:HOH:O	2.54	0.41
1:A:18:ARG:HH21	1:A:36:ASN:HD21	1.68	0.40
2:B:178[B]:ILE:HG23	2:B:179:PRO:HD2	2.03	0.40
2:D:178[B]:ILE:HG23	2:D:179:PRO:HD2	2.02	0.40
1:C:187:TYR:CE2	1:C:577:PRO:HD2	2.57	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	607/596 (102%)	596 (98%)	11 (2%)	0	100	100
1	C	607/596 (102%)	597 (98%)	10 (2%)	0	100	100
2	B	278/283 (98%)	269 (97%)	9 (3%)	0	100	100
2	D	270/283 (95%)	259 (96%)	11 (4%)	0	100	100
All	All	1762/1758 (100%)	1721 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	518/505 (103%)	514 (99%)	4 (1%)	86	62
1	C	518/505 (103%)	510 (98%)	8 (2%)	72	36
2	B	232/233 (100%)	225 (97%)	7 (3%)	48	9
2	D	226/233 (97%)	223 (99%)	3 (1%)	76	41
All	All	1494/1476 (101%)	1472 (98%)	22 (2%)	74	36

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	180	LEU

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Mol	Chain	Res	Type
1	A	261	PHE
1	A	500	ASN
2	B	52	ASP
2	B	66[A]	LEU
2	B	66[B]	LEU
2	B	70	LYS
2	B	74	LYS
2	B	231	LYS
2	B	251	PRO
1	C	17	ARG
1	C	126[A]	LEU
1	C	126[B]	LEU
1	C	261	PHE
1	C	443	ARG
1	C	444	LEU
1	C	450	LYS
1	C	455	LEU
2	D	72	LYS
2	D	150	LYS
2	D	275	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	36	ASN
1	A	115	GLN
1	A	168	GLN
1	A	185	ASN
1	A	228	ASN
1	A	232	ASN
1	A	273	ASN
1	A	432	HIS
1	A	439	ASN
1	A	493	ASN
1	A	500	ASN
2	B	245	ASN
1	C	41	ASN
1	C	125	HIS
1	C	168	GLN
1	C	232	ASN
1	C	273	ASN

