Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:06 PM GMT

PDB ID	:	1NIR
Title	:	OXYDIZED NITRITE REDUCTASE FROM PSEUDOMONAS AERUGINOSA
Authors	:	Nurizzo, D.; Tegoni, M.; Cambillau, C.
Deposited on	:	1997-06-17
Resolution	:	2.15 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 (i) symbol.

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

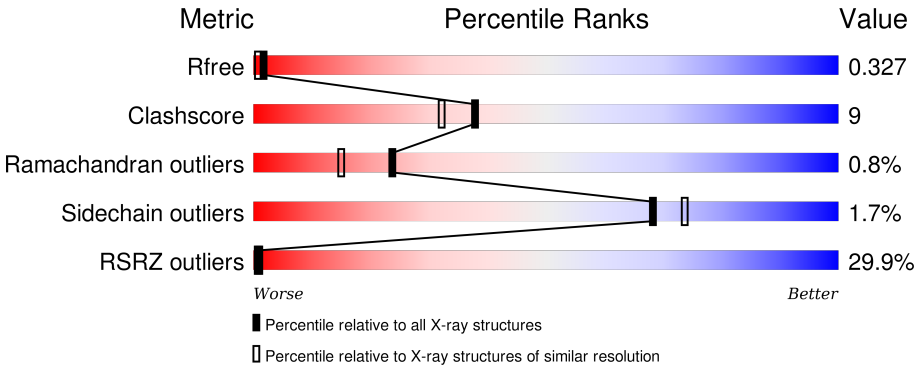
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	543	20% 75% 22%
1	B	543	39% 79% 18%

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	PO4	A	604	-	X	-	-
2	PO4	B	604	-	X	-	-

2 Entry composition

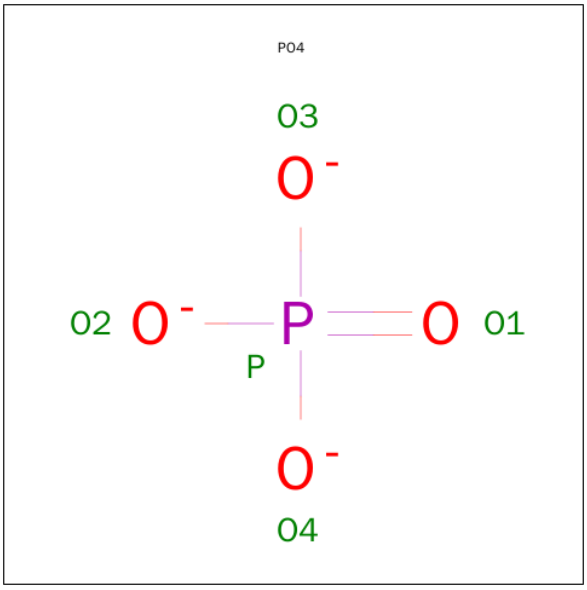
There are 7 unique types of molecules in this entry. The entry contains 9483 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4203	2665	733	793	12			
1	B	539	Total	C	N	O	S	0	0	0
			4212	2671	735	794	12			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

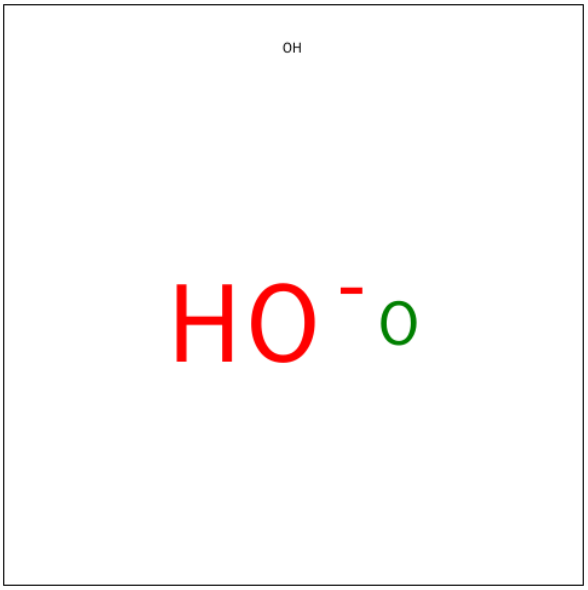


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

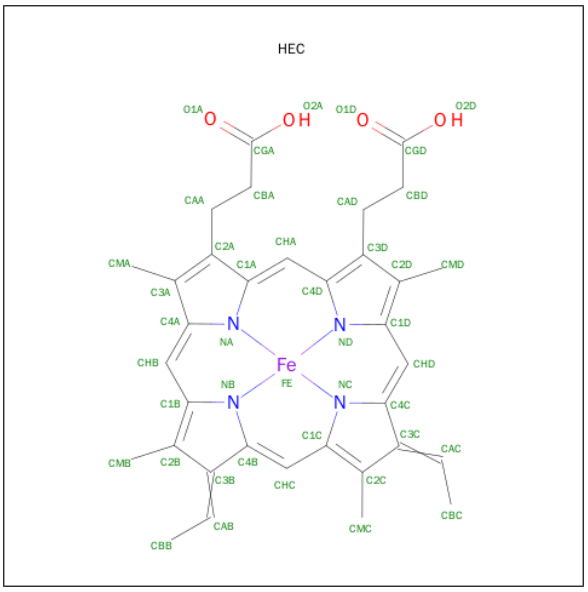
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



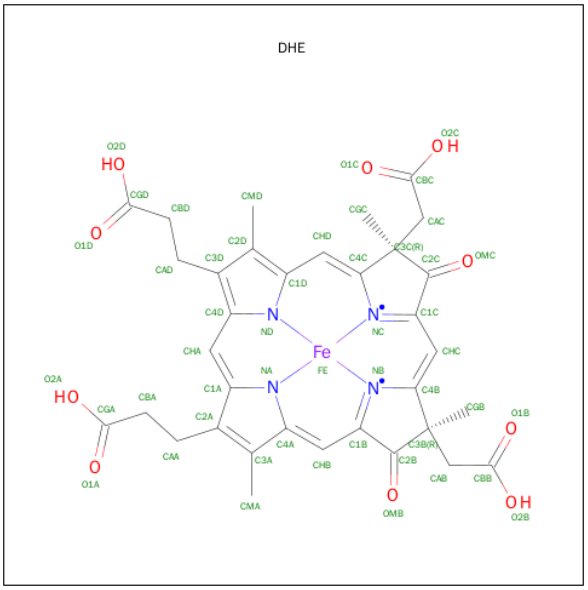
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 6 is HEME D (three-letter code: DHE) (formula: $C_{34}H_{32}FeN_4O_{10}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			49	34	1	4	10		
6	B	1	Total	C	Fe	N	O	0	0
			49	34	1	4	10		

- Molecule 7 is water.

