Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:03 AM GMT

PDB ID	:	2FDY
Title	:	Microsomal P450 2A6 with the inhibitor Adrithiol bound
Authors	:	Yano, J.K.; Stout, C.D.; Johnson, E.F.
Deposited on	:	2005-12-14
Resolution	:	1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
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:

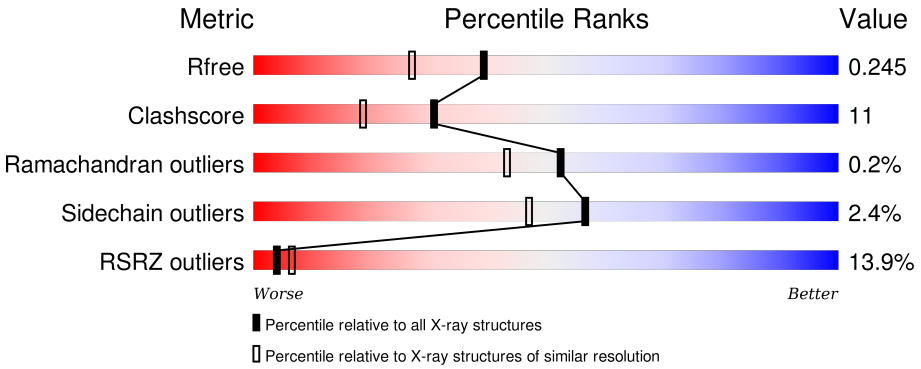
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	476	10% 81% 17%
1	B	476	17% 70% 25%
1	C	476	11% 76% 21%
1	D	476	17% 75% 22%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	D4G	A	501	-	-	-	X
4	D4G	D	501	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16035 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 Cytochrome P450 2A6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3760	2414	650	678	18			
1	B	464	Total	C	N	O	S	0	0	0
			3757	2412	650	677	18			
1	C	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			
1	D	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	CLONING ARTIFACT	UNP P11509
A	24	ALA	-	CLONING ARTIFACT	UNP P11509
A	25	LYS	-	CLONING ARTIFACT	UNP P11509
A	26	LYS	-	CLONING ARTIFACT	UNP P11509
A	27	THR	-	CLONING ARTIFACT	UNP P11509
A	28	SER	-	CLONING ARTIFACT	UNP P11509
A	495	HIS	-	EXPRESSION TAG	UNP P11509
A	496	HIS	-	EXPRESSION TAG	UNP P11509
A	497	HIS	-	EXPRESSION TAG	UNP P11509
A	498	HIS	-	EXPRESSION TAG	UNP P11509
B	23	MET	-	CLONING ARTIFACT	UNP P11509
B	24	ALA	-	CLONING ARTIFACT	UNP P11509
B	25	LYS	-	CLONING ARTIFACT	UNP P11509
B	26	LYS	-	CLONING ARTIFACT	UNP P11509
B	27	THR	-	CLONING ARTIFACT	UNP P11509
B	28	SER	-	CLONING ARTIFACT	UNP P11509
B	495	HIS	-	EXPRESSION TAG	UNP P11509
B	496	HIS	-	EXPRESSION TAG	UNP P11509
B	497	HIS	-	EXPRESSION TAG	UNP P11509
B	498	HIS	-	EXPRESSION TAG	UNP P11509
C	23	MET	-	CLONING ARTIFACT	UNP P11509

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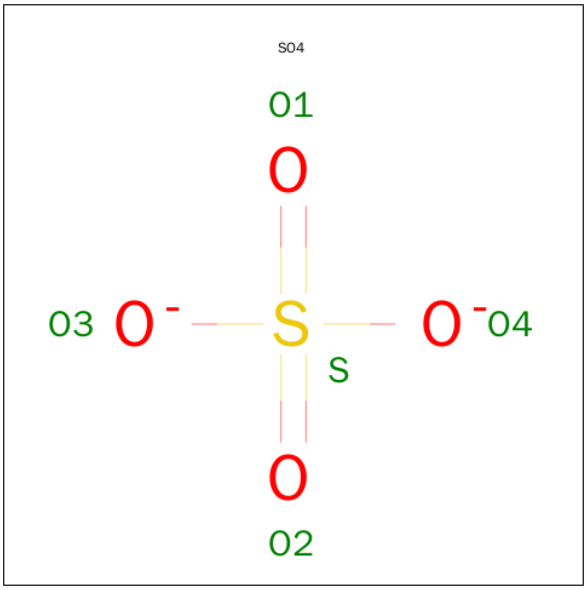
Chain	Residue	Modelled	Actual	Comment	Reference
C	24	ALA	-	CLONING ARTIFACT	UNP P11509
C	25	LYS	-	CLONING ARTIFACT	UNP P11509
C	26	LYS	-	CLONING ARTIFACT	UNP P11509
C	27	THR	-	CLONING ARTIFACT	UNP P11509
C	28	SER	-	CLONING ARTIFACT	UNP P11509
C	495	HIS	-	EXPRESSION TAG	UNP P11509
C	496	HIS	-	EXPRESSION TAG	UNP P11509
C	497	HIS	-	EXPRESSION TAG	UNP P11509
C	498	HIS	-	EXPRESSION TAG	UNP P11509
D	23	MET	-	CLONING ARTIFACT	UNP P11509
D	24	ALA	-	CLONING ARTIFACT	UNP P11509
D	25	LYS	-	CLONING ARTIFACT	UNP P11509
D	26	LYS	-	CLONING ARTIFACT	UNP P11509
D	27	THR	-	CLONING ARTIFACT	UNP P11509
D	28	SER	-	CLONING ARTIFACT	UNP P11509
D	495	HIS	-	EXPRESSION TAG	UNP P11509
D	496	HIS	-	EXPRESSION TAG	UNP P11509
D	497	HIS	-	EXPRESSION TAG	UNP P11509
D	498	HIS	-	EXPRESSION TAG	UNP P11509

