Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 11:34 am GMT

PDB ID	:	3SN5
Title	:	Crystal structure of human CYP7A1 in complex with cholest-4-en-3-one
Authors	:	Strushkevich, N.; Tempel, W.; MacKenzie, F.; Wernimont, A.K.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on	:	2011-06-28
Resolution	:	2.75 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:

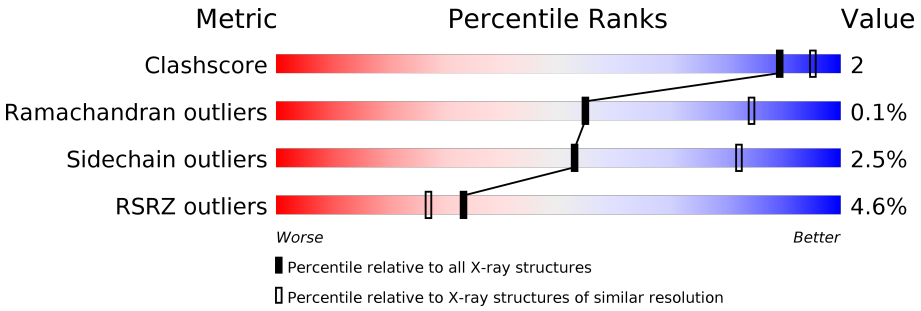
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.75 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))
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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	491	4% 90% 5% 5%
1	B	491	4% 90% 5% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNX	B	2066	-	-	-	X
4	UNX	B	2123	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNX	B	2205	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7401 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 Cholesterol 7-alpha-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3624	2338	608	657	21			
1	B	466	Total	C	N	O	S	0	0	0
			3591	2312	606	652	21			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	EXPRESSION TAG	UNP P22680
A	19	ALA	-	EXPRESSION TAG	UNP P22680
A	20	LYS	-	EXPRESSION TAG	UNP P22680
A	21	LYS	-	EXPRESSION TAG	UNP P22680
A	22	THR	-	EXPRESSION TAG	UNP P22680
A	23	SER	-	EXPRESSION TAG	UNP P22680
A	24	SER	-	EXPRESSION TAG	UNP P22680
A	104	LEU	THR	ENGINEERED MUTATION	UNP P22680
A	504	HIS	-	EXPRESSION TAG	UNP P22680
A	505	HIS	-	EXPRESSION TAG	UNP P22680
A	506	HIS	-	EXPRESSION TAG	UNP P22680
A	507	HIS	-	EXPRESSION TAG	UNP P22680
A	508	HIS	-	EXPRESSION TAG	UNP P22680
B	18	MET	-	EXPRESSION TAG	UNP P22680
B	19	ALA	-	EXPRESSION TAG	UNP P22680
B	20	LYS	-	EXPRESSION TAG	UNP P22680
B	21	LYS	-	EXPRESSION TAG	UNP P22680
B	22	THR	-	EXPRESSION TAG	UNP P22680
B	23	SER	-	EXPRESSION TAG	UNP P22680
B	24	SER	-	EXPRESSION TAG	UNP P22680
B	104	LEU	THR	ENGINEERED MUTATION	UNP P22680
B	504	HIS	-	EXPRESSION TAG	UNP P22680
B	505	HIS	-	EXPRESSION TAG	UNP P22680
B	506	HIS	-	EXPRESSION TAG	UNP P22680
B	507	HIS	-	EXPRESSION TAG	UNP P22680

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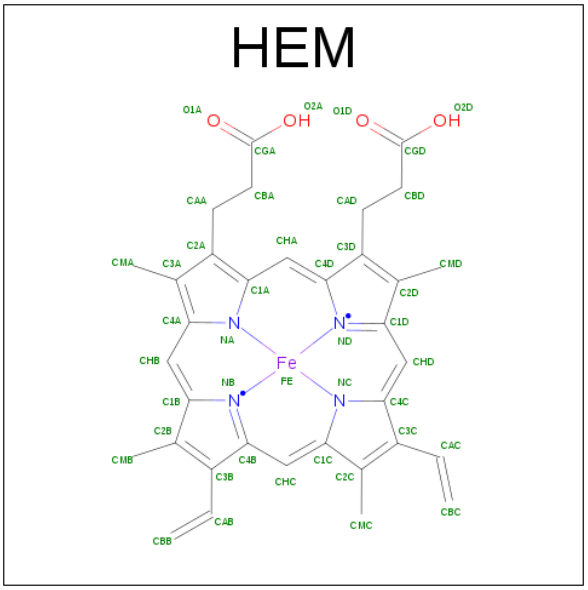
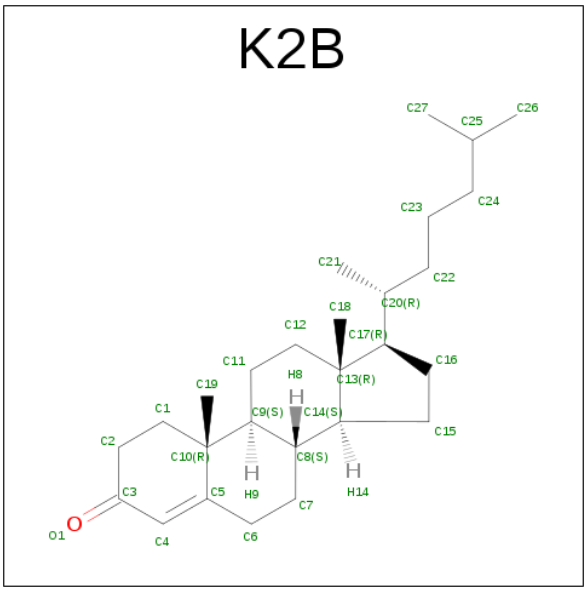
Chain	Residue	Modelled	Actual	Comment	Reference
B	508	HIS	-	EXPRESSION TAG	UNP P22680

