



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 07:18 am BST

PDB ID : 3MYR
Title : Crystal structure of [NiFe] hydrogenase from *Allochromatium vinosum* in its Ni-A state
Authors : Ogata, H.; Kellers, P.; Lubitz, W.
Deposited on : 2010-05-11
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

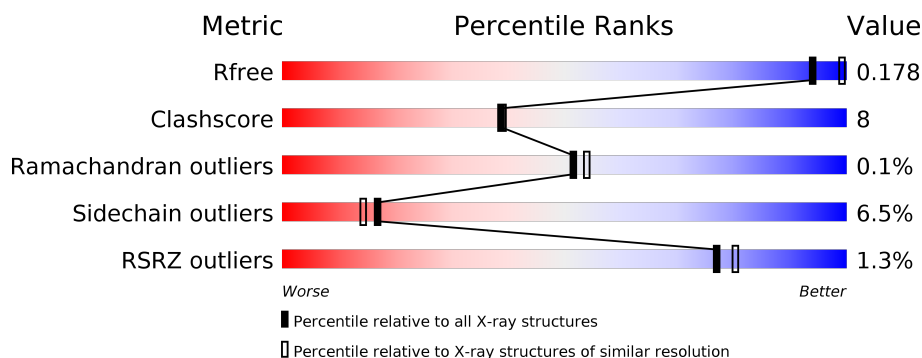
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



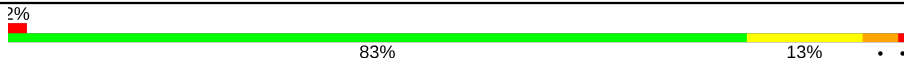

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	269	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>••</div> </div> </div>
1	C	269	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>•</div> </div> </div>
1	E	269	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>
1	G	269	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>••</div> </div> </div>
2	B	561	<div> <div></div> <div> <div>85%</div> <div>12%</div> <div>•</div> </div> </div>
2	D	561	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>•</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	561	 2% 83% 13% . .
2	H	561	 82% 13% . .

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
7	NFV	B	2005	-	-	X	-
7	NFV	D	2005	-	-	X	-
7	NFV	F	2005	-	-	X	-
7	NFV	H	2005	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 27720 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.

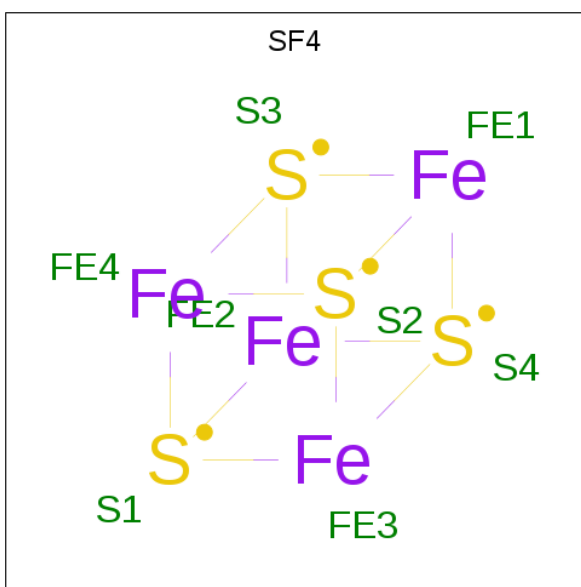
- Molecule 1 is a protein called Hydrogenase (NiFe) small subunit HydA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2038	1293	348	381	16			
1	C	269	Total	C	N	O	S	0	0	0
			2047	1299	349	383	16			
1	E	268	Total	C	N	O	S	0	0	0
			2038	1293	348	381	16			
1	G	268	Total	C	N	O	S	0	0	0
			2038	1293	348	381	16			

- Molecule 2 is a protein called Nickel-dependent hydrogenase large subunit.

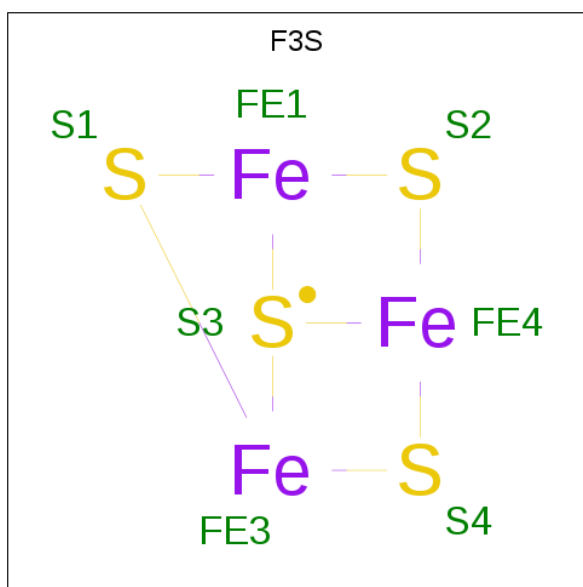
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	559	Total	C	N	O	S	0	0	0
			4363	2765	773	811	14			
2	D	561	Total	C	N	O	S	0	0	0
			4377	2773	775	814	15			
2	F	561	Total	C	N	O	S	0	0	0
			4377	2773	775	814	15			
2	H	559	Total	C	N	O	S	0	0	0
			4363	2765	773	811	14			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



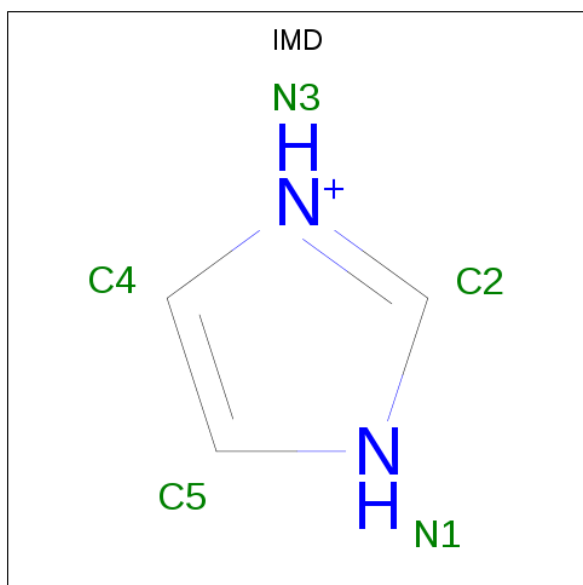
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	1
			10	5	5		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	1
			10	5	5		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	1
			10	5	5		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	1
			10	5	5		
3	G	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			7	3	4		
4	C	1	Total	Fe	S	0	0
			7	3	4		
4	E	1	Total	Fe	S	0	0
			7	3	4		
4	G	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).

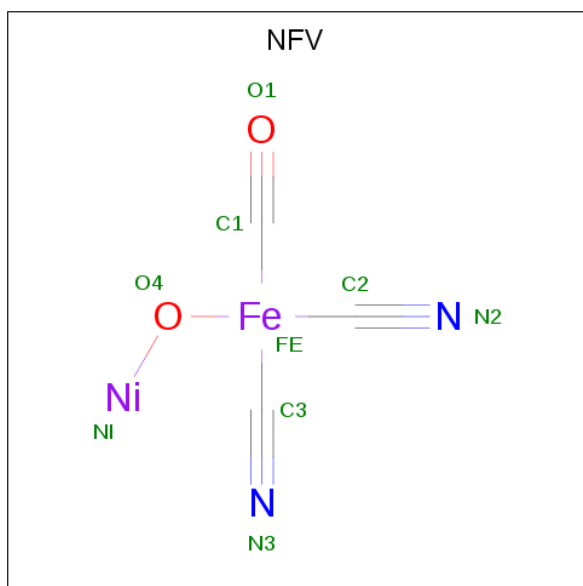


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 5 3 2	0	0
5	G	1	Total C N 5 3 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total Cl 1 1	0	0
6	A	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0
6	E	1	Total Cl 1 1	0	0

- Molecule 7 is NI-FE OXIDIZED ACTIVE CENTER (three-letter code: NFV) (formula: C₃FeN₂NiO₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C Fe N Ni O 9 3 1 2 1 2	0	0
7	D	1	Total C Fe N Ni O 9 3 1 2 1 2	0	0
7	F	1	Total C Fe N Ni O 9 3 1 2 1 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	H	1	Total	C	Fe	N	Ni	O	0	0
			9	3	1	2	1	2		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		

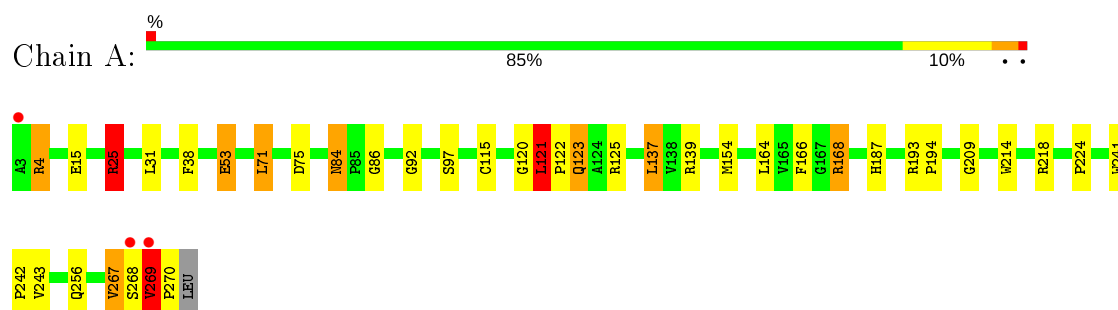
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	199	Total	O	0	0
			199	199		
9	B	379	Total	O	0	0
			379	379		
9	C	157	Total	O	0	0
			157	157		
9	D	281	Total	O	0	0
			281	281		
9	E	115	Total	O	0	0
			115	115		
9	F	286	Total	O	0	0
			286	286		
9	G	179	Total	O	0	0
			179	179		
9	H	329	Total	O	0	0
			329	329		

