



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:16 PM GMT

PDB ID : 4L3Y  
Title : Nitrite complex of TvNiR, high dose data set (NO complex)  
Authors : Trofimov, A.A.; Polyakov, K.M.; Lazarenko, V.A.; Popov, A.N.; Tikhonova, T.V.; Tikhonov, A.V.; Popov, V.O.  
Deposited on : 2013-06-07  
Resolution : 1.95 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](mailto: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.

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

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

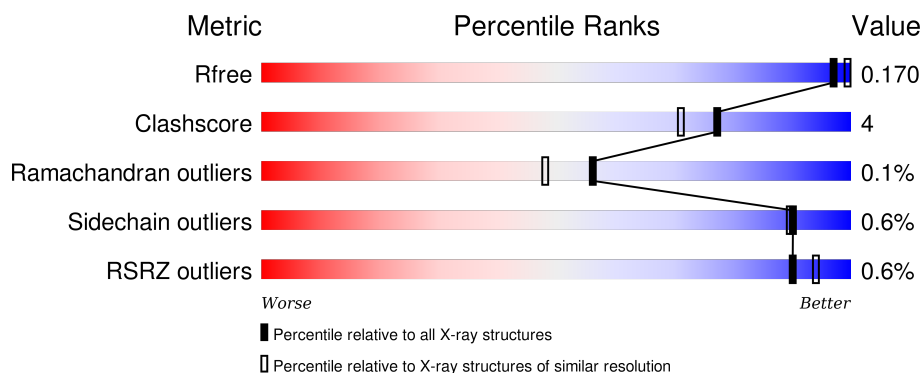
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	520	<div> <div style="width: 93%;"></div> <div style="width: 7%;"></div> </div> <div> <div style="width: 93%;"></div> <div style="width: 7%;"></div> </div>
1	B	520	<div> <div style="width: 95%;"></div> <div style="width: 5%;"></div> </div> <div> <div style="width: 95%;"></div> <div style="width: 5%;"></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	605	-	-	-	X
2	HEC	B	605	-	-	-	X
3	NO2	A	609	-	-	-	X
5	MPD	A	612	-	-	-	X
5	MPD	B	612	-	-	-	X
6	GOL	A	613[A]	-	-	-	X
6	GOL	A	613[B]	-	-	-	X
6	GOL	A	614	-	-	-	X
6	GOL	B	613[A]	-	-	-	X
6	GOL	B	613[B]	-	-	-	X
6	GOL	B	614	-	-	-	X
7	SO4	A	616	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10324 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.

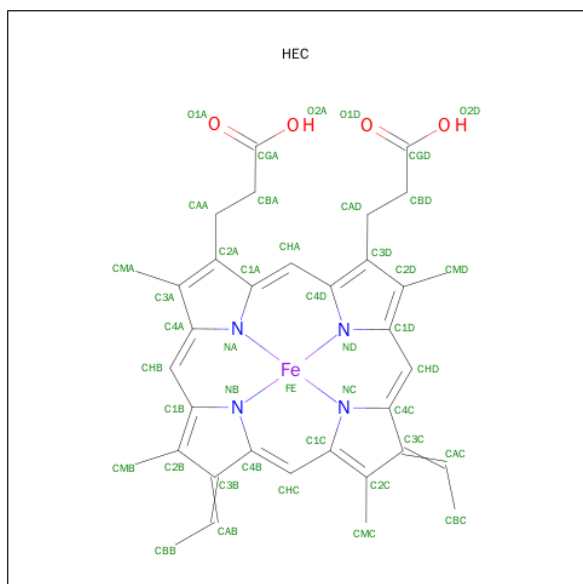
- Molecule 1 is a protein called Eight-heme nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	17	0
			4172	2587	755	796	34			
1	B	520	Total	C	N	O	S	0	16	0
			4179	2591	759	795	34			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	524	VAL	-	EXPRESSION TAG	UNP L0DSL2
B	524	VAL	-	EXPRESSION TAG	UNP L0DSL2

- Molecule 2 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



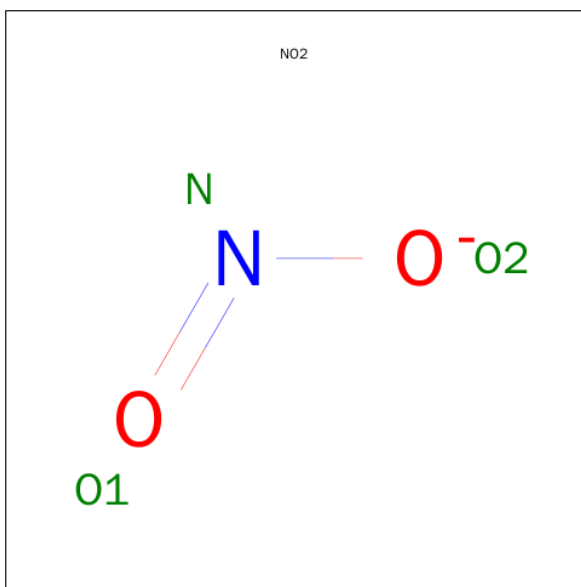
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			38	31	1	4	2		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	1
			47	36	1	4	6		
2	B	1	Total	C	Fe	N	O	0	0
			39	32	1	4	2		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO<sub>2</sub>).

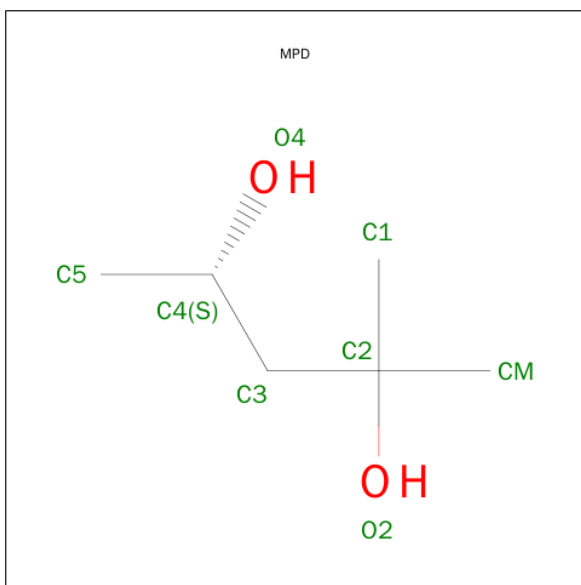


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			2	1	1		
3	A	1	Total	N	O	0	0
			3	1	2		
3	A	1	Total	N	O	0	0
			3	1	2		
3	B	1	Total	N	O	0	0
			2	1	1		
3	B	1	Total	N	O	0	0
			3	1	2		
3	B	1	Total	N	O	0	0
			3	1	2		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		
4	A	2	Total	Ca	0	0
			2	2		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