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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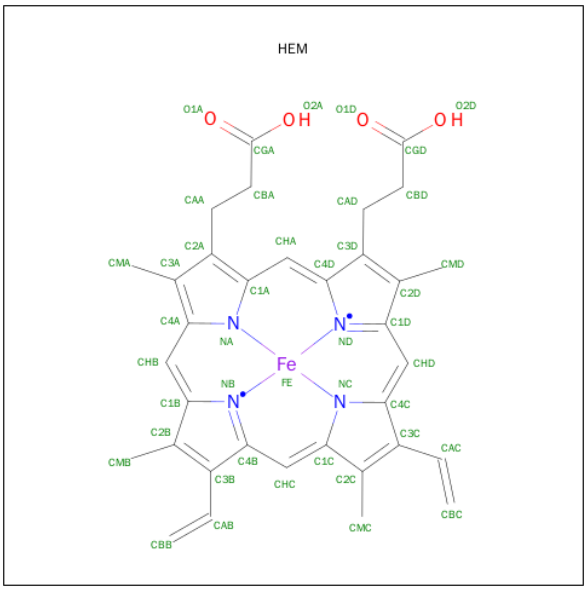
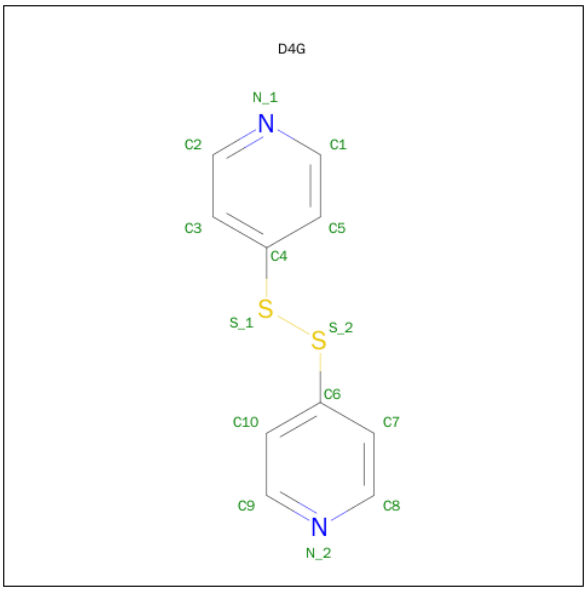
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is 4,4'-DIPYRIDYL DISULFIDE (three-letter code: D4G) (formula: $C_{10}H_8N_2S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N S 14 10 2 2	0	0
4	B	1	Total C N S 14 10 2 2	0	0
4	C	1	Total C N S 14 10 2 2	0	0
4	D	1	Total C N S 14 10 2 2	0	0

- Molecule 5 is water.

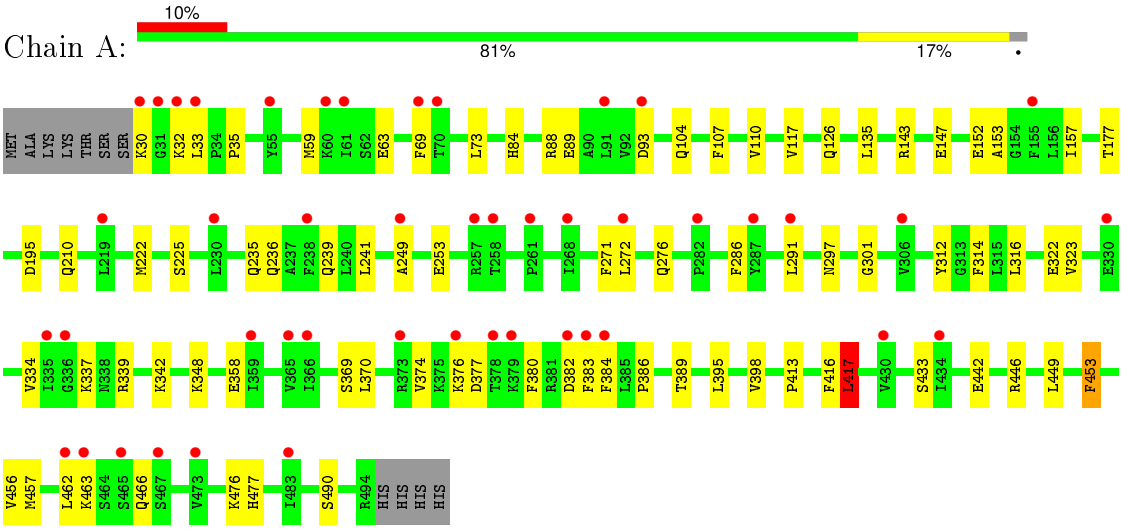
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	232	Total O 232 232	0	0
5	B	139	Total O 139 139	0	0
5	C	224	Total O 224 224	0	0
5	D	178	Total O 178 178	0	0

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.

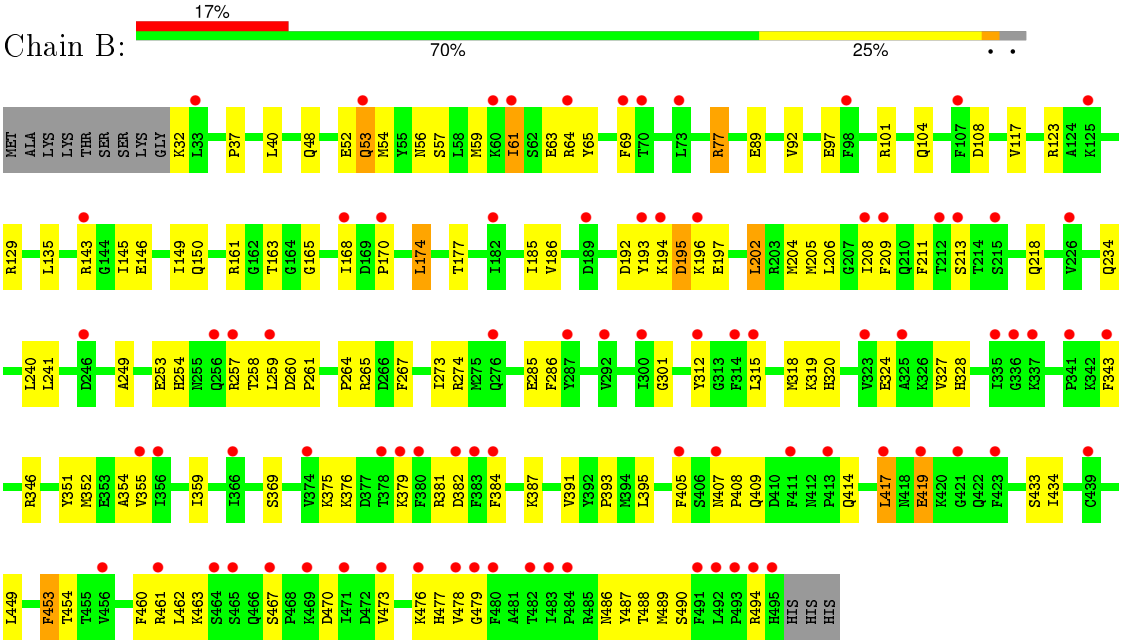
- Molecule 1: Cytochrome P450 2A6

Chain A:

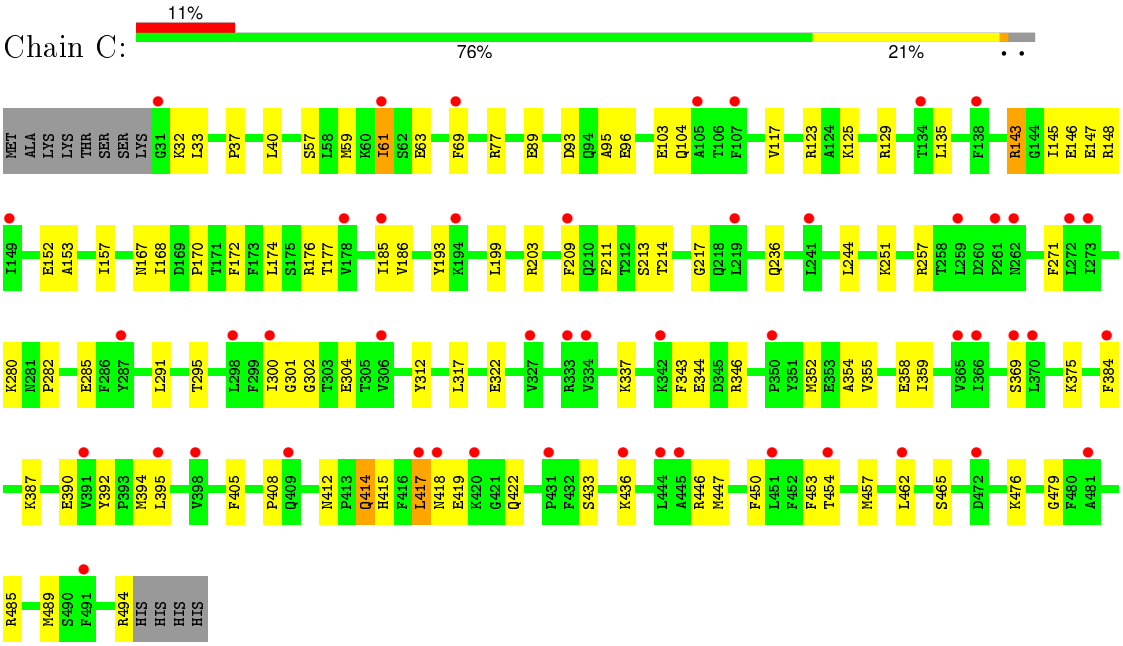


- Molecule 1: Cytochrome P450 2A6

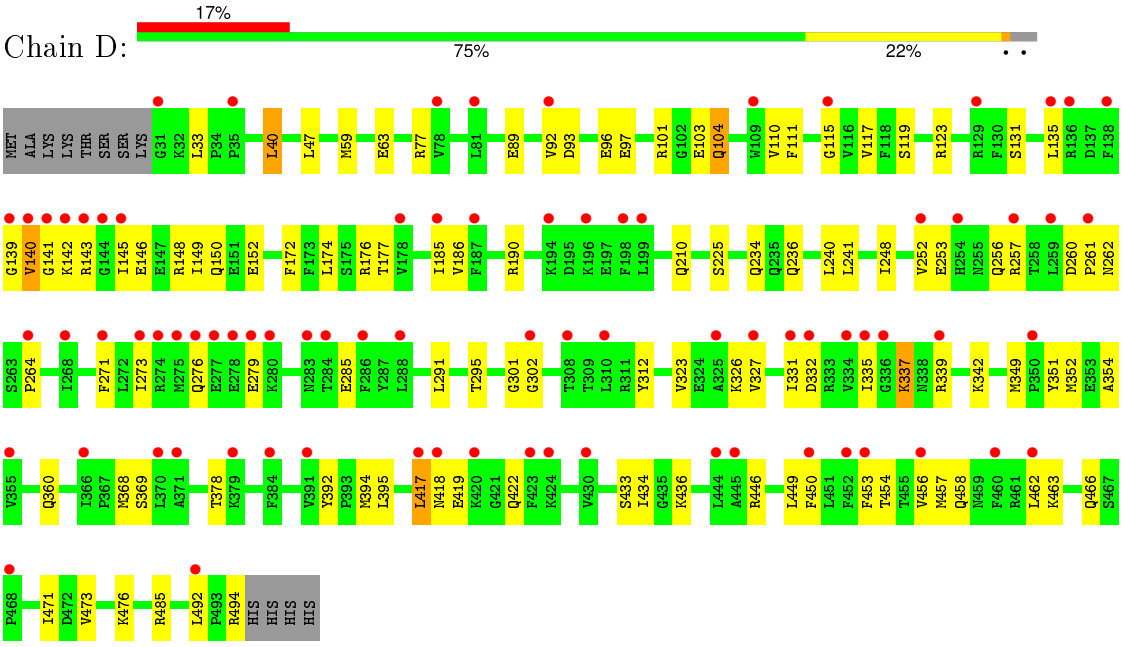
Chain B:



- Molecule 1: Cytochrome P450 2A6



• Molecule 1: Cytochrome P450 2A6



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.20Å 156.62Å 104.00Å 90.00° 91.79° 90.00°	Depositor
Resolution (Å)	42.41 – 1.95 42.40 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (42.41-1.95) 97.5 (42.40-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.49 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.250 0.209 , 0.245	Depositor DCC
R_{free} test set	8053 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.6	EDS
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 171651 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16035	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, D4G, SO4

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	0.37	0/3851	0.59	2/5186 (0.0%)
1	B	0.34	0/3849	0.56	1/5185 (0.0%)
1	C	0.38	0/3842	0.59	1/5175 (0.0%)
1	D	0.36	0/3842	0.59	1/5175 (0.0%)
All	All	0.36	0/15384	0.58	5/20721 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	GLN	N-CA-C	-5.67	95.70	111.00
1	D	104	GLN	N-CA-C	-5.57	95.95	111.00
1	B	104	GLN	N-CA-C	-5.36	96.53	111.00
1	A	417	LEU	CA-CB-CG	5.30	127.50	115.30
1	C	104	GLN	N-CA-C	-5.27	96.78	111.00

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	3760	0	3747	55	0
1	B	3757	0	3738	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3751	0	3734	74	0
1	D	3751	0	3734	89	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	43	0	30	3	0
3	B	43	0	30	2	0
3	C	43	0	30	4	0
3	D	43	0	30	4	0
4	A	14	0	8	4	0
4	B	14	0	8	1	0
4	C	14	0	8	1	0
4	D	14	0	8	3	0
5	A	232	0	0	2	0
5	B	139	0	0	7	0
5	C	224	0	0	4	0
5	D	178	0	0	3	0
All	All	16035	0	15105	331	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 11.