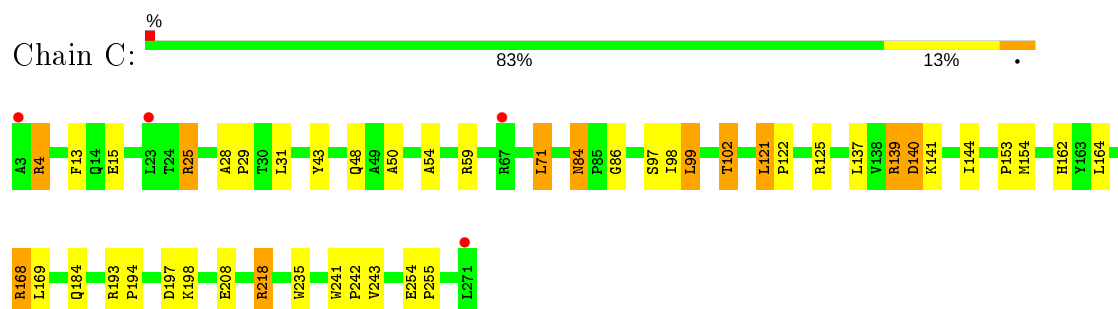
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

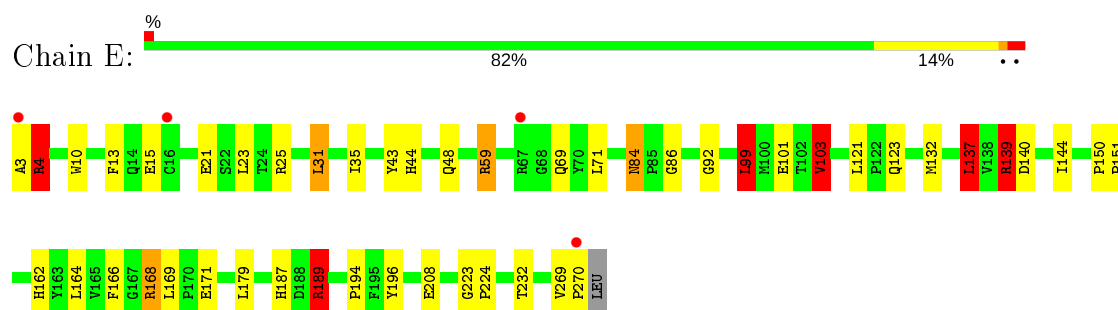
- Molecule 1: Hydrogenase (NiFe) small subunit HydA



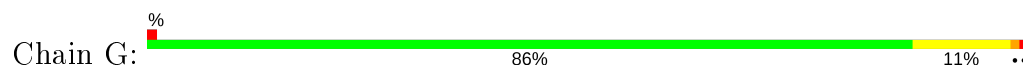
- Molecule 1: Hydrogenase (NiFe) small subunit HydA

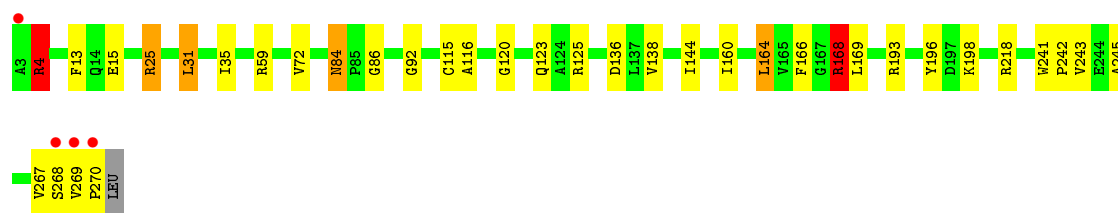


- Molecule 1: Hydrogenase (NiFe) small subunit HydA



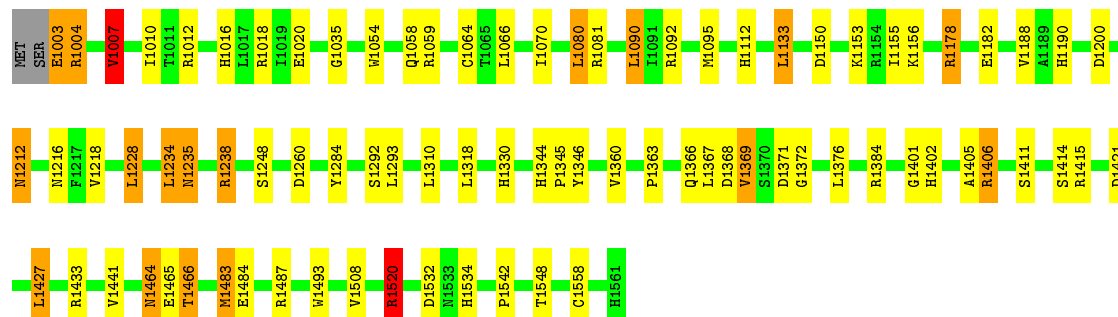
- Molecule 1: Hydrogenase (NiFe) small subunit HydA





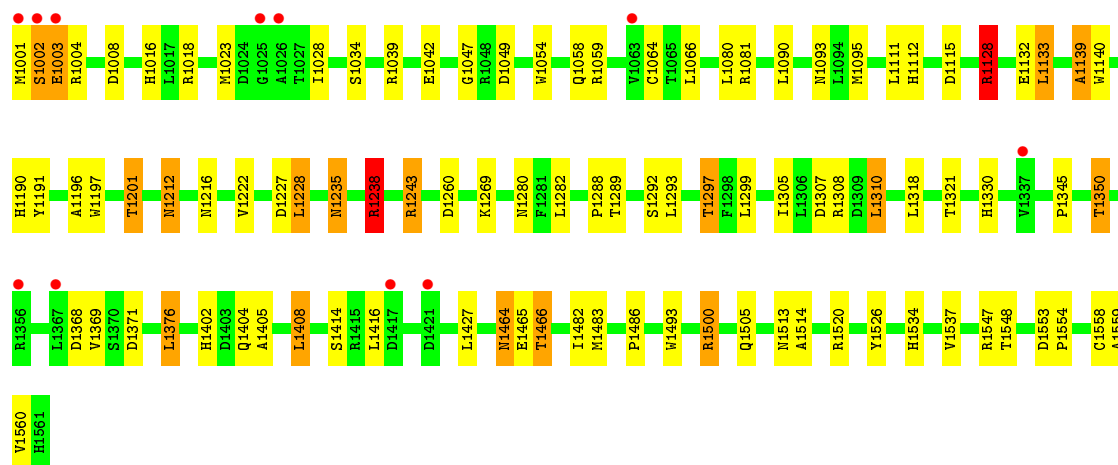
• Molecule 2: Nickel-dependent hydrogenase large subunit

Chain B: 85% 12%



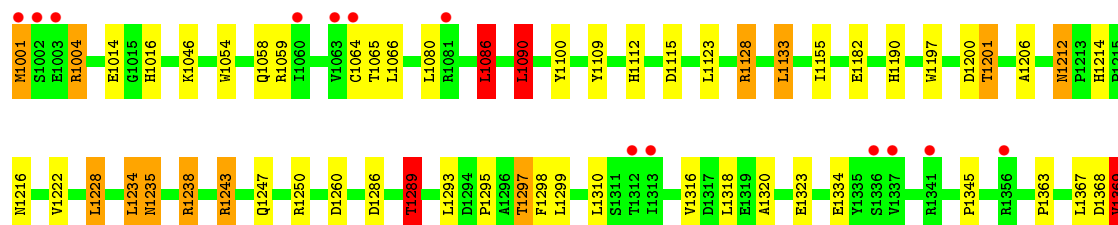
• Molecule 2: Nickel-dependent hydrogenase large subunit

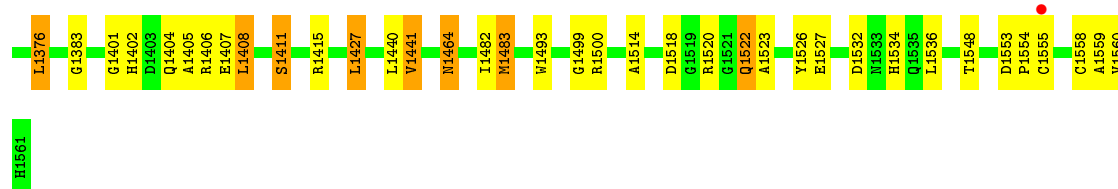
Chain D: 83% 14%



• Molecule 2: Nickel-dependent hydrogenase large subunit

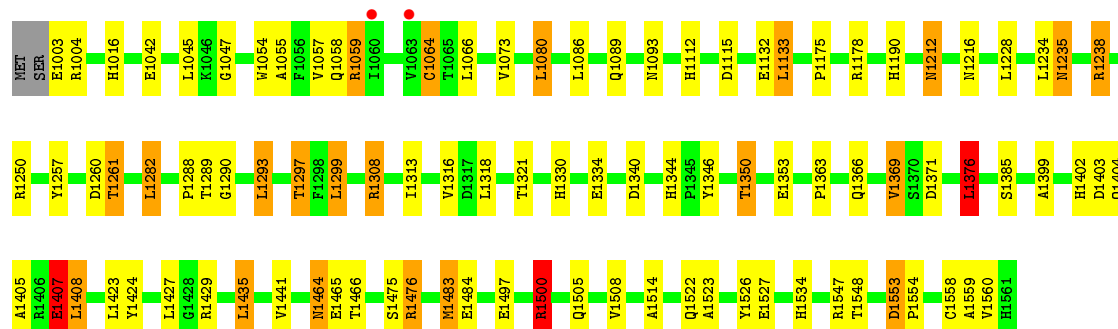
Chain F: 83% 13%





• Molecule 2: Nickel-dependent hydrogenase large subunit

Chain H: 82% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	205.75 Å 216.96 Å 119.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 48.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.10) 99.6 (48.05-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.138 , 0.168 0.151 , 0.178	Depositor DCC
R_{free} test set	15482 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	27720	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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: MG, IMD, CL, SF4, NFV, F3S