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is (8ALPHA,9BETA)-CHOLEST-4-EN-3-ONE (three-letter code: K2B) (formula: $C_{27}H_{44}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 28 27 1	0	0
3	B	1	Total C O 28 27 1	0	0

- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	4	Total X 4 4	0	0
4	A	4	Total X 4 4	0	0

- Molecule 5 is water.

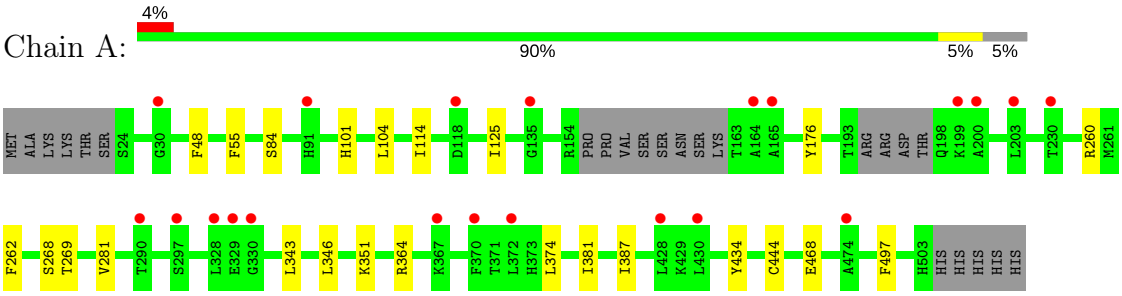
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	20	Total O 20 20	0	0
5	B	16	Total O 16 16	0	0

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

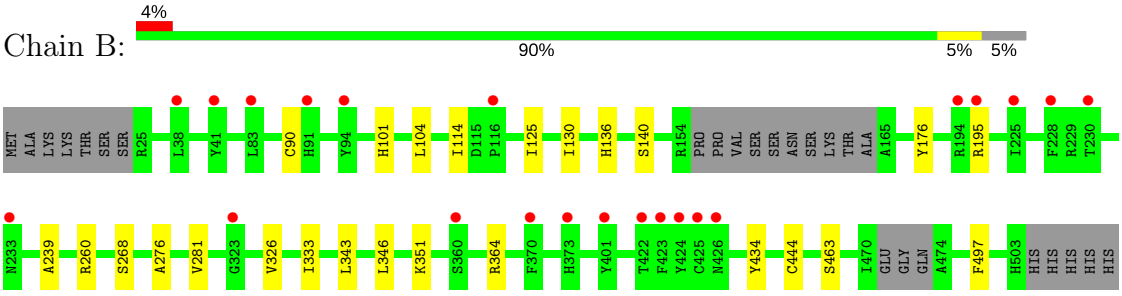
• Molecule 1: Cholesterol 7-alpha-monooxygenase

Chain A:



• Molecule 1: Cholesterol 7-alpha-monooxygenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.16Å 137.63Å 160.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 29.58 – 2.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.75) 100.0 (29.58-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.76Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.182 , 0.220 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	63.7	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 102.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7401	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, HEM, K2B

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	0.45	0/3712	0.61	0/5038
1	B	0.46	0/3680	0.61	0/5003
All	All	0.45	0/7392	0.61	0/10041