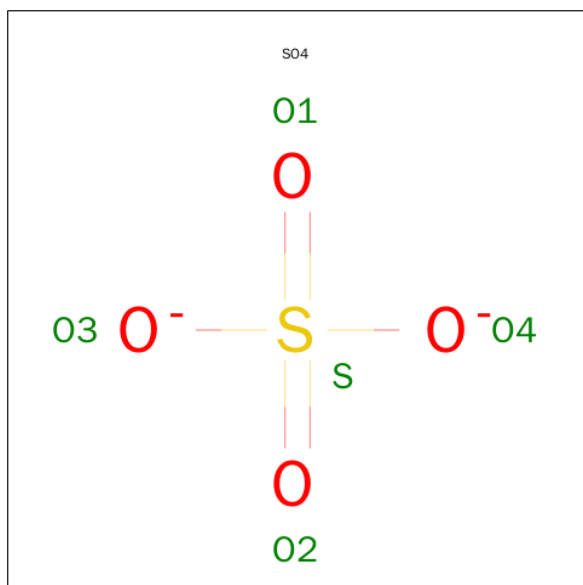
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			7	3	4		
6	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			7	3	4		
6	B	1	Total	C	O	0	1
			7	3	4		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 8 is water.

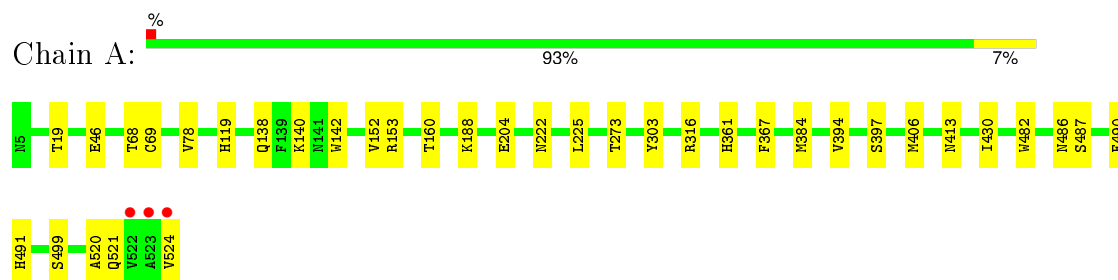
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	594	Total	O	0	0
			594	594		
8	B	617	Total	O	0	0
			617	617		



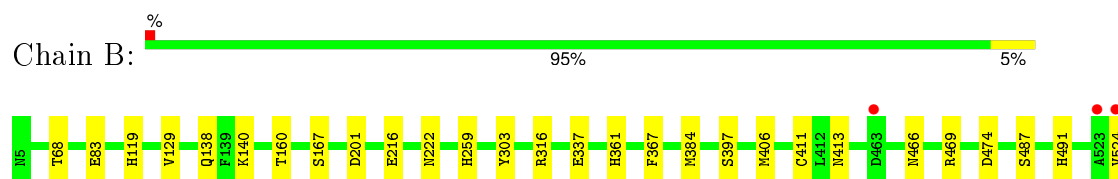
### 3 Residue-property plots

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

- Molecule 1: Eight-heme nitrite reductase



- Molecule 1: Eight-heme nitrite reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.98Å 194.98Å 194.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.08 – 1.95 29.07 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.08-1.95) 99.5 (29.07-1.95)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.151 , 0.170 0.151 , 0.170	Depositor DCC
$R_{free}$ test set	8889 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.3	EDS
Estimated twinning fraction	0.050 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 177422 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10324	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MPD, CA, SO4, HEC, NO2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.72	0/4370	0.76	2/5930 (0.0%)
1	B	0.72	1/4369 (0.0%)	0.76	2/5928 (0.0%)
All	All	0.72	1/8739 (0.0%)	0.76	4/11858 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	GLU	CD-OE1	6.16	1.32	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	LYS	CD-CE-NZ	5.35	124.00	111.70
1	B	411	CYS	CB-CA-C	-5.33	99.74	110.40
1	A	153	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	201	ASP	CB-CG-OD1	5.05	122.85	118.30