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.22	6/2099 (0.3%)	1.04	10/2866 (0.3%)
1	C	1.12	2/2108 (0.1%)	0.96	6/2877 (0.2%)
1	E	1.07	3/2099 (0.1%)	1.00	9/2866 (0.3%)
1	G	1.15	3/2099 (0.1%)	0.99	10/2866 (0.3%)
2	B	1.12	11/4476 (0.2%)	1.00	24/6097 (0.4%)
2	D	1.00	3/4490 (0.1%)	0.97	17/6115 (0.3%)
2	F	1.02	4/4490 (0.1%)	0.94	18/6115 (0.3%)
2	H	1.09	4/4476 (0.1%)	1.01	23/6097 (0.4%)
All	All	1.09	36/26337 (0.1%)	0.99	117/35899 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	G	0	1
All	All	0	3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	GLU	CG-CD	10.78	1.68	1.51
2	B	1003	GLU	CG-CD	-7.87	1.40	1.51
1	C	208	GLU	CG-CD	7.27	1.62	1.51
2	H	1064	CYS	CB-SG	7.07	1.94	1.82
2	B	1465	GLU	CG-CD	6.92	1.62	1.51
2	B	1003	GLU	CB-CG	-6.60	1.39	1.52
2	B	1248	SER	CB-OG	-6.23	1.34	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	21	GLU	CG-CD	6.05	1.61	1.51
2	F	1407	GLU	CG-CD	6.00	1.60	1.51
2	B	1150	ASP	CB-CG	5.99	1.64	1.51
2	F	1182	GLU	CD-OE1	5.96	1.32	1.25
2	B	1182	GLU	CD-OE2	5.91	1.32	1.25
1	A	269	VAL	CA-CB	5.80	1.67	1.54
2	B	1218	VAL	CB-CG1	-5.79	1.40	1.52
1	E	101	GLU	CG-CD	5.77	1.60	1.51
1	E	208	GLU	CG-CD	5.72	1.60	1.51
1	A	53	GLU	CD-OE2	5.70	1.31	1.25
1	C	208	GLU	CB-CG	5.68	1.62	1.52
1	A	53	GLU	CD-OE1	5.67	1.31	1.25
2	H	1407	GLU	CG-CD	5.59	1.60	1.51
2	B	1284	TYR	CD2-CE2	5.47	1.47	1.39
2	D	1139	ALA	CA-CB	5.40	1.63	1.52
2	B	1360	VAL	CB-CG1	5.35	1.64	1.52
2	H	1073	VAL	CB-CG2	5.32	1.64	1.52
1	A	97	SER	CB-OG	-5.30	1.35	1.42
2	F	1206	ALA	CA-CB	5.29	1.63	1.52
1	G	72	VAL	CB-CG1	5.28	1.64	1.52
2	B	1465	GLU	CB-CG	5.25	1.62	1.52
2	B	1182	GLU	CD-OE1	5.24	1.31	1.25
2	D	1196	ALA	CA-CB	5.23	1.63	1.52
2	H	1132	GLU	CG-CD	5.20	1.59	1.51
1	A	38	PHE	CE1-CZ	5.19	1.47	1.37
2	D	1465	GLU	CG-CD	5.17	1.59	1.51
2	F	1109	TYR	CD1-CE1	5.05	1.47	1.39
1	G	245	ALA	CA-CB	5.05	1.63	1.52
1	G	116	ALA	CA-CB	5.03	1.63	1.52

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1128	ARG	NE-CZ-NH2	15.65	128.13	120.30
1	E	189	ARG	NE-CZ-NH2	14.94	127.77	120.30
2	H	1004	ARG	NE-CZ-NH2	-12.68	113.96	120.30
2	D	1128	ARG	NE-CZ-NH1	-11.63	114.48	120.30
1	E	189	ARG	NE-CZ-NH1	-11.24	114.68	120.30
2	B	1487	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	G	168	ARG	NE-CZ-NH2	-9.31	115.64	120.30
2	F	1004	ARG	NE-CZ-NH2	-9.06	115.77	120.30
2	H	1308	ARG	NE-CZ-NH2	-8.98	115.81	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1376	LEU	CB-CG-CD2	8.87	126.08	111.00
2	F	1004	ARG	NE-CZ-NH1	8.81	124.70	120.30
2	B	1004	ARG	NE-CZ-NH2	-8.55	116.03	120.30
2	B	1238	ARG	NE-CZ-NH1	8.42	124.51	120.30
2	D	1243	ARG	NE-CZ-NH2	8.36	124.48	120.30
1	A	137	LEU	CB-CG-CD1	8.33	125.17	111.00
1	G	168	ARG	NE-CZ-NH1	8.18	124.39	120.30
2	H	1004	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	E	140	ASP	CB-CA-C	-7.96	94.49	110.40
2	B	1178	ARG	NE-CZ-NH2	-7.93	116.33	120.30
2	B	1004	ARG	NE-CZ-NH1	7.81	124.21	120.30
2	B	1369	VAL	CG1-CB-CG2	7.72	123.25	110.90
2	D	1308	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	G	59	ARG	NE-CZ-NH2	7.59	124.10	120.30
2	H	1369	VAL	CG1-CB-CG2	7.49	122.88	110.90
2	D	1228	LEU	CB-CG-CD1	7.41	123.60	111.00
2	F	1128	ARG	NE-CZ-NH1	-7.40	116.60	120.30
2	D	1238	ARG	NE-CZ-NH1	7.39	124.00	120.30
2	F	1376	LEU	CB-CG-CD2	7.36	123.51	111.00
2	H	1376	LEU	CB-CG-CD2	7.23	123.29	111.00
2	B	1520	ARG	NE-CZ-NH1	-7.20	116.70	120.30
2	F	1133	LEU	CB-CG-CD1	7.10	123.07	111.00
2	D	1243	ARG	NE-CZ-NH1	-7.00	116.80	120.30
2	H	1238	ARG	NE-CZ-NH2	-6.98	116.81	120.30
2	B	1520	ARG	NE-CZ-NH2	6.88	123.74	120.30
2	B	1007	VAL	CG1-CB-CG2	6.75	121.70	110.90
1	E	99	LEU	CB-CG-CD2	6.74	122.46	111.00
2	D	1238	ARG	NE-CZ-NH2	-6.69	116.96	120.30
2	B	1228	LEU	CB-CG-CD1	6.64	122.29	111.00
2	D	1039	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	E	103	VAL	CG1-CB-CG2	6.57	121.41	110.90
2	B	1238	ARG	NE-CZ-NH2	-6.57	117.02	120.30
2	H	1500	ARG	NE-CZ-NH1	6.47	123.53	120.30
2	D	1133	LEU	CB-CG-CD2	6.44	121.95	111.00
1	G	59	ARG	NE-CZ-NH1	-6.43	117.08	120.30
2	B	1090	LEU	CB-CG-CD1	6.32	121.75	111.00
2	B	1178	ARG	CG-CD-NE	6.30	125.04	111.80
2	B	1318	LEU	CA-CB-CG	-6.30	100.81	115.30
1	A	25	ARG	NE-CZ-NH2	-6.29	117.16	120.30
2	H	1238	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	B	1080	LEU	CB-CG-CD1	6.22	121.58	111.00
2	H	1376	LEU	CA-CB-CG	6.22	129.60	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1133	LEU	CB-CG-CD2	6.20	121.54	111.00
2	B	1234	LEU	CB-CG-CD1	6.19	121.53	111.00
2	B	1133	LEU	CB-CG-CD2	6.12	121.41	111.00
1	G	125	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	C	125	ARG	NE-CZ-NH1	-6.09	117.25	120.30
2	H	1282	LEU	CB-CG-CD2	6.05	121.29	111.00
2	H	1429	ARG	NE-CZ-NH2	-6.01	117.29	120.30
2	D	1308	ARG	CG-CD-NE	-6.00	99.20	111.80
2	B	1487	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	71	LEU	CA-CB-CG	5.96	129.00	115.30
2	H	1435	LEU	CB-CG-CD1	5.95	121.11	111.00
1	E	137	LEU	CB-CG-CD1	5.91	121.05	111.00
2	F	1238	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	218	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	G	31	LEU	CB-CG-CD2	5.87	120.98	111.00
2	F	1369	VAL	CG1-CB-CG2	5.85	120.27	110.90
2	F	1228	LEU	CB-CG-CD1	5.84	120.93	111.00
2	D	1308	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	E	139	ARG	NE-CZ-NH2	-5.75	117.42	120.30
2	F	1376	LEU	CA-CB-CG	5.74	128.51	115.30
1	G	136	ASP	CB-CG-OD1	5.74	123.47	118.30
2	B	1368	ASP	CB-CG-OD1	5.73	123.46	118.30
2	B	1007	VAL	CA-CB-CG2	5.72	119.48	110.90
2	H	1080	LEU	CB-CG-CD1	5.69	120.68	111.00
2	H	1059	ARG	NE-CZ-NH2	-5.68	117.46	120.30
2	F	1090	LEU	CB-CG-CD1	5.67	120.64	111.00
2	H	1500	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	F	1086	LEU	CB-CG-CD2	5.62	120.55	111.00
1	G	4	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	99	LEU	CB-CG-CD2	5.55	120.43	111.00
1	C	154	MET	CA-CB-CG	-5.51	103.93	113.30
2	F	1427	LEU	CB-CG-CD2	5.51	120.37	111.00
1	A	218	ARG	CB-CG-CD	5.49	125.87	111.60
2	F	1234	LEU	CB-CG-CD1	5.48	120.32	111.00
2	F	1059	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	H	1132	GLU	OE1-CD-OE2	-5.46	116.74	123.30
2	H	1308	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	G	138	VAL	CG1-CB-CG2	5.44	119.61	110.90
2	H	1299	LEU	CA-CB-CG	5.44	127.81	115.30
2	F	1289	THR	N-CA-CB	-5.44	99.97	110.30
1	A	218	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	154	MET	CA-CB-CG	-5.37	104.17	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1133	LEU	CB-CG-CD2	5.37	120.12	111.00
1	A	121	LEU	CB-CG-CD2	5.36	120.12	111.00
2	B	1012	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	H	1293	LEU	CB-CG-CD2	5.35	120.10	111.00
2	H	1308	ARG	CG-CD-NE	-5.34	100.58	111.80
2	F	1411	SER	CB-CA-C	-5.33	99.97	110.10
1	A	71	LEU	CB-CG-CD2	5.29	119.99	111.00
2	B	1433	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	C	25	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	197	ASP	CB-CG-OD1	5.24	123.01	118.30
2	B	1369	VAL	CA-CB-CG1	5.19	118.69	110.90
1	G	138	VAL	CA-CB-CG1	5.18	118.68	110.90
2	F	1115	ASP	CB-CG-OD1	-5.18	113.64	118.30
2	H	1376	LEU	CB-CG-CD1	5.17	119.80	111.00
2	B	1427	LEU	CB-CG-CD2	5.16	119.77	111.00
2	H	1553	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	A	75	ASP	CB-CG-OD1	-5.14	113.67	118.30
2	D	1318	LEU	CA-CB-CG	-5.10	103.57	115.30
1	E	59	ARG	NE-CZ-NH2	5.09	122.84	120.30
2	D	1049	ASP	CB-CG-OD1	5.08	122.87	118.30
1	E	31	LEU	CB-CG-CD2	5.07	119.62	111.00
1	A	139	ARG	C-N-CA	-5.06	109.05	121.70
2	D	1227	ASP	CB-CG-OD1	5.05	122.85	118.30
2	D	1128	ARG	CD-NE-CZ	5.01	130.62	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	ARG	Sidechain
1	E	139	ARG	Peptide
1	G	25	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	2038	0	1934	25	0
1	C	2047	0	1945	30	0
1	E	2038	0	1934	32	0
1	G	2038	0	1934	25	0
2	B	4363	0	4242	54	0
2	D	4377	0	4256	77	0
2	F	4377	0	4256	79	0
2	H	4363	0	4242	71	0
3	A	18	0	0	1	0
3	C	18	0	0	1	0
3	E	18	0	0	0	0
3	G	18	0	0	0	0
4	A	7	0	0	0	0
4	C	7	0	0	0	0
4	E	7	0	0	0	0
4	G	7	0	0	0	0
5	A	5	0	5	1	0
5	G	5	0	5	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
7	B	9	0	0	5	0
7	D	9	0	0	5	0
7	F	9	0	0	5	0
7	H	9	0	0	5	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
8	H	1	0	0	0	0
9	A	199	0	0	2	0
9	B	379	0	0	7	0
9	C	157	0	0	5	0
9	D	281	0	0	6	0
9	E	115	0	0	1	0
9	F	286	0	0	9	0
9	G	179	0	0	1	0
9	H	329	0	0	7	0
All	All	27720	0	24753	380	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 8.

