Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:43 PM GMT

PDB ID	:	3RUK
Title	:	Human Cytochrome P450 CYP17A1 in complex with Abiraterone
Authors	:	DeVore, N.M.; Scott, E.E.
Deposited on	:	2011-05-05
Resolution	:	2.60 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:

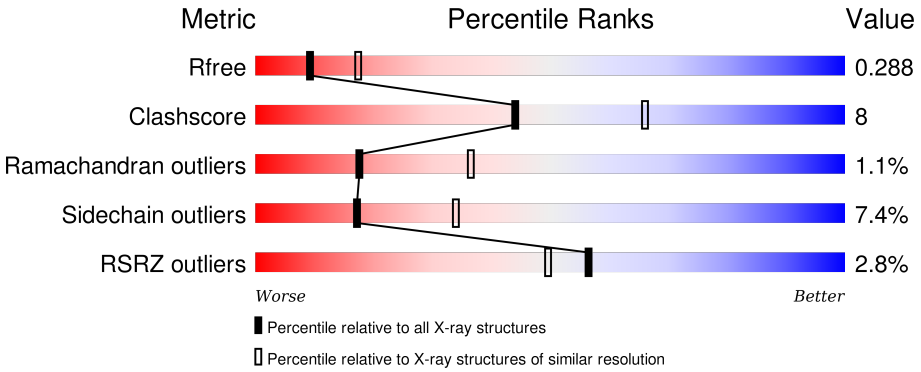
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	494	72% 21% 6%
1	B	494	2% 77% 15% 6%
1	C	494	4% 71% 22%
1	D	494	3% 72% 21%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15332 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 Steroid 17-alpha-hydroxylase/17,20 lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	2	0
			3710	2382	640	673	15			
1	B	465	Total	C	N	O	S	0	0	0
			3708	2380	641	672	15			
1	C	472	Total	C	N	O	S	0	0	0
			3752	2404	650	683	15			
1	D	473	Total	C	N	O	S	0	1	0
			3768	2414	654	685	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	EXPRESSION TAG	UNP P05093
A	20	ALA	-	EXPRESSION TAG	UNP P05093
A	21	LYS	-	EXPRESSION TAG	UNP P05093
A	22	LYS	-	EXPRESSION TAG	UNP P05093
A	23	THR	-	EXPRESSION TAG	UNP P05093
A	509	HIS	-	EXPRESSION TAG	UNP P05093
A	510	HIS	-	EXPRESSION TAG	UNP P05093
A	511	HIS	-	EXPRESSION TAG	UNP P05093
A	512	HIS	-	EXPRESSION TAG	UNP P05093
B	19	MET	-	EXPRESSION TAG	UNP P05093
B	20	ALA	-	EXPRESSION TAG	UNP P05093
B	21	LYS	-	EXPRESSION TAG	UNP P05093
B	22	LYS	-	EXPRESSION TAG	UNP P05093
B	23	THR	-	EXPRESSION TAG	UNP P05093
B	509	HIS	-	EXPRESSION TAG	UNP P05093
B	510	HIS	-	EXPRESSION TAG	UNP P05093
B	511	HIS	-	EXPRESSION TAG	UNP P05093
B	512	HIS	-	EXPRESSION TAG	UNP P05093
C	19	MET	-	EXPRESSION TAG	UNP P05093
C	20	ALA	-	EXPRESSION TAG	UNP P05093
C	21	LYS	-	EXPRESSION TAG	UNP P05093

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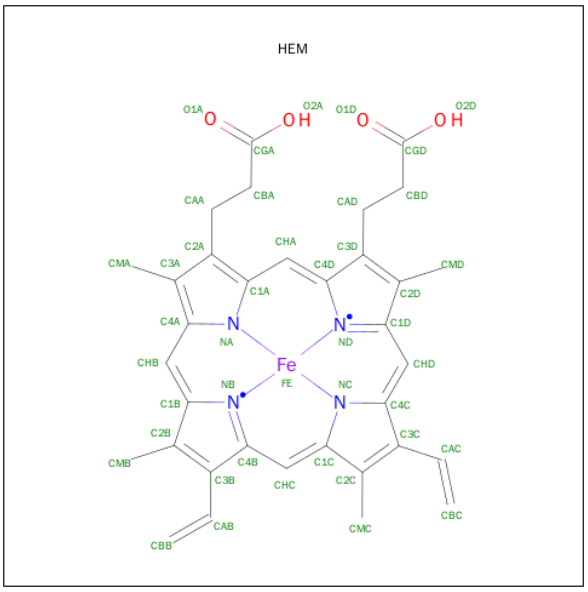
Chain	Residue	Modelled	Actual	Comment	Reference
C	22	LYS	-	EXPRESSION TAG	UNP P05093
C	23	THR	-	EXPRESSION TAG	UNP P05093
C	509	HIS	-	EXPRESSION TAG	UNP P05093
C	510	HIS	-	EXPRESSION TAG	UNP P05093
C	511	HIS	-	EXPRESSION TAG	UNP P05093
C	512	HIS	-	EXPRESSION TAG	UNP P05093
D	19	MET	-	EXPRESSION TAG	UNP P05093
D	20	ALA	-	EXPRESSION TAG	UNP P05093
D	21	LYS	-	EXPRESSION TAG	UNP P05093
D	22	LYS	-	EXPRESSION TAG	UNP P05093
D	23	THR	-	EXPRESSION TAG	UNP P05093
D	509	HIS	-	EXPRESSION TAG	UNP P05093
D	510	HIS	-	EXPRESSION TAG	UNP P05093
D	511	HIS	-	EXPRESSION TAG	UNP P05093
D	512	HIS	-	EXPRESSION TAG	UNP P05093

- 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		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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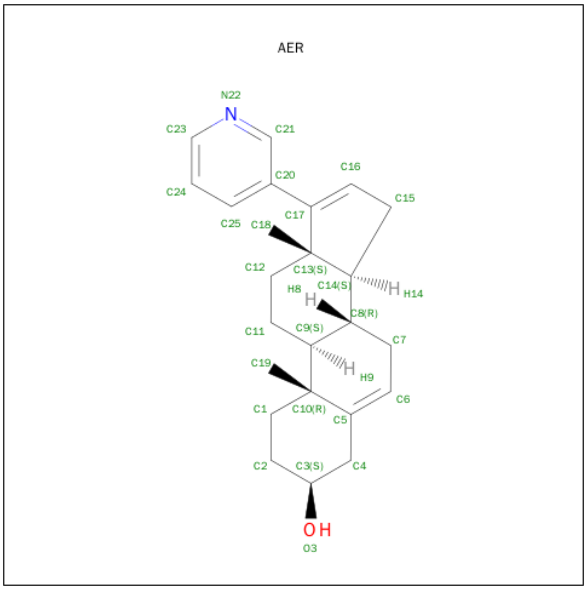
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is ABIRATERONE (three-letter code: AER) (formula: $C_{24}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	24	1	1		
3	B	1	Total	C	N	O	0	0
			26	24	1	1		
3	C	1	Total	C	N	O	0	0
			26	24	1	1		
3	D	1	Total	C	N	O	0	0
			26	24	1	1		

- Molecule 4 is water.