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Mol	Chain	Res	Type
1	C	432	HIS
1	C	439	ASN
1	C	449	HIS
1	C	558	ASN
2	D	245	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0.85	0	5,5,5	1.92	1 (20%)
8	GOL	A	703	-	5,5,5	0.93	0	5,5,5	2.88	2 (40%)
10	F4S	B	301	2	0,9,9	0.00	-	0,15,15	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	0.56	0	5,5,5	1.45	1 (20%)
8	GOL	C	703	-	5,5,5	1.26	0	5,5,5	5.08	4 (80%)
10	F4S	D	301	2	0,9,9	0.00	-	0,15,15	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	F4S	B	301	2	-	0/0/24/24	0/0/3/3
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
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	F4S	D	301	2	-	0/0/24/24	0/0/3/3
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 (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	703	GOL	C3-C2-C1	-6.20	86.82	111.12
8	C	703	GOL	O1-C1-C2	-5.02	85.86	110.18
8	A	702	GOL	O1-C1-C2	-3.20	94.65	110.18
8	A	703	GOL	O1-C1-C2	-3.20	94.67	110.18
8	C	702	GOL	C3-C2-C1	-2.67	100.66	111.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	703	GOL	O2-C2-C1	4.74	130.41	108.65
8	A	703	GOL	O2-C2-C1	5.44	133.57	108.65
8	C	703	GOL	O2-C2-C3	6.53	138.61	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	605	CYN	1	0
8	A	703	GOL	4	0
8	C	703	GOL	1	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%)	-0.29	2 (0%) 94 93	7, 12, 27, 49	0
1	C	595/596 (99%)	-0.17	12 (2%) 68 69	7, 15, 34, 61	0
2	B	273/283 (96%)	-0.19	7 (2%) 59 59	7, 11, 32, 53	0
2	D	267/283 (94%)	-0.11	10 (3%) 45 44	8, 13, 39, 71	0
All	All	1730/1758 (98%)	-0.21	31 (1%) 71 73	7, 13, 32, 71	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	277	THR	8.0
1	A	313	TYR	4.7
1	C	448	ASN	4.5
1	C	313	TYR	4.2
2	B	281	ALA	4.2
2	D	276	ASP	3.7
2	B	283	GLY	3.7
2	B	183[A]	ARG	3.4
2	B	278	GLU	3.0
1	C	39	GLU	2.6
2	D	147	GLY	2.6
2	B	280	ASN	2.6
2	B	71	GLU	2.6
1	C	450	LYS	2.6
1	C	443	ARG	2.5
2	B	279	MET	2.5
2	D	183	ARG	2.5
2	D	275	ARG	2.5
2	D	146	GLY	2.5
2	D	71	GLU	2.5
1	C	3	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	11	PRO	2.4
2	D	73	TYR	2.3
1	A	3	VAL	2.2
1	C	447	PRO	2.2
1	C	299	ALA	2.1
1	C	7	PRO	2.1
2	D	149	ASP	2.1
1	C	2	SER	2.1
1	C	17	ARG	2.0
1	C	444	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	0.43	24.20	7,7,7,7	1
7	O	C	606	1/1	0.97	0.12	13.58	11,11,11,11	1
7	O	A	610	1/1	0.98	0.29	8.60	8,8,8,8	1
7	O	C	609	1/1	0.97	0.14	8.07	8,8,8,8	1
7	O	A	606	1/1	0.88	0.15	6.26	11,11,11,11	1
4	NI	C	602	1/1	1.00	0.09	5.06	14,14,14,14	0
7	O	A	607	1/1	0.88	0.15	3.30	8,8,8,8	1
7	O	C	610	1/1	0.99	0.15	3.13	8,8,8,8	1
7	O	C	607	1/1	0.90	0.15	3.01	9,9,9,9	1
8	GOL	C	703	6/6	0.92	0.13	2.91	19,28,33,39	0
7	O	A	608	1/1	0.96	0.15	2.88	12,12,12,12	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NI	A	602	1/1	1.00	0.10	2.53	12,12,12,12	0
8	GOL	A	702	6/6	0.94	0.09	2.39	21,24,27,41	0
8	GOL	C	702	6/6	0.91	0.10	2.35	23,26,30,39	0
8	GOL	A	703	6/6	0.92	0.12	1.98	19,32,37,42	0
7	O	C	608	1/1	0.96	0.10	0.95	11,11,11,11	1
6	CYN	A	605	2/2	0.98	0.06	0.03	8,8,8,9	0
5	CMO	C	603	2/2	1.00	0.05	-0.49	10,10,10,11	0
5	CMO	A	603	2/2	0.99	0.04	-0.90	7,7,7,10	0
6	CYN	C	605	2/2	0.99	0.04	-1.03	9,9,9,10	0
6	CYN	A	604	2/2	0.99	0.04	-1.12	7,7,7,8	0
9	MG	C	701	1/1	1.00	0.04	-1.58	10,10,10,10	0
3	FE2	C	601	1/1	1.00	0.02	-1.61	10,10,10,10	0
3	FE2	A	601	1/1	1.00	0.02	-1.82	8,8,8,8	0
11	F3S	D	308	7/7	1.00	0.03	-2.02	8,8,8,8	0
9	MG	A	701	1/1	1.00	0.03	-2.30	7,7,7,7	0
12	SF4	D	309	8/8	1.00	0.03	-2.33	8,9,9,9	0
12	SF4	B	309	8/8	1.00	0.03	-2.37	8,8,8,8	0
6	CYN	C	604	2/2	0.99	0.03	-2.55	9,9,9,11	0
11	F3S	B	308	7/7	1.00	0.02	-2.70	7,7,7,7	0
10	F4S	B	301	7/7	1.00	0.02	-3.14	7,7,8,8	0
10	F4S	D	301	7/7	1.00	0.02	-3.58	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.