All (380) 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)
7:H:2005:NFV:C2	7:H:2005:NFV:C1	2.27	1.13
2:D:1464:ASN:HD21	2:D:1466:THR:HG23	1.04	1.12
2:B:1464:ASN:HD21	2:B:1466:THR:HG23	1.09	1.09
7:F:2005:NFV:C2	7:F:2005:NFV:C1	2.30	1.08
1:C:144:ILE:HD11	1:C:169:LEU:HD22	1.32	1.08
1:A:269:VAL:HB	1:A:270:PRO:HD2	1.11	1.06
1:E:25:ARG:HH21	2:F:1212:ASN:HD21	1.11	0.98
1:G:4:ARG:HH11	1:G:4:ARG:HG2	1.27	0.97
7:D:2005:NFV:C2	7:D:2005:NFV:C1	2.43	0.97
2:B:1464:ASN:ND2	2:B:1466:THR:HG23	1.79	0.96
1:A:269:VAL:HB	1:A:270:PRO:CD	1.95	0.96
7:H:2005:NFV:C1	7:H:2005:NFV:C3	2.43	0.95
7:B:2005:NFV:C1	7:B:2005:NFV:C2	2.45	0.94
2:D:1464:ASN:HD21	2:D:1466:THR:CG2	1.80	0.94
7:F:2005:NFV:FE	7:F:2005:NFV:C1	1.50	0.92
2:D:1023:MET:HE2	2:D:1028:ILE:HA	1.51	0.91
7:H:2005:NFV:C1	7:H:2005:NFV:FE	1.52	0.91
7:F:2005:NFV:C3	7:F:2005:NFV:C1	2.47	0.91
1:C:84:ASN:HD22	1:C:86:GLY:H	1.18	0.90
2:D:1023:MET:CE	2:D:1028:ILE:HA	2.02	0.90
1:A:25:ARG:HH21	2:B:1212:ASN:HD21	1.18	0.90
7:D:2005:NFV:FE	7:D:2005:NFV:C1	1.53	0.90
2:B:1058:GLN:HE21	2:B:1066:LEU:H	1.20	0.89
2:H:1297:THR:HG21	9:H:5014:HOH:O	1.72	0.89
2:F:1250:ARG:HD2	9:F:5626:HOH:O	1.73	0.89
2:D:1201:THR:HG22	9:D:3924:HOH:O	1.73	0.88
1:C:25:ARG:HH21	2:D:1212:ASN:HD21	1.20	0.88
2:D:1042:GLU:OE1	2:D:1350:THR:HG21	1.74	0.88
2:F:1402:HIS:HD2	2:F:1405:ALA:H	1.21	0.88
1:E:171:GLU:HG2	1:E:179:LEU:HD12	1.55	0.87
2:F:1190:HIS:HD2	2:F:1260:ASP:OD2	1.58	0.87
7:B:2005:NFV:C1	7:B:2005:NFV:C3	2.52	0.87
7:B:2005:NFV:C1	7:B:2005:NFV:FE	1.57	0.86
2:D:1464:ASN:ND2	2:D:1466:THR:HG23	1.89	0.86
2:H:1042:GLU:OE1	2:H:1350:THR:HG21	1.77	0.85
1:G:84:ASN:HD22	1:G:86:GLY:H	1.20	0.84
2:H:1475:SER:O	2:H:1476:ARG:CD	2.25	0.84
2:H:1058:GLN:HE21	2:H:1066:LEU:H	1.26	0.83
1:C:140:ASP:OD2	9:C:3912:HOH:O	1.97	0.83
1:A:84:ASN:HD22	1:A:86:GLY:H	1.22	0.83
2:H:1475:SER:O	2:H:1476:ARG:HD2	1.78	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1402:HIS:HD2	2:B:1405:ALA:H	1.25	0.82
2:D:1001:MET:HB3	9:D:6067:HOH:O	1.78	0.82
2:H:1289:THR:H	2:H:1297:THR:HG23	1.44	0.82
2:F:1243:ARG:CD	9:F:5196:HOH:O	2.26	0.82
7:D:2005:NFV:C3	7:D:2005:NFV:C1	2.58	0.81
2:F:1123:LEU:HD21	2:F:1155:ILE:HG22	1.63	0.80
2:B:1190:HIS:HD2	2:B:1260:ASP:OD2	1.64	0.80
1:G:25:ARG:HH21	2:H:1212:ASN:HD21	1.30	0.79
1:C:139:ARG:HG3	1:C:139:ARG:HH21	1.48	0.79
1:G:4:ARG:HH11	1:G:4:ARG:CG	1.95	0.79
2:D:1058:GLN:HE21	2:D:1066:LEU:H	1.29	0.78
2:D:1297:THR:HG21	9:D:4025:HOH:O	1.83	0.78
1:G:4:ARG:NH1	1:G:4:ARG:HG2	1.96	0.77
5:A:3002:IMD:H5	9:A:3657:HOH:O	1.84	0.77
2:D:1190:HIS:HD2	2:D:1260:ASP:OD2	1.68	0.76
2:F:1001:MET:HA	2:F:1001:MET:CE	2.15	0.76
2:H:1376:LEU:HD13	2:H:1559:ALA:HB1	1.67	0.76
2:F:1058:GLN:HE21	2:F:1066:LEU:H	1.34	0.76
2:F:1001:MET:CB	2:F:1004:ARG:HH22	1.99	0.75
2:D:1402:HIS:HD2	2:D:1405:ALA:H	1.34	0.75
1:C:98:ILE:O	1:C:102:THR:HG23	1.87	0.74
2:F:1482:ILE:O	2:F:1482:ILE:HD12	1.88	0.74
2:H:1190:HIS:HD2	2:H:1260:ASP:OD2	1.71	0.74
2:D:1289:THR:H	2:D:1297:THR:HG23	1.52	0.73
2:F:1243:ARG:NE	9:F:5196:HOH:O	2.20	0.73
2:D:1003:GLU:HA	2:D:1003:GLU:OE1	1.86	0.73
2:H:1476:ARG:NH1	2:H:1476:ARG:HG3	2.03	0.73
2:D:1534:HIS:HE1	2:D:1548:THR:OG1	1.72	0.72
2:F:1197:TRP:CE2	2:F:1201:THR:HG21	2.23	0.72
2:H:1475:SER:C	2:H:1476:ARG:HD3	2.10	0.72
2:F:1243:ARG:HD2	9:F:5196:HOH:O	1.85	0.72
1:E:84:ASN:HD22	1:E:86:GLY:H	1.38	0.71
2:F:1086:LEU:HD22	2:F:1090:LEU:HD22	1.73	0.71
2:F:1482:ILE:HD12	2:F:1482:ILE:C	2.09	0.71
2:H:1476:ARG:HG3	2:H:1476:ARG:HH11	1.54	0.70
2:H:1534:HIS:HE1	2:H:1548:THR:OG1	1.74	0.70
2:F:1376:LEU:HD13	2:F:1559:ALA:HB1	1.74	0.70
2:H:1350:THR:HG23	2:H:1505:GLN:HE22	1.56	0.70
2:D:1023:MET:HE1	2:D:1028:ILE:HG12	1.74	0.70
1:A:269:VAL:CB	1:A:270:PRO:HD2	2.06	0.70
2:B:1384:ARG:HD3	9:B:3458:HOH:O	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1297:THR:HG21	9:F:5029:HOH:O	1.91	0.70
2:F:1558:CYS:SG	7:F:2005:NFV:C1	2.80	0.69
2:H:1475:SER:O	2:H:1476:ARG:HD3	1.92	0.69
2:H:1402:HIS:HD2	2:H:1405:ALA:H	1.40	0.69
1:G:84:ASN:ND2	1:G:86:GLY:H	1.90	0.69
2:F:1534:HIS:HE1	2:F:1548:THR:OG1	1.75	0.69
2:F:1001:MET:HB2	2:F:1004:ARG:HH12	1.57	0.68
2:F:1197:TRP:CZ2	2:F:1201:THR:HG21	2.30	0.67
2:F:1190:HIS:CD2	2:F:1260:ASP:OD2	2.46	0.67
1:E:92:GLY:O	2:F:1363:PRO:HA	1.95	0.66
2:F:1243:ARG:HH21	2:F:1243:ARG:HG2	1.59	0.66
2:B:1003:GLU:CB	9:B:6104:HOH:O	2.42	0.66
2:H:1558:CYS:SG	7:H:2005:NFV:C1	2.84	0.65
2:D:1128:ARG:HD2	2:D:1132:GLU:OE1	1.96	0.65
2:D:1197:TRP:CE2	2:D:1201:THR:HG21	2.31	0.65
2:D:1558:CYS:SG	7:D:2005:NFV:C1	2.85	0.65
2:B:1520:ARG:HD3	2:B:1520:ARG:N	2.11	0.65
1:C:218:ARG:NH1	9:C:5022:HOH:O	2.30	0.65
2:B:1235:ASN:C	2:B:1235:ASN:HD22	2.00	0.65
2:H:1465:GLU:HG2	9:H:5879:HOH:O	1.97	0.64
2:B:1016:HIS:HD2	9:B:3503:HOH:O	1.80	0.64
2:B:1534:HIS:HE1	2:B:1548:THR:OG1	1.81	0.64
1:G:268:SER:O	1:G:269:VAL:HG23	1.98	0.64
2:F:1001:MET:N	2:F:1367:LEU:O	2.32	0.63
1:C:198:LYS:NZ	9:C:6149:HOH:O	2.22	0.63
1:G:269:VAL:HG13	1:G:270:PRO:CD	2.28	0.63
2:D:1197:TRP:CZ2	2:D:1201:THR:HG21	2.34	0.62
2:D:1190:HIS:HE1	9:D:3516:HOH:O	1.83	0.62
1:G:166:PHE:O	1:G:168:ARG:HD3	2.00	0.62
2:B:1190:HIS:HE1	9:B:5004:HOH:O	1.82	0.62
2:F:1250:ARG:CG	9:F:5626:HOH:O	2.48	0.62
2:F:1402:HIS:CD2	2:F:1405:ALA:H	2.10	0.61
2:F:1376:LEU:HD22	2:F:1560:VAL:CG2	2.30	0.61
2:B:1156:LYS:HD2	9:B:3722:HOH:O	2.00	0.61
2:B:1558:CYS:SG	7:B:2005:NFV:C1	2.89	0.61
2:H:1476:ARG:NH1	2:H:1497:GLU:HG2	2.15	0.61
2:B:1054:TRP:HH2	2:B:1216:ASN:HD22	1.49	0.60
1:E:25:ARG:NH2	2:F:1212:ASN:HD21	1.92	0.60
1:G:144:ILE:HD11	1:G:169:LEU:HD22	1.82	0.60
2:B:1058:GLN:HE21	2:B:1066:LEU:N	1.98	0.60
2:D:1054:TRP:HH2	2:D:1216:ASN:HD22	1.49	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:GLN:HG2	1:E:123:GLN:O	2.00	0.60
1:E:84:ASN:ND2	1:E:86:GLY:H	1.99	0.60
2:H:1350:THR:CG2	2:H:1505:GLN:HE22	2.15	0.60
2:D:1235:ASN:C	2:D:1235:ASN:HD22	2.03	0.59
1:G:269:VAL:HG13	1:G:270:PRO:HD2	1.84	0.59
1:C:98:ILE:O	1:C:102:THR:CG2	2.49	0.59
2:H:1093:ASN:HD21	2:H:1288:PRO:HD2	1.66	0.59
1:C:121:LEU:HB3	1:C:122:PRO:HD3	1.84	0.58
2:B:1190:HIS:CD2	2:B:1260:ASP:OD2	2.51	0.58
2:H:1058:GLN:HE21	2:H:1066:LEU:N	2.01	0.58
2:D:1464:ASN:ND2	2:D:1466:THR:CG2	2.57	0.58
2:H:1376:LEU:HD22	2:H:1560:VAL:CG2	2.32	0.58
2:H:1475:SER:C	2:H:1476:ARG:CD	2.71	0.58
9:B:3350:HOH:O	1:C:162:HIS:HD2	1.87	0.58
2:D:1482:ILE:HD12	2:D:1482:ILE:O	2.03	0.58
1:A:25:ARG:HE	2:B:1212:ASN:ND2	2.02	0.58
1:A:84:ASN:ND2	1:A:86:GLY:H	1.98	0.57
2:D:1376:LEU:HD22	2:D:1560:VAL:CG2	2.35	0.57
1:C:25:ARG:NH2	2:D:1212:ASN:HD21	1.98	0.57
2:H:1235:ASN:HD22	2:H:1235:ASN:C	2.06	0.57
2:F:1190:HIS:HE1	9:F:3522:HOH:O	1.87	0.57
1:E:3:ALA:O	1:E:4:ARG:HB3	2.04	0.56
2:B:1411:SER:O	2:B:1415:ARG:HG3	2.04	0.56
2:H:1190:HIS:CD2	2:H:1260:ASP:OD2	2.57	0.56
2:F:1058:GLN:HG2	2:F:1214:HIS:CD2	2.40	0.56
1:G:92:GLY:O	2:H:1363:PRO:HA	2.05	0.56
2:H:1003:GLU:HB3	2:H:1366:GLN:OE1	2.06	0.56
2:B:1464:ASN:HD22	2:B:1464:ASN:C	2.09	0.56
2:B:1483:MET:HG3	2:B:1484:GLU:N	2.20	0.56
2:D:1350:THR:HG23	2:D:1505:GLN:HE22	1.70	0.56
2:H:1476:ARG:HH11	2:H:1476:ARG:CG	2.14	0.56
2:B:1402:HIS:CD2	2:B:1405:ALA:H	2.16	0.55
1:A:193:ARG:HG2	1:C:194:PRO:HG3	1.88	0.55
2:F:1250:ARG:CD	9:F:5626:HOH:O	2.40	0.55
2:D:1534:HIS:CE1	2:D:1548:THR:OG1	2.56	0.55
2:H:1257:TYR:O	2:H:1261:THR:HG23	2.07	0.55
1:C:25:ARG:HE	2:D:1212:ASN:ND2	2.04	0.55
2:D:1023:MET:CE	2:D:1023:MET:HA	2.36	0.55
2:F:1376:LEU:CD1	2:F:1559:ALA:HB1	2.36	0.55
2:D:1350:THR:CG2	2:D:1505:GLN:HE22	2.20	0.55
2:F:1197:TRP:O	2:F:1201:THR:HG23	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1383:GLY:O	2:F:1522:GLN:NE2	2.40	0.55
2:D:1404:GLN:HG2	2:D:1408:LEU:HD22	1.87	0.55
1:C:241:TRP:CH2	1:C:243:VAL:HB	2.42	0.54
2:H:1334:GLU:OE2	2:H:1353:GLU:HG2	2.06	0.54
1:E:44:HIS:H	1:E:48:GLN:NE2	2.05	0.54
2:D:1482:ILE:HD12	2:D:1482:ILE:C	2.28	0.54
2:F:1001:MET:HE2	2:F:1001:MET:HA	1.87	0.54
2:H:1289:THR:N	2:H:1297:THR:HG23	2.20	0.54
1:E:25:ARG:HH21	2:F:1212:ASN:ND2	1.95	0.54
2:D:1345:PRO:HB2	2:D:1493:TRP:CG	2.43	0.53
2:F:1235:ASN:HD22	2:F:1235:ASN:C	2.09	0.53
2:H:1313:ILE:HD11	2:H:1399:ALA:HB1	1.91	0.53
1:A:166:PHE:O	1:A:168:ARG:HD3	2.09	0.53
2:D:1190:HIS:CD2	2:D:1260:ASP:OD2	2.56	0.52
2:D:1064:CYS:SG	7:D:2005:NFV:C1	2.97	0.52
9:E:3560:HOH:O	2:F:1016:HIS:HD2	1.92	0.52
2:H:1330:HIS:HE1	9:H:5111:HOH:O	1.91	0.52
1:E:162:HIS:HD2	9:H:3606:HOH:O	1.92	0.52
2:F:1247:GLN:HG2	2:F:1250:ARG:NH1	2.24	0.52
2:B:1018:ARG:HD3	2:B:1367:LEU:HD11	1.92	0.52
2:F:1523:ALA:HB1	2:F:1527:GLU:HB2	1.92	0.52
1:A:123:GLN:HE22	1:A:256:GLN:HE21	1.57	0.52
1:A:25:ARG:NH2	2:B:1212:ASN:HD21	1.96	0.52
2:D:1023:MET:HE1	2:D:1028:ILE:HA	1.85	0.52
1:A:269:VAL:CB	1:A:270:PRO:CD	2.80	0.52
2:D:1023:MET:HE2	2:D:1023:MET:HA	1.92	0.52
2:D:1001:MET:HE1	2:D:1369:VAL:HG22	1.92	0.52
2:F:1534:HIS:CE1	2:F:1548:THR:OG1	2.61	0.52
1:G:13:PHE:O	2:H:1016:HIS:HE1	1.93	0.52
2:H:1483:MET:HG3	2:H:1484:GLU:N	2.25	0.52
1:A:115:CYS:HA	1:A:120:GLY:HA3	1.92	0.52
2:F:1001:MET:HG2	2:F:1369:VAL:H	1.75	0.52