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	4172	0	3878	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4179	0	3892	27	0
2	A	339	0	236	9	0
2	B	344	0	214	7	0
3	A	8	0	0	0	0
3	B	8	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	8	0	14	1	0
5	B	8	0	14	3	0
6	A	20	0	18	0	0
6	B	13	0	12	0	0
7	A	5	0	0	0	0
7	B	5	0	0	1	0
8	A	594	0	0	10	0
8	B	617	0	0	13	0
All	All	10324	0	8278	63	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259[B]:HIS:HD2	8:B:956:HOH:O	0.82	1.17
1:A:222[A]:ASN:ND2	8:A:1186:HOH:O	1.85	1.10
1:B:138[B]:GLN:CD	8:B:1128:HOH:O	1.90	1.09
1:B:138[B]:GLN:NE2	8:B:1128:HOH:O	1.85	1.08
1:B:138[B]:GLN:OE1	8:B:1128:HOH:O	1.72	1.07
7:B:615:SO4:O1	8:B:1236:HOH:O	1.72	1.06
1:B:222[B]:ASN:ND2	8:B:1015:HOH:O	1.98	0.94
1:B:222[A]:ASN:OD1	8:B:1150:HOH:O	1.85	0.93
1:B:259[B]:HIS:CD2	8:B:956:HOH:O	1.66	0.92
1:A:204:GLU:OE2	8:A:1064:HOH:O	1.87	0.91
2:B:605:HEC:HMC1	2:B:605:HEC:HBC3	1.56	0.87
1:A:222[B]:ASN:OD1	8:A:1120:HOH:O	1.97	0.81
1:B:138[B]:GLN:NE2	5:B:612:MPD:H32	1.96	0.81
1:A:413:ASN:HB2	8:A:1118:HOH:O	1.84	0.76
1:B:474[A]:ASP:OD2	8:B:1225:HOH:O	2.07	0.73
2:A:605:HEC:HBC3	2:A:605:HEC:HMC1	1.75	0.68
2:A:606:HEC:HBC3	2:A:606:HEC:HMC1	1.77	0.67
1:A:521:GLN:O	1:A:524:VAL:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:HEC:HMC1	2:B:606:HEC:HBC3	1.83	0.60
1:B:413:ASN:HB2	8:B:1148:HOH:O	2.03	0.58
1:B:138[B]:GLN:HE21	5:B:612:MPD:H32	1.68	0.57
1:A:140:LYS:HG2	1:A:160[B]:THR:HG23	1.84	0.57
1:A:19[B]:THR:HG23	8:A:1226:HOH:O	2.03	0.57
1:A:68[B]:THR:HG23	8:A:1228:HOH:O	2.07	0.54
1:A:303:TYR:CE2	2:A:601:HEC:HMC2	2.43	0.54
1:A:140:LYS:HG2	1:A:160[B]:THR:CG2	2.39	0.53
2:B:603:HEC:HMA3	2:B:604[B]:HEC:HBA2	1.91	0.53
1:A:394[B]:VAL:HG12	8:A:950:HOH:O	2.10	0.52
1:B:138[B]:GLN:NE2	5:B:612:MPD:C3	2.70	0.51
1:A:384:MET:HB2	1:A:397:SER:O	2.10	0.51
1:B:129:VAL:HG11	2:B:601:HEC:HMA1	1.93	0.51
2:B:606:HEC:HBD2	2:B:606:HEC:HHA	1.93	0.51
1:B:524:VAL:HG13	8:B:1132:HOH:O	2.11	0.50
1:B:303:TYR:CE2	2:B:601:HEC:HMC2	2.48	0.48
1:A:367:PHE:CZ	2:A:604:HEC:HMC2	2.49	0.47
1:B:466:ASN:HD22	1:B:469:ARG:HD2	1.77	0.47
1:A:273[B]:THR:HG22	8:A:949:HOH:O	2.14	0.47
1:A:68[A]:THR:HG23	1:A:69:CYS:N	2.29	0.47
1:B:466:ASN:ND2	1:B:469:ARG:HH11	2.13	0.47
1:B:384:MET:HB2	1:B:397:SER:O	2.15	0.47
1:B:413:ASN:ND2	8:B:1142:HOH:O	2.48	0.46
1:B:140:LYS:HG2	1:B:160[B]:THR:HG23	1.99	0.45
1:A:487:SER:HB3	1:A:491:HIS:CE1	2.52	0.45
1:A:520:ALA:O	1:A:524:VAL:HG13	2.17	0.45
1:A:225:LEU:HD11	2:A:602:HEC:HMC1	1.99	0.44
1:A:138:GLN:HG2	8:A:1098:HOH:O	2.18	0.44
2:A:603:HEC:HMA3	2:A:604:HEC:HBA2	1.99	0.44
1:A:486:ASN:HB3	2:A:604:HEC:HAA1	2.00	0.44
1:B:487:SER:HB3	1:B:491:HIS:CE1	2.52	0.44
1:B:361:HIS:NE2	3:B:609:NO2:O2	2.39	0.44
1:A:46:GLU:HG3	8:A:1232:HOH:O	2.18	0.43
1:A:486:ASN:HB3	2:A:604:HEC:CAA	2.49	0.42
1:A:430:ILE:HG21	1:A:490:PHE:HA	2.02	0.42
1:B:119:HIS:CD2	2:B:603:HEC:ND	2.88	0.42
1:A:78[A]:VAL:HG12	1:A:152:VAL:HG21	2.02	0.41
1:A:119:HIS:CD2	2:A:603:HEC:ND	2.89	0.41
1:B:337:GLU:HG2	8:B:1252:HOH:O	2.21	0.41
1:A:482:TRP:HE1	1:A:499:SER:CB	2.34	0.41
1:A:142:TRP:CE3	5:A:612:MPD:H11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:SER:HB2	1:B:216[B]:GLU:HG2	2.04	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	535/520 (103%)	508 (95%)	26 (5%)	1 (0%)	52	43
1	B	534/520 (103%)	510 (96%)	24 (4%)	0	100	100
All	All	1069/1040 (103%)	1018 (95%)	50 (5%)	1 (0%)	56	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	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	455/439 (104%)	453 (100%)	2 (0%)	93	93
