Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:32 PM GMT

PDB ID	:	4FAS
Title	:	Complex crystal structure of hydroxylamine oxidoreductase and NE1300 from Nitrosomonas europaea
Authors	:	Cedervall, P.E.; Wilmot, C.M.
Deposited on	:	2012-05-22
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

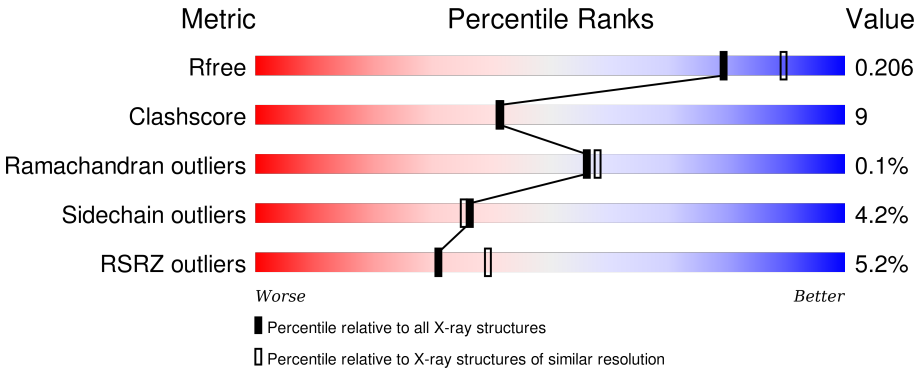
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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. 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 <=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	546	% 77% 14% • 8%
1	B	546	% 76% 14% • 8%
1	C	546	3% 78% 13% • 8%
2	D	69	30% 62% 9% 29%
2	E	69	41% 52% 16% • 29%

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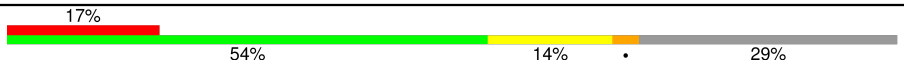
Mol	Chain	Length	Quality of chain
2	F	69	

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
10	NO3	B	617	-	X	-	-
10	NO3	B	618	-	X	-	-
10	NO3	C	619	-	X	-	-
10	NO3	F	101	-	X	-	-
5	PEG	A	610	-	-	-	X
5	PEG	A	611	-	-	-	X
5	PEG	A	614	-	-	-	X
5	PEG	B	610	-	-	-	X
5	PEG	B	612	-	-	-	X
5	PEG	C	610	-	-	-	X
5	PEG	C	613	-	-	-	X
6	PGE	A	615	-	-	-	X
6	PGE	C	614	-	-	-	X
7	EDO	B	616	-	-	-	X
7	EDO	B	621	-	-	-	X
9	PG4	B	614	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 15197 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.

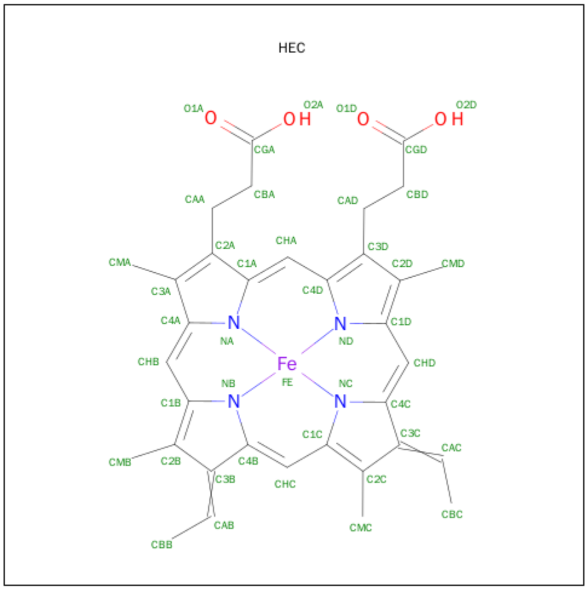
- Molecule 1 is a protein called Hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	0	1	0
			4013	2495	711	775	32			
1	B	502	Total	C	N	O	S	0	1	0
			4005	2491	710	772	32			
1	C	502	Total	C	N	O	S	0	0	0
			4005	2491	710	772	32			

- Molecule 2 is a protein called NE1300.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	49	Total	C	N	O	S	0	0	0
			370	233	63	71	3			
2	E	49	Total	C	N	O	S	0	0	0
			370	233	63	71	3			
2	F	49	Total	C	N	O	S	0	0	0
			370	233	63	71	3			

- Molecule 3 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0

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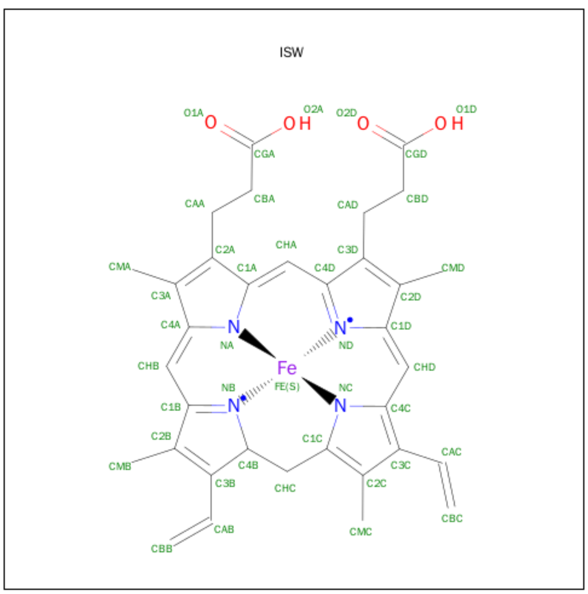
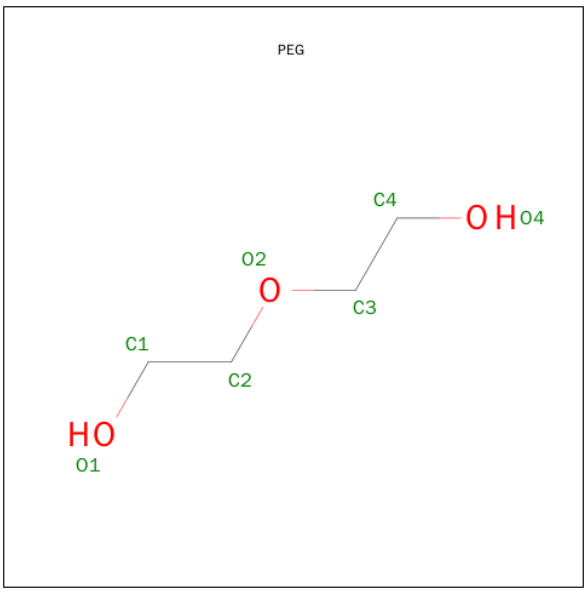
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C Fe N O 43 34 1 4 4	0	0
3	C	1	Total C Fe N O 43 34 1 4 4	0	0
3	C	1	Total C Fe N O 43 34 1 4 4	0	0
3	C	1	Total C Fe N O 43 34 1 4 4	0	0
3	C	1	Total C Fe N O 43 34 1 4 4	0	0
3	C	1	Total C Fe N O 43 34 1 4 4	0	0
3	C	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 4 is {3,3'-[(9S)-8,13-DIETHENYL-3,7,12,17-TETRAMETHYL-9,10-DIHYDROPORPHYRIN-2,18-DIYL-KAPPA 4 N 21 ,N 22 ,N 23 ,N 24]DIPROPANOATO(2-)}IRON (three-letter code: ISW) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Fe N O 43 34 1 4 4	0	0
4	B	1	Total C Fe N O 43 34 1 4 4	0	0
4	C	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0

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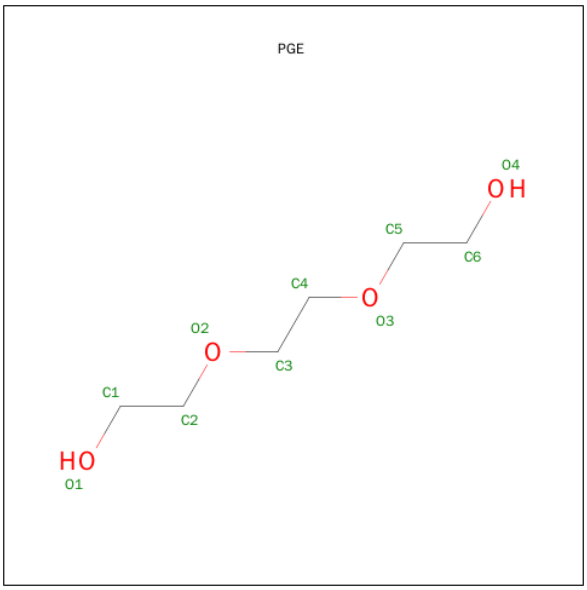
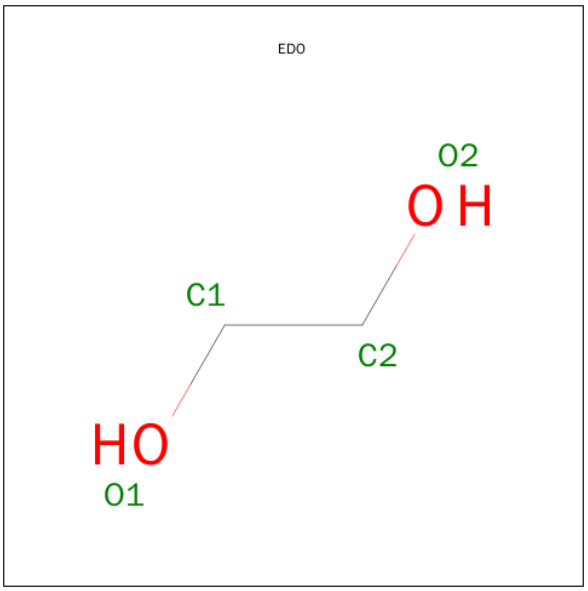
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 6 4	0	0
6	C	1	Total C O 10 6 4	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0

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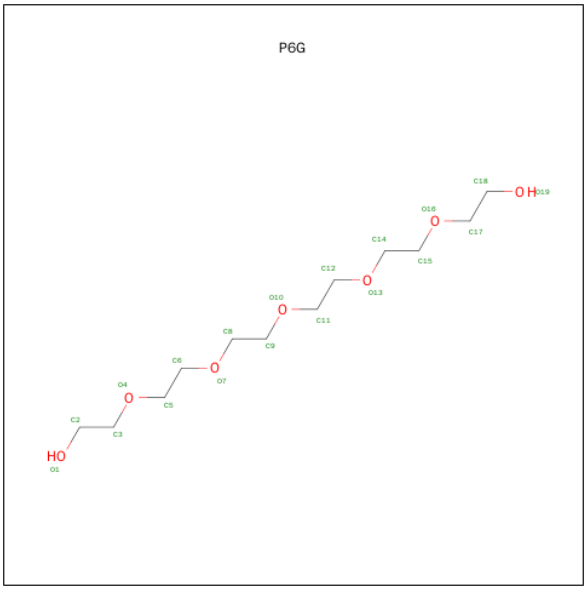
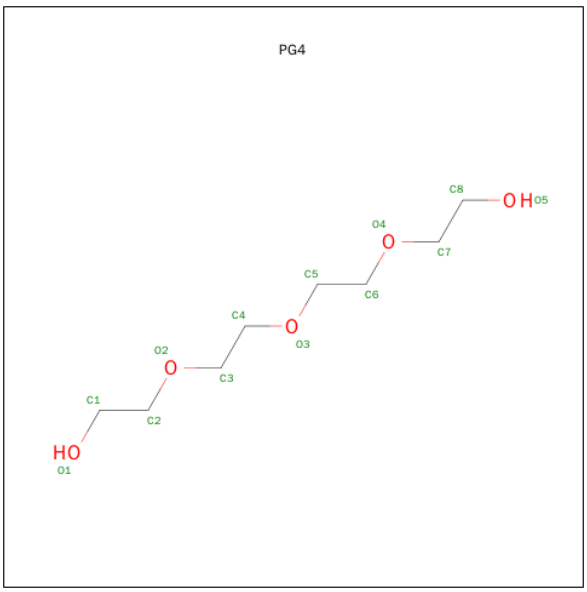
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	0