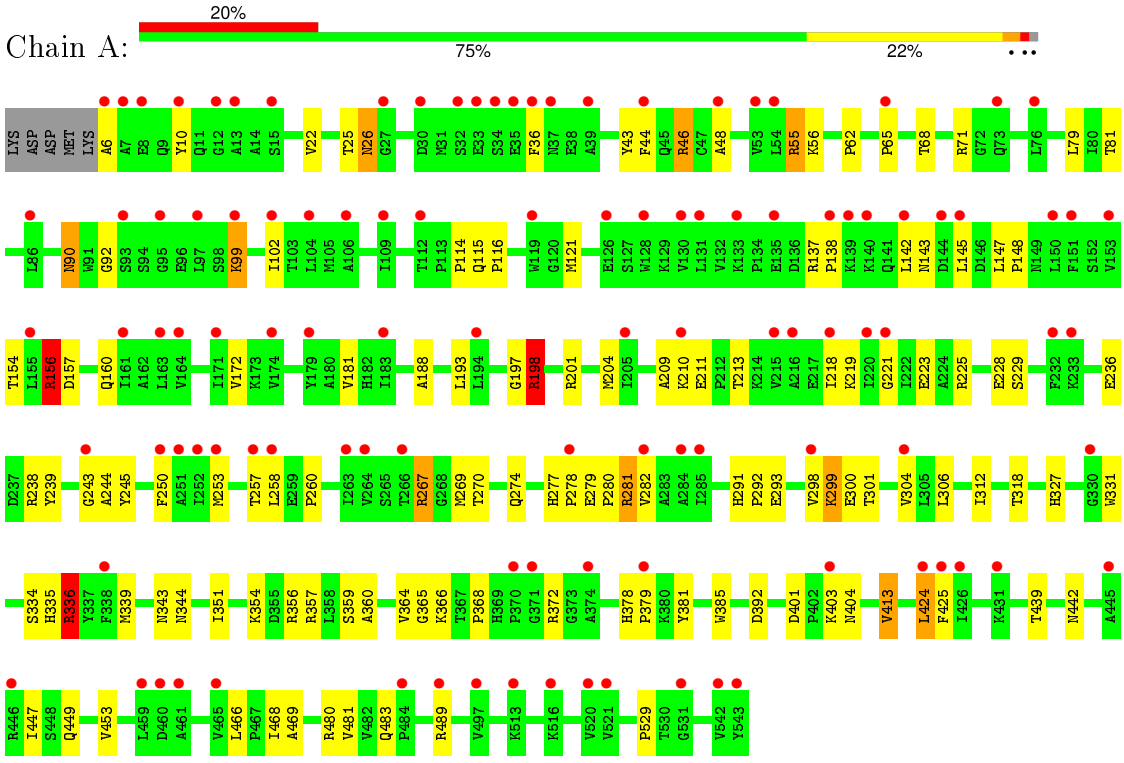
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	449	Total O 449 449	0	0
7	B	421	Total O 421 421	0	0

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.

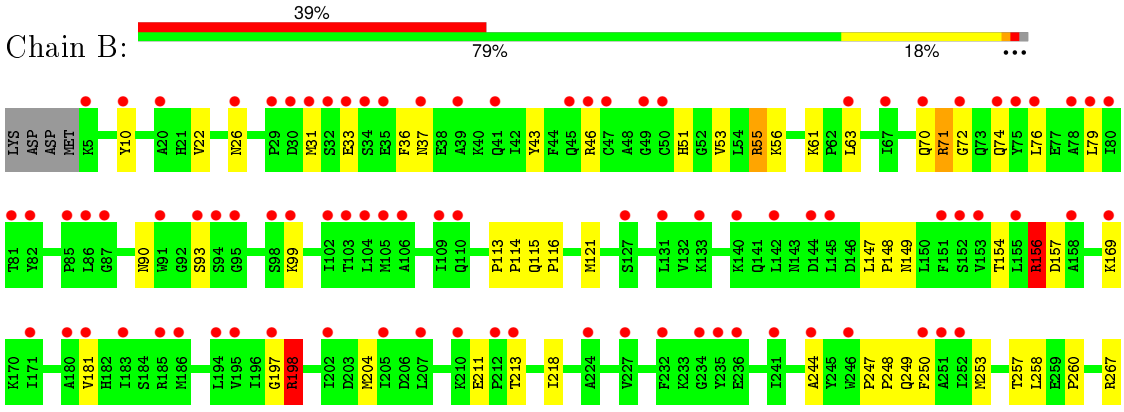
- Molecule 1: NITRITE REDUCTASE

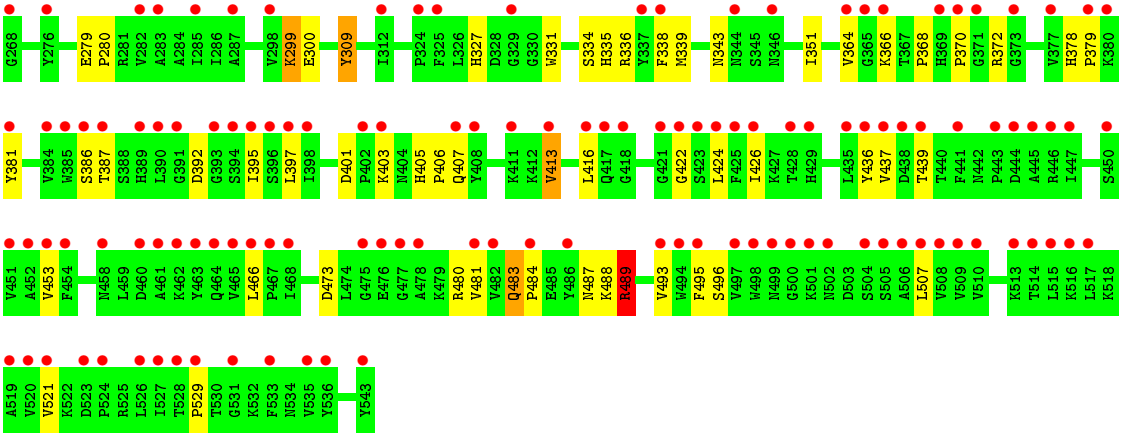
Chain A:



- Molecule 1: NITRITE REDUCTASE

Chain B:




G268 Y276 E279 P280 R281 V282 A283 A284 I285 I286 A287 V298 K299 E300 Y309 I312 P324 F325 L326 H327 D328 G329 G330 W331 S334 H335 R336 Y337 F338 M339 N343 N344 S345 N346 I351 V364 G365 K366 T367 P368 H369 P370 G371 R372 G373 V377 H378 P379 K380
Y381 V384 W385 S386 T387 S388 H389 L390 G391 D392 G393 S394 I395 S396 L397 I398 D401 P402 K403 N404 H405 P406 Q407 Y408 K411 K412 V413 L416 Q417 G418 G421 G422 S423 L424 F425 I426 K427 T428 H429 L435 Y436 V437 D438 T439 T440 F441 N442 P443 D444 A445 R446 I447 S450
V451 A452 V453 F454 N458 L459 D460 A461 K462 Y463 Q464 V465 L466 P467 I468 D473 L474 G475 E476 G477 A478 K479 R480 V481 V482 Q483 P484 E485 Y486 N487 K488 R489 V493 W494 F495 S496 V497 W498 N499 G500 K501 N502 D503 S504 S505 A506 L507 V508 V509 V510 K513 T514 L515 K516 L517 K518
A519 V520 V521 K522 D523 P524 R525 L526 I527 T528 P529 T530 G531 K532 F533 N534 V535 Y536 Y543

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	163.07Å 90.07Å 111.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15 29.48 – 2.13	Depositor EDS
% Data completeness (in resolution range)	89.0 (30.00-2.15) 88.7 (29.48-2.13)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	5.31 (at 2.14Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.209 , 0.242 0.318 , 0.327	Depositor DCC
R_{free} test set	3191 reflections (4.10%)	DCC
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	4 of 91621 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9483	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.40 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.9823e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: HEC, DHE, CL, PO4, OH

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	0.79	1/4308 (0.0%)	1.03	21/5854 (0.4%)
1	B	0.67	2/4317 (0.0%)	0.91	15/5865 (0.3%)
All	All	0.73	3/8625 (0.0%)	0.97	36/11719 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	248	PRO	C-N	-6.38	1.19	1.34
1	B	244	ALA	C-N	-5.06	1.22	1.34
1	A	244	ALA	C-N	-5.02	1.22	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	281	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	B	489	ARG	NE-CZ-NH2	7.59	124.09	120.30
1	A	156	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	A	267	ARG	NE-CZ-NH2	7.49	124.05	120.30
1	A	238	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	B	156	ARG	NE-CZ-NH2	7.45	124.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	201	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	B	480	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	B	336	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	B	372	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	A	372	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	A	225	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	55	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	A	46	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	A	336	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	A	356	ARG	NE-CZ-NH2	7.01	123.80	120.30
1	A	137	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	A	357	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	B	55	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	A	480	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	B	71	ARG	NE-CZ-NH2	6.77	123.68	120.30
1	A	489	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	A	71	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	B	198	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	B	46	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	A	253	MET	CG-SD-CE	6.16	110.05	100.20
1	B	339	MET	CG-SD-CE	6.13	110.00	100.20
1	B	253	MET	CG-SD-CE	6.11	109.97	100.20
1	A	204	MET	CG-SD-CE	6.08	109.93	100.20
1	A	269	MET	CG-SD-CE	6.06	109.90	100.20
1	B	309	TYR	O-C-N	-6.00	113.10	122.70
1	B	31	MET	CG-SD-CE	5.99	109.78	100.20
1	A	339	MET	CG-SD-CE	5.93	109.69	100.20
1	B	244	ALA	O-C-N	-5.77	113.46	122.70
1	B	204	MET	CG-SD-CE	5.36	108.77	100.20
1	A	198	ARG	NE-CZ-NH2	-5.19	117.70	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	TRP	Mainchain
1	B	309	TYR	Mainchain
1	B	483	GLN	Mainchain

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	4203	0	4157	86	0
1	B	4212	0	4169	76	2
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	43	0	30	1	0
5	B	43	0	30	3	0
6	A	49	0	24	3	0
6	B	49	0	24	3	0
7	A	449	0	0	5	1
7	B	421	0	0	7	2
All	All	9483	0	8434	157	5