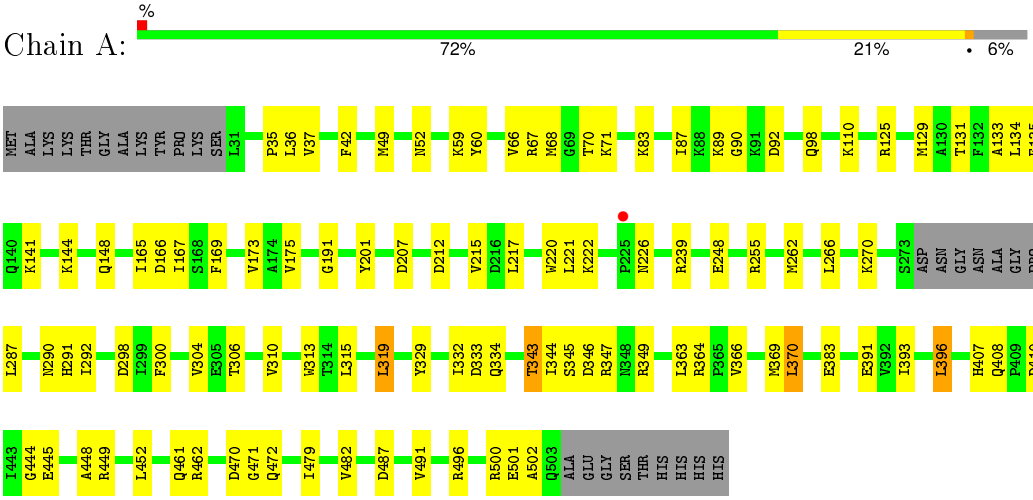
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	22	Total	O	0	0
			22	22		
4	C	23	Total	O	0	0
			23	23		
4	D	30	Total	O	0	0
			30	30		

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.

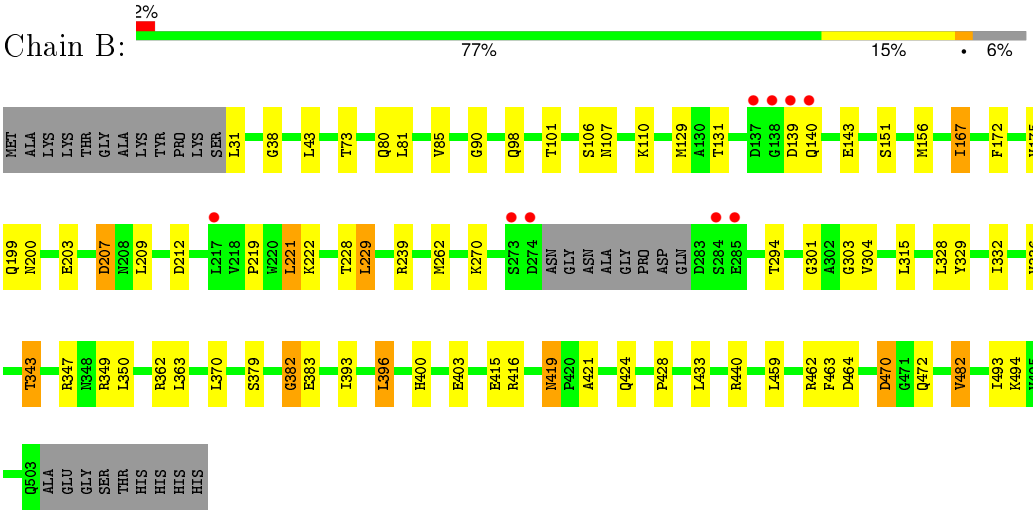
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain A:



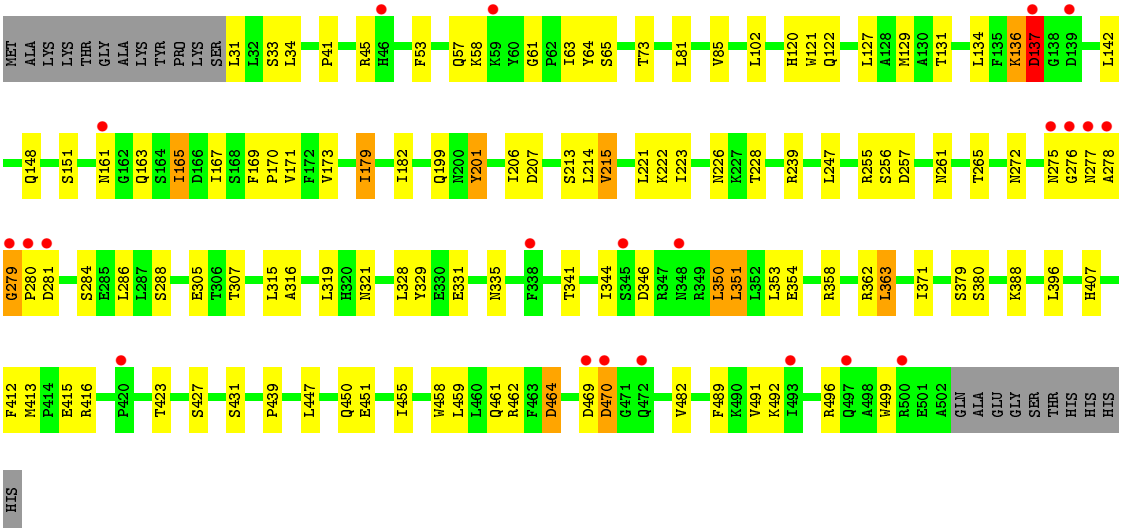
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain B:



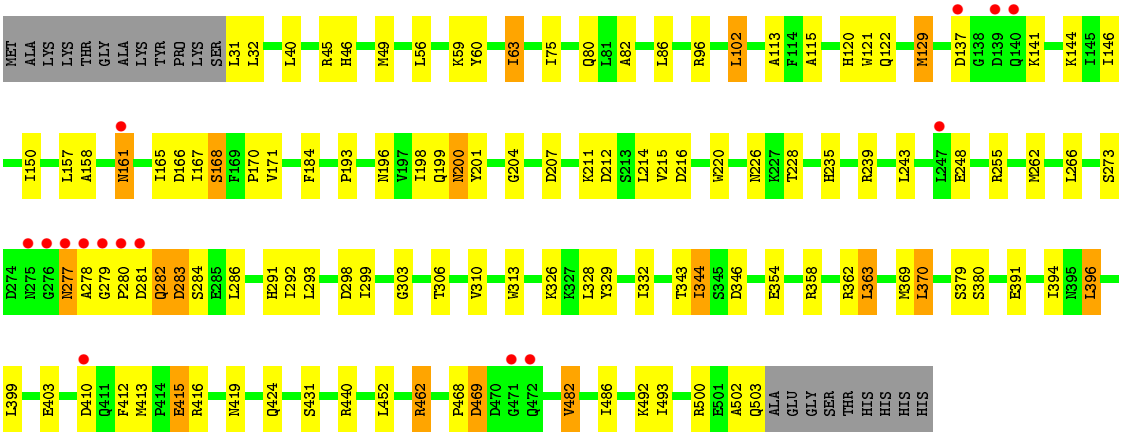
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain C:



- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.81Å 152.10Å 172.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.49 – 2.60 40.49 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.49-2.60) 100.0 (40.49-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.61Å)	Xtriage
Refinement program	REFMAC 6.1.13	Depositor
R, R_{free}	0.218 , 0.291 0.215 , 0.288	Depositor DCC
R_{free} test set	3531 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	5 of 70289 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15332	wwPDB-VP
Average B, all atoms (Å^2)	42.0	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 41.85 % 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 2.2224e-04.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: HEM, AER

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	2/3796 (0.1%)	0.85	3/5139 (0.1%)
1	B	0.77	0/3788	0.83	4/5128 (0.1%)
1	C	0.74	0/3834	0.80	1/5193 (0.0%)
1	D	0.77	0/3854	0.83	2/5220 (0.0%)
All	All	0.77	2/15272 (0.0%)	0.83	10/20680 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	GLU	CB-CG	5.62	1.62	1.52
1	A	383	GLU	CG-CD	5.29	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	212	ASP	CB-CG-OD1	5.94	123.65	118.30
1	D	243	LEU	CA-CB-CG	5.84	128.73	115.30
1	A	333	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	221	LEU	CA-CB-CG	5.39	127.71	115.30
1	D	102	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	212	ASP	N-CA-C	-5.31	96.66	111.00
1	C	279	GLY	C-N-CD	-5.26	109.02	120.60
1	A	166	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	433	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	B	382	GLY	N-CA-C	-5.14	100.25	113.10