1	B	454/439 (103%)	450 (99%)	4 (1%)	84	83
All	All	909/878 (104%)	903 (99%)	6 (1%)	90	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	ARG
1	A	406	MET
1	B	68[A]	THR
1	B	68[B]	THR
1	B	316	ARG
1	B	406	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	B	388	GLN
1	B	413	ASN
1	B	466	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 39 ligands modelled in this entry, 4 are monoatomic - leaving 35 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
2	HEC	A	601	1,8,3	24,50,50	2.15	8 (33%)	19,82,82	2.55	8 (42%)
2	HEC	A	602	1	24,50,50	2.37	8 (33%)	19,82,82	3.08	9 (47%)
2	HEC	A	603	1,4	24,50,50	2.32	12 (50%)	19,82,82	3.01	10 (52%)
2	HEC	A	604	1	24,50,50	2.17	8 (33%)	19,82,82	3.21	9 (47%)
2	HEC	A	605	1	23,45,50	3.27	10 (43%)	18,75,82	2.82	7 (38%)
2	HEC	A	606	1	24,50,50	2.50	10 (41%)	19,82,82	2.85	7 (36%)
2	HEC	A	607	1	24,50,50	2.04	8 (33%)	19,82,82	3.02	8 (42%)
2	HEC	A	608	1	24,50,50	2.38	10 (41%)	19,82,82	2.76	10 (52%)
3	NO2	A	609	2	0,1,2	0.00	-	0,0,1	0.00	-
5	MPD	A	612	-	6,7,7	0.71	0	7,10,10	0.31	0
6	GOL	A	613[A]	-	5,5,5	0.62	0	5,5,5	0.50	0
6	GOL	A	613[B]	-	5,5,5	0.64	0	5,5,5	0.74	0
6	GOL	A	614	-	5,5,5	0.59	0	5,5,5	0.38	0
6	GOL	A	615[A]	-	5,5,5	0.27	0	5,5,5	0.48	0
6	GOL	A	615[B]	-	5,5,5	0.32	0	5,5,5	0.47	0
7	SO4	A	616	-	4,4,4	0.49	0	6,6,6	0.69	0
3	NO2	A	617	-	2,2,2	0.79	0	1,1,1	0.10	0
3	NO2	A	618	-	2,2,2	0.66	0	1,1,1	0.01	0
2	HEC	B	601	1,8,3	24,50,50	2.37	7 (29%)	19,82,82	2.55	5 (26%)
2	HEC	B	602	1	24,50,50	2.14	7 (29%)	19,82,82	3.25	8 (42%)
2	HEC	B	603	1,4	24,50,50	2.29	8 (33%)	19,82,82	3.26	8 (42%)
2	HEC	B	604[A]	-	24,50,50	2.24	9 (37%)	19,82,82	2.96	6 (31%)
2	HEC	B	604[B]	4	24,50,50	2.24	9 (37%)	19,82,82	2.89	5 (26%)
2	HEC	B	605	1	23,46,50	2.46	10 (43%)	17,77,82	2.62	4 (23%)
2	HEC	B	606	1	24,50,50	2.54	9 (37%)	19,82,82	2.80	8 (42%)
2	HEC	B	607	1	24,50,50	2.17	8 (33%)	19,82,82	2.51	5 (26%)
2	HEC	B	608	1	24,50,50	2.68	11 (45%)	19,82,82	3.07	8 (42%)
3	NO2	B	609	2	0,1,2	0.00	-	0,0,1	0.00	-
5	MPD	B	612	-	6,7,7	0.67	0	7,10,10	0.54	0
6	GOL	B	613[A]	-	5,5,5	0.57	0	5,5,5	0.39	0
6	GOL	B	613[B]	-	5,5,5	0.58	0	5,5,5	0.50	0
6	GOL	B	614	-	5,5,5	0.45	0	5,5,5	0.33	0
7	SO4	B	615	-	4,4,4	0.65	0	6,6,6	0.44	0
3	NO2	B	616	-	2,2,2	0.75	0	1,1,1	0.13	0
3	NO2	B	617	-	2,2,2	0.74	0	1,1,1	0.08	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
2	HEC	A	601	1,8,3	-	0/6/54/54	0/0/8/8
2	HEC	A	602	1	-	0/6/54/54	0/0/8/8
2	HEC	A	603	1,4	-	0/6/54/54	0/0/8/8
2	HEC	A	604	1	-	0/6/54/54	0/0/8/8
2	HEC	A	605	1	-	0/3/49/54	0/0/8/8
2	HEC	A	606	1	-	0/6/54/54	0/0/8/8
2	HEC	A	607	1	-	0/6/54/54	0/0/8/8
2	HEC	A	608	1	-	0/6/54/54	0/0/8/8
3	NO2	A	609	2	-	0/0/0/0	0/0/0/0
5	MPD	A	612	-	-	0/5/5/5	0/0/0/0
6	GOL	A	613[A]	-	-	0/4/4/4	0/0/0/0
6	GOL	A	613[B]	-	-	0/4/4/4	0/0/0/0
6	GOL	A	614	-	-	0/4/4/4	0/0/0/0
6	GOL	A	615[A]	-	-	0/4/4/4	0/0/0/0
6	GOL	A	615[B]	-	-	0/4/4/4	0/0/0/0
7	SO4	A	616	-	-	0/0/0/0	0/0/0/0
3	NO2	A	617	-	-	0/0/0/0	0/0/0/0
3	NO2	A	618	-	-	0/0/0/0	0/0/0/0
2	HEC	B	601	1,8,3	-	0/6/54/54	0/0/8/8
2	HEC	B	602	1	-	0/6/54/54	0/0/8/8
2	HEC	B	603	1,4	-	0/6/54/54	0/0/8/8
2	HEC	B	604[A]	-	-	0/6/54/54	0/0/8/8
2	HEC	B	604[B]	4	-	0/6/54/54	0/0/8/8
2	HEC	B	605	1	-	0/3/49/54	0/0/8/8
2	HEC	B	606	1	-	0/6/54/54	0/0/8/8
2	HEC	B	607	1	-	0/6/54/54	0/0/8/8
2	HEC	B	608	1	-	0/6/54/54	0/0/8/8
3	NO2	B	609	2	-	0/0/0/0	0/0/0/0
5	MPD	B	612	-	-	0/5/5/5	0/0/0/0
6	GOL	B	613[A]	-	-	0/4/4/4	0/0/0/0
6	GOL	B	613[B]	-	-	0/4/4/4	0/0/0/0
6	GOL	B	614	-	-	0/4/4/4	0/0/0/0
7	SO4	B	615	-	-	0/0/0/0	0/0/0/0
3	NO2	B	616	-	-	0/0/0/0	0/0/0/0
3	NO2	B	617	-	-	0/0/0/0	0/0/0/0