All (331) 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:C:32:LYS:HB3	1:C:384:PHE:HB3	1.45	0.97
1:D:463:LYS:HD3	1:D:492:LEU:HD11	1.52	0.91
1:B:352:MET:HE3	1:B:454:THR:HG22	1.54	0.87
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.40	0.86
1:B:61:ILE:HD11	1:B:69:PHE:CD1	2.12	0.84
1:B:208:ILE:HD11	1:B:240:LEU:HB2	1.60	0.83
1:C:412:ASN:OD1	1:C:414:GLN:HB2	1.80	0.82
1:B:375:LYS:HE2	5:B:2610:HOH:O	1.82	0.79
1:B:407:ASN:HB3	1:B:409:GLN:HE22	1.47	0.78
1:B:318:MET:HE1	1:B:489:MET:HB2	1.64	0.77
1:B:407:ASN:HB3	1:B:409:GLN:NE2	2.00	0.76
1:B:414:GLN:NE2	1:B:417:LEU:HD23	2.00	0.76
1:C:392:TYR:HB3	1:C:394:MET:CE	2.17	0.75
1:B:258:THR:HG23	1:B:265:ARG:HH22	1.51	0.75
1:A:235:GLN:O	1:A:239:GLN:HG2	1.87	0.74
1:D:418:ASN:HD22	1:D:422:GLN:HB2	1.53	0.73
1:D:392:TYR:HB3	1:D:394:MET:HE3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:PHE:O	1:C:214:THR:HG22	1.87	0.73
1:C:37:PRO:HD3	1:C:61:ILE:HD13	1.73	0.71
1:C:125:LYS:HZ2	1:C:129:ARG:NH2	1.87	0.71
1:C:61:ILE:HD11	1:C:69:PHE:CD1	2.26	0.71
1:D:392:TYR:HB3	1:D:394:MET:CE	2.21	0.70
1:D:326:LYS:HD2	1:D:351:TYR:CE1	2.27	0.69
1:D:418:ASN:ND2	1:D:422:GLN:HB2	2.08	0.69
1:D:101:ARG:HD3	1:D:117:VAL:O	1.93	0.69
1:C:199:LEU:HG	1:C:203:ARG:HH11	1.56	0.69
1:B:463:LYS:HB3	1:B:490:SER:OG	1.94	0.67
1:C:59:MET:O	1:C:63:GLU:HG3	1.93	0.67
1:B:57:SER:O	1:B:61:ILE:HG23	1.95	0.67
1:C:199:LEU:HG	1:C:203:ARG:NH1	2.10	0.67
1:A:89:GLU:O	1:A:93:ASP:HB2	1.95	0.67
1:C:392:TYR:HB3	1:C:394:MET:HE3	1.77	0.66
1:B:108:ASP:HB3	5:B:2613:HOH:O	1.94	0.66
1:C:125:LYS:NZ	1:C:129:ARG:HH22	1.93	0.66
1:B:494:ARG:HH11	1:B:494:ARG:HG3	1.61	0.66
1:B:193:TYR:CD1	1:B:194:LYS:HG2	2.32	0.65
1:C:352:MET:HE3	1:C:454:THR:HG22	1.78	0.64
1:D:142:LYS:O	1:D:145:ILE:HG22	1.98	0.64
1:D:446:ARG:HG2	5:D:673:HOH:O	1.98	0.63
1:A:457:MET:HE1	1:A:462:LEU:HD21	1.79	0.62
1:D:457:MET:HE1	1:D:462:LEU:HD21	1.82	0.62
1:D:123:ARG:HA	1:D:285:GLU:HG3	1.82	0.62
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.80	0.62
1:C:392:TYR:HB3	1:C:394:MET:HE1	1.81	0.62
1:B:414:GLN:HE22	1:B:417:LEU:HD23	1.64	0.61
1:C:433:SER:HB3	3:C:500:HEM:HBA1	1.82	0.61
1:B:433:SER:HB3	3:B:500:HEM:HBA1	1.81	0.61
1:C:214:THR:HG21	5:C:629:HOH:O	2.00	0.61
1:A:152:GLU:HG3	1:A:177:THR:HG23	1.82	0.61
1:D:419:GLU:CD	1:D:419:GLU:H	2.03	0.61
1:B:476:LYS:HE3	1:B:477:HIS:CD2	2.36	0.61
1:C:117:VAL:HG22	3:C:500:HEM:HAD1	1.82	0.60
1:B:143:ARG:HD2	1:B:146:GLU:OE2	2.01	0.60
1:D:148:ARG:HH21	1:D:190:ARG:HB3	1.66	0.60
1:C:125:LYS:HZ2	1:C:129:ARG:HH22	1.47	0.60
1:B:254:HIS:O	1:B:258:THR:HG22	2.02	0.60
1:D:276:GLN:O	1:D:279:GLU:HB2	2.03	0.59
1:B:318:MET:CE	1:B:489:MET:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:THR:CG2	1:B:265:ARG:HH12	2.16	0.58
1:C:450:PHE:O	1:C:454:THR:HG23	2.04	0.58
1:D:135:LEU:HG	1:D:140:VAL:HG21	1.84	0.58
1:D:101:ARG:CD	1:D:117:VAL:O	2.52	0.58
1:D:139:GLY:HA2	1:D:142:LYS:HE2	1.86	0.58
1:A:210:GLN:HE22	1:A:476:LYS:NZ	2.02	0.58
1:B:208:ILE:CD1	1:B:240:LEU:HB2	2.33	0.57
1:A:433:SER:HB3	3:A:500:HEM:HBA1	1.86	0.57
1:B:161:ARG:HG2	1:B:460:PHE:HZ	1.69	0.57
1:B:213:SER:HA	1:B:479:GLY:HA3	1.87	0.57
1:B:258:THR:HG23	1:B:265:ARG:NH2	2.19	0.57
1:D:271:PHE:CG	1:D:291:LEU:HD13	2.38	0.57
1:A:33:LEU:HD21	1:A:386:PRO:HD2	1.86	0.56
1:D:252:VAL:O	1:D:256:GLN:HG3	2.05	0.56
1:D:103:GLU:HG2	1:D:104:GLN:N	2.20	0.56
1:D:456:VAL:HG12	1:D:457:MET:HE3	1.85	0.56
1:C:152:GLU:HG3	1:C:177:THR:HG23	1.87	0.56
1:A:33:LEU:HD23	1:A:384:PHE:O	2.06	0.56
1:D:326:LYS:HD2	1:D:351:TYR:CZ	2.40	0.56
1:A:271:PHE:HB3	1:A:291:LEU:HD13	1.88	0.56
1:C:418:ASN:HB3	1:C:422:GLN:H	1.71	0.55
1:C:355:VAL:O	1:C:359:ILE:HG13	2.05	0.55
1:C:170:PRO:O	1:C:174:LEU:HD13	2.07	0.55
1:B:249:ALA:O	1:B:253:GLU:HG3	2.07	0.55
1:B:407:ASN:CB	1:B:409:GLN:HE22	2.19	0.55
1:C:405:PHE:O	1:C:408:PRO:HD3	2.05	0.55
1:B:77:ARG:NH1	1:B:77:ARG:HG2	2.14	0.54
1:D:323:VAL:O	1:D:327:VAL:HG23	2.06	0.54
1:C:337:LYS:HE2	1:C:494:ARG:NH1	2.22	0.54
1:C:251:LYS:HZ2	1:C:251:LYS:HB3	1.72	0.54
1:B:258:THR:HG23	1:B:265:ARG:HH12	1.72	0.54
1:D:97:GLU:OE1	1:D:378:THR:HG23	2.07	0.54
1:B:196:LYS:O	1:B:196:LYS:HG2	2.06	0.54
1:D:59:MET:O	1:D:63:GLU:HG3	2.08	0.54
1:D:337:LYS:NZ	1:D:337:LYS:HB3	2.23	0.54
1:D:458:GLN:O	1:D:494:ARG:HD3	2.08	0.54
1:C:186:VAL:CG1	1:C:295:THR:HG23	2.37	0.54
1:B:478:VAL:HG11	5:B:2635:HOH:O	2.08	0.54
1:D:186:VAL:CG1	1:D:295:THR:HG23	2.38	0.54
1:C:354:ALA:HB2	1:C:417:LEU:HD13	1.90	0.53
1:A:73:LEU:HB3	1:A:222:MET:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:SER:HB3	1:B:477:HIS:HB3	1.89	0.53
1:B:77:ARG:CG	1:B:77:ARG:HH11	2.17	0.53
1:A:30:LYS:HG3	1:A:32:LYS:H	1.73	0.53
1:D:301:GLY:HA2	4:D:501:D4G:C5	2.39	0.53
1:D:148:ARG:NH2	1:D:190:ARG:HB3	2.22	0.53
1:C:280:LYS:O	1:C:282:PRO:HD3	2.09	0.53
1:B:193:TYR:HD1	1:B:194:LYS:HG2	1.72	0.53
1:A:334:VAL:HG13	1:A:348:LYS:HE2	1.90	0.53
1:D:110:VAL:HG11	1:D:241:LEU:HD22	1.91	0.53
1:B:414:GLN:HA	1:B:417:LEU:HB2	1.91	0.53
1:C:369:SER:HB2	1:C:395:LEU:HG	1.89	0.53
1:C:257:ARG:HH11	1:C:257:ARG:HG2	1.74	0.53