- Molecule 8 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



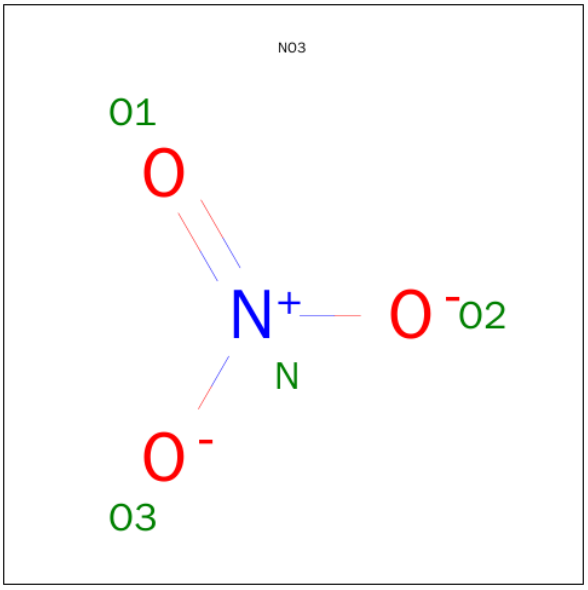
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 19 12 7	0	0

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 13 8 5	0	0

- Molecule 10 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total N O 4 1 3	0	0
10	B	1	Total N O 4 1 3	0	0
10	C	1	Total N O 4 1 3	0	0
10	F	1	Total N O 4 1 3	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	237	Total O 237 237	0	0
11	B	258	Total O 258 258	0	0
11	C	244	Total O 244 244	0	0
11	D	14	Total O 14 14	0	0
11	E	10	Total O 10 10	0	0

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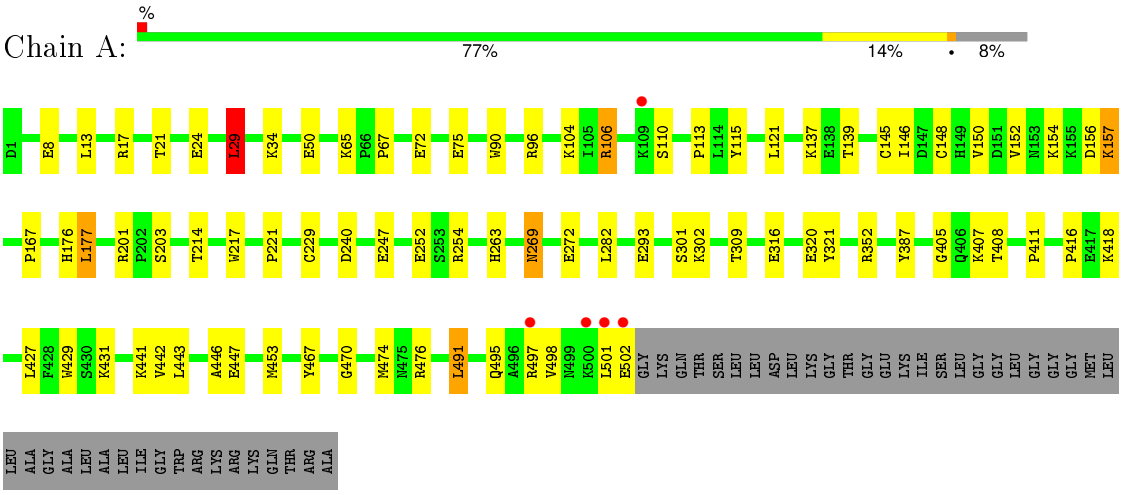
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	F	22	Total O 22 22	0	0

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.

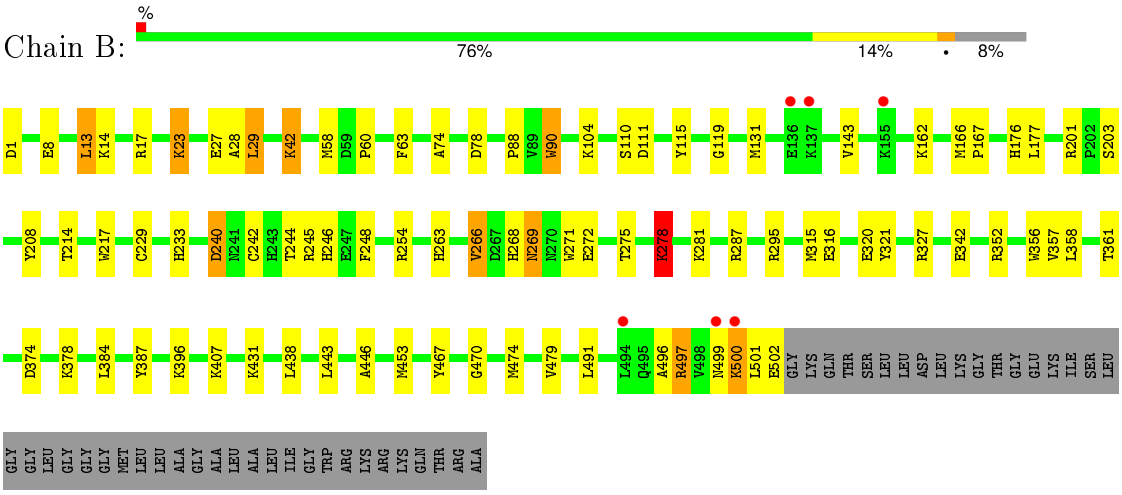
- Molecule 1: Hydroxylamine oxidoreductase

Chain A:



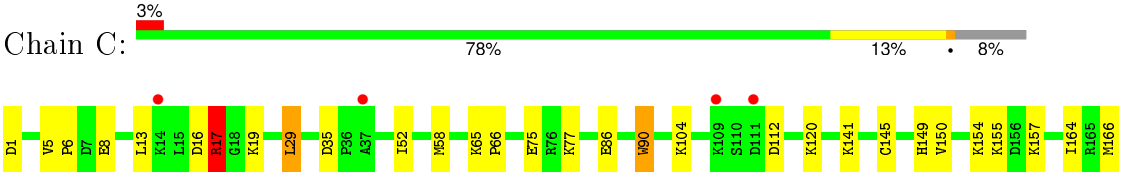
- Molecule 1: Hydroxylamine oxidoreductase

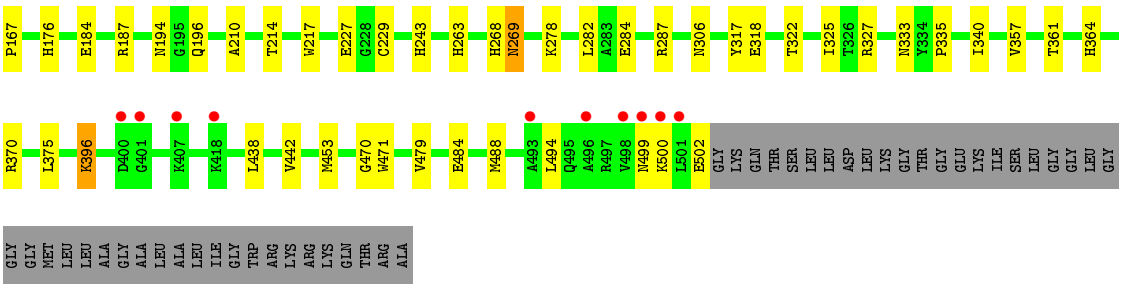
Chain B:



- Molecule 1: Hydroxylamine oxidoreductase

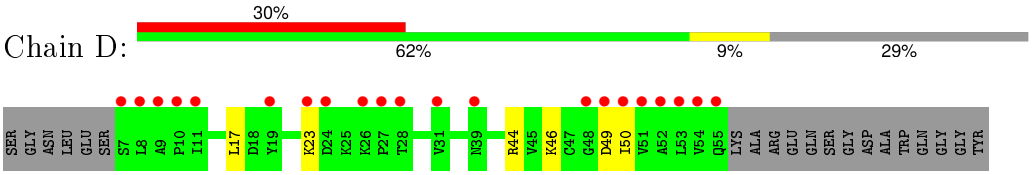
Chain C:





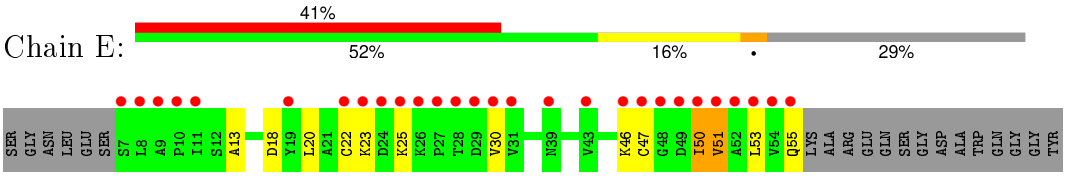
- Molecule 2: NE1300

Chain D:



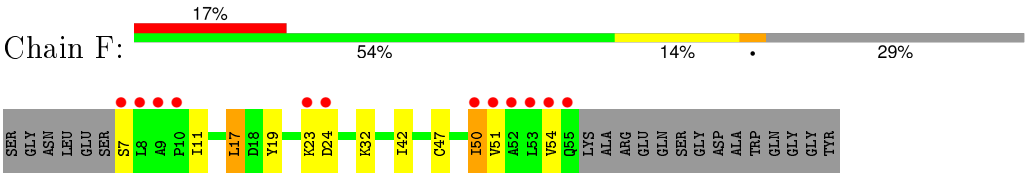
- Molecule 2: NE1300

Chain E:



- Molecule 2: NE1300

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	140.73Å 142.62Å 107.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.89 – 2.10 42.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	79.9 (42.89-2.10) 79.9 (42.89-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.165 , 0.206 0.166 , 0.206	Depositor DCC
R_{free} test set	5071 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 56.4	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 100626 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15197	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PGE, ISW, EDO, PG4, P6G, HEC, PEG, NO3

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	1.07	5/4116 (0.1%)	0.92	8/5578 (0.1%)
1	B	1.10	8/4108 (0.2%)	0.96	11/5567 (0.2%)
1	C	1.07	1/4108 (0.0%)	0.92	5/5567 (0.1%)
2	D	0.78	0/373	0.87	0/502
2	E	0.76	0/373	0.86	0/502
2	F	0.87	0/373	0.96	1/502 (0.2%)
All	All	1.06	14/13451 (0.1%)	0.93	25/18218 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	GLU	CG-CD	5.90	1.60	1.51
1	B	266	VAL	CB-CG1	-5.85	1.40	1.52
1	B	272	GLU	CG-CD	5.78	1.60	1.51
1	B	242	CYS	CB-SG	-5.52	1.72	1.81
1	A	148	CYS	CB-SG	-5.45	1.73	1.81
1	B	320	GLU	CG-CD	5.42	1.60	1.51
1	B	208	TYR	CD1-CE1	5.28	1.47	1.39
1	C	471	TRP	CE3-CZ3	5.26	1.47	1.38
1	A	293	GLU	CG-CD	5.25	1.59	1.51
1	A	72	GLU	CG-CD	5.21	1.59	1.51
1	A	320	GLU	CG-CD	5.18	1.59	1.51
1	B	356	TRP	CE3-CZ3	5.15	1.47	1.38
1	B	272	GLU	CB-CG	5.14	1.61	1.52
1	B	278	LYS	CB-CG	-5.07	1.38	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	ARG	NE-CZ-NH1	6.10	123.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	295	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	58	MET	CG-SD-CE	5.93	109.69	100.20
1	A	254	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	B	17	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	315	MET	CG-SD-CE	5.90	109.63	100.20
1	B	266	VAL	CB-CA-C	-5.88	100.22	111.40
1	A	17	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	177	LEU	CB-CG-CD2	5.73	120.75	111.00
1	C	112	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	111	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	476	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	352	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	438	LEU	CA-CB-CG	5.44	127.82	115.30
1	C	438	LEU	CB-CG-CD1	-5.44	101.75	111.00
2	F	17	LEU	CB-CG-CD1	5.44	120.25	111.00
1	A	29	LEU	CA-CB-CG	5.41	127.73	115.30
1	B	240	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	58	MET	CG-SD-CE	5.39	108.83	100.20
1	A	240	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	327	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	106	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	254	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	35	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	17	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4013	0	3811	59	0
1	B	4005	0	3807	66	0
1	C	4005	0	3808	64	0
2	D	370	0	391	1	0
2	E	370	0	391	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	370	0	391	8	0
3	A	301	0	210	15	0
3	B	301	0	210	17	0
3	C	301	0	210	20	0
4	A	43	0	28	11	0
4	B	43	0	28	14	0
4	C	43	0	28	11	0
5	A	42	0	60	5	0
5	B	28	0	40	4	0
5	C	42	0	60	4	0
5	F	7	0	10	1	0
6	A	10	0	14	2	0
6	C	10	0	14	4	0
7	A	16	0	24	2	0
7	B	20	0	30	0	0
7	C	24	0	36	3	0
8	B	19	0	26	1	0
9	B	13	0	18	1	0
10	B	8	0	0	0	0
10	C	4	0	0	0	0
10	F	4	0	0	0	0
11	A	237	0	0	4	0
11	B	258	0	0	1	0
11	C	244	0	0	3	0
11	D	14	0	0	0	0
11	E	10	0	0	0	0
11	F	22	0	0	1	0
All	All	15197	0	13645	239	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 9.