2:B:1003:GLU:HG3	2:B:1366:GLN:CD	2.31	0.51
2:F:1464:ASN:HD22	2:F:1464:ASN:C	2.14	0.51
1:G:198:LYS:NZ	9:G:5941:HOH:O	2.41	0.51
2:H:1045:LEU:HD11	2:H:1057:VAL:CG1	2.40	0.51
2:D:1464:ASN:HD22	2:D:1464:ASN:C	2.13	0.51
2:D:1514:ALA:HB2	2:D:1526:TYR:CE2	2.46	0.51
1:G:115:CYS:HA	1:G:120:GLY:HA3	1.92	0.51
1:G:269:VAL:CG1	1:G:270:PRO:CD	2.87	0.51
2:D:1002:SER:OG	2:D:1003:GLU:N	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1385:SER:H	2:H:1522:GLN:NE2	2.08	0.51
2:B:1508:VAL:HG11	2:B:1558:CYS:HB3	1.93	0.51
1:C:84:ASN:ND2	1:C:86:GLY:H	1.97	0.51
1:E:166:PHE:O	1:E:168:ARG:HD3	2.09	0.51
2:F:1001:MET:HG2	2:F:1368:ASP:HA	1.92	0.51
1:C:139:ARG:HG3	1:C:139:ARG:NH2	2.18	0.51
2:F:1286:ASP:OD1	2:F:1483:MET:HG2	2.11	0.51
2:B:1003:GLU:HG3	2:B:1366:GLN:OE1	2.11	0.51
2:D:1376:LEU:HD13	2:D:1559:ALA:HB1	1.93	0.51
1:A:241:TRP:CH2	1:A:243:VAL:HB	2.47	0.50
2:H:1330:HIS:HD2	2:H:1371:ASP:O	1.93	0.50
2:F:1058:GLN:HE21	2:F:1066:LEU:N	2.06	0.50
2:B:1003:GLU:HB3	9:B:6104:HOH:O	2.07	0.50
2:F:1401:GLY:HA2	2:F:1406:ARG:HE	1.76	0.50
2:D:1058:GLN:HE21	2:D:1066:LEU:N	2.02	0.50
2:H:1054:TRP:HH2	2:H:1216:ASN:HD22	1.59	0.49
2:D:1330:HIS:HD2	2:D:1371:ASP:O	1.96	0.49
2:F:1289:THR:H	2:F:1297:THR:HG23	1.77	0.49
1:C:184:GLN:HA	1:C:184:GLN:HE21	1.78	0.49
2:F:1001:MET:HB2	2:F:1004:ARG:HH22	1.74	0.49
1:C:193:ARG:HA	3:C:2002:SF4:S3	2.53	0.49
1:E:43:TYR:HA	1:E:48:GLN:HE22	1.77	0.49
2:H:1514:ALA:HB2	2:H:1526:TYR:CE2	2.48	0.49
1:E:187:HIS:CB	1:E:224:PRO:HA	2.43	0.48
1:G:84:ASN:HD22	1:G:86:GLY:N	1.99	0.48
2:H:1403:ASP:O	2:H:1407:GLU:HG3	2.13	0.48
2:H:1289:THR:HG22	2:H:1297:THR:HG23	1.95	0.48
1:A:125:ARG:NH2	9:A:5571:HOH:O	2.46	0.48
2:H:1115:ASP:HB3	2:H:1547:ARG:HG3	1.94	0.48
1:G:25:ARG:HE	2:H:1212:ASN:ND2	2.10	0.48
2:B:1155:ILE:CD1	2:B:1188:VAL:HG11	2.44	0.48
2:D:1402:HIS:CD2	2:D:1405:ALA:H	2.23	0.48
2:F:1197:TRP:CE2	2:F:1201:THR:CG2	2.96	0.48
2:B:1330:HIS:HD2	2:B:1371:ASP:O	1.96	0.48
2:D:1093:ASN:HD21	2:D:1288:PRO:HD2	1.79	0.48
2:H:1376:LEU:HD22	2:H:1560:VAL:HG23	1.96	0.48
2:F:1064:CYS:SG	7:F:2005:NFV:C1	3.02	0.48
2:D:1047:GLY:O	2:D:1500:ARG:HD3	2.13	0.47
2:D:1222:VAL:HB	9:D:3210:HOH:O	2.14	0.47
2:D:1115:ASP:HB3	2:D:1547:ARG:HG3	1.96	0.47
2:F:1318:LEU:HD13	2:F:1482:ILE:HG21	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:HA	3:A:2002:SF4:S3	2.55	0.47
2:B:1235:ASN:ND2	2:B:1238:ARG:H	2.11	0.47
2:F:1376:LEU:HD22	2:F:1560:VAL:HG22	1.96	0.47
2:F:1054:TRP:HH2	2:F:1216:ASN:HD22	1.63	0.47
2:D:1376:LEU:HD22	2:D:1560:VAL:HG22	1.97	0.47
2:H:1313:ILE:HD11	2:H:1399:ALA:CB	2.44	0.47
2:D:1128:ARG:HD3	2:D:1128:ARG:O	2.15	0.47
2:D:1001:MET:HE2	2:D:1368:ASP:HA	1.96	0.47
2:F:1320:ALA:HB3	2:F:1323:GLU:HG3	1.96	0.47
2:B:1344:HIS:CD2	2:B:1346:TYR:H	2.32	0.47
2:F:1482:ILE:CD1	2:F:1482:ILE:C	2.79	0.47
1:E:194:PRO:HG3	1:G:193:ARG:HG2	1.96	0.46
1:C:139:ARG:HD3	9:C:5077:HOH:O	2.16	0.46
1:C:168:ARG:NH2	9:C:5866:HOH:O	2.45	0.46
2:D:1008:ASP:HB2	2:D:1018:ARG:HG3	1.97	0.46
2:H:1016:HIS:HD2	9:H:3609:HOH:O	1.98	0.46
2:H:1344:HIS:CD2	2:H:1346:TYR:H	2.33	0.46
2:H:1235:ASN:ND2	2:H:1238:ARG:H	2.13	0.46
2:H:1514:ALA:HB2	2:H:1526:TYR:CZ	2.51	0.46
1:E:189:ARG:HD3	1:E:232:THR:HG21	1.98	0.46
2:F:1514:ALA:HB2	2:F:1526:TYR:CE2	2.50	0.46
1:G:196:TYR:OH	1:G:270:PRO:HG2	2.16	0.46
2:B:1344:HIS:HD2	2:B:1346:TYR:H	1.63	0.46
2:B:1534:HIS:CE1	2:B:1548:THR:OG1	2.66	0.46
2:H:1190:HIS:HE1	9:H:3370:HOH:O	1.99	0.46
2:H:1534:HIS:CE1	2:H:1548:THR:OG1	2.63	0.46
2:B:1007:VAL:HG22	2:B:1010:ILE:HD13	1.98	0.45
2:D:1305:ILE:HD13	2:D:1310:LEU:HD12	1.98	0.45
2:F:1222:VAL:HB	9:F:3222:HOH:O	2.15	0.45
2:F:1376:LEU:HD22	2:F:1560:VAL:HG23	1.99	0.45
2:H:1308:ARG:HD3	2:H:1424:TYR:CG	2.51	0.45
1:E:187:HIS:HB2	1:E:224:PRO:HA	1.99	0.45
2:F:1295:PRO:HA	2:F:1298:PHE:CD1	2.52	0.45
2:H:1055:ALA:O	2:H:1059:ARG:HD3	2.16	0.45
2:H:1058:GLN:NE2	2:H:1066:LEU:H	2.06	0.45
1:E:223:GLY:N	1:E:224:PRO:CD	2.80	0.45
2:H:1523:ALA:HB1	2:H:1527:GLU:HB2	1.99	0.45
1:A:25:ARG:HH21	2:B:1212:ASN:ND2	2.00	0.45
2:D:1553:ASP:N	2:D:1554:PRO:HD3	2.32	0.45
2:F:1238:ARG:HD2	2:F:1238:ARG:HA	1.88	0.45
1:E:99:LEU:O	1:E:103:VAL:HB	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:PHE:O	2:F:1016:HIS:HE1	2.00	0.44
2:D:1018:ARG:HB3	2:D:1034:SER:HB3	2.00	0.44
2:B:1155:ILE:HD11	2:B:1188:VAL:HG11	1.99	0.44
1:C:50:ALA:HB1	1:C:54:ALA:HB3	1.99	0.44
2:D:1016:HIS:HD2	9:D:3703:HOH:O	2.00	0.44
2:D:1280:ASN:ND2	2:D:1307:ASP:H	2.16	0.44
1:E:25:ARG:HE	2:F:1212:ASN:ND2	2.15	0.44
1:G:25:ARG:HH21	2:H:1212:ASN:ND2	2.07	0.44
2:D:1464:ASN:ND2	2:D:1466:THR:H	2.15	0.44
2:H:1175:PRO:O	2:H:1178:ARG:NH1	2.50	0.44
2:H:1508:VAL:HG11	2:H:1558:CYS:HB3	1.99	0.44
2:D:1001:MET:O	2:D:1002:SER:CB	2.66	0.44
2:F:1001:MET:HB2	2:F:1004:ARG:NH1	2.29	0.44
1:G:241:TRP:CH2	1:G:243:VAL:HB	2.53	0.43
2:H:1464:ASN:C	2:H:1464:ASN:HD22	2.22	0.43
2:H:1047:GLY:O	2:H:1500:ARG:HD3	2.19	0.43
1:A:121:LEU:HB3	1:A:122:PRO:HD3	2.00	0.43
2:B:1178:ARG:CG	2:B:1178:ARG:HH21	2.30	0.43
2:B:1464:ASN:ND2	2:B:1466:THR:H	2.16	0.43
2:H:1340:ASP:HB2	9:H:6019:HOH:O	2.18	0.43
2:D:1066:LEU:CD1	2:D:1095:MET:HB3	2.48	0.43
2:D:1197:TRP:CE2	2:D:1201:THR:CG2	3.02	0.43
2:B:1092:ARG:HA	2:B:1095:MET:HE2	2.01	0.43
1:C:43:TYR:CD1	1:C:59:ARG:HB2	2.54	0.43
2:H:1064:CYS:SG	7:H:2005:NFV:C1	3.07	0.43
1:C:13:PHE:O	2:D:1016:HIS:HE1	2.01	0.43
2:F:1100:TYR:CD2	2:F:1440:LEU:CD1	3.02	0.43
1:E:43:TYR:CD1	1:E:59:ARG:HB2	2.54	0.42
2:F:1250:ARG:HA	2:F:1441:VAL:HG21	2.01	0.42
2:F:1499:GLY:O	2:F:1500:ARG:HD2	2.19	0.42
2:H:1404:GLN:HG2	2:H:1408:LEU:HD22	2.01	0.42
1:A:187:HIS:HB3	1:A:224:PRO:HA	2.01	0.42
2:B:1064:CYS:SG	7:B:2005:NFV:C1	3.07	0.42
1:E:10:TRP:CZ3	1:E:23:LEU:HD22	2.54	0.42
2:F:1518:ASP:OD2	2:F:1522:GLN:HG3	2.19	0.42
2:B:1035:GLY:HA3	2:B:1376:LEU:CD1	2.50	0.42
2:B:1532:ASP:O	2:B:1534:HIS:HD2	2.02	0.42
2:D:1139:ALA:O	2:D:1140:TRP:C	2.56	0.42
1:E:132:MET:HE1	1:E:137:LEU:HD13	2.01	0.42
1:G:25:ARG:NH2	2:H:1212:ASN:HD21	2.08	0.42
1:A:267:VAL:HG13	1:A:268:SER:N	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1513:ASN:HB3	2:D:1526:TYR:CE1	2.54	0.42
2:F:1553:ASP:N	2:F:1554:PRO:HD3	2.34	0.42
2:D:1464:ASN:ND2	2:D:1464:ASN:C	2.72	0.42
1:E:139:ARG:HD3	1:E:139:ARG:HA	1.75	0.42
1:E:196:TYR:C	1:E:196:TYR:CD2	2.92	0.42
2:F:1001:MET:HB3	2:F:1004:ARG:HH22	1.81	0.42
2:F:1345:PRO:HB2	2:F:1493:TRP:CD2	2.54	0.42
2:B:1330:HIS:C	2:B:1372:GLY:HA2	2.40	0.42
2:D:1002:SER:O	2:D:1003:GLU:CB	2.67	0.42
2:F:1190:HIS:HD2	2:F:1260:ASP:CG	2.21	0.42
2:H:1464:ASN:ND2	2:H:1466:THR:H	2.18	0.42
2:D:1269:LYS:HE2	2:D:1416:LEU:O	2.20	0.42
1:E:144:ILE:HD11	1:E:169:LEU:HD22	2.00	0.42
2:F:1001:MET:CB	2:F:1004:ARG:NH2	2.76	0.42
1:G:35:ILE:HD13	1:G:35:ILE:HG21	1.78	0.42
2:D:1514:ALA:HB2	2:D:1526:TYR:CZ	2.55	0.42
1:A:194:PRO:HG3	1:C:193:ARG:HG2	2.02	0.41
2:D:1197:TRP:O	2:D:1201:THR:HG23	2.20	0.41
1:E:150:PRO:HB2	1:E:151:PRO:HD2	2.02	0.41
1:E:48:GLN:HE21	1:E:48:GLN:HB2	1.70	0.41
1:E:84:ASN:HD22	1:E:86:GLY:N	2.10	0.41
2:H:1553:ASP:N	2:H:1554:PRO:HD3	2.35	0.41
2:B:1066:LEU:HD21	2:B:1070:ILE:HD12	2.01	0.41
1:C:121:LEU:HD12	2:D:1059:ARG:HB3	2.03	0.41
1:E:269:VAL:HA	1:E:270:PRO:HD3	1.75	0.41
2:F:1243:ARG:HH21	2:F:1243:ARG:CG	2.30	0.41
2:H:1238:ARG:HA	2:H:1238:ARG:HD2	1.76	0.41
2:B:1004:ARG:HD2	2:B:1020:GLU:HB3	2.02	0.41
2:D:1238:ARG:HD2	2:D:1238:ARG:HA	1.75	0.41
2:H:1089:GLN:HG2	2:H:1290:GLY:O	2.20	0.41
1:A:92:GLY:O	2:B:1363:PRO:HA	2.20	0.41
2:F:1404:GLN:HG2	2:F:1408:LEU:HD22	2.02	0.41
1:A:121:LEU:HD12	2:B:1059:ARG:HB3	2.02	0.41
2:D:1345:PRO:HB2	2:D:1493:TRP:CD2	2.56	0.41
2:F:1014:GLU:HB3	2:F:1555:CYS:HA	2.03	0.41
2:B:1345:PRO:HB2	2:B:1493:TRP:CD2	2.56	0.41
2:B:1345:PRO:HB2	2:B:1493:TRP:CG	2.56	0.41
2:D:1001:MET:CE	2:D:1004:ARG:HH22	2.34	0.41
2:B:1464:ASN:C	2:B:1464:ASN:ND2	2.75	0.40
1:C:153:PRO:HD3	1:C:235:TRP:CZ3	2.56	0.40
2:F:1065:THR:OG1	2:F:1214:HIS:HD2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:ILE:HG22	1:G:164:LEU:HD22	2.03	0.40
1:A:187:HIS:CB	1:A:224:PRO:HA	2.51	0.40
1:A:209:GLY:HA2	1:A:214:TRP:CD2	2.56	0.40
2:B:1238:ARG:HA	2:B:1238:ARG:HD2	1.93	0.40
2:B:1401:GLY:HA2	2:B:1406:ARG:HE	1.86	0.40
1:C:254:GLU:HA	1:C:255:PRO:HD3	1.87	0.40
1:E:35:ILE:HG21	1:E:35:ILE:HD13	1.85	0.40
1:C:28:ALA:HA	1:C:29:PRO:HA	1.99	0.40
1:C:48:GLN:HB2	1:C:48:GLN:HE21	1.54	0.40
2:F:1532:ASP:O	2:F:1534:HIS:HD2	2.04	0.40
2:H:1250:ARG:HA	2:H:1441:VAL:HG21	2.03	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	266/269 (99%)	254 (96%)	11 (4%)	1 (0%)	34	32
1	C	267/269 (99%)	259 (97%)	7 (3%)	1 (0%)	34	32
1	E	266/269 (99%)	256 (96%)	9 (3%)	1 (0%)	34	32
1	G	266/269 (99%)	254 (96%)	12 (4%)	0	100	100
2	B	557/561 (99%)	546 (98%)	11 (2%)	0	100	100
2	D	559/561 (100%)	539 (96%)	19 (3%)	1 (0%)	47	49
2	F	559/561 (100%)	540 (97%)	19 (3%)	0	100	100
2	H	557/561 (99%)	543 (98%)	14 (2%)	0	100	100
All	All	3297/3320 (99%)	3191 (97%)	102 (3%)	4 (0%)	51	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	C	4	ARG
2	D	1002	SER
1	E	4	ARG