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	3710	0	3784	64	0
1	B	3708	0	3779	39	0
1	C	3752	0	3814	61	0
1	D	3768	0	3829	81	0
2	A	43	0	30	10	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	5	0
3	A	26	0	31	4	0
3	B	26	0	31	1	0
3	C	26	0	31	0	0
3	D	26	0	31	2	0
4	A	43	0	0	1	0
4	B	22	0	0	0	0
4	C	23	0	0	1	0
4	D	30	0	0	0	0
All	All	15332	0	15450	243	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (243) 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:D:277:ASN:ND2	1:D:280:PRO:HG2	1.67	1.10
1:D:277:ASN:ND2	1:D:280:PRO:HB2	1.68	1.09
1:D:277:ASN:CG	1:D:280:PRO:HG2	1.78	1.03
1:D:277:ASN:HD21	1:D:280:PRO:HB2	1.25	1.02
1:D:277:ASN:H	1:D:277:ASN:ND2	1.52	1.00
1:D:277:ASN:HD22	1:D:277:ASN:H	1.09	0.99
1:D:277:ASN:ND2	1:D:280:PRO:CB	2.29	0.95
1:D:277:ASN:ND2	1:D:280:PRO:CG	2.30	0.94
1:C:169:PHE:O	1:C:173:VAL:HG23	1.73	0.89
1:A:479:ILE:HD11	1:A:487:ASP:OD1	1.74	0.88
1:D:306:THR:HB	2:D:600:HEM:HBB2	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:ASN:HD21	1:D:280:PRO:CB	1.90	0.85
1:C:120:HIS:CD2	1:C:286:LEU:HD22	2.13	0.83
1:A:125:ARG:O	1:A:129:MET:HG3	1.80	0.82
1:C:275:ASN:O	1:C:277:ASN:N	2.13	0.81
1:D:266:LEU:HD13	1:D:292:ILE:HG23	1.63	0.79
1:A:66:VAL:CG1	1:A:68:MET:HE2	2.13	0.79
1:D:413:MET:O	1:D:416:ARG:HG2	1.82	0.78
1:A:306:THR:O	1:A:310:VAL:HG23	1.84	0.78
1:B:419:ASN:HD21	1:B:421:ALA:HB3	1.51	0.76
1:C:354:GLU:O	1:C:358:ARG:HG3	1.84	0.75
1:C:226:ASN:OD1	1:C:228:THR:HG23	1.85	0.75
1:D:279:GLY:N	1:D:280:PRO:HD2	2.02	0.75
1:C:470:ASP:HA	4:C:14:HOH:O	1.85	0.75
1:A:407:HIS:O	1:A:408:GLN:HB2	1.85	0.75
1:D:502:ALA:O	1:D:503:GLN:HG2	1.87	0.75
1:D:370:LEU:HD21	1:D:396:LEU:HG	1.69	0.74
1:D:158:ALA:O	1:D:161:ASN:HB2	1.88	0.74
1:D:115:ALA:O	1:D:440:ARG:NH2	2.20	0.73
1:D:277:ASN:O	1:D:281:ASP:HB2	1.89	0.72
1:D:167:ILE:HD12	1:D:171:VAL:HG21	1.71	0.71
2:C:600:HEM:HBC2	2:C:600:HEM:HHD	1.74	0.70
1:D:419:ASN:ND2	1:D:424:GLN:HG2	2.07	0.70
1:A:141:LYS:HB3	1:A:144:LYS:HG3	1.75	0.69
1:A:167:ILE:HD11	1:A:315:LEU:HD12	1.74	0.68
1:D:167:ILE:HD12	1:D:171:VAL:CG2	2.23	0.68
1:C:315:LEU:O	1:C:319:LEU:HD13	1.94	0.67
1:B:209:LEU:HD23	1:B:482:VAL:HG21	1.75	0.67
1:A:445:GLU:O	1:A:449:ARG:HG3	1.94	0.67
1:D:277:ASN:N	1:D:277:ASN:ND2	2.29	0.66
1:A:461:GLN:O	1:A:496:ARG:HD3	1.96	0.65
1:D:277:ASN:HD22	1:D:277:ASN:N	1.81	0.65
1:D:281:ASP:O	1:D:283:ASP:N	2.30	0.65
1:D:157:LEU:HD22	1:D:493:ILE:HD13	1.78	0.65
1:D:279:GLY:H	1:D:280:PRO:HD2	1.61	0.64
1:D:362:ARG:NH2	1:D:363:LEU:HG	2.11	0.64
1:D:440:ARG:NH1	2:D:600:HEM:O2D	2.31	0.64
1:D:226:ASN:OD1	1:D:228:THR:HG23	1.97	0.64
1:A:319:LEU:HD21	1:A:491:VAL:HG12	1.81	0.63
1:A:370:LEU:HD21	1:A:396:LEU:HG	1.80	0.62
1:C:455:ILE:O	1:C:459:LEU:HD13	2.00	0.62
1:C:277:ASN:O	1:C:279:GLY:N	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:HIS:CD2	1:C:286:LEU:CD2	2.84	0.61
1:A:500:ARG:C	1:A:502:ALA:H	2.03	0.61
1:D:196:ASN:O	1:D:200:ASN:HB2	2.01	0.61
1:A:201:TYR:CE1	1:A:239:ARG:HG2	2.36	0.61
1:D:279:GLY:N	1:D:280:PRO:CD	2.64	0.60
1:A:462:ARG:O	1:A:496:ARG:HG3	2.01	0.60
1:A:366:VAL:HG21	2:A:600:HEM:HMB2	1.84	0.60
2:A:600:HEM:C1D	3:A:601:AER:H21	2.37	0.60
1:C:136:LYS:O	1:C:137:ASP:HB3	2.03	0.59
1:B:470:ASP:OD2	1:B:472:GLN:HB2	2.03	0.58
1:A:442:CYS:SG	2:A:600:HEM:NC	2.76	0.58
1:D:310:VAL:HG11	1:D:452:LEU:HD13	1.85	0.58
1:B:497:GLN:OE1	1:B:497:GLN:HA	2.04	0.58
2:A:600:HEM:CMB	2:A:600:HEM:HBB2	2.34	0.58
1:C:167:ILE:HD11	1:C:315:LEU:HD12	1.86	0.58
1:C:53:PHE:O	1:C:64:TYR:OH	2.22	0.57
1:B:38:GLY:HA3	1:D:40:LEU:HD23	1.87	0.57
1:B:362:ARG:HA	1:B:400:HIS:HD1	1.69	0.57
1:C:201:TYR:CE1	1:C:239:ARG:HG2	2.39	0.57
1:D:328:LEU:O	1:D:332:ILE:HG22	2.04	0.57
1:C:167:ILE:O	1:C:171:VAL:HG23	2.05	0.57
1:A:442:CYS:SG	2:A:600:HEM:NB	2.78	0.56
1:B:332:ILE:HA	1:B:350:LEU:HD21	1.88	0.56
1:C:277:ASN:C	1:C:279:GLY:H	2.07	0.56
1:A:366:VAL:CG2	2:A:600:HEM:HMB2	2.36	0.56
1:C:214:LEU:O	1:C:215:VAL:HG22	2.05	0.56
1:A:169:PHE:O	1:A:173:VAL:HG23	2.06	0.56
1:A:175:VAL:HG23	1:A:304:VAL:HA	1.87	0.56
1:A:67:ARG:HH21	1:C:41:PRO:HA	1.71	0.55
1:D:96:ARG:CZ	1:D:440:ARG:HD3	2.37	0.55
1:D:419:ASN:HD22	1:D:424:GLN:HG2	1.72	0.55
1:B:362:ARG:NH2	1:B:363:LEU:HG	2.22	0.54
1:D:214:LEU:O	1:D:215:VAL:HG22	2.07	0.54
1:D:113:ALA:HA	2:D:600:HEM:HAD1	1.88	0.54
1:D:303:GLY:HA2	2:D:600:HEM:HMC3	1.89	0.54
1:A:442:CYS:SG	2:A:600:HEM:NA	2.80	0.54
1:B:362:ARG:HA	1:B:400:HIS:ND1	2.23	0.54
1:A:220:TRP:HB3	1:C:223:ILE:CG2	2.38	0.54
1:A:165:ILE:HD12	1:A:167:ILE:HG22	1.90	0.53
3:A:601:AER:H18B	3:A:601:AER:H25	1.89	0.53
1:A:212:ASP:HB3	4:A:550:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:MET:O	1:C:416:ARG:HD2	2.09	0.53
1:B:419:ASN:ND2	1:B:421:ALA:H	2.07	0.53
1:D:468:PRO:HA	1:D:492:LYS:HB2	1.90	0.53
2:A:600:HEM:HMB2	2:A:600:HEM:HBB2	1.90	0.53
1:A:266:LEU:HB3	1:A:292:ILE:HG12	1.90	0.53
1:D:146:ILE:HG22	1:D:150:ILE:HD12	1.90	0.53
1:A:35:PRO:HG2	1:C:63:ILE:O	2.09	0.53
1:B:464:ASP:OD1	1:B:496:ARG:HG2	2.10	0.52
1:D:165:ILE:HD12	1:D:167:ILE:HG22	1.91	0.52
1:D:120[A]:HIS:CD2	1:D:286:LEU:HD22	2.44	0.52
1:C:201:TYR:CE1	1:C:239:ARG:CG	2.92	0.52
1:C:496:ARG:HB2	1:C:499:TRP:HB2	1.90	0.52
1:C:121:TRP:HZ2	1:C:439:PRO:O	1.91	0.52
1:B:203:GLU:O	1:B:207:ASP:HB2	2.10	0.52
1:D:141:LYS:HB3	1:D:144:LYS:HG3	1.90	0.52
1:C:206:ILE:HD11	1:C:305:GLU:HG3	1.92	0.52
1:C:65:SER:HA	1:C:73:THR:O	2.10	0.51
1:C:379:SER:OG	1:C:380:SER:N	2.43	0.51
1:D:370:LEU:CD2	1:D:396:LEU:HG	2.40	0.51
1:C:81:LEU:O	1:C:85:VAL:HG23	2.10	0.51
1:A:67:ARG:NH2	1:C:41:PRO:HB3	2.25	0.51
1:C:163:GLN:O	1:C:492:LYS:HA	2.11	0.50
1:C:328:LEU:HD22	1:C:353:LEU:HD13	1.93	0.50
1:D:354:GLU:O	1:D:358:ARG:HG3	2.11	0.50
1:A:133:ALA:C	1:A:135:PHE:H	2.15	0.50
1:C:169:PHE:HB3	1:C:170:PRO:HD3	1.93	0.50