All (239) 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)
4:A:608:ISW:HBAA	3:B:605:HEC:O1D	1.65	0.96
4:B:608:ISW:HBAA	3:C:606:HEC:O1D	1.66	0.95
1:B:497:ARG:HH11	1:B:497:ARG:HB2	1.31	0.95
1:B:497:ARG:HH11	1:B:497:ARG:CB	1.80	0.94
5:A:614:PEG:H42	4:C:601:ISW:HMAA	1.49	0.93
1:B:13:LEU:HD21	1:B:29:LEU:HD13	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD11	1:A:29:LEU:HD13	1.55	0.89
1:B:104:LYS:HE3	5:B:609:PEG:H22	1.54	0.87
1:A:495:GLN:HG2	1:C:494:LEU:HD13	1.61	0.81
1:C:13:LEU:HD11	1:C:29:LEU:HD13	1.64	0.80
1:B:104:LYS:CE	5:B:609:PEG:H22	2.12	0.79
2:E:30:VAL:HG22	2:E:46:LYS:HA	1.64	0.79
3:C:608:HEC:HMB1	3:C:608:HEC:HBB3	1.65	0.78
1:B:497:ARG:CG	1:B:497:ARG:HH11	1.96	0.77
3:A:605:HEC:O1D	4:C:601:ISW:HBAA	1.83	0.77
1:B:119:GLY:HA3	8:B:613:P6G:H61	1.68	0.75
1:A:407:LYS:HE3	5:A:613:PEG:H11	1.69	0.74
4:A:608:ISW:HMB	4:A:608:ISW:HBB	1.70	0.74
1:B:497:ARG:HB2	1:B:497:ARG:NH1	2.03	0.73
1:C:269:ASN:HD22	1:C:269:ASN:H	1.36	0.71
1:A:405:GLY:HA2	1:A:408:THR:CG2	2.21	0.70
1:A:407:LYS:CE	5:A:613:PEG:H11	2.21	0.70
2:D:46:LYS:HB3	2:D:49:ASP:OD2	1.90	0.70
1:A:405:GLY:HA2	1:A:408:THR:HG22	1.73	0.69
3:B:601:HEC:CAA	3:B:602:HEC:HMA3	2.22	0.69
1:B:497:ARG:CB	1:B:497:ARG:NH1	2.56	0.69
1:C:396:LYS:HE2	1:C:396:LYS:HA	1.74	0.69
1:A:8:GLU:OE1	1:A:8:GLU:N	2.28	0.67
3:C:602:HEC:HMC1	3:C:602:HEC:HBC3	1.78	0.66
1:A:431:LYS:HE3	11:F:212:HOH:O	1.95	0.66
1:B:8:GLU:OE1	1:B:8:GLU:N	2.20	0.66
1:C:104:LYS:NZ	6:C:614:PGE:H42	2.11	0.65
3:C:602:HEC:CAA	3:C:603:HEC:HMA3	2.26	0.65
1:A:498:VAL:O	1:A:502:GLU:HG3	1.96	0.64
3:B:606:HEC:HMC1	3:B:606:HEC:HBC3	1.80	0.64
1:B:248:PHE:O	3:B:603:HEC:HBA1	1.98	0.64
1:A:214:THR:HG21	4:C:601:ISW:HMBA	1.81	0.63
1:C:13:LEU:CD1	1:C:29:LEU:HD13	2.28	0.62
1:B:13:LEU:CD2	1:B:29:LEU:HD13	2.27	0.62
1:C:90:TRP:HA	1:C:90:TRP:CE3	2.33	0.62
4:B:608:ISW:HMB	4:B:608:ISW:HBB	1.81	0.62
3:A:605:HEC:O2A	4:C:601:ISW:O2D	2.18	0.62
3:B:601:HEC:HBB3	3:B:601:HEC:HMB1	1.82	0.62
1:A:34:LYS:NZ	11:A:832:HOH:O	2.32	0.62
3:B:607:HEC:HMB1	3:B:607:HEC:HBB3	1.82	0.61
1:B:374:ASP:OD1	1:B:378:LYS:HE2	2.01	0.61
1:A:316:GLU:HB2	1:A:321:TYR:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASN:H	1:A:269:ASN:HD22	1.48	0.60
1:C:333:ASN:O	1:C:335:PRO:HD3	2.01	0.60
1:C:19:LYS:NZ	7:C:617:EDO:H21	2.17	0.59
1:C:86:GLU:HG3	3:C:602:HEC:HMD3	1.84	0.59
3:B:601:HEC:HAA2	3:B:602:HEC:HMA3	1.84	0.59
4:A:608:ISW:HHC	1:B:229:CYS:SG	2.42	0.59
4:B:608:ISW:HMBA	1:C:214:THR:HG21	1.84	0.59
1:C:13:LEU:HD11	1:C:29:LEU:CD1	2.31	0.59
1:B:387:TYR:CE1	1:B:446:ALA:HB2	2.38	0.58
1:B:269:ASN:HD22	1:B:269:ASN:H	1.50	0.58
1:C:194:ASN:HB3	2:F:7:SER:HB3	1.86	0.57
1:A:201:ARG:NE	4:C:601:ISW:O1A	2.29	0.57
1:A:229:CYS:SG	4:C:601:ISW:HHC	2.45	0.57
3:C:606:HEC:HBB3	3:C:606:HEC:HMB1	1.87	0.56
1:C:90:TRP:HE3	1:C:90:TRP:HA	1.71	0.56
2:F:11:ILE:HD13	2:F:54:VAL:HG22	1.87	0.56
4:C:601:ISW:HBB	4:C:601:ISW:HMB	1.87	0.55
1:B:23:LYS:HG3	1:B:131:MET:HA	1.88	0.55
1:A:495:GLN:HG2	1:C:494:LEU:CD1	2.32	0.55
3:C:608:HEC:HBB3	3:C:608:HEC:CMB	2.37	0.55
3:A:601:HEC:CAA	3:A:602:HEC:HMA3	2.37	0.55
4:B:608:ISW:HHC	1:C:229:CYS:SG	2.46	0.54
1:B:501:LEU:HD11	1:C:502:GLU:HG2	1.88	0.54
1:A:407:LYS:NZ	5:A:613:PEG:H11	2.21	0.54
1:A:501:LEU:HD11	1:B:502:GLU:HG3	1.88	0.54
1:C:104:LYS:HZ2	6:C:614:PGE:H42	1.72	0.54
1:B:90:TRP:CE3	1:B:90:TRP:HA	2.43	0.54
4:A:608:ISW:O2A	1:B:201:ARG:NE	2.35	0.53
1:B:497:ARG:HH11	1:B:497:ARG:HG3	1.71	0.53
1:A:75:GLU:OE2	1:A:157:LYS:HE2	2.09	0.53
4:B:608:ISW:C3A	5:C:610:PEG:H32	2.39	0.53
1:B:316:GLU:HB2	1:B:321:TYR:CE2	2.43	0.52
4:A:608:ISW:HMBA	1:B:214:THR:HG21	1.92	0.52
1:B:357:VAL:O	1:B:361:THR:HG23	2.10	0.52
1:C:1:ASP:HB3	1:C:17:ARG:O	2.10	0.52
3:A:602:HEC:HMC1	3:A:602:HEC:HBC3	1.92	0.52
4:A:608:ISW:HBB	4:A:608:ISW:CMB	2.38	0.51
1:C:19:LYS:HZ1	7:C:617:EDO:H21	1.74	0.51
1:C:484:GLU:HG2	1:C:488:MET:HE2	1.92	0.51
3:C:603:HEC:HMC1	3:C:603:HEC:HBC3	1.93	0.51
1:B:1:ASP:OD2	9:B:614:PG4:O1	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:608:ISW:HMD	1:C:263:HIS:CE1	2.45	0.51
1:C:75:GLU:HG3	1:C:157:LYS:HG2	1.93	0.51
1:B:453:MET:SD	1:B:474:MET:CE	2.99	0.51
4:A:608:ISW:HMB	4:A:608:ISW:CBB	2.40	0.50
1:B:453:MET:HB2	1:B:470:GLY:HA2	1.93	0.50
1:C:488:MET:HE1	11:C:877:HOH:O	2.11	0.50
1:A:104:LYS:NZ	6:A:615:PGE:H1	2.26	0.50
2:F:32:LYS:HD2	5:F:102:PEG:H22	1.94	0.50
1:B:90:TRP:HE3	1:B:90:TRP:HA	1.77	0.50
1:A:427:LEU:HD11	1:A:447:GLU:HG3	1.92	0.49
2:E:50:ILE:HD13	2:E:50:ILE:O	2.12	0.49
1:B:479:VAL:HG22	11:C:726:HOH:O	2.11	0.49
3:C:603:HEC:HBB3	3:C:603:HEC:HMB1	1.95	0.49
1:B:203:SER:O	3:B:605:HEC:HBD1	2.13	0.49
3:B:604:HEC:HMC1	3:B:604:HEC:HBC3	1.95	0.49
1:A:217:TRP:HB2	4:C:601:ISW:HMB	1.94	0.49
3:A:602:HEC:HMB1	3:A:602:HEC:HBB3	1.94	0.49
3:C:605:HEC:HBC3	3:C:605:HEC:HMC1	1.93	0.49
1:A:309:THR:C	3:A:606:HEC:HMC3	2.33	0.49
3:A:601:HEC:CBC	3:A:601:HEC:HMC1	2.42	0.49
1:B:496:ALA:O	1:B:500:LYS:HE2	2.13	0.48
1:C:184:GLU:OE1	1:C:187:ARG:NE	2.43	0.48
4:A:608:ISW:O1A	1:B:201:ARG:NH1	2.35	0.48
1:C:453:MET:HB2	1:C:470:GLY:HA2	1.95	0.48
4:A:608:ISW:HMB	1:B:217:TRP:HB2	1.95	0.48
1:B:176:HIS:CG	3:B:604:HEC:HMA1	2.49	0.48
1:B:60:PRO:HB3	1:B:166:MET:HB2	1.95	0.48
1:A:387:TYR:CE1	1:A:446:ALA:HB2	2.49	0.48
1:C:484:GLU:HG2	1:C:488:MET:CE	2.44	0.48
1:C:8:GLU:N	1:C:8:GLU:OE1	2.46	0.47
1:C:66:PRO:HB3	1:C:164:ILE:HB	1.96	0.47
1:B:431:LYS:NZ	11:B:914:HOH:O	2.44	0.47
3:C:602:HEC:HMC1	3:C:602:HEC:CBC	2.44	0.47
1:C:484:GLU:CG	1:C:488:MET:HE2	2.44	0.47
1:A:453:MET:SD	1:A:474:MET:CE	3.03	0.47
1:B:271:TRP:O	1:B:275:THR:HG23	2.14	0.47
1:A:453:MET:HB2	1:A:470:GLY:HA2	1.96	0.47
1:A:104:LYS:HZ3	6:A:615:PGE:H1	1.80	0.47
1:C:141:LYS:HB3	5:C:612:PEG:H22	1.97	0.47
4:A:608:ISW:HMD	1:B:263:HIS:CE1	2.49	0.47
1:A:495:GLN:CG	1:C:494:LEU:HD13	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ASN:HD22	1:C:269:ASN:N	2.05	0.47
2:F:50:ILE:O	2:F:50:ILE:HD13	2.14	0.47
3:A:604:HEC:HHA	3:A:604:HEC:HAA2	1.69	0.47
1:C:120:LYS:HE2	3:C:605:HEC:HAA1	1.97	0.46
1:B:233:HIS:CE1	3:B:605:HEC:HMD1	2.50	0.46
1:C:284:GLU:O	1:C:287:ARG:HG2	2.15	0.46
1:A:150:VAL:HG11	1:A:154:LYS:HD3	1.97	0.46
2:F:19:TYR:CE2	2:F:23:LYS:HE2	2.50	0.46
3:A:603:HEC:CAA	3:A:604:HEC:HBA1	2.46	0.46
1:B:110:SER:HA	1:B:115:TYR:CG	2.51	0.46
1:A:13:LEU:CD1	1:A:29:LEU:HD13	2.38	0.46
1:C:375:LEU:C	1:C:375:LEU:HD23	2.36	0.46
1:A:106:ARG:HG3	1:A:121:LEU:HD21	1.97	0.45
1:A:106:ARG:NH2	1:A:139:THR:HB	2.31	0.45
1:A:411:PRO:HG3	1:A:431:LYS:HG3	1.98	0.45
1:B:74:ALA:HB1	1:B:78:ASP:HB2	1.99	0.45
1:A:50:GLU:OE1	2:F:32:LYS:NZ	2.48	0.45
1:C:196:GLN:HG2	1:C:340:ILE:HD13	1.98	0.45
1:B:13:LEU:HG	1:B:28:ALA:HB1	1.98	0.45
1:A:302:LYS:NZ	7:A:617:EDO:H12	2.32	0.45
1:A:21:THR:OG1	1:A:24:GLU:HG3	2.17	0.45
1:A:467:TYR:HD2	4:A:608:ISW:HMCA	1.81	0.45
1:C:1:ASP:OD1	1:C:17:ARG:NE	2.40	0.45
1:B:407:LYS:HA	1:B:407:LYS:HD3	1.71	0.45
3:C:607:HEC:HMB1	3:C:607:HEC:HBB3	1.99	0.44
2:F:47:CYS:O	2:F:51:VAL:HG23	2.17	0.44
3:B:605:HEC:HMC1	3:B:605:HEC:HBC3	1.99	0.44
1:C:176:HIS:CG	3:C:605:HEC:HMA1	2.52	0.44
4:B:608:ISW:O2D	3:C:606:HEC:O2A	2.35	0.44
2:E:30:VAL:HG22	2:E:46:LYS:CA	2.42	0.44
1:A:263:HIS:CE1	4:C:601:ISW:HMD	2.52	0.44
1:B:269:ASN:HD22	1:B:269:ASN:N	2.12	0.44
1:A:146:ILE:O	1:A:150:VAL:HB	2.18	0.44
1:B:162:LYS:HB2	1:B:162:LYS:HE3	1.77	0.44
4:B:608:ISW:C3A	5:C:610:PEG:C3	2.96	0.44
1:C:52:ILE:HD11	1:C:227:GLU:HG2	2.00	0.44
1:B:167:PRO:HG2	3:B:602:HEC:CHD	2.48	0.44
1:A:156:ASP:N	1:A:156:ASP:OD1	2.49	0.44
3:A:601:HEC:HMC1	3:A:601:HEC:HBC3	2.00	0.43
1:C:243:HIS:CE1	3:C:605:HEC:NB	2.85	0.43
1:B:384:LEU:HD23	2:E:13:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:608:ISW:HMB	1:C:217:TRP:HB2	2.00	0.43
1:C:484:GLU:OE2	1:C:488:MET:HE2	2.17	0.43
1:C:361:THR:HA	1:C:364:HIS:O	2.18	0.43
3:A:605:HEC:HBB3	3:A:605:HEC:HMB1	2.00	0.43
3:A:601:HEC:HBB3	3:A:601:HEC:HMB1	2.01	0.43
1:C:396:LYS:CA	1:C:396:LYS:HE2	2.34	0.43
1:C:453:MET:HB2	1:C:470:GLY:CA	2.48	0.43
11:A:775:HOH:O	1:C:479:VAL:HG22	2.17	0.43
1:A:221:PRO:HB3	2:F:42:ILE:HG12	2.00	0.43
1:A:176:HIS:HA	11:A:804:HOH:O	2.18	0.43
1:B:491:LEU:HD13	1:B:491:LEU:O	2.18	0.43
1:B:104:LYS:NZ	5:B:609:PEG:H22	2.34	0.43
1:A:96:ARG:HH22	1:C:306:ASN:HB3	1.83	0.43
1:A:157:LYS:CD	1:A:157:LYS:H	2.31	0.43
1:B:23:LYS:O	1:B:27:GLU:HG3	2.19	0.43
1:B:42:LYS:HD2	1:B:63:PHE:CZ	2.53	0.43
1:A:203:SER:O	3:A:605:HEC:HBD1	2.18	0.43
1:C:104:LYS:HZ3	6:C:614:PGE:H42	1.83	0.43
1:B:275:THR:O	1:B:281:LYS:HG2	2.18	0.43
1:A:110:SER:HA	1:A:115:TYR:CG	2.54	0.43
4:B:608:ISW:HMAB	1:C:210:ALA:HB1	2.01	0.42
2:E:22:CYS:O	2:E:23:LYS:C	2.57	0.42
1:C:278:LYS:HA	1:C:278:LYS:HD3	1.80	0.42
1:C:166:MET:HA	1:C:167:PRO:HD3	1.93	0.42
1:A:167:PRO:HG2	3:A:602:HEC:CHD	2.49	0.42
1:A:113:PRO:HA	5:A:612:PEG:H21	2.00	0.42
2:E:47:CYS:O	2:E:51:VAL:HB	2.19	0.42
1:C:145:CYS:O	1:C:149:HIS:HB2	2.20	0.42
2:E:20:LEU:HD23	2:E:20:LEU:HA	1.68	0.42
1:C:150:VAL:HG11	1:C:154:LYS:HE2	2.01	0.42
3:B:606:HEC:HBB3	3:B:606:HEC:HMB1	2.02	0.42
1:B:176:HIS:CD2	3:B:603:HEC:NB	2.86	0.42
1:B:453:MET:SD	1:B:474:MET:HE1	2.60	0.42
1:A:96:ARG:NH2	1:C:306:ASN:HB3	2.34	0.42
1:C:327:ARG:HB2	11:C:727:HOH:O	2.19	0.42
1:C:370:ARG:HB3	7:C:616:EDO:H21	2.02	0.42
1:C:104:LYS:HD2	6:C:614:PGE:H2	2.00	0.41
1:A:214:THR:CG2	4:C:601:ISW:HMBA	2.50	0.41
1:B:278:LYS:HD3	1:B:278:LYS:HA	1.60	0.41
4:B:608:ISW:HMBA	1:C:214:THR:CG2	2.50	0.41
2:E:18:ASP:HB2	2:E:50:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:VAL:O	1:C:361:THR:HG23	2.20	0.41
3:C:604:HEC:HBC3	3:C:604:HEC:HMC1	2.02	0.41
1:B:245:ARG:HA	1:B:246:HIS:HA	1.87	0.41
1:B:467:TYR:HD2	4:B:608:ISW:HMCA	1.86	0.41
1:B:143:VAL:HG22	3:B:603:HEC:HBC2	2.02	0.41
1:C:317:TYR:O	1:C:318:GLU:C	2.57	0.41
4:B:608:ISW:HBAA	3:C:606:HEC:CGD	2.44	0.41
5:B:612:PEG:H21	5:B:612:PEG:H41	1.59	0.41
1:A:252:GLU:OE2	1:C:282:LEU:HD21	2.20	0.41
1:A:429:TRP:CZ2	1:A:431:LYS:HB3	2.56	0.41
1:B:143:VAL:HG21	3:B:603:HEC:CHD	2.51	0.41
3:A:604:HEC:HMC1	3:A:604:HEC:HBC3	2.02	0.41
1:A:416:PRO:O	7:A:619:EDO:H11	2.21	0.41
1:A:491:LEU:CD2	1:B:491:LEU:HD21	2.51	0.41
1:A:152:VAL:HG23	11:A:720:HOH:O	2.21	0.41
1:C:325:ILE:HD13	3:C:606:HEC:C3A	2.51	0.40
1:B:42:LYS:HD2	1:B:63:PHE:HZ	1.85	0.40
2:E:55:GLN:N	2:E:55:GLN:CD	2.74	0.40
1:B:240:ASP:O	1:B:244:THR:HA	2.21	0.40
3:C:602:HEC:HHB	3:C:602:HEC:HMA1	1.92	0.40
1:A:441:LYS:HE3	1:A:441:LYS:HB2	1.90	0.40
1:C:5:VAL:HA	1:C:6:PRO:HD3	1.83	0.40
1:A:491:LEU:HD21	1:B:491:LEU:HD21	2.03	0.40
4:B:608:ISW:HMAA	5:C:610:PEG:H31	2.04	0.40
1:A:201:ARG:HH21	4:C:601:ISW:CGA	2.33	0.40
1:B:271:TRP:CZ2	1:B:275:THR:HG21	2.57	0.40
1:B:13:LEU:HD21	1:B:29:LEU:CD1	2.34	0.40
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.87	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	501/546 (92%)	482 (96%)	19 (4%)	0	100	100
1	B	500/546 (92%)	483 (97%)	16 (3%)	1 (0%)	52	53
1	C	500/546 (92%)	478 (96%)	21 (4%)	1 (0%)	52	53
2	D	47/69 (68%)	45 (96%)	2 (4%)	0	100	100
2	E	47/69 (68%)	44 (94%)	3 (6%)	0	100	100
2	F	47/69 (68%)	45 (96%)	2 (4%)	0	100	100
All	All	1642/1845 (89%)	1577 (96%)	63 (4%)	2 (0%)	56	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	HIS
1	C	268	HIS