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	604	HEC	C4B-NB	-2.85	1.32	1.36
2	B	605	HEC	C4B-NB	-2.44	1.33	1.36
2	A	603	HEC	C4C-NC	-2.40	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	606	HEC	C4C-NC	-2.36	1.33	1.36
2	A	604	HEC	C4C-NC	-2.26	1.33	1.36
2	B	608	HEC	C1A-NA	-2.20	1.33	1.36
2	B	604[B]	HEC	C4B-NB	-2.19	1.33	1.36
2	B	604[A]	HEC	C4B-NB	-2.19	1.33	1.36
2	A	603	HEC	C1A-NA	-2.06	1.33	1.36
2	B	603	HEC	C3C-C4C	2.04	1.47	1.42
2	A	601	HEC	C4D-CHA	2.06	1.45	1.39
2	A	604	HEC	C1B-CHB	2.06	1.45	1.39
2	A	604	HEC	C3C-C4C	2.09	1.47	1.42
2	A	607	HEC	C3C-C4C	2.10	1.47	1.42
2	A	605	HEC	C1C-CHC	2.12	1.45	1.39
2	B	601	HEC	C3C-C4C	2.14	1.47	1.42
2	B	608	HEC	C1B-CHB	2.14	1.45	1.39
2	B	601	HEC	C3B-C4B	2.16	1.47	1.42
2	B	606	HEC	C4D-CHA	2.21	1.45	1.39
2	B	601	HEC	C1B-CHB	2.21	1.45	1.39
2	A	602	HEC	C3C-C4C	2.22	1.47	1.42
2	B	604[B]	HEC	C3C-C4C	2.26	1.47	1.42
2	B	604[A]	HEC	C3C-C4C	2.26	1.47	1.42
2	B	603	HEC	C1B-CHB	2.26	1.46	1.39
2	A	608	HEC	C1D-CHD	2.27	1.46	1.39
2	B	607	HEC	C4D-CHA	2.27	1.46	1.39
2	B	602	HEC	C4D-CHA	2.27	1.46	1.39
2	B	603	HEC	C1C-CHC	2.29	1.46	1.39
2	B	605	HEC	C3B-C4B	2.30	1.48	1.42
2	A	601	HEC	C3B-C4B	2.32	1.48	1.42
2	A	608	HEC	C1B-CHB	2.32	1.46	1.39
2	A	602	HEC	C1C-CHC	2.33	1.46	1.39
2	A	606	HEC	C4D-CHA	2.33	1.46	1.39
2	B	602	HEC	C1C-CHC	2.33	1.46	1.39
2	A	607	HEC	C1D-CHD	2.35	1.46	1.39
2	A	603	HEC	C3C-C4C	2.38	1.48	1.42
2	A	607	HEC	C3D-C2D	2.38	1.44	1.37
2	B	602	HEC	C1B-CHB	2.41	1.46	1.39
2	A	607	HEC	C1C-CHC	2.42	1.46	1.39
2	A	601	HEC	C1C-CHC	2.44	1.46	1.39
2	A	603	HEC	C1D-CHD	2.45	1.46	1.39
2	A	603	HEC	C2A-C3A	2.45	1.44	1.37
2	B	606	HEC	C1C-CHC	2.45	1.46	1.39
2	B	608	HEC	C1D-CHD	2.46	1.46	1.39
2	A	606	HEC	C1C-CHC	2.49	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	606	HEC	C1D-CHD	2.51	1.46	1.39
2	A	608	HEC	C1C-CHC	2.52	1.46	1.39
2	B	604[B]	HEC	C1C-CHC	2.55	1.46	1.39
2	B	604[A]	HEC	C1C-CHC	2.55	1.46	1.39
2	B	604[B]	HEC	C1B-CHB	2.55	1.46	1.39
2	B	604[A]	HEC	C1B-CHB	2.55	1.46	1.39
2	B	606	HEC	C3C-C4C	2.56	1.48	1.42
2	A	603	HEC	C1C-CHC	2.57	1.46	1.39
2	B	605	HEC	C1B-CHB	2.59	1.47	1.39
2	A	603	HEC	C3B-C4B	2.60	1.48	1.42
2	B	602	HEC	C3D-C2D	2.60	1.45	1.37
2	A	604	HEC	C3D-C2D	2.61	1.45	1.37
2	A	607	HEC	C1B-CHB	2.61	1.47	1.39
2	A	603	HEC	C1B-CHB	2.64	1.47	1.39
2	B	605	HEC	C3D-C2D	2.65	1.50	1.41
2	B	606	HEC	C2A-C3A	2.66	1.45	1.37
2	A	602	HEC	C4D-CHA	2.66	1.47	1.39
2	B	608	HEC	C3B-C4B	2.67	1.48	1.42
2	A	605	HEC	C1B-CHB	2.68	1.47	1.39
2	B	604[B]	HEC	C3B-C4B	2.68	1.48	1.42
2	B	604[A]	HEC	C3B-C4B	2.68	1.48	1.42
2	B	608	HEC	C1C-CHC	2.69	1.47	1.39
2	B	607	HEC	C3D-C2D	2.71	1.45	1.37
2	B	608	HEC	C4D-CHA	2.71	1.47	1.39
2	B	604[B]	HEC	C3D-C2D	2.73	1.45	1.37
2	B	604[A]	HEC	C3D-C2D	2.73	1.45	1.37
2	B	602	HEC	C2A-C3A	2.73	1.45	1.37
2	A	608	HEC	C4D-CHA	2.73	1.47	1.39
2	B	606	HEC	C1B-CHB	2.74	1.47	1.39
2	B	606	HEC	C3B-C4B	2.75	1.49	1.42
2	B	607	HEC	C2A-C3A	2.78	1.45	1.37
2	A	601	HEC	C1B-CHB	2.78	1.47	1.39
2	B	607	HEC	C1C-CHC	2.83	1.47	1.39
2	B	607	HEC	C1B-CHB	2.83	1.47	1.39
2	A	607	HEC	C2A-C3A	2.83	1.46	1.37
2	A	606	HEC	C3C-C4C	2.84	1.49	1.42
2	A	601	HEC	C3D-C2D	2.85	1.46	1.37
2	B	603	HEC	C4D-CHA	2.90	1.47	1.39
2	B	607	HEC	C3B-C4B	2.90	1.49	1.42
2	A	605	HEC	C4D-CHA	2.91	1.49	1.43
2	A	608	HEC	C3C-C4C	2.92	1.49	1.42
2	A	602	HEC	C1D-CHD	2.93	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	608	HEC	C3B-C4B	2.99	1.49	1.42
2	A	603	HEC	C4D-CHA	2.99	1.48	1.39
2	B	608	HEC	C2A-C3A	3.00	1.46	1.37
2	B	603	HEC	C2A-C3A	3.01	1.46	1.37
2	A	601	HEC	C2A-C3A	3.02	1.46	1.37
2	A	606	HEC	C3B-C4B	3.07	1.49	1.42
2	A	602	HEC	C2A-C3A	3.07	1.46	1.37
2	B	603	HEC	C3D-C2D	3.17	1.47	1.37
2	B	601	HEC	C3D-C2D	3.18	1.47	1.37
2	A	604	HEC	C2A-C3A	3.20	1.47	1.37
2	B	601	HEC	C2A-C3A	3.23	1.47	1.37
2	B	608	HEC	C3D-C2D	3.26	1.47	1.37
2	A	606	HEC	C2A-C3A	3.29	1.47	1.37
2	B	605	HEC	C1D-CHD	3.32	1.49	1.39
2	A	606	HEC	C3D-C2D	3.33	1.47	1.37
2	A	603	HEC	C3D-C2D	3.34	1.47	1.37
2	B	606	HEC	C3D-C2D	3.34	1.47	1.37
2	A	608	HEC	C3D-C2D	3.35	1.47	1.37
2	B	605	HEC	C3C-C4C	3.37	1.50	1.42
2	A	608	HEC	C2A-C3A	3.38	1.47	1.37
2	B	605	HEC	C4D-CHA	3.38	1.49	1.39
2	A	605	HEC	C1D-CHD	3.46	1.49	1.39
2	A	602	HEC	C3D-C2D	3.50	1.48	1.37
2	A	605	HEC	C3C-C4C	3.51	1.50	1.42
2	B	608	HEC	C3C-C4C	3.54	1.50	1.42
2	B	604[B]	HEC	C2A-C3A	3.66	1.48	1.37
2	B	604[A]	HEC	C2A-C3A	3.66	1.48	1.37
2	A	605	HEC	C2A-C3A	3.79	1.48	1.37
2	B	605	HEC	C2A-C3A	3.80	1.48	1.37
2	A	605	HEC	C3D-C2D	4.26	1.50	1.38
2	B	604[B]	HEC	C3B-C2B	4.30	1.45	1.40
2	B	604[A]	HEC	C3B-C2B	4.30	1.45	1.40
2	A	601	HEC	C3B-C2B	4.51	1.45	1.40
2	A	604	HEC	C3B-C2B	4.52	1.45	1.40
2	B	602	HEC	C3B-C2B	4.60	1.45	1.40
2	B	605	HEC	C3B-C2B	4.64	1.45	1.40
2	B	607	HEC	C3C-C2C	4.77	1.45	1.40
2	A	607	HEC	C3B-C2B	5.01	1.46	1.40
2	A	607	HEC	C3C-C2C	5.10	1.46	1.40
2	A	603	HEC	C3B-C2B	5.13	1.46	1.40
2	A	608	HEC	C3B-C2B	5.15	1.46	1.40
2	A	603	HEC	C3C-C2C	5.17	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEC	C3C-C2C	5.31	1.46	1.40
2	A	602	HEC	C3B-C2B	5.33	1.46	1.40
2	B	607	HEC	C3B-C2B	5.61	1.46	1.40
2	B	601	HEC	C3C-C2C	5.64	1.46	1.40
2	A	605	HEC	C3B-C2B	5.73	1.46	1.40
2	B	602	HEC	C3C-C2C	5.75	1.46	1.40
2	B	603	HEC	C3B-C2B	5.78	1.46	1.40
2	A	601	HEC	C3C-C2C	5.79	1.46	1.40
2	A	604	HEC	C3C-C2C	5.88	1.46	1.40
2	B	605	HEC	C3C-C2C	6.13	1.47	1.40
2	A	608	HEC	C3C-C2C	6.16	1.47	1.40
2	B	603	HEC	C3C-C2C	6.17	1.47	1.40
2	A	606	HEC	C3C-C2C	6.20	1.47	1.40
2	A	606	HEC	C3B-C2B	6.35	1.47	1.40
2	B	608	HEC	C3B-C2B	6.43	1.47	1.40
2	B	604[B]	HEC	C3C-C2C	6.44	1.47	1.40
2	B	604[A]	HEC	C3C-C2C	6.44	1.47	1.40
2	A	602	HEC	C3C-C2C	6.54	1.47	1.40
2	B	606	HEC	C3B-C2B	6.64	1.47	1.40
2	B	601	HEC	C3B-C2B	6.81	1.47	1.40
2	B	606	HEC	C3C-C2C	7.08	1.48	1.40
2	B	608	HEC	C3C-C2C	7.10	1.48	1.40
2	A	605	HEC	C3D-C4D	9.80	1.51	1.39