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 (157) 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:488:LYS:HB3	7:B:1008:HOH:O	1.62	0.98
1:A:277:HIS:O	1:A:280:PRO:HD3	1.84	0.78
1:A:114:PRO:HB2	1:B:22:VAL:HG12	1.64	0.78
1:B:211:GLU:O	1:B:213:THR:HG23	1.87	0.75
1:B:489:ARG:HG2	7:B:1008:HOH:O	1.88	0.73
1:A:257:THR:O	1:A:258:LEU:HB2	1.88	0.72
1:A:364:VAL:CG2	1:A:368:PRO:HG3	2.21	0.70
1:A:22:VAL:HG12	1:B:114:PRO:HB2	1.75	0.68
1:A:278:PRO:HG3	7:A:947:HOH:O	1.93	0.67
1:A:219:LYS:HE3	1:A:221:GLY:O	1.95	0.67
1:A:147:LEU:HB2	1:A:148:PRO:HD3	1.77	0.66
1:A:43:TYR:OH	1:A:55:ARG:HG2	1.96	0.66
1:B:364:VAL:CG2	1:B:368:PRO:HG3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:TYR:OH	1:B:327:HIS:HE1	1.81	0.63
1:B:487:ASN:HD21	1:B:489:ARG:HG3	1.63	0.63
1:B:401:ASP:HB3	1:B:405:HIS:HB2	1.81	0.63
1:B:257:THR:O	1:B:258:LEU:HB2	1.99	0.62
1:A:228:GLU:HG3	1:A:229:SER:N	2.15	0.60
1:B:489:ARG:HD2	7:B:815:HOH:O	2.00	0.60
1:B:343:ASN:HA	1:B:368:PRO:HD2	1.82	0.60
1:B:395:ILE:HB	1:B:416:LEU:HB2	1.82	0.60
1:B:484:PRO:HB3	1:B:495:PHE:CE2	2.37	0.60
1:A:364:VAL:HG21	1:A:368:PRO:HG3	1.84	0.59
1:A:55:ARG:NH2	7:A:789:HOH:O	2.29	0.59
1:A:36:PHE:HZ	1:A:114:PRO:HG3	1.67	0.59
1:A:90:ASN:H	1:A:90:ASN:HD22	1.50	0.59
1:B:53:VAL:HG11	1:B:116:PRO:HG2	1.85	0.58
1:A:25:THR:O	1:A:26:ASN:HB2	2.03	0.58
1:A:304:VAL:HG11	1:A:351:ILE:HG12	1.86	0.57
1:B:99:LYS:O	1:B:99:LYS:HD3	2.04	0.57
1:B:507:LEU:HB2	1:B:521:VAL:HB	1.86	0.57
1:A:364:VAL:HG23	1:A:368:PRO:HG3	1.86	0.56
1:A:279:GLU:O	1:A:279:GLU:HG2	2.04	0.56
1:A:291:HIS:O	1:A:293:GLU:N	2.38	0.56
1:A:327:HIS:HE1	1:B:10:TYR:OH	1.88	0.56
1:A:211:GLU:O	1:A:213:THR:HG23	2.06	0.55
1:B:55:ARG:NH2	7:B:693:HOH:O	2.27	0.55
1:B:61:LYS:HD2	1:B:71:ARG:NH2	2.22	0.55
5:A:601:HEC:HMC1	5:A:601:HEC:HBC3	1.87	0.55
1:A:366:LYS:HE3	1:A:392:ASP:OD2	2.08	0.54
1:B:453:VAL:HG21	1:B:466:LEU:HD22	1.90	0.53
1:B:364:VAL:HG21	1:B:368:PRO:HG3	1.91	0.53
1:A:90:ASN:H	1:A:90:ASN:ND2	2.07	0.53
1:B:198:ARG:HH22	6:B:602:DHE:CBB	2.21	0.53
1:A:381:TYR:CD1	1:A:413:VAL:HG22	2.43	0.53
1:B:381:TYR:CD1	1:B:413:VAL:HG22	2.44	0.53
1:B:299:LYS:NZ	1:B:327:HIS:HD2	2.06	0.52
1:B:72:GLY:O	1:B:76:LEU:HG	2.10	0.52
1:B:250:PHE:C	1:B:250:PHE:CD1	2.83	0.52
1:B:36:PHE:HZ	1:B:114:PRO:HG3	1.75	0.51
1:B:378:HIS:CG	1:B:379:PRO:HD2	2.46	0.51
1:B:51:HIS:O	1:B:55:ARG:HA	2.11	0.51
5:B:601:HEC:HMC1	5:B:601:HEC:HBC3	1.92	0.51
1:A:181:VAL:HA	1:A:197:GLY:HA2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:ILE:HG13	1:B:437:VAL:HG22	1.93	0.51
1:B:366:LYS:HD2	1:B:392:ASP:OD2	2.10	0.51
1:B:56:LYS:HE2	7:B:1003:HOH:O	2.10	0.51
1:B:405:HIS:N	1:B:406:PRO:HD3	2.26	0.50
1:A:439:THR:OG1	1:A:442:ASN:HB2	2.11	0.50
1:A:6:ALA:HB1	1:B:422:GLY:HA2	1.94	0.50
1:A:270:THR:O	1:A:274:GLN:HA	2.11	0.50
1:B:148:PRO:HB2	1:B:488:LYS:HE2	1.94	0.50
1:A:306:LEU:HB2	1:A:318:THR:HB	1.94	0.50
1:B:147:LEU:HB2	1:B:148:PRO:HD3	1.95	0.49
1:A:381:TYR:CD2	1:A:413:VAL:HG13	2.48	0.49
1:A:209:ALA:O	1:A:210:LYS:C	2.51	0.49
1:A:114:PRO:HB2	1:B:22:VAL:CG1	2.39	0.48
1:B:55:ARG:HB3	1:B:63:LEU:HB2	1.94	0.48
1:A:267:ARG:NH1	7:A:1040:HOH:O	2.44	0.48
1:B:386:SER:HB3	1:B:397:LEU:HD23	1.95	0.48
1:A:298:VAL:HG12	1:A:301:THR:OG1	2.14	0.48
1:A:188:ALA:HB3	1:A:236:GLU:HG2	1.95	0.48
1:B:334:SER:O	1:B:335:HIS:HB2	2.13	0.48
1:A:10:TYR:OH	1:B:327:HIS:CE1	2.64	0.48
1:B:299:LYS:HZ1	1:B:327:HIS:HD2	1.62	0.47
1:B:436:TYR:CE1	1:B:493:VAL:HG21	2.49	0.47
1:B:250:PHE:O	1:B:250:PHE:CD1	2.68	0.47
1:B:181:VAL:HA	1:B:197:GLY:HA2	1.95	0.47
1:A:343:ASN:OD1	1:A:344:ASN:N	2.43	0.47
1:A:378:HIS:CG	1:A:379:PRO:HD2	2.49	0.47