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	430/459 (94%)	414 (96%)	16 (4%)	41	41
1	B	429/459 (94%)	410 (96%)	19 (4%)	35	33
1	C	429/459 (94%)	416 (97%)	13 (3%)	48	51
2	D	43/57 (75%)	39 (91%)	4 (9%)	11	7
2	E	43/57 (75%)	39 (91%)	4 (9%)	11	7
2	F	43/57 (75%)	40 (93%)	3 (7%)	19	15
All	All	1417/1548 (92%)	1358 (96%)	59 (4%)	36	35

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	65	LYS
1	A	67	PRO

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Mol	Chain	Res	Type
1	A	90	TRP
1	A	137	LYS
1	A	145	CYS
1	A	157	LYS
1	A	177	LEU
1	A	247	GLU
1	A	269	ASN
1	A	301	SER
1	A	418	LYS
1	A	442	VAL
1	A	443	LEU
1	A	491	LEU
1	A	497	ARG
1	B	13	LEU
1	B	14	LYS
1	B	23	LYS
1	B	29	LEU
1	B	42	LYS
1	B	88	PRO
1	B	90	TRP
1	B	177	LEU
1	B	266	VAL
1	B	269	ASN
1	B	278	LYS
1	B	287	ARG
1	B	342	GLU
1	B	358	LEU
1	B	396	LYS
1	B	443	LEU
1	B	497	ARG
1	B	499	ASN
1	B	500	LYS
1	C	16	ASP
1	C	17	ARG
1	C	29	LEU
1	C	65	LYS
1	C	77	LYS
1	C	90	TRP
1	C	155	LYS
1	C	269	ASN
1	C	322	THR
1	C	396	LYS