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	HEC	CBB-CAB-C3B	-9.96	105.22	127.35
2	B	603	HEC	CBB-CAB-C3B	-8.31	108.88	127.35
2	B	601	HEC	CBB-CAB-C3B	-8.13	109.28	127.35
2	A	604	HEC	CBB-CAB-C3B	-7.90	109.80	127.35
2	A	602	HEC	CBB-CAB-C3B	-7.70	110.24	127.35
2	A	607	HEC	CBB-CAB-C3B	-7.65	110.35	127.35
2	B	608	HEC	CBB-CAB-C3B	-7.51	110.67	127.35
2	B	604[B]	HEC	CBB-CAB-C3B	-7.39	110.93	127.35
2	B	604[A]	HEC	CBB-CAB-C3B	-7.39	110.93	127.35
2	A	603	HEC	CBB-CAB-C3B	-7.28	111.18	127.35
2	A	604	HEC	CBA-CAA-C2A	-7.11	99.78	112.53
2	A	601	HEC	CBB-CAB-C3B	-7.11	111.54	127.35
2	B	607	HEC	CBB-CAB-C3B	-6.92	111.97	127.35
2	B	603	HEC	CBC-CAC-C3C	-6.76	112.32	127.35
2	B	605	HEC	CBA-CAA-C2A	-6.76	100.41	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	608	HEC	CBC-CAC-C3C	-6.35	113.25	127.35
2	A	602	HEC	CAD-CBD-CGD	-6.20	101.39	112.75
2	B	606	HEC	CAA-CBA-CGA	-6.05	101.66	112.75
2	A	605	HEC	CBA-CAA-C2A	-6.01	101.76	112.53
2	A	606	HEC	CBC-CAC-C3C	-5.99	114.04	127.35
2	A	606	HEC	CBB-CAB-C3B	-5.93	114.17	127.35
2	B	606	HEC	CBB-CAB-C3B	-5.82	114.42	127.35
2	A	603	HEC	CBC-CAC-C3C	-5.81	114.44	127.35
2	B	604[A]	HEC	CBA-CAA-C2A	-5.62	102.45	112.53
2	A	608	HEC	CBB-CAB-C3B	-5.57	114.98	127.35
2	A	607	HEC	CBA-CAA-C2A	-5.53	102.61	112.53
2	A	605	HEC	C4D-C3D-C2D	-5.49	101.92	106.42
2	B	604[B]	HEC	CBD-CAD-C3D	-5.45	102.75	112.53
2	B	604[A]	HEC	CBD-CAD-C3D	-5.45	102.75	112.53
2	A	605	HEC	CBB-CAB-C3B	-5.44	115.27	127.35
2	B	604[B]	HEC	CBA-CAA-C2A	-5.40	102.84	112.53
2	B	605	HEC	CBC-CAC-C3C	-5.38	115.41	127.35
2	B	608	HEC	CBD-CAD-C3D	-5.36	102.92	112.53
2	A	606	HEC	CAA-CBA-CGA	-5.36	102.93	112.75
2	B	608	HEC	CBC-CAC-C3C	-5.33	115.51	127.35
2	A	604	HEC	CBD-CAD-C3D	-5.07	103.44	112.53
2	B	608	HEC	CBA-CAA-C2A	-5.07	103.44	112.53
2	B	607	HEC	CBA-CAA-C2A	-4.92	103.70	112.53
2	A	603	HEC	CBA-CAA-C2A	-4.92	103.71	112.53
2	B	604[B]	HEC	CBC-CAC-C3C	-4.92	116.43	127.35
2	B	604[A]	HEC	CBC-CAC-C3C	-4.92	116.43	127.35
2	A	602	HEC	CBC-CAC-C3C	-4.89	116.49	127.35
2	B	605	HEC	CBB-CAB-C3B	-4.84	116.61	127.35
2	B	603	HEC	CBA-CAA-C2A	-4.71	104.09	112.53
2	B	606	HEC	CBC-CAC-C3C	-4.70	116.90	127.35
2	B	603	HEC	CBD-CAD-C3D	-4.52	104.42	112.53
2	B	602	HEC	CBC-CAC-C3C	-4.41	117.56	127.35
2	A	605	HEC	CBC-CAC-C3C	-4.39	117.59	127.35
2	A	607	HEC	CAD-CBD-CGD	-4.38	104.72	112.75
2	A	607	HEC	CBC-CAC-C3C	-4.29	117.82	127.35
2	A	601	HEC	CBC-CAC-C3C	-4.23	117.95	127.35
2	B	607	HEC	CAD-CBD-CGD	-4.15	105.15	112.75
2	B	602	HEC	CAD-CBD-CGD	-4.12	105.19	112.75
2	A	606	HEC	CBA-CAA-C2A	-4.06	105.26	112.53
2	B	602	HEC	CAA-CBA-CGA	-3.98	105.45	112.75
2	A	608	HEC	CAD-CBD-CGD	-3.97	105.47	112.75
2	A	602	HEC	CAA-CBA-CGA	-3.94	105.53	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	HEC	CBD-CAD-C3D	-3.88	105.57	112.53
2	B	602	HEC	C4C-C3C-C2C	-3.69	102.36	106.35
2	A	608	HEC	CBD-CAD-C3D	-3.62	106.03	112.53
2	A	604	HEC	CBC-CAC-C3C	-3.53	119.50	127.35
2	A	608	HEC	CAA-CBA-CGA	-3.53	106.28	112.75
2	A	607	HEC	CBD-CAD-C3D	-3.53	106.20	112.53
2	B	601	HEC	CBC-CAC-C3C	-3.47	119.63	127.35
2	B	606	HEC	CBA-CAA-C2A	-3.42	106.41	112.53
2	A	602	HEC	C4C-C3C-C2C	-3.14	102.97	106.35
2	A	601	HEC	CBA-CAA-C2A	-3.09	107.00	112.53
2	B	601	HEC	CBD-CAD-C3D	-2.90	107.32	112.53
2	A	606	HEC	C4B-C3B-C2B	-2.83	103.30	106.35