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	213/214 (100%)	199 (93%)	14 (7%)	16	14
1	C	214/214 (100%)	197 (92%)	17 (8%)	12	9
1	E	213/214 (100%)	200 (94%)	13 (6%)	18	16
1	G	213/214 (100%)	203 (95%)	10 (5%)	26	25
2	B	452/454 (100%)	426 (94%)	26 (6%)	20	17
2	D	454/454 (100%)	421 (93%)	33 (7%)	14	11
2	F	454/454 (100%)	421 (93%)	33 (7%)	14	11
2	H	452/454 (100%)	424 (94%)	28 (6%)	18	15
All	All	2665/2672 (100%)	2491 (94%)	174 (6%)	17	14

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	15	GLU
1	A	31	LEU
1	A	53	GLU
1	A	71	LEU
1	A	84	ASN
1	A	121	LEU
1	A	123	GLN
1	A	137	LEU
1	A	164	LEU
1	A	168	ARG
1	A	242	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	267	VAL
1	A	269	VAL
2	B	1007	VAL
2	B	1080	LEU
2	B	1081	ARG
2	B	1090	LEU
2	B	1112	HIS
2	B	1133	LEU
2	B	1153	LYS
2	B	1200	ASP
2	B	1212	ASN
2	B	1228	LEU
2	B	1234	LEU
2	B	1235	ASN
2	B	1292	SER
2	B	1293	LEU
2	B	1310	LEU
2	B	1369	VAL
2	B	1406	ARG
2	B	1414	SER
2	B	1421	ASP
2	B	1427	LEU
2	B	1441	VAL
2	B	1464	ASN
2	B	1466	THR
2	B	1483	MET
2	B	1520	ARG
2	B	1542	PRO
1	C	4	ARG
1	C	15	GLU
1	C	31	LEU
1	C	71	LEU
1	C	84	ASN
1	C	97	SER
1	C	99	LEU
1	C	102	THR
1	C	121	LEU
1	C	137	LEU
1	C	139	ARG
1	C	140	ASP
1	C	141	LYS
1	C	164	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	168	ARG
1	C	218	ARG
1	C	242	PRO
2	D	1003	GLU
2	D	1080	LEU
2	D	1081	ARG
2	D	1090	LEU
2	D	1111	LEU
2	D	1112	HIS
2	D	1128	ARG
2	D	1133	LEU
2	D	1191	TYR
2	D	1201	THR
2	D	1212	ASN
2	D	1228	LEU
2	D	1235	ASN
2	D	1238	ARG
2	D	1243	ARG
2	D	1282	LEU
2	D	1292	SER
2	D	1293	LEU
2	D	1297	THR
2	D	1299	LEU
2	D	1310	LEU
2	D	1321	THR
2	D	1350	THR
2	D	1408	LEU
2	D	1414	SER
2	D	1427	LEU
2	D	1464	ASN
2	D	1466	THR
2	D	1483	MET
2	D	1486	PRO
2	D	1500	ARG
2	D	1520	ARG
2	D	1537	VAL
1	E	4	ARG
1	E	15	GLU
1	E	31	LEU
1	E	69	GLN
1	E	71	LEU
1	E	84	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	99	LEU
1	E	103	VAL
1	E	121	LEU
1	E	137	LEU
1	E	164	LEU
1	E	168	ARG
1	E	189	ARG
2	F	1001	MET
2	F	1046	LYS
2	F	1080	LEU
2	F	1086	LEU
2	F	1090	LEU
2	F	1112	HIS
2	F	1128	ARG
2	F	1133	LEU
2	F	1200	ASP
2	F	1201	THR
2	F	1212	ASN
2	F	1228	LEU
2	F	1234	LEU
2	F	1235	ASN
2	F	1243	ARG
2	F	1289	THR
2	F	1293	LEU
2	F	1297	THR
2	F	1299	LEU
2	F	1310	LEU
2	F	1316	VAL
2	F	1334	GLU
2	F	1369	VAL
2	F	1408	LEU
2	F	1411	SER
2	F	1415	ARG
2	F	1427	LEU
2	F	1441	VAL
2	F	1464	ASN
2	F	1483	MET
2	F	1520	ARG
2	F	1522	GLN
2	F	1536	LEU
1	G	4	ARG
1	G	15	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	31	LEU
1	G	84	ASN
1	G	123	GLN
1	G	164	LEU
1	G	168	ARG
1	G	218	ARG
1	G	242	PRO
1	G	267	VAL
2	H	1080	LEU
2	H	1086	LEU
2	H	1112	HIS
2	H	1133	LEU
2	H	1212	ASN
2	H	1228	LEU
2	H	1234	LEU
2	H	1235	ASN
2	H	1261	THR
2	H	1282	LEU
2	H	1293	LEU
2	H	1297	THR
2	H	1299	LEU
2	H	1316	VAL
2	H	1318	LEU
2	H	1321	THR
2	H	1350	THR
2	H	1369	VAL
2	H	1376	LEU
2	H	1407	GLU
2	H	1408	LEU
2	H	1423	LEU
2	H	1427	LEU
2	H	1435	LEU
2	H	1464	ASN
2	H	1476	ARG
2	H	1483	MET
2	H	1500	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	123	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	162	HIS
2	B	1016	HIS
2	B	1030	GLN
2	B	1058	GLN
2	B	1089	GLN
2	B	1093	ASN
2	B	1112	HIS
2	B	1152	GLN
2	B	1169	ASN
2	B	1190	HIS
2	B	1212	ASN
2	B	1214	HIS
2	B	1216	ASN
2	B	1235	ASN
2	B	1330	HIS
2	B	1344	HIS
2	B	1402	HIS
2	B	1445	GLN
2	B	1454	ASN
2	B	1464	ASN
2	B	1533	ASN
2	B	1534	HIS
2	B	1535	GLN
1	C	27	HIS
1	C	48	GLN
1	C	84	ASN
1	C	162	HIS
1	C	184	GLN
2	D	1016	HIS
2	D	1030	GLN
2	D	1058	GLN
2	D	1093	ASN
2	D	1112	HIS
2	D	1135	GLN
2	D	1152	GLN
2	D	1169	ASN
2	D	1190	HIS
2	D	1212	ASN
2	D	1214	HIS
2	D	1216	ASN
2	D	1235	ASN
2	D	1280	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	1330	HIS
2	D	1344	HIS
2	D	1402	HIS
2	D	1454	ASN
2	D	1464	ASN
2	D	1505	GLN
2	D	1533	ASN
2	D	1534	HIS
2	D	1535	GLN
1	E	48	GLN
1	E	69	GLN
1	E	84	ASN
1	E	162	HIS
1	E	184	GLN
2	F	1016	HIS
2	F	1058	GLN
2	F	1093	ASN
2	F	1112	HIS
2	F	1135	GLN
2	F	1152	GLN
2	F	1169	ASN
2	F	1190	HIS
2	F	1212	ASN
2	F	1214	HIS
2	F	1216	ASN
2	F	1235	ASN
2	F	1330	HIS
2	F	1344	HIS
2	F	1402	HIS
2	F	1454	ASN
2	F	1464	ASN
2	F	1533	ASN
2	F	1534	HIS
2	F	1535	GLN
1	G	84	ASN
1	G	123	GLN
1	G	184	GLN
2	H	1016	HIS
2	H	1030	GLN
2	H	1058	GLN
2	H	1093	ASN
2	H	1112	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	1169	ASN
2	H	1190	HIS
2	H	1212	ASN
2	H	1214	HIS
2	H	1216	ASN
2	H	1235	ASN
2	H	1330	HIS
2	H	1344	HIS
2	H	1402	HIS
2	H	1445	GLN
2	H	1454	ASN
2	H	1464	ASN
2	H	1522	GLN
2	H	1533	ASN
2	H	1534	HIS
2	H	1535	GLN