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Mol	Chain	Res	Type
1	C	442	VAL
1	C	499	ASN
1	C	500	LYS
2	D	17	LEU
2	D	23	LYS
2	D	44	ARG
2	D	50	ILE
2	E	25	LYS
2	E	50	ILE
2	E	51	VAL
2	E	53	LEU
2	F	17	LEU
2	F	24	ASP
2	F	50	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	ASN
1	A	343	ASN
1	A	448	ASN
1	A	461	ASN
1	A	489	GLN
1	B	269	ASN
1	B	448	ASN
1	B	461	ASN
1	C	269	ASN
1	C	448	ASN
1	C	461	ASN
1	C	495	GLN
1	C	499	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)

64 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEC	A	601	1	24,50,50	1.32	4 (16%)	19,82,82	2.49	5 (26%)
3	HEC	A	602	1	24,50,50	1.70	5 (20%)	19,82,82	2.91	6 (31%)
3	HEC	A	603	1	24,50,50	1.34	2 (8%)	19,82,82	2.51	5 (26%)
3	HEC	A	604	1	24,50,50	1.62	5 (20%)	19,82,82	3.40	6 (31%)
3	HEC	A	605	1	24,50,50	1.40	3 (12%)	19,82,82	2.70	8 (42%)
3	HEC	A	606	1	24,50,50	1.53	7 (29%)	19,82,82	3.08	6 (31%)
3	HEC	A	607	1	24,50,50	1.68	6 (25%)	19,82,82	3.25	10 (52%)
4	ISW	A	608	1	29,50,50	2.96	12 (41%)	23,82,82	4.29	10 (43%)
5	PEG	A	609	-	6,6,6	0.22	0	5,5,5	1.00	0
5	PEG	A	610	-	6,6,6	0.27	0	5,5,5	1.05	0
5	PEG	A	611	-	6,6,6	0.64	0	5,5,5	0.49	0
5	PEG	A	612	-	6,6,6	0.53	0	5,5,5	0.29	0
5	PEG	A	613	-	6,6,6	0.55	0	5,5,5	0.52	0
5	PEG	A	614	-	6,6,6	0.75	0	5,5,5	0.79	0
6	PGE	A	615	-	9,9,9	0.67	0	8,8,8	0.78	0
7	EDO	A	616	-	3,3,3	0.62	0	2,2,2	1.07	0
7	EDO	A	617	-	3,3,3	0.68	0	2,2,2	0.41	0
7	EDO	A	618	-	3,3,3	0.47	0	2,2,2	0.27	0
7	EDO	A	619	-	3,3,3	0.57	0	2,2,2	0.41	0
3	HEC	B	601	1	24,50,50	1.60	6 (25%)	19,82,82	2.80	7 (36%)
3	HEC	B	602	1	24,50,50	1.70	4 (16%)	19,82,82	2.48	8 (42%)
3	HEC	B	603	1	24,50,50	1.48	4 (16%)	19,82,82	2.88	9 (47%)
3	HEC	B	604	1	24,50,50	1.34	5 (20%)	19,82,82	3.21	6 (31%)
3	HEC	B	605	1	24,50,50	1.52	5 (20%)	19,82,82	2.29	7 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEC	B	606	1	24,50,50	1.49	5 (20%)	19,82,82	2.48	4 (21%)
3	HEC	B	607	1	24,50,50	1.58	6 (25%)	19,82,82	2.70	7 (36%)
4	ISW	B	608	1	29,50,50	3.50	13 (44%)	23,82,82	4.09	11 (47%)
5	PEG	B	609	-	6,6,6	0.46	0	5,5,5	0.88	0
5	PEG	B	610	-	6,6,6	0.50	0	5,5,5	0.48	0
5	PEG	B	611	-	6,6,6	0.34	0	5,5,5	0.94	0
5	PEG	B	612	-	6,6,6	0.69	0	5,5,5	0.67	0
8	P6G	B	613	-	18,18,18	0.49	0	17,17,17	0.74	0
9	PG4	B	614	-	12,12,12	0.62	0	11,11,11	0.91	0
7	EDO	B	615	-	3,3,3	0.63	0	2,2,2	0.10	0
7	EDO	B	616	-	3,3,3	0.50	0	2,2,2	0.49	0
10	NO3	B	617	-	3,3,3	3.14	3 (100%)	3,3,3	0.62	0
10	NO3	B	618	-	3,3,3	3.65	3 (100%)	3,3,3	0.45	0
7	EDO	B	619	-	3,3,3	0.27	0	2,2,2	0.80	0
7	EDO	B	620	-	3,3,3	0.74	0	2,2,2	0.45	0
7	EDO	B	621	-	3,3,3	0.49	0	2,2,2	0.23	0
4	ISW	C	601	1	29,50,50	3.23	16 (55%)	23,82,82	3.85	8 (34%)
3	HEC	C	602	1	24,50,50	1.42	4 (16%)	19,82,82	2.84	7 (36%)
3	HEC	C	603	1	24,50,50	1.54	5 (20%)	19,82,82	2.41	7 (36%)
3	HEC	C	604	1	24,50,50	1.49	5 (20%)	19,82,82	2.94	5 (26%)
3	HEC	C	605	1	24,50,50	1.66	4 (16%)	19,82,82	3.28	7 (36%)
3	HEC	C	606	1	24,50,50	1.27	3 (12%)	19,82,82	2.55	6 (31%)
3	HEC	C	607	1	24,50,50	1.55	4 (16%)	19,82,82	2.34	6 (31%)
3	HEC	C	608	1	24,50,50	1.33	4 (16%)	19,82,82	3.01	9 (47%)
5	PEG	C	609	-	6,6,6	0.48	0	5,5,5	0.44	0
5	PEG	C	610	-	6,6,6	0.74	0	5,5,5	0.61	0
5	PEG	C	611	-	6,6,6	0.56	0	5,5,5	0.59	0
5	PEG	C	612	-	6,6,6	0.46	0	5,5,5	0.83	0
5	PEG	C	613	-	6,6,6	0.65	0	5,5,5	0.84	0
6	PGE	C	614	-	9,9,9	0.36	0	8,8,8	1.01	0
7	EDO	C	615	-	3,3,3	0.46	0	2,2,2	0.31	0
7	EDO	C	616	-	3,3,3	0.21	0	2,2,2	0.83	0
7	EDO	C	617	-	3,3,3	0.53	0	2,2,2	0.40	0
7	EDO	C	618	-	3,3,3	0.73	0	2,2,2	0.13	0
10	NO3	C	619	-	3,3,3	3.40	3 (100%)	3,3,3	0.36	0
7	EDO	C	620	-	3,3,3	0.82	0	2,2,2	0.39	0
7	EDO	C	621	-	3,3,3	0.56	0	2,2,2	0.51	0
5	PEG	C	622	-	6,6,6	0.95	0	5,5,5	1.11	0
10	NO3	F	101	-	3,3,3	3.57	3 (100%)	3,3,3	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PEG	F	102	-	6,6,6	0.58	0	5,5,5	0.68	0

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	HEC	A	601	1	-	0/6/54/54	0/0/8/8
3	HEC	A	602	1	-	0/6/54/54	0/0/8/8
3	HEC	A	603	1	-	0/6/54/54	0/0/8/8
3	HEC	A	604	1	-	0/6/54/54	0/0/8/8
3	HEC	A	605	1	-	0/6/54/54	0/0/8/8
3	HEC	A	606	1	-	0/6/54/54	0/0/8/8
3	HEC	A	607	1	-	0/6/54/54	0/0/8/8
4	ISW	A	608	1	-	0/8/74/74	0/0/8/8
5	PEG	A	609	-	-	0/4/4/4	0/0/0/0
5	PEG	A	610	-	-	0/4/4/4	0/0/0/0
5	PEG	A	611	-	-	0/4/4/4	0/0/0/0
5	PEG	A	612	-	-	0/4/4/4	0/0/0/0
5	PEG	A	613	-	-	0/4/4/4	0/0/0/0
5	PEG	A	614	-	-	0/4/4/4	0/0/0/0
6	PGE	A	615	-	-	0/7/7/7	0/0/0/0
7	EDO	A	616	-	-	0/1/1/1	0/0/0/0
7	EDO	A	617	-	-	0/1/1/1	0/0/0/0
7	EDO	A	618	-	-	0/1/1/1	0/0/0/0
7	EDO	A	619	-	-	0/1/1/1	0/0/0/0
3	HEC	B	601	1	-	0/6/54/54	0/0/8/8
3	HEC	B	602	1	-	0/6/54/54	0/0/8/8
3	HEC	B	603	1	-	0/6/54/54	0/0/8/8
3	HEC	B	604	1	-	0/6/54/54	0/0/8/8
3	HEC	B	605	1	-	0/6/54/54	0/0/8/8
3	HEC	B	606	1	-	0/6/54/54	0/0/8/8
3	HEC	B	607	1	-	0/6/54/54	0/0/8/8
4	ISW	B	608	1	-	0/8/74/74	0/0/8/8
5	PEG	B	609	-	-	0/4/4/4	0/0/0/0
5	PEG	B	610	-	-	0/4/4/4	0/0/0/0
5	PEG	B	611	-	-	0/4/4/4	0/0/0/0
5	PEG	B	612	-	-	0/4/4/4	0/0/0/0
8	P6G	B	613	-	-	0/16/16/16	0/0/0/0
9	PG4	B	614	-	-	0/10/10/10	0/0/0/0
7	EDO	B	615	-	-	0/1/1/1	0/0/0/0
7	EDO	B	616	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NO3	B	617	-	-	0/0/0/0	0/0/0/0
10	NO3	B	618	-	-	0/0/0/0	0/0/0/0
7	EDO	B	619	-	-	0/1/1/1	0/0/0/0
7	EDO	B	620	-	-	0/1/1/1	0/0/0/0
7	EDO	B	621	-	-	0/1/1/1	0/0/0/0
4	ISW	C	601	1	-	0/8/74/74	0/0/8/8
3	HEC	C	602	1	-	0/6/54/54	0/0/8/8
3	HEC	C	603	1	-	0/6/54/54	0/0/8/8
3	HEC	C	604	1	-	0/6/54/54	0/0/8/8
3	HEC	C	605	1	-	0/6/54/54	0/0/8/8
3	HEC	C	606	1	-	0/6/54/54	0/0/8/8
3	HEC	C	607	1	-	0/6/54/54	0/0/8/8
3	HEC	C	608	1	-	0/6/54/54	0/0/8/8
5	PEG	C	609	-	-	0/4/4/4	0/0/0/0
5	PEG	C	610	-	-	0/4/4/4	0/0/0/0
5	PEG	C	611	-	-	0/4/4/4	0/0/0/0
5	PEG	C	612	-	-	0/4/4/4	0/0/0/0
5	PEG	C	613	-	-	0/4/4/4	0/0/0/0
6	PGE	C	614	-	-	0/7/7/7	0/0/0/0
7	EDO	C	615	-	-	0/1/1/1	0/0/0/0
7	EDO	C	616	-	-	0/1/1/1	0/0/0/0
7	EDO	C	617	-	-	0/1/1/1	0/0/0/0
7	EDO	C	618	-	-	0/1/1/1	0/0/0/0
10	NO3	C	619	-	-	0/0/0/0	0/0/0/0
7	EDO	C	620	-	-	0/1/1/1	0/0/0/0
7	EDO	C	621	-	-	0/1/1/1	0/0/0/0
5	PEG	C	622	-	-	0/4/4/4	0/0/0/0
10	NO3	F	101	-	-	0/0/0/0	0/0/0/0
5	PEG	F	102	-	-	0/4/4/4	0/0/0/0