1:A:424:LEU:HB3	1:A:425:PHE:CD2	2.49	0.47
1:B:370:PRO:HB3	1:B:387:THR:HB	1.97	0.47
1:A:145:LEU:HD11	1:A:172:VAL:HG11	1.97	0.47
1:B:79:LEU:HD13	5:B:601:HEC:HAA1	1.97	0.47
1:A:439:THR:HG23	1:A:447:ILE:O	2.15	0.47
1:B:381:TYR:CD1	1:B:413:VAL:CG2	2.99	0.46
1:B:279:GLU:N	1:B:280:PRO:HD3	2.30	0.46
1:A:198:ARG:NH2	6:A:602:DHE:O2B	2.47	0.46
1:A:219:LYS:HE2	7:A:857:HOH:O	2.16	0.46
1:A:250:PHE:CD1	1:A:250:PHE:C	2.89	0.46
1:B:378:HIS:ND1	1:B:379:PRO:HD2	2.30	0.46
1:A:160:GLN:NE2	7:A:1031:HOH:O	2.49	0.46
1:A:223:GLU:HG2	1:A:245:TYR:HB2	1.97	0.46
1:B:267:ARG:NH1	7:B:787:HOH:O	2.46	0.46
1:A:154:THR:O	1:A:529:PRO:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:TYR:CZ	6:B:602:DHE:HGB2	2.51	0.45
1:A:331:TRP:HB3	1:A:335:HIS:HA	1.99	0.45
1:B:331:TRP:HB3	1:B:335:HIS:HA	1.98	0.45
1:B:364:VAL:HG23	1:B:368:PRO:HG3	1.97	0.45
1:A:218:ILE:HD11	1:A:260:PRO:HG3	1.98	0.45
1:A:449:GLN:HB3	1:A:469:ALA:HB3	1.99	0.45
1:A:299:LYS:NZ	1:A:327:HIS:HD2	2.14	0.45
1:B:198:ARG:NH2	6:B:602:DHE:O2B	2.50	0.44
1:A:401:ASP:OD2	1:A:404:ASN:HB2	2.18	0.44
1:A:138:PRO:HB3	1:A:142:LEU:HD11	1.99	0.44
1:A:299:LYS:HB3	1:A:300:GLU:OE1	2.18	0.44
1:A:468:ILE:HB	1:A:481:VAL:HG21	1.99	0.44
6:A:602:DHE:O2C	6:A:602:DHE:C2C	2.65	0.44
1:A:239:TYR:CE1	1:A:312:ILE:HD12	2.52	0.44
1:B:43:TYR:OH	1:B:55:ARG:HG2	2.18	0.44
1:B:113:PRO:HA	1:B:114:PRO:HD3	1.90	0.44
1:A:359:SER:O	1:A:360:ALA:HB2	2.17	0.44
1:B:218:ILE:HD11	1:B:260:PRO:HG3	1.99	0.44
1:A:44:PHE:HA	1:A:48:ALA:HB2	1.99	0.44
1:A:223:GLU:O	1:A:245:TYR:N	2.51	0.44
1:B:299:LYS:HB3	1:B:300:GLU:OE1	2.18	0.44
1:A:334:SER:O	1:A:335:HIS:HB2	2.18	0.44
1:A:243:GLY:HA3	1:A:282:VAL:HG11	1.99	0.43
1:A:453:VAL:HG21	1:A:466:LEU:HD22	2.00	0.43
1:A:281:ARG:HD2	1:A:300:GLU:OE2	2.19	0.43
1:A:156:ARG:HB3	1:A:157:ASP:H	1.62	0.43
1:A:99:LYS:HE2	1:A:102:ILE:HD12	2.00	0.43
1:A:381:TYR:HB3	1:A:413:VAL:HG21	2.01	0.43
1:A:279:GLU:N	1:A:280:PRO:HD3	2.32	0.43
1:B:436:TYR:CZ	1:B:493:VAL:HG21	2.54	0.43
1:B:33:GLU:HG2	1:B:37:ASN:ND2	2.34	0.43
1:A:279:GLU:N	1:A:280:PRO:CD	2.82	0.42
1:B:115:GLN:HA	1:B:116:PRO:HD3	1.90	0.42
1:A:336:ARG:NH1	1:A:354:LYS:HB3	2.34	0.42
1:B:403:LYS:HG3	7:B:822:HOH:O	2.19	0.42
1:B:90:ASN:HD22	1:B:93:SER:HB2	1.84	0.42
1:A:81:THR:HG23	1:A:92:GLY:HA3	2.00	0.42
1:B:149:ASN:HB2	1:B:488:LYS:HE3	2.01	0.42
1:A:280:PRO:HB3	1:A:301:THR:HG23	2.01	0.42
1:B:79:LEU:HD13	5:B:601:HEC:CAA	2.50	0.42
1:B:405:HIS:N	1:B:406:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASN:OD1	1:A:145:LEU:HB2	2.20	0.42
1:B:154:THR:O	1:B:529:PRO:HA	2.19	0.42
1:A:115:GLN:HA	1:A:116:PRO:HD3	1.90	0.42
1:B:487:ASN:HD21	1:B:489:ARG:CG	2.31	0.41
1:B:338:PHE:HB3	1:B:351:ILE:HB	2.01	0.41
1:A:56:LYS:HG2	1:A:62:PRO:HB3	2.01	0.41
1:B:381:TYR:CG	1:B:413:VAL:HG21	2.55	0.41
1:A:188:ALA:CB	1:A:236:GLU:HG2	2.50	0.41
1:A:299:LYS:HZ1	1:A:327:HIS:CD2	2.38	0.41
1:A:336:ARG:HH11	1:A:354:LYS:HB3	1.85	0.41
1:A:327:HIS:CE1	1:B:10:TYR:OH	2.70	0.41
1:A:198:ARG:HH22	6:A:602:DHE:CBB	2.34	0.41
1:A:403:LYS:HB2	1:A:403:LYS:NZ	2.35	0.41
1:B:121:MET:SD	1:B:260:PRO:HB2	2.61	0.41
1:A:121:MET:SD	1:A:260:PRO:HB2	2.61	0.41
1:B:247:PRO:O	1:B:249:GLN:HG2	2.21	0.41
1:A:65:PRO:HA	1:A:68:THR:OG1	2.21	0.41
1:B:156:ARG:HB3	1:B:157:ASP:H	1.79	0.41
1:A:364:VAL:HB	1:A:365:GLY:H	1.69	0.40
1:A:228:GLU:CG	1:A:229:SER:N	2.83	0.40
1:B:481:VAL:HA	1:B:496:SER:O	2.22	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLN:NE2	1:B:473:ASP:O[3_556]	1.93	0.27
7:A:616:HOH:O	7:A:772:HOH:O[3_545]	2.01	0.19
7:B:706:HOH:O	7:B:874:HOH:O[3_546]	2.07	0.13
1:B:74:GLN:OE1	1:B:169:LYS:O[3_556]	2.08	0.12
7:B:768:HOH:O	7:B:898:HOH:O[3_556]	2.18	0.02