1:C:214:THR:CG2	1:C:217:GLY:H	2.22	0.53
1:B:264:PRO:HG3	1:B:273:ILE:CD1	2.39	0.53
1:C:103:GLU:HG2	1:C:390:GLU:OE2	2.09	0.53
1:D:271:PHE:HB3	1:D:291:LEU:HD13	1.91	0.52
1:B:163:THR:HG21	1:B:168:ILE:HD13	1.91	0.52
1:C:57:SER:O	1:C:61:ILE:HG23	2.09	0.52
1:A:297:ASN:HA	4:A:501:D4G:N_2	2.25	0.52
1:D:143:ARG:HH11	1:D:143:ARG:HG3	1.75	0.52
1:D:360:GLN:HG2	5:D:523:HOH:O	2.08	0.52
1:B:351:TYR:O	1:B:355:VAL:HG23	2.10	0.52
1:B:37:PRO:HB2	1:B:48:GLN:NE2	2.25	0.52
1:B:97:GLU:HG3	5:B:2534:HOH:O	2.09	0.52
1:B:61:ILE:HD11	1:B:69:PHE:CE1	2.44	0.52
1:C:271:PHE:HB3	1:C:291:LEU:HD13	1.92	0.52
1:C:95:ALA:HB1	1:C:436:LYS:HD3	1.91	0.51
1:B:409:GLN:CD	1:B:409:GLN:H	2.13	0.51
1:A:107:PHE:CE2	4:A:501:D4G:H10	2.46	0.51
1:B:161:ARG:HG3	1:B:161:ARG:HH11	1.76	0.51
1:B:354:ALA:CB	1:B:417:LEU:HD13	2.41	0.51
1:A:30:LYS:HG3	1:A:32:LYS:HB3	1.91	0.51
1:C:453:PHE:O	1:C:457:MET:HG2	2.11	0.51
1:C:172:PHE:O	1:C:176:ARG:HG3	2.11	0.50
1:B:381:ARG:O	1:B:382:ASP:HB2	2.11	0.50
1:A:322:GLU:HG2	1:A:323:VAL:N	2.26	0.50
1:D:172:PHE:O	1:D:176:ARG:HG3	2.11	0.50
1:B:355:VAL:O	1:B:359:ILE:HG13	2.12	0.50
1:D:253:GLU:O	1:D:257:ARG:HG2	2.11	0.50
1:A:457:MET:CE	1:A:462:LEU:HD21	2.41	0.50
1:C:301:GLY:HA2	4:C:501:D4G:C5	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:ASP:OD1	1:D:337:LYS:HD3	2.11	0.50
1:D:352:MET:HE3	1:D:454:THR:HG22	1.93	0.49
1:B:92:VAL:HG23	1:B:434:ILE:HD12	1.94	0.49
1:B:354:ALA:HB2	1:B:417:LEU:HD13	1.94	0.49
1:A:84:HIS:HB2	1:A:398:VAL:HG13	1.95	0.49
1:B:59:MET:O	1:B:63:GLU:HG3	2.12	0.49
1:B:61:ILE:HD12	1:B:61:ILE:O	2.12	0.49
1:D:339:ARG:NH1	1:D:342:LYS:HE2	2.26	0.49
1:D:264:PRO:HG3	1:D:273:ILE:CD1	2.43	0.49
1:B:204:MET:O	1:B:208:ILE:HG12	2.12	0.49
1:C:476:LYS:HB2	1:C:485:ARG:HA	1.94	0.49
1:C:343:PHE:CE1	1:C:447:MET:HA	2.48	0.49
1:A:143:ARG:O	1:A:147:GLU:HG3	2.12	0.49
1:B:64:ARG:HD3	1:B:65:TYR:CE2	2.48	0.48
1:C:244:LEU:HD13	1:C:300:ILE:HD11	1.94	0.48
1:D:148:ARG:HH12	1:D:152:GLU:HB2	1.78	0.48
1:B:319:LYS:HD3	1:B:473:VAL:HG11	1.96	0.48
1:D:449:LEU:O	1:D:453:PHE:HB2	2.13	0.48
1:B:319:LYS:HD3	1:B:473:VAL:CG1	2.43	0.48
1:C:446:ARG:HG2	1:C:446:ARG:HH11	1.78	0.48
1:B:170:PRO:HB2	1:B:174:LEU:HD22	1.96	0.48
1:B:461:ARG:HB2	1:B:461:ARG:HH11	1.79	0.48
1:A:413:PRO:O	1:A:417:LEU:HD22	2.13	0.48
1:C:214:THR:HG23	1:C:217:GLY:H	1.79	0.48
1:B:494:ARG:NH1	1:B:494:ARG:HG3	2.29	0.48
1:D:131:SER:O	1:D:135:LEU:HB2	2.13	0.48
1:D:456:VAL:HG12	1:D:457:MET:CE	2.43	0.48
1:D:466:GLN:CG	1:D:471:ILE:HG12	2.44	0.47
1:D:453:PHE:O	1:D:457:MET:HG2	2.13	0.47
1:C:251:LYS:NZ	1:C:251:LYS:HB3	2.30	0.47
1:D:332:ASP:OD2	1:D:494:ARG:NH2	2.45	0.47
1:B:89:GLU:CD	1:B:381:ARG:HH21	2.17	0.47
1:C:143:ARG:O	1:C:147:GLU:HG3	2.14	0.47
1:C:352:MET:CE	1:C:454:THR:HG22	2.42	0.47
1:D:248:ILE:O	1:D:252:VAL:HG23	2.14	0.47
1:B:449:LEU:O	1:B:453:PHE:HB2	2.14	0.47
1:A:337:LYS:HD2	1:A:337:LYS:N	2.29	0.47
1:C:89:GLU:O	1:C:93:ASP:HB2	2.15	0.47
1:D:89:GLU:O	1:D:93:ASP:HB2	2.13	0.47
1:B:165:GLY:O	1:B:490:SER:HB2	2.14	0.47
1:D:332:ASP:CG	1:D:494:ARG:HH22	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:PRO:O	1:A:69:PHE:HB2	2.14	0.47
1:B:54:MET:HG3	1:B:218:GLN:OE1	2.15	0.47
1:D:392:TYR:HB3	1:D:394:MET:HE1	1.96	0.47
1:B:123:ARG:HA	1:B:285:GLU:HG3	1.97	0.47
1:A:272:LEU:O	1:A:276:GLN:HG3	2.14	0.47
1:A:466:GLN:HG2	5:A:2575:HOH:O	2.15	0.47
1:A:225:SER:HB2	1:D:225:SER:HB2	1.96	0.47
1:D:433:SER:HB3	3:D:500:HEM:HBA1	1.98	0.47
1:D:369:SER:HB2	1:D:395:LEU:HG	1.97	0.46
1:D:327:VAL:O	1:D:331:ILE:HG13	2.15	0.46
1:D:96:GLU:OE1	1:D:436:LYS:NZ	2.49	0.46
1:A:59:MET:O	1:A:63:GLU:HG3	2.15	0.46
1:C:213:SER:HA	1:C:479:GLY:HA3	1.97	0.46
1:D:476:LYS:HB2	1:D:485:ARG:HA	1.97	0.46
1:B:145:ILE:CD1	1:B:185:ILE:HD11	2.46	0.46
1:A:210:GLN:HE22	1:A:476:LYS:HZ3	1.64	0.46
1:B:64:ARG:HH11	1:B:64:ARG:HG2	1.81	0.46
1:A:442:GLU:O	1:A:446:ARG:HG3	2.15	0.46
1:D:354:ALA:HB2	1:D:417:LEU:HD13	1.98	0.45
1:C:344:GLU:HG3	5:C:551:HOH:O	2.16	0.45
1:B:53:GLN:HG3	1:B:56:ASN:HD22	1.81	0.45
1:B:208:ILE:HD11	1:B:240:LEU:CB	2.39	0.45
1:A:301:GLY:HA2	4:A:501:D4G:C5	2.46	0.45
1:D:186:VAL:HG11	1:D:295:THR:HG23	1.98	0.45
1:C:358:GLU:CD	1:C:415:HIS:HD1	2.19	0.45
1:D:271:PHE:CB	1:D:291:LEU:HD13	2.46	0.45
1:D:260:ASP:O	1:D:262:ASN:N	2.50	0.45
1:C:462:LEU:HD22	1:C:489:MET:HE1	1.97	0.45
1:D:145:ILE:HD13	1:D:185:ILE:HD11	1.99	0.45
1:C:186:VAL:HG11	1:C:295:THR:HG23	1.97	0.45
1:D:92:VAL:HG23	1:D:434:ILE:HD12	1.99	0.45
1:A:449:LEU:O	1:A:453:PHE:HB2	2.16	0.45
1:A:380:PHE:O	1:A:383:PHE:HB2	2.17	0.45
1:D:457:MET:CE	1:D:462:LEU:HD21	2.45	0.45
1:B:32:LYS:HE2	1:B:384:PHE:HB2	1.99	0.45
1:B:77:ARG:CG	1:B:77:ARG:NH1	2.77	0.44
1:A:476:LYS:HE2	1:A:477:HIS:NE2	2.32	0.44
1:D:352:MET:CE	1:D:454:THR:HG22	2.46	0.44
1:B:405:PHE:O	1:B:408:PRO:HD3	2.17	0.44
1:A:456:VAL:HG12	1:A:457:MET:CE	2.47	0.44
1:A:249:ALA:O	1:A:253:GLU:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LYS:HZ1	1:C:129:ARG:HH12	1.65	0.44
1:B:328:HIS:HB3	1:B:494:ARG:NH2	2.33	0.44
1:B:324:GLU:OE2	1:B:462:LEU:HG	2.18	0.44