1:A:370:LEU:CD2	1:A:396:LEU:HG	2.42	0.50
1:D:120[B]:HIS:CE1	1:D:291:HIS:ND1	2.80	0.50
1:D:198:ILE:HA	1:D:201:TYR:CE2	2.47	0.50
1:A:500:ARG:O	1:A:502:ALA:N	2.44	0.50
1:B:440:ARG:NH1	2:B:600:HEM:O2D	2.36	0.50
1:D:166:ASP:OD1	1:D:168:SER:OG	2.31	0.49
1:A:407:HIS:CG	1:A:407:HIS:O	2.66	0.49
1:C:362:ARG:NH2	1:C:363:LEU:HG	2.27	0.49
1:D:63:ILE:HA	1:D:75:ILE:O	2.12	0.49
1:C:255:ARG:NH2	1:C:257:ASP:OD1	2.45	0.49
1:A:59:LYS:HD3	1:A:60:TYR:CZ	2.48	0.48
1:C:407:HIS:O	1:C:416:ARG:NH2	2.46	0.48
1:D:45:ARG:O	1:D:46:HIS:HB2	2.13	0.48
1:A:66:VAL:HG11	1:A:217:LEU:HD11	1.94	0.48
1:D:211:LYS:HB2	1:D:220:TRP:HZ3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:LEU:O	1:B:332:ILE:HG22	2.13	0.48
1:C:341:THR:HB	1:C:458:TRP:CZ2	2.48	0.48
1:B:167:ILE:HD11	1:B:315:LEU:HD12	1.95	0.48
1:C:461:GLN:O	1:C:461:GLN:HG2	2.14	0.48
1:C:201:TYR:CZ	1:C:239:ARG:HG2	2.49	0.48
1:B:81:LEU:O	1:B:85:VAL:HG23	2.13	0.48
1:A:363:LEU:O	1:A:364:ARG:HD3	2.12	0.48
1:C:371:ILE:HD12	2:C:600:HEM:HAA1	1.95	0.48
1:A:66:VAL:HG13	1:A:68:MET:HE2	1.95	0.48
1:A:89:LYS:HG2	1:A:92:ASP:OD2	2.13	0.48
1:A:444:GLY:HA3	2:A:600:HEM:C3C	2.49	0.47
1:B:396:LEU:HD21	1:B:433:LEU:HB2	1.96	0.47
1:C:165:ILE:HD12	1:C:167:ILE:HG22	1.95	0.47
1:A:408:GLN:HE22	1:D:193:PRO:HD3	1.79	0.47
1:C:329:TYR:OH	1:C:464:ASP:HA	2.14	0.47
1:A:167:ILE:HD11	1:A:315:LEU:CD1	2.43	0.47
1:A:110:LYS:HD3	1:A:291:HIS:CD2	2.50	0.47
1:C:131:THR:HG22	1:C:131:THR:O	2.14	0.47
1:D:216:ASP:HB3	1:D:391:GLU:OE1	2.14	0.47
1:B:143:GLU:OE2	1:B:343:THR:HB	2.14	0.47
1:C:179:ILE:HD12	1:C:179:ILE:HA	1.74	0.47
1:C:272:ASN:O	1:C:277:ASN:CB	2.63	0.46
1:C:58:LYS:HE3	1:C:58:LYS:HB2	1.74	0.46
1:D:462:ARG:O	1:D:462:ARG:HG3	2.16	0.46
1:D:201:TYR:CE1	1:D:239:ARG:HG2	2.51	0.46
1:A:407:HIS:O	1:A:408:GLN:CB	2.59	0.46
1:D:399:LEU:O	1:D:431:SER:OG	2.32	0.46
1:C:331:GLU:O	1:C:335:ASN:HB2	2.16	0.46
1:C:319:LEU:HD21	1:C:491:VAL:HG12	1.97	0.46
1:A:175:VAL:CG2	1:A:304:VAL:HA	2.46	0.46
1:A:270:LYS:HD3	1:A:287:LEU:HB2	1.98	0.45
1:A:369:MET:O	1:A:370:LEU:C	2.55	0.45
1:A:37:VAL:HG22	1:C:65:SER:O	2.16	0.45
1:D:313:TRP:CE3	1:D:486:ILE:HD12	2.51	0.45
1:D:121:TRP:O	1:D:122:GLN:C	2.55	0.45
1:A:191:GLY:HA3	1:B:191:GLY:CA	2.47	0.45
1:B:329:TYR:CD1	1:B:496:ARG:NH1	2.85	0.45
1:B:239:ARG:HD2	1:B:239:ARG:C	2.37	0.45
1:D:262:MET:SD	1:D:299:ILE:HG13	2.57	0.44
1:B:107:ASN:O	1:B:110:LYS:HG3	2.17	0.44
1:D:343:THR:O	1:D:346:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ASN:ND2	1:C:412:PHE:CD2	2.85	0.44
1:A:298:ASP:HA	3:A:601:AER:H7	2.00	0.43
1:B:131:THR:HG21	1:B:262:MET:HB2	2.00	0.43
1:C:182:ILE:O	1:C:261:ASN:HB2	2.18	0.43
1:D:363:LEU:HD11	1:D:412:PHE:HA	2.01	0.43
1:C:127:LEU:HD22	1:C:265:THR:HG22	1.99	0.43
1:B:303:GLY:HA2	2:B:600:HEM:HMC2	2.01	0.43
1:C:307:THR:HG21	1:C:451:GLU:OE1	2.19	0.43
1:D:326:LYS:HA	1:D:329:TYR:HD2	1.82	0.43
1:D:282:GLN:C	1:D:284:SER:H	2.22	0.43
1:A:407:HIS:CD2	1:A:407:HIS:O	2.71	0.43
1:A:500:ARG:C	1:A:502:ALA:N	2.72	0.43
1:D:214:LEU:HD11	1:D:482:VAL:HG12	2.00	0.42
1:D:379:SER:OG	1:D:380:SER:N	2.49	0.42
1:D:56:LEU:HD22	1:D:60:TYR:HD2	1.82	0.42
1:D:226:ASN:CG	1:D:228:THR:HG23	2.40	0.42
1:A:313:TRP:CZ3	1:A:364:ARG:HG3	2.54	0.42
1:A:448:ALA:O	1:A:452:LEU:HG	2.18	0.42
1:B:496:ARG:O	1:B:497:GLN:C	2.58	0.42
1:C:142:LEU:HD11	1:C:447:LEU:HD13	2.00	0.42
1:A:343:THR:O	1:A:346:ASP:HB2	2.19	0.42
1:D:298:ASP:HA	3:D:601:AER:H7	2.02	0.42
1:B:301:GLY:HA3	3:B:601:AER:H7	2.01	0.42
1:D:201:TYR:CE1	1:D:239:ARG:CG	3.02	0.42
1:B:219:PRO:HB2	1:B:222:LYS:HD3	2.00	0.42
1:C:346:ASP:O	1:C:350:LEU:HB2	2.19	0.42
2:A:600:HEM:ND	3:A:601:AER:H21	2.32	0.42
1:D:129:MET:HA	1:D:129:MET:CE	2.50	0.42
1:A:220:TRP:CG	1:C:223:ILE:HG23	2.55	0.42
1:A:83:LYS:HG2	1:A:87:ILE:HD12	2.02	0.42
1:B:462:ARG:HD2	1:B:499:TRP:CE2	2.55	0.41
1:B:156:MET:SD	1:B:190:ASN:ND2	2.93	0.41
1:A:391:GLU:HG2	1:A:393:ILE:HD12	2.01	0.41
1:C:316:ALA:HB2	1:C:489:PHE:CZ	2.55	0.41
1:C:462:ARG:HG2	1:C:462:ARG:O	2.20	0.41
1:D:500:ARG:O	1:D:502:ALA:O	2.38	0.41
1:B:416:ARG:O	1:B:428:PRO:HG3	2.19	0.41
1:D:273:SER:HB2	1:D:281:ASP:O	2.20	0.41
1:B:464:ASP:HB2	1:B:494:LYS:HB2	2.03	0.41
1:A:329:TYR:O	1:A:332:ILE:HG22	2.20	0.41
1:A:42:PHE:CD2	1:A:52:ASN:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:ILE:HD12	1:C:450:GLN:HG2	2.03	0.41
1:D:299:ILE:HG23	2:D:600:HEM:HBC1	2.02	0.41
1:A:462:ARG:C	1:A:496:ARG:HG3	2.41	0.41
1:D:86:LEU:HD21	1:D:394:ILE:HG13	2.01	0.41
1:D:502:ALA:C	1:D:503:GLN:HG2	2.40	0.41
1:A:344:ILE:HA	1:A:344:ILE:HD13	1.98	0.41
1:C:57:GLN:HG2	1:C:61:GLY:O	2.20	0.41
1:B:336:VAL:HG13	1:B:340:ARG:NH1	2.35	0.41
1:D:204:GLY:HA3	1:D:235:HIS:CD2	2.56	0.41
1:B:382:GLY:O	1:B:383:GLU:HG2	2.20	0.41
1:D:344:ILE:HD13	1:D:344:ILE:HA	1.94	0.41
1:B:73:THR:CG2	1:B:393:ILE:HD12	2.50	0.41
1:B:106:SER:O	1:B:294:THR:HG21	2.21	0.41
1:A:131:THR:HG21	1:A:262:MET:HB2	2.02	0.40
1:D:167:ILE:HD12	1:D:171:VAL:HG23	2.03	0.40
1:B:315:LEU:HD23	1:B:315:LEU:HA	1.93	0.40
1:C:351:LEU:HG	1:C:351:LEU:H	1.73	0.40
1:A:363:LEU:HD22	1:A:364:ARG:NH1	2.35	0.40
1:D:82:ALA:O	1:D:86:LEU:HG	2.22	0.40
1:B:229:LEU:HD12	1:B:229:LEU:HA	1.95	0.40
1:D:415:GLU:H	1:D:415:GLU:CD	2.25	0.40
1:C:272:ASN:O	1:C:277:ASN:HB3	2.21	0.40
1:B:175:VAL:HG23	1:B:304:VAL:HA	2.02	0.40
1:B:463:PHE:C	1:B:496:ARG:HG3	2.41	0.40
3:D:601:AER:H18B	3:D:601:AER:H25	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	462/494 (94%)	424 (92%)	32 (7%)	6 (1%)	15 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	461/494 (93%)	432 (94%)	26 (6%)	3 (1%)	26 51
1	C	470/494 (95%)	423 (90%)	40 (8%)	7 (2%)	13 26
1	D	472/494 (96%)	436 (92%)	31 (7%)	5 (1%)	17 36
All	All	1865/1976 (94%)	1715 (92%)	129 (7%)	21 (1%)	17 36