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	536/543 (99%)	496 (92%)	35 (6%)	5 (1%)	21 13
1	B	537/543 (99%)	502 (94%)	31 (6%)	4 (1%)	26 18
All	All	1073/1086 (99%)	998 (93%)	66 (6%)	9 (1%)	24 15

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	156	ARG
1	A	299	LYS
1	B	156	ARG
1	B	299	LYS
1	B	26	ASN
1	B	483	GLN
1	A	292	PRO
1	A	483	GLN

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	453/458 (99%)	444 (98%)	9 (2%)	63 67
1	B	454/458 (99%)	448 (99%)	6 (1%)	76 82
All	All	907/916 (99%)	892 (98%)	15 (2%)	68 74

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

Mol	Chain	Res	Type
1	A	46	ARG
1	A	79	LEU
1	A	90	ASN
1	A	99	LYS

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Mol	Chain	Res	Type
1	A	193	LEU
1	A	198	ARG
1	A	336	ARG
1	A	413	VAL
1	A	424	LEU
1	B	198	ARG
1	B	407	GLN
1	B	413	VAL
1	B	424	LEU
1	B	439	THR
1	B	489	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	111	HIS
1	A	115	GLN
1	A	160	GLN
1	A	274	GLN
1	A	327	HIS
1	A	344	ASN
1	B	73	GLN
1	B	90	ASN
1	B	110	GLN
1	B	115	GLN
1	B	160	GLN
1	B	289	HIS
1	B	314	ASN
1	B	327	HIS
1	B	344	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic and 2 are modelled with single atom - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	HEC	A	601	1	24,50,50	1.91	4 (16%)	19,82,82	1.76	4 (21%)
6	DHE	A	602	1,4	29,56,56	1.98	8 (27%)	27,94,94	3.09	10 (37%)
2	PO4	A	604	-	4,4,4	2.39	4 (100%)	6,6,6	0.27	0
5	HEC	B	601	1	24,50,50	1.61	3 (12%)	19,82,82	1.06	1 (5%)
6	DHE	B	602	1,4	29,56,56	1.92	9 (31%)	27,94,94	3.09	11 (40%)
2	PO4	B	604	-	4,4,4	2.47	4 (100%)	6,6,6	0.33	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
5	HEC	A	601	1	-	0/6/54/54	0/0/8/8
6	DHE	A	602	1,4	-	0/12/108/108	0/0/8/8
2	PO4	A	604	-	-	0/0/0/0	0/0/0/0
5	HEC	B	601	1	-	0/6/54/54	0/0/8/8
6	DHE	B	602	1,4	-	0/12/108/108	0/0/8/8
2	PO4	B	604	-	-	0/0/0/0	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	HEC	C3C-C2C	-5.97	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	HEC	C3B-C2B	-5.36	1.35	1.40
6	B	602	DHE	CAB-C3B	-4.91	1.48	1.56
6	A	602	DHE	CAB-C3B	-4.82	1.48	1.56
6	A	602	DHE	CAC-C3C	-4.49	1.49	1.56
5	B	601	HEC	C3B-C2B	-4.40	1.36	1.40
5	B	601	HEC	C3C-C2C	-4.17	1.36	1.40
6	A	602	DHE	CBD-CAD	-3.50	1.29	1.53
6	B	602	DHE	CAC-C3C	-3.50	1.50	1.56
6	B	602	DHE	CBD-CAD	-3.47	1.29	1.53
6	B	602	DHE	CAD-C3D	-2.84	1.47	1.52
6	A	602	DHE	CAD-C3D	-2.80	1.47	1.52
6	B	602	DHE	FE-NC	2.03	2.08	1.97
2	B	604	PO4	P-O1	2.08	1.61	1.52
6	A	602	DHE	FE-NC	2.16	2.08	1.97
2	A	604	PO4	P-O2	2.22	1.61	1.53
5	A	601	HEC	C4C-NC	2.27	1.39	1.36
2	A	604	PO4	P-O1	2.32	1.62	1.52
2	A	604	PO4	P-O3	2.38	1.62	1.53
2	B	604	PO4	P-O4	2.38	1.62	1.53
6	B	602	DHE	CHB-C1B	2.46	1.39	1.35
5	A	601	HEC	C4A-NA	2.48	1.40	1.36
5	B	601	HEC	C4A-NA	2.48	1.40	1.36
2	A	604	PO4	P-O4	2.61	1.62	1.53
6	A	602	DHE	FE-NB	2.66	2.06	1.95
2	B	604	PO4	P-O2	2.67	1.63	1.53
2	B	604	PO4	P-O3	2.69	1.63	1.53
6	B	602	DHE	FE-NB	2.89	2.07	1.95
6	B	602	DHE	CGB-C3B	3.08	1.61	1.54
6	A	602	DHE	CGC-C3C	3.13	1.61	1.54
6	A	602	DHE	CGB-C3B	3.35	1.61	1.54
6	B	602	DHE	CGC-C3C	3.43	1.62	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	601	HEC	CBB-CAB-C3B	-3.96	118.55	127.35
5	A	601	HEC	CBC-CAC-C3C	-3.35	119.92	127.35
5	A	601	HEC	CBD-CAD-C3D	-3.25	106.70	112.53
5	A	601	HEC	CAD-C3D-C4D	-2.95	123.80	127.01
6	B	602	DHE	CMA-C3A-C4A	-2.76	123.80	128.36
6	A	602	DHE	CMA-C3A-C4A	-2.66	123.96	128.36
6	B	602	DHE	CMD-C2D-C1D	-2.61	124.04	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	601	HEC	CBC-CAC-C3C	-2.26	122.32	127.35
6	B	602	DHE	CAD-C3D-C4D	-2.26	124.55	127.01
6	A	602	DHE	CMD-C2D-C1D	-2.21	124.70	128.36
6	B	602	DHE	CAA-C2A-C1A	-2.20	124.62	127.01
6	A	602	DHE	CAA-C2A-C1A	-2.11	124.71	127.01
6	B	602	DHE	CHC-C1C-NC	2.07	126.86	124.45
6	A	602	DHE	CHC-C1C-NC	2.16	126.97	124.45
6	B	602	DHE	CHB-C1B-NB	2.34	126.91	124.42
6	B	602	DHE	CAA-CBA-CGA	2.63	117.56	112.75
6	A	602	DHE	CAA-CBA-CGA	2.75	117.78	112.75
6	A	602	DHE	CHB-C1B-NB	3.10	127.71	124.42
6	A	602	DHE	C1C-NC-C4C	6.50	110.91	105.00
6	B	602	DHE	C1C-NC-C4C	6.57	110.98	105.00
6	B	602	DHE	C1B-NB-C4B	6.69	110.53	106.90
6	A	602	DHE	C1B-NB-C4B	6.99	110.69	106.90
6	B	602	DHE	CAD-CBD-CGD	7.20	125.93	112.75
6	A	602	DHE	CBD-CAD-C3D	7.28	125.58	112.53
6	A	602	DHE	CAD-CBD-CGD	7.81	127.07	112.75
6	B	602	DHE	CBD-CAD-C3D	8.11	127.06	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	HEC	1	0
6	A	602	DHE	3	0
5	B	601	HEC	3	0
6	B	602	DHE	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	538/543 (99%)	1.26	110 (20%)	1	2	22, 36, 54, 71	0
1	B	539/543 (99%)	1.86	212 (39%)	0	1	23, 37, 56, 72	0
All	All	1077/1086 (99%)	1.56	322 (29%)	1	1	22, 36, 55, 72	0