1:C:176:ARG:NH1	1:C:193:TYR:HB3	2.33	0.44
1:D:450:PHE:O	1:D:454:THR:HG23	2.18	0.44
1:D:335:ILE:HG12	1:D:339:ARG:HH22	1.82	0.44
1:B:101:ARG:HD3	1:B:117:VAL:O	2.18	0.44
1:B:208:ILE:HD12	1:B:241:LEU:HG	2.00	0.44
1:C:302:GLY:HA2	3:C:500:HEM:HMC2	2.00	0.44
1:B:352:MET:HG2	1:B:454:THR:HG22	2.00	0.44
1:A:30:LYS:C	1:A:32:LYS:H	2.21	0.44
1:B:40:LEU:HD11	1:D:47:LEU:HD21	1.99	0.44
1:C:143:ARG:CZ	1:C:147:GLU:HG2	2.48	0.44
1:B:168:ILE:O	1:B:488:THR:HA	2.18	0.43
1:A:110:VAL:HG11	1:A:241:LEU:HD22	2.00	0.43
1:C:168:ILE:O	1:C:168:ILE:HD12	2.18	0.43
1:B:146:GLU:O	1:B:150:GLN:HG3	2.18	0.43
1:B:145:ILE:HA	1:B:145:ILE:HD12	1.93	0.43
1:D:146:GLU:O	1:D:150:GLN:HG3	2.19	0.43
1:A:117:VAL:HG21	4:A:501:D4G:H8	1.99	0.43
1:D:271:PHE:CD2	1:D:291:LEU:HD13	2.54	0.43
1:D:152:GLU:HG3	1:D:177:THR:HG23	2.01	0.43
1:B:258:THR:HG23	1:B:265:ARG:NH1	2.34	0.43
1:B:433:SER:CB	3:B:500:HEM:HBA1	2.48	0.43
1:A:271:PHE:CB	1:A:291:LEU:HD13	2.47	0.43
1:D:337:LYS:HB3	1:D:337:LYS:HZ3	1.82	0.43
1:D:143:ARG:HG3	1:D:143:ARG:NH1	2.34	0.43
1:A:369:SER:HB2	1:A:395:LEU:HG	2.01	0.43
1:B:343:PHE:CE1	1:B:346:ARG:HD3	2.54	0.43
1:D:236:GLN:O	1:D:240:LEU:HG	2.19	0.43
1:B:467:SER:HB3	1:B:470:ASP:OD2	2.18	0.43
1:B:206:LEU:HA	1:B:206:LEU:HD12	1.90	0.43
1:C:145:ILE:HD13	1:C:185:ILE:HD11	2.01	0.43
1:B:211:PHE:C	1:B:213:SER:H	2.22	0.42
1:A:271:PHE:CG	1:A:291:LEU:HD13	2.54	0.42
1:C:168:ILE:C	1:C:168:ILE:HD12	2.39	0.42
1:B:462:LEU:HD22	1:B:489:MET:CE	2.49	0.42
1:A:117:VAL:HG22	3:A:500:HEM:HAD1	2.01	0.42
1:A:30:LYS:CD	1:A:32:LYS:HB3	2.50	0.42
1:C:375:LYS:O	1:C:387:LYS:HG3	2.19	0.42
1:D:40:LEU:HA	1:D:40:LEU:HD12	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:GLU:HB2	5:C:710:HOH:O	2.20	0.42
1:B:376:LYS:HA	1:B:387:LYS:CG	2.50	0.42
1:D:326:LYS:HB3	1:D:351:TYR:CE2	2.55	0.42
1:C:418:ASN:OD1	1:C:419:GLU:N	2.53	0.42
1:B:379:LYS:HE3	1:B:382:ASP:HA	2.01	0.42
1:C:343:PHE:O	1:C:346:ARG:HG2	2.19	0.42
1:D:115:GLY:O	1:D:119:SER:HB3	2.20	0.42
1:B:327:VAL:HG13	1:B:352:MET:CE	2.49	0.42
1:D:111:PHE:CE1	4:D:501:D4G:H9	2.55	0.42
1:B:194:LYS:HD3	1:B:194:LYS:HA	1.86	0.42
1:C:433:SER:CB	3:C:500:HEM:HBA1	2.50	0.42
1:B:145:ILE:HD11	1:B:185:ILE:HD11	2.01	0.42
1:B:52:GLU:HG2	1:B:52:GLU:O	2.18	0.42
1:B:319:LYS:HG2	1:B:320:HIS:CE1	2.55	0.42
1:A:88:ARG:HD3	5:A:2694:HOH:O	2.20	0.42
1:C:209:PHE:CG	1:C:304:GLU:HG2	2.55	0.42
1:D:145:ILE:O	1:D:149:ILE:HG13	2.19	0.42
1:B:161:ARG:HG3	5:B:2543:HOH:O	2.19	0.42
1:B:129:ARG:HG3	1:B:129:ARG:HH11	1.84	0.42
1:D:473:VAL:HG22	5:D:584:HOH:O	2.20	0.42
1:C:418:ASN:N	1:C:422:GLN:O	2.45	0.41
1:A:314:PHE:CE2	1:A:457:MET:HE1	2.56	0.41
1:B:195:ASP:OD1	1:B:197:GLU:N	2.45	0.41
1:A:153:ALA:O	1:A:157:ILE:HG12	2.20	0.41
1:B:202:LEU:HD22	1:B:206:LEU:HD22	2.01	0.41
1:A:376:LYS:O	1:A:377:ASP:C	2.58	0.41
1:D:368:MET:HB3	1:D:394:MET:CE	2.50	0.41
1:D:331:ILE:HG12	1:D:349:MET:CE	2.50	0.41
1:B:301:GLY:HA2	4:B:501:D4G:C5	2.50	0.41
1:C:375:LYS:HE2	5:C:561:HOH:O	2.20	0.41
1:B:205:MET:O	1:B:209:PHE:HD1	2.02	0.41
1:D:141:GLY:H	1:D:145:ILE:HG21	1.86	0.41
1:C:417:LEU:HA	1:C:417:LEU:HD12	1.91	0.41
1:D:264:PRO:HG3	1:D:273:ILE:HD12	2.03	0.41
1:B:260:ASP:HA	1:B:261:PRO:HD2	1.88	0.41
1:C:167:ASN:HD21	1:C:465:SER:HB3	1.85	0.41
1:D:33:LEU:HD11	1:D:77:ARG:CZ	2.50	0.41
1:B:77:ARG:NH1	5:B:2537:HOH:O	2.53	0.41
1:B:318:MET:HE3	1:B:462:LEU:HB3	2.02	0.41
1:A:314:PHE:HE2	1:A:457:MET:CE	2.34	0.41
1:B:145:ILE:O	1:B:149:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ALA:O	1:C:157:ILE:HG12	2.21	0.41
1:A:374:VAL:O	1:A:374:VAL:HG23	2.21	0.41
1:A:358:GLU:OE1	1:A:358:GLU:HA	2.21	0.41
1:A:339:ARG:NH1	1:A:342:LYS:HZ2	2.19	0.41
1:B:101:ARG:CD	1:B:117:VAL:O	2.69	0.41
1:A:126:GLN:HG3	1:A:286:PHE:CE2	2.57	0.41
1:C:33:LEU:HD11	1:C:77:ARG:CZ	2.51	0.41
1:B:315:LEU:HD13	1:B:487:TYR:CD2	2.56	0.41
1:B:419:GLU:HG3	1:B:419:GLU:H	1.61	0.41
1:D:257:ARG:HD3	1:D:257:ARG:N	2.36	0.40
1:B:274:ARG:NH1	1:B:286:PHE:CE2	2.89	0.40
1:A:463:LYS:HB3	1:A:490:SER:HB2	2.02	0.40
3:D:500:HEM:NA	4:D:501:D4G:H2	2.35	0.40
1:B:259:LEU:HD12	1:B:260:ASP:H	1.86	0.40
1:D:117:VAL:HG22	3:D:500:HEM:HAD1	2.03	0.40
1:D:302:GLY:HA2	3:D:500:HEM:HMC2	2.03	0.40
1:B:264:PRO:HG3	1:B:273:ILE:HD12	2.04	0.40
1:A:374:VAL:HG22	1:A:389:THR:N	2.36	0.40
1:B:186:VAL:HA	1:B:267:PHE:HB3	2.03	0.40
1:B:257:ARG:HG2	1:B:257:ARG:O	2.22	0.40
1:B:369:SER:HB2	1:B:395:LEU:HG	2.02	0.40
1:D:139:GLY:O	1:D:140:VAL:C	2.60	0.40
1:A:433:SER:CB	3:A:500:HEM:HBA1	2.51	0.40
1:C:317:LEU:HD13	1:C:457:MET:CE	2.51	0.40
1:A:416:PHE:O	1:A:417:LEU:HD13	2.22	0.40
1:B:177:THR:HG23	5:B:2520:HOH:O	2.21	0.40
1:B:391:VAL:O	1:B:393:PRO:HD3	2.22	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	463/476 (97%)	444 (96%)	18 (4%)	1 (0%)	52	43
1	B	462/476 (97%)	438 (95%)	23 (5%)	1 (0%)	52	43
1	C	462/476 (97%)	450 (97%)	12 (3%)	0	100	100
1	D	462/476 (97%)	439 (95%)	21 (4%)	2 (0%)	39	27
All	All	1849/1904 (97%)	1771 (96%)	74 (4%)	4 (0%)	52	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	140	VAL
1	B	192	ASP
1	A	195	ASP
1	D	261	PRO