2	B	606	HEC	C4C-C3C-C2C	-2.83	103.30	106.35
2	B	601	HEC	CBA-CAA-C2A	-2.80	107.50	112.53
2	A	603	HEC	C4C-C3C-C2C	-2.80	103.33	106.35
2	A	606	HEC	CBD-CAD-C3D	-2.74	107.62	112.53
2	A	601	HEC	CBD-CAD-C3D	-2.71	107.66	112.53
2	B	603	HEC	C4C-C3C-C2C	-2.70	103.44	106.35
2	A	607	HEC	C4C-C3C-C2C	-2.67	103.47	106.35
2	B	607	HEC	CBC-CAC-C3C	-2.67	121.41	127.35
2	A	601	HEC	C4C-C3C-C2C	-2.61	103.54	106.35
2	A	608	HEC	C4B-C3B-C2B	-2.60	103.54	106.35
2	A	603	HEC	CAA-CBA-CGA	-2.55	108.07	112.75
2	B	606	HEC	C4B-C3B-C2B	-2.51	103.64	106.35
2	A	606	HEC	C4C-C3C-C2C	-2.41	103.75	106.35
2	A	608	HEC	C4C-C3C-C2C	-2.28	103.89	106.35
2	B	607	HEC	C4B-C3B-C2B	-2.28	103.89	106.35
2	B	608	HEC	C4B-C3B-C2B	-2.26	103.91	106.35
2	B	606	HEC	CBD-CAD-C3D	-2.25	108.50	112.53
2	A	608	HEC	CBA-CAA-C2A	-2.22	108.56	112.53
2	B	603	HEC	CAA-CBA-CGA	-2.19	108.73	112.75
2	B	608	HEC	C4C-C3C-C2C	-2.19	103.99	106.35
2	A	604	HEC	C4C-C3C-C2C	-2.15	104.03	106.35
2	A	604	HEC	C4B-C3B-C2B	-2.09	104.10	106.35
2	B	603	HEC	CAD-CBD-CGD	-2.09	108.92	112.75
2	B	608	HEC	CAA-CBA-CGA	-2.06	108.97	112.75
2	A	608	HEC	CMC-C2C-C1C	-2.03	125.01	128.36
2	A	607	HEC	CAD-C3D-C4D	2.01	129.19	127.01
2	A	603	HEC	CAD-C3D-C4D	2.04	129.22	127.01
2	A	601	HEC	CAD-CBD-CGD	2.04	116.48	112.75
2	A	603	HEC	C3B-C4B-NB	2.05	114.82	110.94
2	B	604[B]	HEC	CMA-C3A-C2A	2.08	129.59	125.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	604[A]	HEC	CMA-C3A-C2A	2.08	129.59	125.24
2	A	603	HEC	C3C-C4C-NC	2.09	114.88	110.94
2	A	605	HEC	CMA-C3A-C2A	2.10	129.63	125.24
2	A	601	HEC	C3C-C4C-NC	2.12	114.94	110.94
2	A	604	HEC	CAA-CBA-CGA	2.18	116.75	112.75
2	A	604	HEC	C3B-C4B-NB	2.21	115.13	110.94
2	A	602	HEC	C3B-C4B-NB	2.23	115.15	110.94
2	A	608	HEC	C3B-C4B-NB	2.23	115.16	110.94
2	A	601	HEC	CAD-C3D-C4D	2.33	129.54	127.01
2	B	602	HEC	C3B-C4B-NB	2.34	115.36	110.94
2	B	601	HEC	CMD-C2D-C3D	2.36	130.18	125.24
2	A	602	HEC	C3C-C4C-NC	2.36	115.41	110.94
2	B	605	HEC	CAD-C3D-C2D	2.39	130.03	125.14
2	A	602	HEC	CMD-C2D-C3D	2.44	130.35	125.24
2	A	605	HEC	CMD-C2D-C3D	2.47	129.50	124.84
2	B	604[A]	HEC	CAA-CBA-CGA	2.49	117.32	112.75
2	B	608	HEC	CMA-C3A-C2A	2.53	130.52	125.24
2	A	607	HEC	C3C-C4C-NC	2.57	115.79	110.94
2	A	602	HEC	CMA-C3A-C2A	2.66	130.81	125.24
2	B	602	HEC	C3C-C4C-NC	2.71	116.06	110.94
2	A	603	HEC	CMA-C3A-C2A	2.81	131.10	125.24
2	B	603	HEC	CMA-C3A-C2A	2.82	131.13	125.24
2	B	606	HEC	CAD-C3D-C4D	3.02	130.28	127.01
2	B	602	HEC	CMA-C3A-C2A	3.26	132.04	125.24
2	A	605	HEC	C3D-C4D-ND	3.32	114.41	110.36
2	A	604	HEC	CAD-C3D-C4D	3.36	130.66	127.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEC	1	0
2	A	602	HEC	1	0
2	A	603	HEC	2	0
2	A	604	HEC	4	0
2	A	605	HEC	1	0
2	A	606	HEC	1	0
5	A	612	MPD	1	0
2	B	601	HEC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	603	HEC	2	0
2	B	604[B]	HEC	1	0
2	B	605	HEC	1	0
2	B	606	HEC	2	0
3	B	609	NO2	1	0
5	B	612	MPD	3	0
7	B	615	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	520/520 (100%)	-0.48	3 (0%) 90 94	10, 15, 29, 55	1 (0%)
1	B	520/520 (100%)	-0.54	3 (0%) 90 94	8, 13, 27, 50	0
All	All	1040/1040 (100%)	-0.51	6 (0%) 90 94	8, 14, 28, 55	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	524	VAL	5.5
1	A	524	VAL	4.1
1	A	523	ALA	3.4
1	B	523	ALA	3.3
1	B	463[A]	ASP	2.6
1	A	522	VAL	2.2