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	GLU
1	C	276	GLY
1	C	278	ALA
1	C	280	PRO
1	D	282	GLN
1	A	134	LEU
1	A	370	LEU
1	A	471	GLY
1	C	284	SER
1	C	415	GLU
1	D	469	ASP
1	C	137	ASP
1	C	288	SER
1	D	278	ALA
1	D	283	ASP
1	D	370	LEU
1	B	370	LEU
1	B	497	GLN
1	B	90	GLY
1	A	90	GLY
1	A	215	VAL

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	416/436 (95%)	390 (94%)	26 (6%)	22 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	415/436 (95%)	384 (92%)	31 (8%)	17 33
1	C	419/436 (96%)	382 (91%)	37 (9%)	12 24
1	D	421/436 (97%)	390 (93%)	31 (7%)	17 34
All	All	1671/1744 (96%)	1546 (92%)	125 (8%)	17 33

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	49	MET
1	A	70	THR
1	A	71	LYS
1	A	98	GLN
1	A	137[A]	ASP
1	A	137[B]	ASP
1	A	139	ASP
1	A	148	GLN
1	A	207	ASP
1	A	221	LEU
1	A	222	LYS
1	A	226	ASN
1	A	248	GLU
1	A	255	ARG
1	A	290	ASN
1	A	300	PHE
1	A	319	LEU
1	A	334	GLN
1	A	343	THR
1	A	345	SER
1	A	347	ARG
1	A	349	ARG
1	A	396	LEU
1	A	410	ASP
1	A	482	VAL
1	B	31	LEU
1	B	43	LEU
1	B	80	GLN
1	B	98	GLN
1	B	101	THR
1	B	129	MET
1	B	139	ASP

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Mol	Chain	Res	Type
1	B	140	GLN
1	B	151	SER
1	B	167	ILE
1	B	172	PHE
1	B	199	GLN
1	B	200	ASN
1	B	207	ASP
1	B	221	LEU
1	B	228	THR
1	B	229	LEU
1	B	270	LYS
1	B	343	THR
1	B	347	ARG
1	B	349	ARG
1	B	379	SER
1	B	396	LEU
1	B	403	GLU
1	B	415	GLU
1	B	419	ASN
1	B	424	GLN
1	B	459	LEU
1	B	470	ASP
1	B	482	VAL
1	B	493	ILE
1	C	31	LEU
1	C	33	SER
1	C	34	LEU
1	C	45	ARG
1	C	102	LEU
1	C	122	GLN
1	C	129	MET
1	C	134	LEU
1	C	136	LYS
1	C	137	ASP
1	C	148	GLN
1	C	151	SER
1	C	161	ASN
1	C	165	ILE
1	C	179	ILE
1	C	199	GLN
1	C	201	TYR
1	C	207	ASP

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Mol	Chain	Res	Type
1	C	213	SER
1	C	215	VAL
1	C	221	LEU
1	C	222	LYS
1	C	247	LEU
1	C	256	SER
1	C	281	ASP
1	C	350	LEU
1	C	351	LEU
1	C	363	LEU
1	C	388	LYS
1	C	396	LEU
1	C	423	THR
1	C	427	SER
1	C	431	SER
1	C	464	ASP
1	C	469	ASP
1	C	470	ASP
1	C	482	VAL
1	D	31	LEU
1	D	32	LEU
1	D	49	MET
1	D	59	LYS
1	D	63	ILE
1	D	80	GLN
1	D	102	LEU
1	D	129	MET
1	D	137	ASP
1	D	161	ASN
1	D	168	SER
1	D	170	PRO
1	D	184	PHE
1	D	199	GLN
1	D	200	ASN
1	D	207	ASP
1	D	212	ASP
1	D	248	GLU
1	D	255	ARG
1	D	277	ASN
1	D	293	LEU
1	D	344	ILE
1	D	363	LEU

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Mol	Chain	Res	Type
1	D	369	MET
1	D	396	LEU
1	D	403	GLU
1	D	410	ASP
1	D	415	GLU
1	D	462	ARG
1	D	469	ASP
1	D	482	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	407	HIS
1	A	408	GLN
1	C	321	ASN
1	D	277	ASN
1	D	321	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

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	600	1,3	30,50,50	2.72	8 (26%)	24,82,82	2.94	12 (50%)
3	AER	A	601	2	30,30,30	1.82	3 (10%)	45,47,47	2.33	14 (31%)
2	HEM	B	600	1,3	30,50,50	2.51	10 (33%)	24,82,82	2.91	12 (50%)
3	AER	B	601	2	30,30,30	1.69	3 (10%)	45,47,47	2.05	10 (22%)
2	HEM	C	600	1,3	30,50,50	2.68	9 (30%)	24,82,82	2.54	11 (45%)
3	AER	C	601	2	30,30,30	1.64	1 (3%)	45,47,47	2.25	10 (22%)
2	HEM	D	600	1,3	30,50,50	2.31	11 (36%)	24,82,82	2.65	10 (41%)
3	AER	D	601	2	30,30,30	1.92	4 (13%)	45,47,47	2.12	11 (24%)