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	412/422 (98%)	404 (98%)	8 (2%)	65	58
1	B	412/422 (98%)	399 (97%)	13 (3%)	46	33
1	C	411/422 (97%)	400 (97%)	11 (3%)	52	41
1	D	411/422 (97%)	404 (98%)	7 (2%)	68	63
All	All	1646/1688 (98%)	1607 (98%)	39 (2%)	57	47

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU
1	A	236	GLN
1	A	312	TYR
1	A	316	LEU
1	A	370	LEU
1	A	382	ASP
1	A	417	LEU

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Mol	Chain	Res	Type
1	A	453	PHE
1	B	53	GLN
1	B	61	ILE
1	B	77	ARG
1	B	135	LEU
1	B	174	LEU
1	B	195	ASP
1	B	202	LEU
1	B	234	GLN
1	B	312	TYR
1	B	417	LEU
1	B	419	GLU
1	B	453	PHE
1	B	486	ASN
1	C	40	LEU
1	C	61	ILE
1	C	96	GLU
1	C	135	LEU
1	C	143	ARG
1	C	146	GLU
1	C	148	ARG
1	C	236	GLN
1	C	312	TYR
1	C	414	GLN
1	C	417	LEU
1	D	40	LEU
1	D	174	LEU
1	D	210	GLN
1	D	234	GLN
1	D	312	TYR
1	D	337	LYS
1	D	417	LEU