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3624	0	3438	13	0
1	B	3591	0	3377	12	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0
3	A	28	0	44	6	0
3	B	28	0	44	6	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	20	0	0	0	0
5	B	16	0	0	0	0
All	All	7401	0	6963	32	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 2.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:VAL:HG11	3:A:1429:K2B:H231	1.72	0.71
1:B:281:VAL:HG11	3:B:1429:K2B:H231	1.74	0.69
1:B:114:ILE:HD13	3:B:1429:K2B:H273	1.82	0.61
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.83	0.60
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.83	0.60
2:B:601:HEM:HHD	2:B:601:HEM:HBC2	1.83	0.59
2:A:601:HEM:HBC2	2:A:601:HEM:HHD	1.85	0.59
1:A:84:SER:HB3	1:A:374:LEU:HD22	1.83	0.59
1:B:326:VAL:HG21	1:B:463:SER:HB3	1.84	0.59
1:A:114:ILE:HD13	3:A:1429:K2B:H273	1.86	0.58
1:A:262:PHE:HE2	1:B:130:ILE:HG12	1.71	0.56
2:A:601:HEM:HAD1	3:A:1429:K2B:H161	1.93	0.48
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.45	0.45
1:B:239:ALA:O	1:B:276:ALA:HB1	2.17	0.45
1:A:343:LEU:HD13	1:A:346:LEU:HD12	1.99	0.45
3:B:1429:K2B:H121	3:B:1429:K2B:H212	2.00	0.44
3:A:1429:K2B:H121	3:A:1429:K2B:H212	1.98	0.44
1:A:269:THR:HG21	1:B:90:CYS:HA	1.99	0.44
1:A:262:PHE:CE2	1:B:130:ILE:HG12	2.51	0.43
2:B:601:HEM:HAD1	3:B:1429:K2B:H161	1.99	0.43
1:B:343:LEU:HD13	1:B:346:LEU:HD12	1.99	0.43
1:A:381:ILE:HG21	1:A:387:ILE:HD11	2.01	0.43
2:B:601:HEM:HBB2	2:B:601:HEM:CMB	2.46	0.43
1:A:125:ILE:HD13	3:A:1429:K2B:H241	2.01	0.42
1:A:444:CYS:HB2	2:A:601:HEM:NA	2.35	0.42
1:A:351:LYS:HG2	1:A:434:TYR:CZ	2.54	0.42
1:B:351:LYS:HG2	1:B:434:TYR:CZ	2.55	0.41
1:A:125:ILE:HG21	3:A:1429:K2B:H262	2.02	0.41
1:B:125:ILE:HG21	3:B:1429:K2B:H262	2.03	0.41
1:B:444:CYS:HB2	2:B:601:HEM:NA	2.36	0.41
1:B:125:ILE:HD13	3:B:1429:K2B:H241	2.03	0.41
1:A:48:PHE:HD1	1:A:55:PHE:CD2	2.39	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	462/491 (94%)	453 (98%)	9 (2%)	0	100 100
1	B	460/491 (94%)	447 (97%)	12 (3%)	1 (0%)	51 81
All	All	922/982 (94%)	900 (98%)	21 (2%)	1 (0%)	55 84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	195	ARG

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	363/433 (84%)	355 (98%)	8 (2%)	57 85
1	B	359/433 (83%)	349 (97%)	10 (3%)	49 79
All	All	722/866 (83%)	704 (98%)	18 (2%)	53 82

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	104	LEU
1	A	176	TYR
1	A	260	ARG
1	A	268	SER

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Mol	Chain	Res	Type
1	A	364	ARG
1	A	468	GLU
1	A	497	PHE
1	B	101	HIS
1	B	104	LEU
1	B	136	HIS
1	B	140	SER
1	B	176	TYR
1	B	260	ARG
1	B	268	SER
1	B	333	ILE
1	B	364	ARG
1	B	497	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	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 12 ligands modelled in this entry, 8 are unknown - leaving 4 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	$\#\|Z\| > 2$
3	K2B	A	1429	-	31,31,31	1.05	2 (6%)	48,48,48	1.12	5 (10%)
2	HEM	A	601	1	28,50,50	1.17	4 (14%)	17,82,82	1.61	4 (23%)
3	K2B	B	1429	-	31,31,31	1.13	2 (6%)	48,48,48	1.06	5 (10%)
2	HEM	B	601	1	28,50,50	1.29	3 (10%)	17,82,82	1.69	5 (29%)

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	K2B	A	1429	-	-	0/10/68/68	0/4/4/4
2	HEM	A	601	1	-	0/6/54/54	0/0/8/8
3	K2B	B	1429	-	-	0/10/68/68	0/4/4/4
2	HEM	B	601	1	-	0/6/54/54	0/0/8/8