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	HEM	A	600	1,3	-	0/10/54/54	0/0/8/8
3	AER	A	601	2	-	0/4/62/62	0/5/5/5
2	HEM	B	600	1,3	-	0/10/54/54	0/0/8/8
3	AER	B	601	2	-	0/4/62/62	0/5/5/5
2	HEM	C	600	1,3	-	0/10/54/54	0/0/8/8
3	AER	C	601	2	-	0/4/62/62	0/5/5/5
2	HEM	D	600	1,3	-	0/10/54/54	0/0/8/8
3	AER	D	601	2	-	0/4/62/62	0/5/5/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	HEM	C3B-C4B	-11.09	1.41	1.51
2	C	600	HEM	C3B-C4B	-9.43	1.43	1.51
2	D	600	HEM	C3B-C4B	-7.02	1.45	1.51
2	B	600	HEM	C3B-C4B	-6.42	1.46	1.51
2	C	600	HEM	C3D-C4D	-6.01	1.43	1.51
2	D	600	HEM	C3D-C4D	-5.83	1.44	1.51
2	B	600	HEM	C3D-C4D	-5.01	1.45	1.51
2	A	600	HEM	C3D-C4D	-4.67	1.45	1.51
2	C	600	HEM	C2C-C1C	-4.53	1.44	1.52
2	A	600	HEM	C2C-C1C	-3.64	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	HEM	C2C-C1C	-3.60	1.45	1.52
2	B	600	HEM	C2C-C1C	-3.48	1.46	1.52
3	D	601	AER	C10-C9	-3.28	1.50	1.56
3	A	601	AER	C13-C17	-3.12	1.49	1.52
2	C	600	HEM	C2B-C1B	-3.04	1.41	1.51
2	A	600	HEM	C2D-C1D	-2.59	1.43	1.51
2	B	600	HEM	C2B-C1B	-2.23	1.44	1.51
2	D	600	HEM	C2D-C1D	-2.21	1.44	1.51
2	A	600	HEM	C2B-C1B	-2.20	1.44	1.51
2	D	600	HEM	C2B-C1B	-2.09	1.45	1.51
3	B	601	AER	C13-C17	-2.05	1.50	1.52
2	A	600	HEM	FE-NC	2.01	2.03	1.95
2	B	600	HEM	C3B-CAB	2.07	1.55	1.51
3	D	601	AER	C15-C16	2.09	1.53	1.50
2	C	600	HEM	C3C-CAC	2.13	1.55	1.51
3	A	601	AER	C20-C17	2.14	1.51	1.48
2	D	600	HEM	CMA-C3A	2.15	1.56	1.51
2	D	600	HEM	FE-ND	2.20	2.09	1.97
2	D	600	HEM	C3C-CAC	2.39	1.55	1.51
2	C	600	HEM	C1C-NC	2.41	1.39	1.36
2	A	600	HEM	CAA-C2A	2.50	1.56	1.52
3	B	601	AER	C20-C17	2.51	1.52	1.48
2	B	600	HEM	CMA-C3A	2.54	1.56	1.51
2	C	600	HEM	C4C-NC	2.57	1.39	1.36
2	D	600	HEM	FE-NC	2.62	2.06	1.95
2	D	600	HEM	FE-NB	2.62	2.11	1.97
2	D	600	HEM	C1C-NC	2.69	1.39	1.36
2	C	600	HEM	FE-ND	2.77	2.12	1.97
2	B	600	HEM	FE-NB	3.25	2.14	1.97
3	D	601	AER	C20-C17	3.28	1.53	1.48
2	B	600	HEM	C4C-NC	3.52	1.40	1.36
2	A	600	HEM	FE-ND	3.68	2.16	1.97
2	C	600	HEM	FE-NB	3.84	2.17	1.97
2	B	600	HEM	C1C-NC	4.45	1.41	1.36
2	B	600	HEM	FE-ND	4.75	2.22	1.97
3	B	601	AER	C16-C17	7.92	1.51	1.33
3	C	601	AER	C16-C17	8.01	1.51	1.33
3	D	601	AER	C16-C17	8.44	1.52	1.33
3	A	601	AER	C16-C17	8.48	1.52	1.33