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	HEC	C4B-NB	-4.73	1.30	1.36
3	A	604	HEC	C1A-NA	-4.12	1.31	1.36
3	C	605	HEC	C3C-C2C	-4.09	1.36	1.40
3	B	602	HEC	C3B-C2B	-4.02	1.36	1.40
3	A	607	HEC	C3B-C2B	-3.99	1.36	1.40
3	C	607	HEC	C3B-C2B	-3.94	1.36	1.40
3	A	605	HEC	C3B-C2B	-3.85	1.36	1.40
3	B	605	HEC	C3C-C2C	-3.83	1.36	1.40
3	B	603	HEC	C1A-NA	-3.68	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEC	C3B-C2B	-3.57	1.37	1.40
3	A	602	HEC	C3B-C4B	-3.29	1.35	1.42
3	C	606	HEC	C3B-C2B	-3.26	1.37	1.40
3	C	604	HEC	C3B-C2B	-3.25	1.37	1.40
3	A	604	HEC	C4B-NB	-3.16	1.32	1.36
3	A	602	HEC	C3C-C2C	-3.11	1.37	1.40
3	B	601	HEC	C4A-NA	-3.10	1.32	1.36
3	C	608	HEC	C4A-NA	-3.06	1.32	1.36
3	B	604	HEC	C4B-NB	-2.90	1.32	1.36
3	B	607	HEC	C3C-C2C	-2.81	1.37	1.40
3	C	605	HEC	C1A-NA	-2.77	1.32	1.36
3	A	604	HEC	C3C-C2C	-2.76	1.37	1.40
3	B	601	HEC	C3C-C2C	-2.75	1.37	1.40
3	C	603	HEC	C3C-C2C	-2.75	1.37	1.40
4	C	601	ISW	CAD-C3D	-2.70	1.47	1.52
3	B	607	HEC	C1A-NA	-2.65	1.33	1.36
3	C	602	HEC	C4A-NA	-2.60	1.33	1.36
3	C	607	HEC	C1A-NA	-2.57	1.33	1.36
3	C	606	HEC	C4A-NA	-2.57	1.33	1.36
3	C	603	HEC	C3B-C4B	-2.57	1.37	1.42
3	A	603	HEC	C4B-NB	-2.52	1.33	1.36
4	C	601	ISW	C1D-ND	-2.47	1.33	1.36
3	B	605	HEC	C3B-C2B	-2.42	1.38	1.40
3	A	606	HEC	C3B-C2B	-2.38	1.38	1.40
3	A	601	HEC	C1A-NA	-2.37	1.33	1.36
3	B	604	HEC	C4C-NC	-2.37	1.33	1.36
3	B	607	HEC	C4C-NC	-2.31	1.33	1.36
3	B	606	HEC	C3C-C4C	-2.30	1.37	1.42
3	B	604	HEC	C3C-C2C	-2.29	1.38	1.40
3	B	606	HEC	C4C-NC	-2.26	1.33	1.36
3	B	602	HEC	C3C-C2C	-2.24	1.38	1.40
3	A	606	HEC	C3C-C2C	-2.22	1.38	1.40
3	A	601	HEC	C3C-C4C	-2.20	1.38	1.42
4	B	608	ISW	C1D-ND	-2.18	1.33	1.36
3	C	608	HEC	C3B-C2B	-2.16	1.38	1.40
3	B	605	HEC	C4A-NA	-2.12	1.33	1.36
3	C	604	HEC	C1A-NA	-2.11	1.33	1.36
3	B	605	HEC	C1A-NA	-2.11	1.33	1.36
3	A	607	HEC	C4A-NA	-2.02	1.33	1.36
3	B	605	HEC	C4C-NC	-2.01	1.34	1.36
3	B	602	HEC	C1A-NA	-2.01	1.34	1.36
3	A	605	HEC	C1C-CHC	2.01	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	ISW	CHC-C4B	2.03	1.55	1.53
3	C	607	HEC	C1B-CHB	2.04	1.45	1.39
3	B	606	HEC	C4D-CHA	2.04	1.45	1.39
3	A	607	HEC	CMA-C3A	2.06	1.56	1.51
3	B	601	HEC	C1B-CHB	2.07	1.45	1.39
4	C	601	ISW	C4C-CHD	2.08	1.45	1.39
3	C	608	HEC	C4D-CHA	2.10	1.45	1.39
3	A	602	HEC	C1B-CHB	2.12	1.45	1.39
3	C	608	HEC	C1D-CHD	2.12	1.45	1.39
3	C	602	HEC	C4D-CHA	2.16	1.45	1.39
3	C	603	HEC	C4B-NB	2.17	1.39	1.36
3	A	601	HEC	C1B-CHB	2.19	1.45	1.39
3	B	601	HEC	C4D-CHA	2.21	1.45	1.39
3	C	606	HEC	C4D-CHA	2.22	1.46	1.39
3	A	606	HEC	CMA-C3A	2.23	1.56	1.51
3	A	604	HEC	C4D-CHA	2.25	1.46	1.39
3	C	602	HEC	C1D-CHD	2.26	1.46	1.39
3	B	604	HEC	C1B-CHB	2.27	1.46	1.39
3	A	604	HEC	CAD-C3D	2.27	1.55	1.52
3	A	606	HEC	C1C-CHC	2.27	1.46	1.39
3	C	604	HEC	C3C-C2C	2.28	1.43	1.40
3	B	604	HEC	C3D-C2D	2.29	1.44	1.37
3	B	603	HEC	C1C-CHC	2.30	1.46	1.39
3	B	607	HEC	C3D-C2D	2.35	1.44	1.37
3	B	607	HEC	C1C-CHC	2.35	1.46	1.39
3	C	604	HEC	C1D-CHD	2.36	1.46	1.39
3	A	606	HEC	CAA-C2A	2.36	1.56	1.52
3	B	607	HEC	C4D-CHA	2.38	1.46	1.39
3	A	607	HEC	C4D-CHA	2.39	1.46	1.39
4	C	601	ISW	C3C-CAC	2.39	1.52	1.47
4	C	601	ISW	CHB-C1B	2.40	1.46	1.41
3	A	601	HEC	C1D-CHD	2.41	1.46	1.39
3	A	603	HEC	C1D-CHD	2.42	1.46	1.39
3	A	606	HEC	C1D-CHD	2.43	1.46	1.39
3	C	603	HEC	C1B-CHB	2.44	1.46	1.39
3	A	605	HEC	C4D-CHA	2.50	1.46	1.39
3	C	605	HEC	C4B-NB	2.52	1.40	1.36
3	B	603	HEC	C1B-CHB	2.53	1.46	1.39
4	C	601	ISW	C1B-C2B	2.56	1.49	1.44
3	A	607	HEC	CMD-C2D	2.57	1.56	1.51
3	B	606	HEC	C3D-C2D	2.58	1.45	1.37
3	A	606	HEC	CMD-C2D	2.61	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	HEC	C1C-CHC	2.64	1.47	1.39
3	C	604	HEC	C1B-CHB	2.65	1.47	1.39
3	C	602	HEC	C1C-CHC	2.66	1.47	1.39
4	A	608	ISW	C1B-C2B	2.66	1.49	1.44
4	A	608	ISW	FE-NB	2.68	2.10	1.97
3	C	603	HEC	C4D-CHA	2.71	1.47	1.39
10	B	617	NO3	O3-N	2.72	1.39	1.25
3	A	602	HEC	C3D-C2D	2.73	1.45	1.37
3	B	603	HEC	C1D-CHD	2.73	1.47	1.39
4	B	608	ISW	CHB-C1B	2.78	1.47	1.41
4	A	608	ISW	CBC-CAC	2.79	1.48	1.28
3	C	605	HEC	C4D-CHA	2.80	1.47	1.39
3	C	607	HEC	C1D-CHD	2.85	1.47	1.39
10	C	619	NO3	O2-N	2.87	1.40	1.25
3	B	606	HEC	C1C-CHC	2.96	1.48	1.39
10	B	618	NO3	O3-N	2.98	1.40	1.25
4	A	608	ISW	CAB-C3B	2.99	1.51	1.46
3	A	607	HEC	C1C-CHC	3.01	1.48	1.39
4	B	608	ISW	CAB-C3B	3.01	1.52	1.46
10	F	101	NO3	O2-N	3.09	1.41	1.25
4	C	601	ISW	FE-NB	3.17	2.12	1.97
10	C	619	NO3	O3-N	3.20	1.41	1.25
4	B	608	ISW	FE-NB	3.24	2.12	1.97
10	B	618	NO3	O2-N	3.25	1.42	1.25
10	F	101	NO3	O3-N	3.29	1.42	1.25
10	B	617	NO3	O1-N	3.31	1.37	1.24
10	B	617	NO3	O2-N	3.35	1.42	1.25
3	B	601	HEC	C1D-CHD	3.41	1.49	1.39
4	B	608	ISW	CBC-CAC	3.51	1.54	1.28
4	B	608	ISW	C4C-CHD	3.53	1.49	1.39
4	B	608	ISW	C3D-C2D	3.58	1.48	1.37
4	C	601	ISW	C3D-C2D	3.60	1.48	1.37
4	C	601	ISW	CBC-CAC	3.63	1.55	1.28
4	A	608	ISW	C4C-CHD	3.87	1.50	1.39
4	B	608	ISW	CBB-CAB	3.88	1.49	1.30
4	A	608	ISW	C1B-NB	3.91	1.31	1.28
4	C	601	ISW	C4D-CHA	4.01	1.50	1.39
10	C	619	NO3	O1-N	4.03	1.40	1.24
4	C	601	ISW	C2A-C3A	4.17	1.50	1.37
10	F	101	NO3	O1-N	4.22	1.41	1.24
4	A	608	ISW	C4D-CHA	4.41	1.52	1.39
10	B	618	NO3	O1-N	4.52	1.43	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	608	ISW	C2A-C3A	4.53	1.51	1.37
4	A	608	ISW	C3D-C2D	4.54	1.51	1.37
4	C	601	ISW	CBB-CAB	4.58	1.53	1.30
4	A	608	ISW	C3C-C2C	4.60	1.46	1.40
4	A	608	ISW	CBB-CAB	4.83	1.54	1.30
4	B	608	ISW	C4D-CHA	4.84	1.53	1.39
4	B	608	ISW	C2A-C3A	5.14	1.52	1.37
4	C	601	ISW	C1B-NB	5.40	1.32	1.28
4	B	608	ISW	C1B-NB	5.63	1.33	1.28
4	C	601	ISW	C3C-C2C	5.98	1.48	1.40
4	B	608	ISW	C3C-C2C	6.96	1.49	1.40
4	A	608	ISW	C1C-C2C	8.50	1.48	1.37
4	C	601	ISW	C1C-C2C	9.95	1.50	1.37
4	B	608	ISW	C1C-C2C	11.45	1.52	1.37