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 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 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
7	NFV	F	2005	2	3,8,8	1.95	1 (33%)	-		
7	NFV	D	2005	2	3,8,8	2.81	1 (33%)	-		
4	F3S	A	2003	1	0,9,9	0.00	-	-		
3	SF4	G	2002	1	0,12,12	0.00	-	-		
3	SF4	C	2002	1	0,12,12	0.00	-	-		
3	SF4	C	2001[B]	1	0,12,12	0.00	-	-		
5	IMD	A	3002	-	3,5,5	0.71	0	4,5,5	0.38	0
3	SF4	G	2001[B]	1	0,12,12	0.00	-	-		
3	SF4	C	2001[A]	1	0,12,12	0.00	-	-		
3	SF4	G	2001[A]	1	0,12,12	0.00	-	-		
4	F3S	E	2003	1	0,9,9	0.00	-	-		
7	NFV	H	2005	2	3,8,8	2.36	2 (66%)	-		
4	F3S	C	2003	1	0,9,9	0.00	-	-		
3	SF4	A	2002	1	0,12,12	0.00	-	-		
7	NFV	B	2005	2	3,8,8	3.16	2 (66%)	-		
5	IMD	G	3001	-	3,5,5	0.53	0	4,5,5	0.86	0
3	SF4	A	2001[A]	1	0,12,12	0.00	-	-		
3	SF4	A	2001[B]	1	0,12,12	0.00	-	-		
3	SF4	E	2002	1	0,12,12	0.00	-	-		
3	SF4	E	2001[A]	1	0,12,12	0.00	-	-		
3	SF4	E	2001[B]	1	0,12,12	0.00	-	-		
4	F3S	G	2003	1	0,9,9	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	G	2001[B]	1	-	-	0/6/5/5
3	SF4	E	2001[A]	1	-	-	0/6/5/5
3	SF4	C	2001[A]	1	-	-	0/6/5/5
5	IMD	G	3001	-	-	-	0/1/1/1
4	F3S	C	2003	1	-	-	0/3/3/3
3	SF4	G	2001[A]	1	-	-	0/6/5/5
4	F3S	E	2003	1	-	-	0/3/3/3
3	SF4	A	2001[A]	1	-	-	0/6/5/5
4	F3S	A	2003	1	-	-	0/3/3/3
3	SF4	A	2001[B]	1	-	-	0/6/5/5
3	SF4	E	2001[B]	1	-	-	0/6/5/5
3	SF4	G	2002	1	-	-	0/6/5/5
5	IMD	A	3002	-	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	E	2002	1	-	-	0/6/5/5
3	SF4	C	2002	1	-	-	0/6/5/5
3	SF4	A	2002	1	-	-	0/6/5/5
3	SF4	C	2001[B]	1	-	-	0/6/5/5
4	F3S	G	2003	1	-	-	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2005	NFV	O1-C1	4.40	1.24	1.16
7	D	2005	NFV	O1-C1	4.17	1.24	1.16
7	H	2005	NFV	O1-C1	3.08	1.22	1.16
7	F	2005	NFV	O1-C1	2.75	1.21	1.16
7	B	2005	NFV	C2-N2	2.58	1.18	1.13
7	H	2005	NFV	C3-N3	2.50	1.18	1.13