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	AER	C15-C16-C17	-10.88	102.75	112.43
3	B	601	AER	C15-C16-C17	-9.87	103.65	112.43
3	C	601	AER	C15-C16-C17	-8.80	104.60	112.43
3	D	601	AER	C15-C16-C17	-7.23	106.00	112.43
2	B	600	HEM	CAA-CBA-CGA	-5.39	102.86	112.75
2	A	600	HEM	C3B-CAB-CBB	-5.32	116.29	124.46
2	D	600	HEM	CAA-CBA-CGA	-5.01	103.56	112.75
2	B	600	HEM	CAA-C2A-C1A	-4.94	121.64	127.01
2	A	600	HEM	CAA-C2A-C1A	-4.58	122.04	127.01
3	C	601	AER	C9-C8-C14	-4.20	103.54	109.06
3	A	601	AER	C12-C13-C14	-3.79	103.32	108.99
2	B	600	HEM	C3B-CAB-CBB	-3.40	119.24	124.46
3	A	601	AER	C4-C5-C6	-3.31	114.95	120.57
3	D	601	AER	C11-C9-C10	-3.21	108.86	113.11
2	C	600	HEM	CMA-C3A-C4A	-3.13	123.18	128.36
2	B	600	HEM	C3B-C4B-NB	-3.11	105.67	111.63
3	A	601	AER	C20-C21-N22	-2.84	119.43	123.52
2	D	600	HEM	C3B-C4B-NB	-2.72	106.42	111.63
3	B	601	AER	C7-C6-C5	-2.61	119.41	125.01
3	D	601	AER	C18-C13-C12	-2.58	107.92	111.12
3	A	601	AER	C9-C8-C14	-2.57	105.67	109.06
2	B	600	HEM	C2C-C1C-NC	-2.57	105.88	110.21
3	A	601	AER	C19-C10-C1	-2.41	105.81	109.43
2	C	600	HEM	C3B-C4B-NB	-2.41	107.03	111.63
3	B	601	AER	C18-C13-C17	-2.40	103.91	108.50
3	D	601	AER	C14-C13-C17	-2.40	97.92	100.57
2	D	600	HEM	CAA-C2A-C1A	-2.29	124.52	127.01
2	C	600	HEM	CAA-CBA-CGA	-2.29	108.55	112.75
2	A	600	HEM	C3C-CAC-CBC	-2.25	121.01	124.46
2	A	600	HEM	CMA-C3A-C4A	-2.21	124.71	128.36
2	A	600	HEM	C3B-C4B-NB	-2.20	107.43	111.63
3	C	601	AER	C1-C10-C9	-2.18	105.84	108.64
3	B	601	AER	C4-C5-C6	-2.18	116.87	120.57
3	C	601	AER	C12-C13-C14	-2.17	105.75	108.99
3	B	601	AER	C19-C10-C5	-2.06	105.18	108.36
3	C	601	AER	C12-C13-C17	-2.03	116.50	118.39
3	D	601	AER	C1-C10-C9	-2.02	106.05	108.64
3	A	601	AER	C18-C13-C17	-2.02	104.64	108.50
2	B	600	HEM	CMD-C2D-C3D	2.05	123.41	114.35
2	A	600	HEM	C2D-C3D-C4D	2.10	105.06	101.50
3	B	601	AER	C12-C11-C9	2.11	116.65	113.10
3	B	601	AER	C14-C15-C16	2.11	105.51	101.84
3	D	601	AER	C23-N22-C21	2.12	120.74	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	HEM	C4B-CHC-C1C	2.14	129.41	125.82
3	A	601	AER	C13-C17-C16	2.18	112.36	110.35
3	C	601	AER	C7-C8-C9	2.19	112.70	109.71
3	B	601	AER	C13-C17-C20	2.22	127.41	123.06
3	C	601	AER	C19-C10-C9	2.41	114.75	111.67
3	B	601	AER	C18-C13-C12	2.43	114.14	111.12
2	C	600	HEM	C2D-C3D-C4D	2.43	105.62	101.50
3	D	601	AER	C19-C10-C5	2.51	112.26	108.36
3	A	601	AER	C19-C10-C5	2.52	112.26	108.36
3	C	601	AER	C13-C17-C16	2.55	112.69	110.35
3	A	601	AER	C23-N22-C21	2.60	121.64	116.84
3	A	601	AER	C14-C15-C16	2.62	106.39	101.84
2	C	600	HEM	CBA-CAA-C2A	2.70	117.36	112.53
3	D	601	AER	C11-C9-C8	2.81	115.82	111.74
2	C	600	HEM	CMD-C2D-C3D	2.86	126.98	114.35
3	D	601	AER	C7-C8-C9	2.95	113.73	109.71
2	D	600	HEM	CMD-C2D-C3D	2.98	127.53	114.35
3	A	601	AER	C18-C13-C14	2.98	117.79	112.94
2	D	600	HEM	C2C-C1C-CHC	3.03	128.29	123.68
3	B	601	AER	C4-C5-C10	3.21	121.10	116.43
3	A	601	AER	C15-C14-C13	3.33	106.75	104.07
2	C	600	HEM	CMC-C2C-C3C	3.42	125.07	116.53
3	C	601	AER	C1-C2-C3	3.43	115.99	110.43
3	A	601	AER	C4-C5-C10	3.74	121.88	116.43
2	B	600	HEM	CMC-C2C-C3C	3.76	125.92	116.53
3	D	601	AER	C18-C13-C14	3.85	119.20	112.94
2	D	600	HEM	CAD-C3D-C4D	3.89	126.18	112.47
2	A	600	HEM	CMD-C2D-C3D	3.92	131.67	114.35
2	D	600	HEM	CMB-C2B-C3B	4.02	126.56	116.53
2	C	600	HEM	CAD-C3D-C4D	4.02	126.66	112.47
2	B	600	HEM	CMB-C2B-C3B	4.09	126.74	116.53
2	D	600	HEM	CMC-C2C-C3C	4.25	127.15	116.53
2	D	600	HEM	C3B-C4B-CHC	4.37	129.31	123.16
2	A	600	HEM	CAD-C3D-C4D	4.45	128.18	112.47
2	A	600	HEM	CBA-CAA-C2A	4.59	120.75	112.53
2	B	600	HEM	CAD-C3D-C4D	4.60	128.69	112.47
2	A	600	HEM	CMC-C2C-C3C	4.61	128.03	116.53
2	A	600	HEM	CAD-C3D-C2D	4.71	126.76	113.22
2	C	600	HEM	C3B-C4B-CHC	4.74	129.84	123.16
2	C	600	HEM	CMB-C2B-C3B	4.82	128.55	116.53
2	B	600	HEM	CAD-C3D-C2D	4.83	127.11	113.22
2	B	600	HEM	C3B-C4B-CHC	4.87	130.01	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	HEM	CMB-C2B-C3B	5.00	129.02	116.53
2	C	600	HEM	CAD-C3D-C2D	5.03	127.69	113.22
2	D	600	HEM	CAD-C3D-C2D	5.52	129.10	113.22
3	D	601	AER	C15-C14-C13	7.06	109.74	104.07
3	C	601	AER	C15-C14-C13	7.51	110.10	104.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	10	0
3	A	601	AER	4	0
2	B	600	HEM	2	0
3	B	601	AER	1	0
2	C	600	HEM	2	0
2	D	600	HEM	5	0
3	D	601	AER	2	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	464/494 (93%)	-0.25	3 (0%)	90	88	19, 38, 62, 72	0
1	B	465/494 (94%)	-0.19	12 (2%)	59	53	20, 38, 60, 73	0
1	C	472/494 (95%)	0.08	22 (4%)	35	28	26, 44, 72, 82	0
1	D	473/494 (95%)	0.00	15 (3%)	51	44	25, 42, 65, 78	0
All	All	1874/1976 (94%)	-0.09	52 (2%)	56	49	19, 40, 67, 82	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	278	ALA	8.5
1	D	279	GLY	8.1
1	D	277	ASN	7.2
1	D	280	PRO	6.5
1	C	279	GLY	6.4
1	C	278	ALA	5.7
1	C	277	ASN	5.5
1	B	139	ASP	5.5
1	C	276	GLY	4.8
1	D	139	ASP	4.5
1	C	280	PRO	4.5
1	A	139	ASP	4.4
1	D	276	GLY	4.1
1	C	281	ASP	3.4
1	B	284	SER	3.2
1	B	274	ASP	3.1
1	D	140	GLN	3.1
1	D	471	GLY	3.0
1	D	472	GLN	3.0
1	C	420	PRO	2.9
1	C	137	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	348	ASN	2.8
1	C	139	ASP	2.8
1	C	469	ASP	2.8
1	C	472	GLN	2.7
1	D	281	ASP	2.7
1	A	225	PRO	2.6
1	C	46	HIS	2.5
1	C	161	ASN	2.5
1	D	275	ASN	2.5
1	D	247	LEU	2.5
1	C	493	ILE	2.4
1	C	275	ASN	2.4
1	B	285	GLU	2.3
1	B	217	LEU	2.3
1	D	137	ASP	2.3
1	D	161	ASN	2.3
1	C	500	ARG	2.2
1	C	345	SER	2.2
1	B	138	GLY	2.2
1	B	273	SER	2.2
1	C	59	LYS	2.2
1	C	470	ASP	2.2
1	B	337	GLY	2.2
1	B	498	ALA	2.2
1	C	338	PHE	2.1
1	C	497	GLN	2.1
1	D	410	ASP	2.1
1	B	338	PHE	2.1
1	A	138	GLY	2.0
1	B	140	GLN	2.0
1	B	137	ASP	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

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
3	AER	C	601	26/26	0.97	0.23	0.85	26,30,31,32	0
2	HEM	B	600	43/43	0.98	0.19	0.64	19,24,28,31	0
3	AER	B	601	26/26	0.97	0.18	0.40	26,30,31,32	0
3	AER	D	601	26/26	0.96	0.18	0.37	21,27,29,30	0
2	HEM	A	600	43/43	0.98	0.15	0.20	18,27,31,36	0
2	HEM	C	600	43/43	0.98	0.20	0.04	21,30,35,38	0
3	AER	A	601	26/26	0.97	0.15	-0.06	27,31,34,34	0
2	HEM	D	600	43/43	0.98	0.16	-0.54	21,27,33,41	0

6.5 Other polymers

There are no such residues in this entry.