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

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

### 6.3 Carbohydrates [i](#)

There are no 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	GOL	A	613[B]	6/6	0.96	0.11	10.25	15,16,17,18	1
6	GOL	A	613[A]	6/6	0.96	0.11	10.25	14,16,17,18	1
6	GOL	A	614	6/6	0.97	0.13	7.72	20,25,26,28	0
7	SO4	A	616	5/5	0.93	0.19	7.69	26,27,29,30	5
5	MPD	A	612	8/8	0.91	0.17	5.91	21,26,27,28	0
6	GOL	B	614	6/6	0.98	0.11	5.61	19,23,24,28	0
6	GOL	B	613[A]	6/6	0.96	0.10	4.77	12,15,16,16	1
6	GOL	B	613[B]	6/6	0.96	0.10	4.77	13,15,16,17	1
3	NO2	A	609	2/3	0.99	0.17	2.88	13,13,13,14	2
5	MPD	B	612	8/8	0.93	0.12	2.46	18,21,22,22	0
2	HEC	B	605	39/43	0.96	0.13	2.34	19,26,44,50	0
2	HEC	A	605	38/43	0.95	0.14	2.06	21,29,44,47	0
2	HEC	B	604[A]	43/43	0.99	0.08	1.19	8,8,9,10	4
2	HEC	B	604[B]	43/43	0.99	0.08	1.19	8,8,10,13	4
2	HEC	A	604	43/43	0.99	0.08	1.17	9,10,13,19	0
3	NO2	B	609	2/3	0.99	0.11	1.10	10,10,10,10	2
2	HEC	B	602	43/43	0.98	0.09	0.86	8,9,16,21	0
2	HEC	B	607	43/43	0.98	0.10	0.83	9,10,22,29	0
2	HEC	A	601	43/43	0.99	0.10	0.78	9,11,12,13	0
2	HEC	A	607	43/43	0.98	0.09	0.63	9,11,23,34	0
2	HEC	A	603	43/43	0.99	0.10	0.43	8,9,10,12	0
2	HEC	B	603	43/43	0.99	0.09	0.39	7,7,9,11	0
2	HEC	B	601	43/43	0.99	0.09	0.38	7,9,10,11	0
2	HEC	B	606	43/43	0.99	0.08	0.21	9,11,13,14	0
2	HEC	A	602	43/43	0.98	0.08	0.19	9,11,17,21	0
2	HEC	A	606	43/43	0.99	0.07	-0.12	11,12,14,14	0
2	HEC	A	608	43/43	0.99	0.07	-0.40	11,13,17,22	0
2	HEC	B	608	43/43	0.98	0.08	-0.44	12,16,18,22	0
3	NO2	B	617	3/3	0.99	0.05	-0.86	13,13,13,14	3
3	NO2	A	618	3/3	0.98	0.07	-0.99	17,17,17,18	3
3	NO2	A	617	3/3	0.99	0.05	-1.05	23,23,24,25	3
4	CA	A	610	1/1	1.00	0.04	-2.22	17,17,17,17	0
4	CA	B	610	1/1	1.00	0.02	-3.61	16,16,16,16	0
6	GOL	A	615[B]	6/6	0.66	0.29	-	37,48,56,56	1
4	CA	A	611	1/1	0.98	0.05	-	14,14,14,14	1
4	CA	B	611	1/1	0.98	0.06	-	12,12,12,12	1
3	NO2	B	616	3/3	0.98	0.07	-	21,21,22,23	3
7	SO4	B	615	5/5	0.94	0.17	-	21,21,22,23	5
6	GOL	A	615[A]	6/6	0.66	0.29	-	36,48,56,56	1

## 6.5 Other polymers

There are no such residues in this entry.