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1429	K2B	C4-C3	-3.07	1.38	1.45
3	B	1429	K2B	C4-C3	-2.74	1.39	1.45
2	A	601	HEM	C3C-C2C	-2.30	1.37	1.40
2	A	601	HEM	C4A-NA	2.14	1.40	1.36
2	B	601	HEM	C4A-NA	2.23	1.40	1.36
2	A	601	HEM	C1C-NC	2.43	1.39	1.36
2	A	601	HEM	C4C-NC	2.68	1.39	1.36
2	B	601	HEM	C1C-NC	2.72	1.40	1.36
3	A	1429	K2B	C4-C5	3.04	1.38	1.34
3	B	1429	K2B	C4-C5	3.73	1.39	1.34
2	B	601	HEM	C4C-NC	4.46	1.42	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	HEM	CAA-CBA-CGA	-2.87	107.76	112.66
2	A	601	HEM	CAA-CBA-CGA	-2.67	108.11	112.66
2	B	601	HEM	C4A-C3A-C2A	-2.61	105.18	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	HEM	CMD-C2D-C1D	-2.51	124.61	128.46
3	A	1429	K2B	C6-C5-C4	-2.43	116.85	120.87
3	B	1429	K2B	C15-C14-C8	-2.34	115.35	119.07
3	B	1429	K2B	C6-C5-C4	-2.28	117.10	120.87
3	A	1429	K2B	C15-C14-C8	-2.26	115.47	119.07
3	B	1429	K2B	C17-C13-C14	-2.23	97.40	100.07
2	B	601	HEM	CMD-C2D-C1D	-2.07	125.28	128.46
3	A	1429	K2B	C17-C13-C14	-2.04	97.63	100.07
2	A	601	HEM	C3B-C4B-NB	2.01	111.81	109.21
2	B	601	HEM	CMD-C2D-C3D	2.05	128.82	124.94
3	B	1429	K2B	C6-C5-C10	2.20	120.83	116.76
3	A	1429	K2B	C6-C5-C10	2.35	121.11	116.76
2	B	601	HEM	CMB-C2B-C3B	2.38	129.31	124.89
3	B	1429	K2B	C2-C3-C4	2.47	120.64	116.74
3	A	1429	K2B	C2-C3-C4	2.86	121.25	116.74
2	A	601	HEM	CMB-C2B-C3B	2.91	130.29	124.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1429	K2B	6	0
2	A	601	HEM	5	0
3	B	1429	K2B	6	0
2	B	601	HEM	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	468/491 (95%)	0.18	21 (4%)	34	28	43, 74, 115, 170	0
1	B	466/491 (94%)	0.17	22 (4%)	32	26	36, 77, 123, 190	0
All	All	934/982 (95%)	0.17	43 (4%)	33	27	36, 75, 121, 190	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	LEU	4.1
1	B	425	CYS	3.9
1	A	200	ALA	3.8
1	B	424	TYR	3.7
1	A	329	GLU	3.6
1	B	426	ASN	3.5
1	B	423	PHE	3.3
1	A	330	GLY	3.2
1	A	370	PHE	3.2
1	B	94	TYR	3.1
1	A	165	ALA	3.1
1	B	373	HIS	3.0
1	A	30	GLY	2.9
1	B	91	HIS	2.9
1	B	225	ILE	2.8
1	A	199	LYS	2.8
1	A	372	LEU	2.8
1	B	228	PHE	2.8
1	B	195	ARG	2.8
1	A	203	LEU	2.8
1	A	430	LEU	2.7
1	A	164	ALA	2.6
1	B	116	PRO	2.6
1	B	370	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	401	TYR	2.6
1	A	290	THR	2.5
1	A	91	HIS	2.5
1	A	230	THR	2.5
1	A	297	SER	2.5
1	B	323	GLY	2.4
1	B	38	LEU	2.4
1	A	428	LEU	2.3
1	B	360	SER	2.2
1	A	135	GLY	2.1
1	B	194	ARG	2.1
1	A	118	ASP	2.1
1	B	83	LEU	2.1
1	B	230	THR	2.1
1	B	422	THR	2.1
1	B	233	ASN	2.0
1	B	41	TYR	2.0
1	A	474	ALA	2.0
1	A	367	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
4	UNX	B	2205	1/1	0.54	0.79	39.12	1,1,1,1	1
4	UNX	B	2066	1/1	0.48	0.69	19.98	1,1,1,1	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	UNX	B	2123	1/1	0.54	0.73	12.47	1,1,1,1	1
4	UNX	A	2205	1/1	0.88	0.22	1.13	1,1,1,1	1
3	K2B	A	1429	28/28	0.95	0.24	0.89	32,54,67,107	0
3	K2B	B	1429	28/28	0.95	0.20	0.18	34,53,79,112	0
2	HEM	A	601	43/43	0.98	0.17	-0.38	48,50,59,61	0
2	HEM	B	601	43/43	0.98	0.15	-0.78	48,50,61,63	0
4	UNX	A	2134	1/1	0.36	1.07	-	1,1,1,1	1
4	UNX	A	2051	1/1	0.57	0.42	-	1,1,1,1	1
4	UNX	A	2491	1/1	0.06	5.80	-	1,1,1,1	1
4	UNX	B	2491	1/1	-0.12	5.81	-	1,1,1,1	1

6.5 Other polymers (i)

There are no such residues in this entry.