All (322) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	LYS	6.2
1	B	475	GLY	5.9
1	B	446	ARG	5.6
1	A	104	LEU	5.6
1	B	32	SER	5.3
1	B	93	SER	5.0
1	A	513	LYS	5.0
1	A	210	LYS	4.8
1	A	446	ARG	4.7
1	B	408	TYR	4.7
1	A	130	VAL	4.7
1	A	140	LYS	4.6
1	A	93	SER	4.6
1	B	498	TRP	4.5
1	A	445	ALA	4.5
1	B	494	TRP	4.5
1	B	436	TYR	4.5
1	B	517	LEU	4.4
1	B	453	VAL	4.4
1	B	454	PHE	4.4
1	B	144	ASP	4.4
1	B	510	VAL	4.3
1	B	495	PHE	4.3
1	A	205	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	131	LEU	4.3
1	B	513	LYS	4.2
1	B	478	ALA	4.2
1	A	128	TRP	4.2
1	B	95	GLY	4.2
1	B	424	LEU	4.2
1	B	467	PRO	4.2
1	B	465	VAL	4.1
1	B	370	PRO	4.1
1	B	514	THR	4.1
1	B	26	ASN	4.1
1	A	142	LEU	4.0
1	B	385	TRP	4.0
1	B	526	LEU	3.9
1	B	477	GLY	3.9
1	B	379	PRO	3.8
1	B	519	ALA	3.8
1	B	484	PRO	3.8
1	B	435	LEU	3.8
1	B	476	GLU	3.7
1	A	27	GLY	3.7
1	B	462	LYS	3.7
1	B	426	ILE	3.7
1	B	527	ILE	3.7
1	B	86	LEU	3.7
1	B	533	PHE	3.6
1	B	451	VAL	3.6
1	B	72	GLY	3.6
1	B	437	VAL	3.6
1	B	509	VAL	3.6
1	B	82	TYR	3.6
1	B	497	VAL	3.6
1	B	312	ILE	3.5
1	B	41	GLN	3.5
1	B	380	LYS	3.5
1	A	424	LEU	3.5
1	A	95	GLY	3.4
1	B	393	GLY	3.4
1	B	104	LEU	3.4
1	B	460	ASP	3.4
1	B	461	ALA	3.4
1	B	421	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	389	HIS	3.4
1	B	466	LEU	3.4
1	B	515	LEU	3.4
1	B	443	PRO	3.3
1	B	155	LEU	3.3
1	B	171	ILE	3.3
1	B	63	LEU	3.3
1	B	500	GLY	3.3
1	A	144	ASP	3.3
1	B	76	LEU	3.3
1	B	391	GLY	3.2
1	B	486	TYR	3.2
1	B	329	GLY	3.2
1	B	506	ALA	3.2
1	A	232	PHE	3.2
1	B	94	SER	3.2
1	B	140	LYS	3.2
1	B	502	ASN	3.1
1	B	395	ILE	3.1
1	A	460	ASP	3.1
1	A	425	PHE	3.1
1	B	151	PHE	3.1
1	B	87	GLY	3.1
1	A	285	ILE	3.1
1	B	103	THR	3.1
1	A	403	LYS	3.0
1	A	431	LYS	3.0
1	B	183	ILE	3.0
1	A	163	LEU	3.0
1	B	298	VAL	3.0
1	B	377	VAL	3.0
1	B	482	VAL	3.0
1	B	181	VAL	3.0
1	B	344	ASN	3.0
1	A	33	GLU	3.0
1	B	78	ALA	3.0
1	B	75	TYR	3.0
1	B	536	TYR	3.0
1	A	371	GLY	2.9
1	B	507	LEU	2.9
1	B	74	GLN	2.9
1	A	250	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	458	ASN	2.9
1	B	33	GLU	2.9
1	B	202	ILE	2.9
1	B	463	TYR	2.9
1	B	371	GLY	2.9
1	B	85	PRO	2.9
1	B	425	PHE	2.9
1	B	102	ILE	2.9
1	B	398	ILE	2.9
1	B	227	VAL	2.9
1	B	364	VAL	2.9
1	B	106	ALA	2.9
1	A	171	ILE	2.8
1	B	30	ASP	2.8
1	B	464	GLN	2.8
1	A	489	ARG	2.8
1	A	37	ASN	2.8
1	A	7	ALA	2.8
1	A	543	TYR	2.8
1	B	29	PRO	2.8
1	A	13	ALA	2.8
1	A	216	ALA	2.8
1	B	441	PHE	2.8
1	B	524	PRO	2.8
1	A	86	LEU	2.8
1	B	282	VAL	2.8
1	A	374	ALA	2.8
1	B	394	SER	2.7
1	A	284	ALA	2.7
1	B	46	ARG	2.7
1	B	452	ALA	2.7
1	A	218	ILE	2.7
1	B	390	LEU	2.7
1	A	126	GLU	2.7
1	A	278	PRO	2.7
1	B	285	ILE	2.7
1	A	461	ALA	2.7
1	A	215	VAL	2.7
1	B	153	VAL	2.7
1	A	35	GLU	2.7
1	B	241	ILE	2.7
1	A	266	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	80	ILE	2.6
1	B	468	ILE	2.6
1	B	387	THR	2.6
1	B	543	TYR	2.6
1	B	407	GLN	2.6
1	B	384	VAL	2.6
1	B	417	GLN	2.6
1	B	450	SER	2.6
1	B	81	THR	2.6
1	A	531	GLY	2.6
1	B	169	LYS	2.6
1	A	39	ALA	2.6
1	A	220	ILE	2.6
1	A	164	VAL	2.6
1	A	131	LEU	2.6
1	B	445	ALA	2.6
1	A	10	TYR	2.5
1	A	76	LEU	2.5
1	B	397	LEU	2.5
1	B	520	VAL	2.5
1	B	523	ASP	2.5
1	A	12	GLY	2.5
1	B	365	GLY	2.5
1	B	250	PHE	2.5
1	B	207	LEU	2.5
1	B	416	LEU	2.5