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	2005	NFV	5	0
7	D	2005	NFV	5	0
3	C	2002	SF4	1	0
5	A	3002	IMD	1	0
7	H	2005	NFV	5	0
3	A	2002	SF4	1	0
7	B	2005	NFV	5	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	268/269 (99%)	-0.36	3 (1%) 80 84	14, 22, 39, 78	0
1	C	269/269 (100%)	-0.33	4 (1%) 73 77	15, 27, 45, 62	0
1	E	268/269 (99%)	-0.33	4 (1%) 73 77	20, 31, 49, 76	0
1	G	268/269 (99%)	-0.45	4 (1%) 73 77	17, 25, 43, 87	0
2	B	559/561 (99%)	-0.60	0 100 100	16, 25, 40, 55	0
2	D	561/561 (100%)	-0.30	11 (1%) 65 69	19, 32, 50, 84	0
2	F	561/561 (100%)	-0.32	14 (2%) 57 62	20, 31, 47, 80	0
2	H	559/561 (99%)	-0.47	2 (0%) 92 93	19, 28, 44, 58	0
All	All	3313/3320 (99%)	-0.40	42 (1%) 77 80	14, 28, 47, 87	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1002	SER	5.0
1	G	3	ALA	5.0
1	E	3	ALA	4.6
2	F	1001	MET	4.6
1	G	270	PRO	4.3
2	D	1001	MET	4.2
1	G	269	VAL	4.1
2	D	1002	SER	3.9
1	G	268	SER	3.6
2	D	1003	GLU	3.6
1	C	271	LEU	3.5
1	C	3	ALA	3.4
2	F	1337	VAL	3.2
1	A	269	VAL	3.2
2	F	1063	VAL	3.1
1	A	3	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	1337	VAL	3.0
2	F	1356	ARG	2.9
2	D	1063	VAL	2.8
2	D	1026	ALA	2.7
2	D	1356	ARG	2.7
2	D	1025	GLY	2.7
1	C	67	ARG	2.7
2	F	1336	SER	2.7
1	E	67	ARG	2.7
2	F	1003	GLU	2.5
1	E	270	PRO	2.5
2	H	1063	VAL	2.4
2	F	1312	THR	2.3
2	F	1060	ILE	2.3
1	A	268	SER	2.2
2	F	1064	CYS	2.2
2	F	1341	ARG	2.2
2	H	1060	ILE	2.2
1	C	23	LEU	2.2
2	D	1417	ASP	2.1
2	D	1421	ASP	2.1
2	F	1081	ARG	2.1
1	E	16	CYS	2.1
2	F	1555	CYS	2.1
2	D	1367	LEU	2.0
2	F	1313	ILE	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. 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(\AA^2)	Q<0.9
5	IMD	A	3002	5/5	0.93	0.11	37,38,39,42	0
5	IMD	G	3001	5/5	0.94	0.11	38,39,40,42	0
8	MG	B	2006	1/1	0.96	0.03	13,13,13,13	0
8	MG	D	2006	1/1	0.96	0.09	17,17,17,17	0
8	MG	H	2006	1/1	0.96	0.04	16,16,16,16	0
8	MG	F	2006	1/1	0.97	0.06	18,18,18,18	0
3	SF4	E	2001[A]	8/8	0.98	0.07	18,22,23,27	2
3	SF4	E	2001[B]	8/8	0.98	0.07	19,22,24,27	2
3	SF4	E	2002	8/8	0.98	0.04	14,16,18,18	0
7	NFV	D	2005	9/9	0.99	0.07	13,17,19,22	0
3	SF4	G	2002	8/8	0.99	0.03	14,15,15,15	0
6	CL	E	2004	1/1	0.99	0.13	24,24,24,24	0
3	SF4	C	2001[B]	8/8	0.99	0.08	16,19,22,26	2
6	CL	C	2004	1/1	0.99	0.12	20,20,20,20	0
3	SF4	A	2001[A]	8/8	0.99	0.11	15,18,21,21	2
7	NFV	F	2005	9/9	0.99	0.06	15,18,21,22	0
3	SF4	A	2001[B]	8/8	0.99	0.11	15,19,21,22	2
3	SF4	G	2001[B]	8/8	0.99	0.10	18,20,22,26	2
3	SF4	C	2001[A]	8/8	0.99	0.08	16,18,22,22	2
6	CL	A	2004	1/1	0.99	0.09	20,20,20,20	0
3	SF4	G	2001[A]	8/8	0.99	0.10	16,20,22,24	2
4	F3S	G	2003	7/7	0.99	0.04	14,15,16,16	0
4	F3S	E	2003	7/7	0.99	0.05	16,17,18,19	0
7	NFV	H	2005	9/9	1.00	0.09	13,15,20,22	0
4	F3S	A	2003	7/7	1.00	0.07	12,13,14,16	0
6	CL	G	2004	1/1	1.00	0.12	21,21,21,21	0
3	SF4	C	2002	8/8	1.00	0.04	14,15,16,17	0
4	F3S	C	2003	7/7	1.00	0.07	14,15,16,16	0
3	SF4	A	2002	8/8	1.00	0.04	12,13,14,14	0
7	NFV	B	2005	9/9	1.00	0.10	13,16,20,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.