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	601	ISW	C3C-CAC-CBC	-10.22	105.42	126.32
4	B	608	ISW	C3C-CAC-CBC	-9.92	106.02	126.32
4	A	608	ISW	CBB-CAB-C3B	-9.47	112.28	126.36
4	A	608	ISW	C3C-CAC-CBC	-9.32	107.25	126.32
3	C	604	HEC	CBB-CAB-C3B	-9.07	107.19	127.35
3	B	604	HEC	CBB-CAB-C3B	-9.07	107.20	127.35
4	A	608	ISW	C1B-C2B-C3B	-8.88	99.53	106.97
3	C	606	HEC	CBB-CAB-C3B	-8.87	107.64	127.35
3	A	602	HEC	CBB-CAB-C3B	-8.84	107.71	127.35
4	B	608	ISW	CBB-CAB-C3B	-8.41	113.87	126.36
3	B	607	HEC	CBB-CAB-C3B	-8.35	108.79	127.35
3	C	608	HEC	CBB-CAB-C3B	-8.33	108.83	127.35
3	C	605	HEC	CBC-CAC-C3C	-8.27	108.97	127.35
3	A	606	HEC	CBB-CAB-C3B	-8.24	109.04	127.35
3	B	606	HEC	CBB-CAB-C3B	-7.83	109.95	127.35
4	C	601	ISW	C1B-C2B-C3B	-7.81	100.42	106.97
3	B	601	HEC	CBB-CAB-C3B	-7.56	110.55	127.35
3	C	605	HEC	CBB-CAB-C3B	-7.53	110.61	127.35
4	C	601	ISW	CBB-CAB-C3B	-7.53	115.16	126.36
3	A	606	HEC	CBC-CAC-C3C	-7.39	110.93	127.35
3	C	602	HEC	CBB-CAB-C3B	-7.30	111.12	127.35
3	A	607	HEC	CBC-CAC-C3C	-7.22	111.30	127.35
3	B	602	HEC	CBB-CAB-C3B	-7.07	111.65	127.35
3	A	604	HEC	CAA-C2A-C1A	-7.04	119.36	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	603	HEC	CBC-CAC-C3C	-7.03	111.72	127.35
3	A	604	HEC	CBB-CAB-C3B	-6.98	111.85	127.35
3	A	604	HEC	CBD-CAD-C3D	-6.63	100.64	112.53
3	A	605	HEC	CBB-CAB-C3B	-6.54	112.83	127.35
4	B	608	ISW	C1B-C2B-C3B	-6.51	101.52	106.97
3	B	604	HEC	CBC-CAC-C3C	-6.49	112.94	127.35
3	B	604	HEC	CBD-CAD-C3D	-6.48	100.92	112.53
3	C	603	HEC	CBB-CAB-C3B	-6.45	113.03	127.35
3	A	601	HEC	CBB-CAB-C3B	-6.41	113.12	127.35
3	A	607	HEC	CBB-CAB-C3B	-6.39	113.16	127.35
3	C	604	HEC	CBC-CAC-C3C	-6.29	113.38	127.35
3	A	607	HEC	CAD-C3D-C4D	-6.25	120.22	127.01
3	B	603	HEC	CAA-CBA-CGA	-6.03	101.70	112.75
3	C	602	HEC	CBC-CAC-C3C	-6.00	114.02	127.35
3	B	603	HEC	CBB-CAB-C3B	-5.98	114.06	127.35
3	A	601	HEC	CBC-CAC-C3C	-5.91	114.21	127.35
3	C	607	HEC	CBB-CAB-C3B	-5.88	114.28	127.35
3	C	605	HEC	CBD-CAD-C3D	-5.86	102.02	112.53
3	A	603	HEC	CBB-CAB-C3B	-5.70	114.69	127.35
4	B	608	ISW	CAD-CBD-CGD	-5.66	102.37	112.75
3	B	603	HEC	CBC-CAC-C3C	-5.37	115.42	127.35
3	A	604	HEC	CBC-CAC-C3C	-5.33	115.50	127.35
4	A	608	ISW	CAD-CBD-CGD	-5.31	103.01	112.75
3	A	602	HEC	CBC-CAC-C3C	-5.31	115.55	127.35
4	C	601	ISW	CAD-CBD-CGD	-5.15	103.31	112.75
3	C	608	HEC	CMC-C2C-C1C	-5.06	119.98	128.36
3	B	605	HEC	CBC-CAC-C3C	-4.97	116.31	127.35
3	B	601	HEC	CBA-CAA-C2A	-4.95	103.67	112.53
3	B	606	HEC	CBC-CAC-C3C	-4.69	116.94	127.35
3	B	607	HEC	CBC-CAC-C3C	-4.65	117.02	127.35
3	A	605	HEC	CBA-CAA-C2A	-4.58	104.31	112.53
3	C	607	HEC	CBD-CAD-C3D	-4.47	104.52	112.53
3	B	602	HEC	CBC-CAC-C3C	-4.33	117.73	127.35
3	A	601	HEC	CMC-C2C-C1C	-4.29	121.26	128.36
3	B	601	HEC	CMD-C2D-C1D	-4.27	121.31	128.36
3	C	608	HEC	CBC-CAC-C3C	-4.17	118.08	127.35
3	C	605	HEC	CAD-C3D-C4D	-4.17	122.48	127.01
3	B	605	HEC	CBB-CAB-C3B	-4.14	118.14	127.35
3	A	606	HEC	CMB-C2B-C1B	-4.09	121.59	128.36
3	A	605	HEC	CMC-C2C-C1C	-4.06	121.64	128.36
3	B	605	HEC	CBA-CAA-C2A	-4.02	105.32	112.53
3	B	603	HEC	CAD-CBD-CGD	-4.00	105.41	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	HEC	CAD-CBD-CGD	-3.93	105.54	112.75
3	B	606	HEC	CMB-C2B-C1B	-3.92	121.88	128.36
4	A	608	ISW	CHB-C1B-NB	-3.92	119.88	124.47
3	A	605	HEC	CBC-CAC-C3C	-3.78	118.94	127.35
3	A	607	HEC	CMC-C2C-C1C	-3.66	122.31	128.36
3	C	603	HEC	CMB-C2B-C1B	-3.63	122.36	128.36
3	C	607	HEC	CBC-CAC-C3C	-3.52	119.54	127.35
3	C	604	HEC	CAA-CBA-CGA	-3.52	106.30	112.75
3	C	602	HEC	CMC-C2C-C1C	-3.49	122.59	128.36
3	A	604	HEC	CMB-C2B-C1B	-3.47	122.62	128.36
3	A	605	HEC	C4C-C3C-C2C	-3.30	102.79	106.35
3	A	606	HEC	CAD-C3D-C4D	-3.20	123.53	127.01
3	C	602	HEC	CBA-CAA-C2A	-3.16	106.87	112.53
3	A	606	HEC	CBD-CAD-C3D	-3.14	106.89	112.53
3	B	603	HEC	CBA-CAA-C2A	-3.12	106.93	112.53
3	B	605	HEC	CAD-CBD-CGD	-3.09	107.08	112.75
3	B	607	HEC	CBD-CAD-C3D	-3.07	107.03	112.53
3	B	607	HEC	CMB-C2B-C1B	-3.05	123.31	128.36
3	A	601	HEC	CBA-CAA-C2A	-3.03	107.10	112.53
3	B	601	HEC	CBC-CAC-C3C	-3.01	120.67	127.35
3	C	606	HEC	CBA-CAA-C2A	-2.96	107.23	112.53
3	A	605	HEC	CBD-CAD-C3D	-2.96	107.23	112.53
3	C	604	HEC	CMC-C2C-C1C	-2.95	123.48	128.36
3	C	606	HEC	CBD-CAD-C3D	-2.88	107.37	112.53
3	B	602	HEC	CBD-CAD-C3D	-2.84	107.44	112.53
3	C	603	HEC	CBC-CAC-C3C	-2.82	121.08	127.35
3	A	607	HEC	CBA-CAA-C2A	-2.82	107.47	112.53
3	C	607	HEC	CBA-CAA-C2A	-2.78	107.55	112.53
3	A	602	HEC	CAA-CBA-CGA	-2.76	107.69	112.75
3	A	603	HEC	CAA-C2A-C1A	-2.75	124.02	127.01
3	C	607	HEC	CMB-C2B-C1B	-2.68	123.93	128.36
3	C	602	HEC	CAD-CBD-CGD	-2.64	107.92	112.75
3	B	605	HEC	C4C-C3C-C2C	-2.63	103.52	106.35
4	B	608	ISW	CHB-C1B-NB	-2.60	121.42	124.47
3	B	603	HEC	CMB-C2B-C1B	-2.60	124.07	128.36
3	C	606	HEC	CBC-CAC-C3C	-2.57	121.63	127.35
3	A	607	HEC	CMB-C2B-C1B	-2.57	124.11	128.36
3	B	604	HEC	CMB-C2B-C1B	-2.57	124.11	128.36
3	C	608	HEC	C4B-C3B-C2B	-2.50	103.66	106.35
3	C	603	HEC	CAD-C3D-C4D	-2.47	124.32	127.01
3	C	606	HEC	CAD-CBD-CGD	-2.46	108.23	112.75
3	C	608	HEC	CMB-C2B-C1B	-2.44	124.33	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	607	HEC	CMC-C2C-C1C	-2.44	124.33	128.36
4	A	608	ISW	C3C-C2C-C1C	-2.42	103.62	106.51
3	B	602	HEC	CAD-CBD-CGD	-2.40	108.34	112.75
3	A	603	HEC	CMD-C2D-C1D	-2.37	124.44	128.36
3	C	603	HEC	CAA-C2A-C3A	-2.37	122.25	129.00
3	C	607	HEC	CMD-C2D-C1D	-2.36	124.46	128.36
4	B	608	ISW	CBD-CAD-C3D	-2.36	108.30	112.53
3	B	603	HEC	CMD-C2D-C1D	-2.36	124.47	128.36
3	B	602	HEC	C4C-C3C-C2C	-2.35	103.81	106.35
3	C	608	HEC	CAD-CBD-CGD	-2.31	108.51	112.75
3	C	605	HEC	CMB-C2B-C1B	-2.30	124.56	128.36
3	A	603	HEC	CBD-CAD-C3D	-2.30	108.41	112.53
3	B	605	HEC	CMC-C2C-C1C	-2.29	124.58	128.36
3	A	605	HEC	CMB-C2B-C1B	-2.23	124.67	128.36
3	A	602	HEC	CAA-C2A-C3A	-2.16	122.83	129.00
3	C	608	HEC	CBA-CAA-C2A	-2.15	108.67	112.53
3	B	607	HEC	CAD-CBD-CGD	-2.14	108.82	112.75
3	B	604	HEC	C4B-C3B-C2B	-2.11	104.08	106.35
3	A	607	HEC	CBD-CAD-C3D	-2.10	108.77	112.53
3	B	606	HEC	CBD-CAD-C3D	-2.08	108.80	112.53
3	C	603	HEC	C4B-C3B-C2B	-2.08	104.11	106.35
3	A	607	HEC	CAA-C2A-C3A	-2.08	123.08	129.00
3	B	603	HEC	CMC-C2C-C1C	-2.07	124.93	128.36
3	B	602	HEC	C4B-C3B-C2B	-2.03	104.17	106.35
3	C	605	HEC	CMC-C2C-C1C	-2.01	125.03	128.36
3	C	608	HEC	CBD-CAD-C3D	-2.00	108.94	112.53
3	B	603	HEC	CMA-C3A-C2A	2.01	129.43	125.24
4	B	608	ISW	CHB-C1B-C2B	2.01	128.20	124.83
3	A	601	HEC	CMA-C3A-C2A	2.02	129.47	125.24
4	C	601	ISW	CAD-C3D-C4D	2.11	129.30	127.01
3	C	606	HEC	CMA-C3A-C2A	2.13	129.69	125.24
3	B	601	HEC	CBD-CAD-C3D	2.19	116.45	112.53
4	C	601	ISW	CMA-C3A-C2A	2.19	129.82	125.24
3	C	605	HEC	CMA-C3A-C2A	2.32	130.09	125.24
3	B	602	HEC	CAD-C3D-C4D	2.34	129.54	127.01
3	C	604	HEC	CAD-C3D-C4D	2.35	129.56	127.01
3	B	605	HEC	CAD-C3D-C4D	2.46	129.68	127.01
3	B	607	HEC	CMD-C2D-C3D	2.48	130.42	125.24
3	A	606	HEC	CMD-C2D-C3D	2.56	130.59	125.24
4	A	608	ISW	CMC-C2C-C3C	2.69	130.34	125.09
3	B	604	HEC	CBA-CAA-C2A	2.70	117.37	112.53
4	A	608	ISW	CMB-C2B-C1B	2.72	129.23	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	602	HEC	CMA-C3A-C2A	2.74	130.96	125.24
3	B	602	HEC	CBA-CAA-C2A	2.80	117.55	112.53
3	B	601	HEC	CMD-C2D-C3D	2.84	131.18	125.24
3	A	607	HEC	CMD-C2D-C3D	3.01	131.53	125.24
4	B	608	ISW	CMA-C3A-C2A	3.02	131.55	125.24
3	A	605	HEC	CAA-C2A-C1A	3.09	130.36	127.01
4	A	608	ISW	CMD-C2D-C3D	3.54	132.65	125.24
4	B	608	ISW	CMD-C2D-C3D	3.62	132.80	125.24
3	A	607	HEC	CAA-C2A-C1A	3.89	131.23	127.01
3	A	602	HEC	CAA-C2A-C1A	3.99	131.34	127.01
3	A	602	HEC	CBA-CAA-C2A	4.03	119.75	112.53
4	B	608	ISW	C3C-C4C-NC	4.09	114.50	109.21
4	C	601	ISW	C3C-C4C-NC	4.11	114.52	109.21
3	C	602	HEC	CBD-CAD-C3D	4.16	119.99	112.53
3	A	604	HEC	CBA-CAA-C2A	4.29	120.22	112.53
3	C	608	HEC	CAA-C2A-C1A	4.29	131.67	127.01
3	C	603	HEC	CAA-C2A-C1A	4.69	132.10	127.01
4	C	601	ISW	C4B-NB-C1B	6.88	113.51	107.32
4	A	608	ISW	C4B-NB-C1B	8.47	114.94	107.32
4	B	608	ISW	C4B-NB-C1B	8.68	115.13	107.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