1	A	34	SER	2.5
1	B	428	THR	2.5
1	B	508	VAL	2.5
1	B	418	GLY	2.5
1	A	99	LYS	2.5
1	B	516	LYS	2.5
1	B	20	ALA	2.5
1	A	330	GLY	2.5
1	A	153	VAL	2.5
1	B	91	TRP	2.5
1	B	158	ALA	2.5
1	B	366	LYS	2.5
1	A	426	ILE	2.5
1	B	447	ILE	2.5
1	A	36	PHE	2.4
1	B	252	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	413	VAL	2.4
1	B	47	CYS	2.4
1	A	6	ALA	2.4
1	B	127	SER	2.4
1	A	151	PHE	2.4
1	A	179	TYR	2.4
1	B	521	VAL	2.4
1	A	133	LYS	2.4
1	B	423	SER	2.4
1	B	268	GLY	2.4
1	B	210	LYS	2.4
1	A	109	ILE	2.4
1	A	484	PRO	2.4
1	B	402	PRO	2.4
1	A	155	LEU	2.4
1	A	379	PRO	2.4
1	A	119	TRP	2.4
1	A	145	LEU	2.4
1	A	542	VAL	2.3
1	B	197	GLY	2.3
1	A	106	ALA	2.3
1	B	251	ALA	2.3
1	A	102	ILE	2.3
1	A	32	SER	2.3
1	A	257	THR	2.3
1	B	325	PHE	2.3
1	B	381	TYR	2.3
1	B	244	ALA	2.3
1	B	195	VAL	2.3
1	B	531	GLY	2.3
1	B	438	ASP	2.3
1	A	65	PRO	2.3
1	B	37	ASN	2.3
1	A	516	LYS	2.3
1	B	99	LYS	2.3
1	B	105	MET	2.3
1	B	186	MET	2.3
1	B	246	TRP	2.3
1	B	439	THR	2.3
1	A	150	LEU	2.3
1	B	79	LEU	2.3
1	B	49	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	232	PHE	2.2
1	A	135	GLU	2.2
1	A	174	VAL	2.2
1	B	213	THR	2.2
1	A	30	ASP	2.2
1	B	67	ILE	2.2
1	B	505	SER	2.2
1	A	298	VAL	2.2
1	A	243	GLY	2.2
1	B	283	ALA	2.2
1	B	10	TYR	2.2
1	B	276	TYR	2.2
1	A	53	VAL	2.2
1	A	304	VAL	2.2
1	B	403	LYS	2.2
1	A	263	ILE	2.2
1	B	145	LEU	2.2
1	A	338	PHE	2.2
1	B	501	LYS	2.2
1	B	396	SER	2.2
1	A	264	VAL	2.2
1	B	535	VAL	2.2
1	B	180	ALA	2.2
1	B	411	LYS	2.2
1	B	504	SER	2.2
1	B	444	ASP	2.2
1	B	236	GLU	2.2
1	A	282	VAL	2.2
1	A	138	PRO	2.2
1	A	54	LEU	2.1
1	A	258	LEU	2.1
1	B	142	LEU	2.1
1	A	8	GLU	2.1
1	B	528	THR	2.1
1	B	481	VAL	2.1
1	A	253	MET	2.1
1	A	459	LEU	2.1
1	A	48	ALA	2.1
1	A	251	ALA	2.1
1	B	224	ALA	2.1
1	A	139	LYS	2.1
1	A	497	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	520	VAL	2.1
1	A	521	VAL	2.1
1	B	324	PRO	2.1
1	B	529	PRO	2.1
1	B	31	MET	2.1
1	B	369	HIS	2.1
1	B	34	SER	2.1
1	B	386	SER	2.1
1	B	45	GLN	2.1
1	B	493	VAL	2.1
1	A	112	THR	2.1
1	A	252	ILE	2.1
1	B	70	GLN	2.1
1	B	133	LYS	2.1
1	B	337	TYR	2.1
1	A	465	VAL	2.1
1	B	109	ILE	2.1
1	A	194	LEU	2.1
1	B	194	LEU	2.1
1	B	185	ARG	2.1
1	A	221	GLY	2.1
1	B	110	GLN	2.1
1	B	234	GLY	2.1
1	B	287	ALA	2.1
1	B	422	GLY	2.1
1	B	98	SER	2.1
1	A	44	PHE	2.1
1	B	50	CYS	2.1
1	A	233	LYS	2.0
1	A	370	PRO	2.0
1	B	499	ASN	2.0
1	A	15	SER	2.0
1	B	39	ALA	2.0
1	B	152	SER	2.0
1	B	338	PHE	2.0
1	B	212	PRO	2.0
1	B	346	ASN	2.0
1	A	161	ILE	2.0
1	A	183	ILE	2.0
1	B	205	ILE	2.0
1	A	97	LEU	2.0
1	B	35	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	73	GLN	2.0
1	B	429	HIS	2.0
1	B	235	TYR	2.0
1	B	373	GLY	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	HEC	B	601	43/43	0.81	0.26	0.63	24,31,34,41	0
5	HEC	A	601	43/43	0.92	0.16	-0.31	24,29,38,42	0
6	DHE	A	602	49/49	0.90	0.19	-0.49	22,29,36,47	0
6	DHE	B	602	49/49	0.85	0.22	-0.75	25,30,39,50	0
3	CL	A	605	1/1	0.83	0.17	-2.70	28,28,28,28	0
3	CL	B	605	1/1	0.94	0.12	-3.40	27,27,27,27	0
4	OH	A	603	1/1	0.98	0.33	-	36,36,36,36	0
2	PO4	A	604	5/5	0.81	0.24	-	75,75,78,78	0
2	PO4	B	604	5/5	0.89	0.20	-	82,82,84,85	0
4	OH	B	603	1/1	0.71	0.36	-	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.