39 monomers are involved in 105 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	HEC	4	0
3	A	602	HEC	4	0
3	A	603	HEC	1	0
3	A	604	HEC	3	0
3	A	605	HEC	4	0
3	A	606	HEC	1	0
4	A	608	ISW	11	0
5	A	612	PEG	1	0
5	A	613	PEG	3	0
5	A	614	PEG	1	0
6	A	615	PGE	2	0
7	A	617	EDO	1	0
7	A	619	EDO	1	0
3	B	601	HEC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	HEC	3	0
3	B	603	HEC	4	0
3	B	604	HEC	2	0
3	B	605	HEC	4	0
3	B	606	HEC	2	0
3	B	607	HEC	1	0
4	B	608	ISW	14	0
5	B	609	PEG	3	0
5	B	612	PEG	1	0
8	B	613	P6G	1	0
9	B	614	PG4	1	0
4	C	601	ISW	11	0
3	C	602	HEC	5	0
3	C	603	HEC	3	0
3	C	604	HEC	1	0
3	C	605	HEC	4	0
3	C	606	HEC	5	0
3	C	607	HEC	1	0
3	C	608	HEC	2	0
5	C	610	PEG	3	0
5	C	612	PEG	1	0
6	C	614	PGE	4	0
7	C	616	EDO	1	0
7	C	617	EDO	2	0
5	F	102	PEG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	502/546 (91%)	-0.22	5 (0%) 84 87	17, 33, 52, 88	0
1	B	502/546 (91%)	-0.28	6 (1%) 81 85	18, 34, 53, 80	0
1	C	502/546 (91%)	-0.04	14 (2%) 56 64	18, 35, 55, 82	0
2	D	49/69 (71%)	1.91	21 (42%) 0 0	39, 58, 89, 96	0
2	E	49/69 (71%)	2.52	28 (57%) 0 0	36, 64, 94, 101	0
2	F	49/69 (71%)	1.11	12 (24%) 1 1	35, 48, 72, 84	0
All	All	1653/1845 (89%)	-0.00	86 (5%) 31 39	17, 35, 63, 101	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	53	LEU	8.0
2	F	54	VAL	7.3
2	E	54	VAL	6.8
2	E	51	VAL	6.5
2	D	54	VAL	6.4
2	F	53	LEU	6.1
2	D	51	VAL	6.1
2	E	30	VAL	5.6
2	F	8	LEU	4.9
2	E	8	LEU	4.8
2	E	50	ILE	4.8
2	D	52	ALA	4.8
2	E	53	LEU	4.8
2	E	52	ALA	4.7
2	F	55	GLN	4.7
1	C	496	ALA	4.6
2	E	28	THR	4.6
2	E	55	GLN	4.5
2	D	55	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
2	E	11	ILE	4.3
2	E	9	ALA	4.2
2	D	8	LEU	4.1
2	E	24	ASP	4.0
2	D	27	PRO	4.0
2	E	19	TYR	4.0
2	D	7	SER	3.8
2	E	48	GLY	3.8
1	C	500	LYS	3.8
2	F	52	ALA	3.8
2	E	29	ASP	3.7
2	D	50	ILE	3.7
2	E	49	ASP	3.6
2	F	50	ILE	3.5
2	E	47	CYS	3.5
2	E	27	PRO	3.5
1	C	401	GLY	3.5
1	A	500	LYS	3.4
2	D	23	LYS	3.4
2	E	31	VAL	3.3
2	D	24	ASP	3.2
2	E	46	LYS	3.1
2	F	51	VAL	3.0
2	E	10	PRO	3.0
2	F	24	ASP	3.0
2	E	26	LYS	2.9
1	C	499	ASN	2.9
2	E	43	VAL	2.8
2	E	22	CYS	2.8
1	A	501	LEU	2.8
1	C	498	VAL	2.8
2	D	19	TYR	2.7
2	E	25	LYS	2.7
2	F	7	SER	2.7
1	C	493	ALA	2.7
2	D	28	THR	2.7
2	F	23	LYS	2.7
1	B	499	ASN	2.7
2	D	9	ALA	2.6
2	F	9	ALA	2.6
2	D	10	PRO	2.6
2	D	26	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	11	ILE	2.5
1	B	494	LEU	2.5
1	C	37	ALA	2.5
1	B	155	LYS	2.5
2	E	39	ASN	2.4
1	C	400	ASP	2.3
2	E	23	LYS	2.3
1	C	111	ASP	2.3
2	E	7	SER	2.3
2	D	31	VAL	2.3
1	B	137	LYS	2.2
1	C	418	LYS	2.2
1	C	501	LEU	2.2
1	C	407	LYS	2.2
2	D	48	GLY	2.2
1	B	500	LYS	2.2
2	F	10	PRO	2.1
1	C	14	LYS	2.1
2	D	39	ASN	2.1
1	A	109	LYS	2.1
1	A	502	GLU	2.1
1	B	136	GLU	2.1
2	D	49	ASP	2.1
1	A	497	ARG	2.0
1	C	109	LYS	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, 95^{th} 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
5	PEG	B	612	7/7	0.77	0.24	15.38	63,68,69,71	0
5	PEG	A	614	7/7	0.80	0.26	10.82	54,61,63,64	0
5	PEG	C	610	7/7	0.81	0.24	8.86	54,58,61,63	0
5	PEG	B	610	7/7	0.81	0.18	5.08	58,59,63,66	0
7	EDO	B	621	4/4	0.94	0.16	4.97	51,52,52,53	0
5	PEG	C	613	7/7	0.86	0.17	3.91	50,55,60,61	0
5	PEG	A	610	7/7	0.94	0.25	3.85	56,57,64,67	0
7	EDO	B	616	4/4	0.80	0.20	3.75	60,61,62,63	0
5	PEG	A	611	7/7	0.92	0.19	3.48	53,55,57,59	0
9	PG4	B	614	13/13	0.87	0.16	3.30	43,50,64,65	0
6	PGE	A	615	10/10	0.88	0.18	3.27	52,55,62,62	0
6	PGE	C	614	10/10	0.91	0.16	2.07	49,52,54,57	0
5	PEG	C	609	7/7	0.91	0.17	1.90	55,59,59,61	0
8	P6G	B	613	19/19	0.87	0.16	1.77	54,60,64,65	0
3	HEC	B	607	43/43	0.99	0.13	1.58	15,21,31,36	0
5	PEG	C	622	7/7	0.83	0.24	1.44	43,48,50,51	0
3	HEC	B	606	43/43	0.99	0.13	1.43	15,21,25,26	0
5	PEG	C	611	7/7	0.82	0.20	1.35	54,60,63,64	0
3	HEC	B	605	43/43	0.99	0.11	1.33	17,24,30,36	0
4	ISW	A	608	43/43	0.96	0.11	1.17	21,32,46,47	0
3	HEC	C	608	43/43	0.99	0.14	1.14	16,21,32,33	0
3	HEC	A	605	43/43	0.99	0.15	1.10	17,23,37,39	0
3	HEC	C	605	43/43	0.99	0.11	1.00	17,25,30,32	0
3	HEC	A	606	43/43	0.99	0.12	1.00	17,23,29,30	0
3	HEC	A	602	43/43	0.98	0.11	0.92	20,24,29,34	0
4	ISW	C	601	43/43	0.95	0.14	0.91	20,32,47,50	0
5	PEG	A	612	7/7	0.88	0.18	0.89	56,58,61,64	0
5	PEG	A	613	7/7	0.86	0.21	0.89	56,57,58,60	0
3	HEC	A	603	43/43	0.98	0.10	0.66	20,28,32,34	0
3	HEC	C	606	43/43	0.99	0.12	0.63	17,22,33,44	0
4	ISW	B	608	43/43	0.95	0.14	0.56	22,34,51,56	0
3	HEC	A	607	43/43	0.99	0.10	0.55	20,24,30,32	0
3	HEC	A	604	43/43	0.99	0.12	0.53	20,25,31,36	0
3	HEC	B	604	43/43	0.99	0.10	0.38	15,24,28,33	0
5	PEG	B	609	7/7	0.92	0.12	0.37	46,48,52,52	0
3	HEC	C	603	43/43	0.98	0.10	0.34	18,25,28,31	0
3	HEC	C	607	43/43	0.99	0.12	0.34	16,22,28,32	0
3	HEC	A	601	43/43	0.98	0.10	0.17	21,29,33,44	0
7	EDO	B	620	4/4	0.80	0.14	0.06	46,51,52,55	0
3	HEC	B	603	43/43	0.98	0.09	-0.06	23,29,33,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	HEC	C	604	43/43	0.98	0.10	-0.11	20,25,29,31	0
10	NO3	B	617	4/4	0.93	0.12	-0.29	51,53,54,56	0
7	EDO	B	619	4/4	0.95	0.10	-0.33	45,47,49,50	0
3	HEC	B	601	43/43	0.98	0.09	-0.57	26,34,43,48	0
3	HEC	C	602	43/43	0.98	0.09	-0.59	25,34,39,43	0
3	HEC	B	602	43/43	0.99	0.09	-0.68	21,26,31,33	0
7	EDO	C	617	4/4	0.93	0.09	-0.77	42,45,46,49	0
7	EDO	A	616	4/4	0.88	0.13	-1.30	44,46,46,50	0
7	EDO	C	621	4/4	0.92	0.16	-	41,42,44,45	0
5	PEG	B	611	7/7	0.91	0.12	-	60,61,61,62	0
10	NO3	F	101	4/4	0.80	0.28	-	70,71,71,71	0
7	EDO	A	618	4/4	0.93	0.10	-	42,46,46,52	0
10	NO3	C	619	4/4	0.83	0.24	-	72,72,72,72	0
7	EDO	A	619	4/4	0.95	0.19	-	44,45,48,49	0
7	EDO	C	615	4/4	0.91	0.12	-	50,51,52,55	0
7	EDO	A	617	4/4	0.74	0.25	-	63,63,63,65	0
7	EDO	B	615	4/4	0.83	0.17	-	50,51,51,55	0
7	EDO	C	618	4/4	0.84	0.17	-	51,52,53,55	0
5	PEG	C	612	7/7	0.85	0.14	-	54,56,58,60	0
7	EDO	C	620	4/4	0.87	0.14	-	48,48,49,51	0
7	EDO	C	616	4/4	0.92	0.14	-	40,45,46,50	0
5	PEG	F	102	7/7	0.88	0.24	-	50,51,54,56	0
10	NO3	B	618	4/4	0.78	0.25	-	67,68,68,69	0
5	PEG	A	609	7/7	0.93	0.13	-	44,45,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.