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	48	GLN
1	A	126	GLN
1	A	210	GLN
1	B	56	ASN
1	B	320	HIS
1	B	409	GLN

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Mol	Chain	Res	Type
1	B	412	ASN
1	B	414	GLN
1	B	466	GLN
1	C	409	GLN
1	C	414	GLN
1	D	256	GLN
1	D	276	GLN
1	D	340	GLN
1	D	409	GLN
1	D	418	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

11 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	SO4	A	2502	-	4,4,4	0.28	0	6,6,6	0.08	0
2	SO4	A	2503	-	4,4,4	0.23	0	6,6,6	0.06	0
3	HEM	A	500	1,4	30,50,50	3.80	11 (36%)	24,82,82	2.62	9 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	D4G	A	501	3	15,15,15	1.92	6 (40%)	18,18,18	1.95	7 (38%)
2	SO4	B	2504	-	4,4,4	0.26	0	6,6,6	0.11	0
3	HEM	B	500	1,4	30,50,50	3.75	13 (43%)	24,82,82	2.71	10 (41%)
4	D4G	B	501	3	15,15,15	1.91	5 (33%)	18,18,18	1.98	8 (44%)
3	HEM	C	500	1,4	30,50,50	3.74	13 (43%)	24,82,82	2.71	9 (37%)
4	D4G	C	501	3	15,15,15	1.89	7 (46%)	18,18,18	1.99	7 (38%)
3	HEM	D	500	1,4	30,50,50	3.65	13 (43%)	24,82,82	2.76	10 (41%)
4	D4G	D	501	3	15,15,15	1.91	6 (40%)	18,18,18	1.92	7 (38%)

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	SO4	A	2502	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2503	-	-	0/0/0/0	0/0/0/0
3	HEM	A	500	1,4	-	0/10/54/54	0/0/8/8
4	D4G	A	501	3	-	0/5/5/5	0/2/2/2
2	SO4	B	2504	-	-	0/0/0/0	0/0/0/0
3	HEM	B	500	1,4	-	0/10/54/54	0/0/8/8
4	D4G	B	501	3	-	0/5/5/5	0/2/2/2
3	HEM	C	500	1,4	-	0/10/54/54	0/0/8/8
4	D4G	C	501	3	-	0/5/5/5	0/2/2/2
3	HEM	D	500	1,4	-	0/10/54/54	0/0/8/8
4	D4G	D	501	3	-	0/5/5/5	0/2/2/2

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	C3B-C4B	-11.12	1.41	1.51
3	C	500	HEM	C3B-C4B	-10.68	1.42	1.51
3	B	500	HEM	C3B-C4B	-10.53	1.42	1.51
3	D	500	HEM	C3B-C4B	-9.53	1.43	1.51
3	B	500	HEM	C3D-C4D	-8.65	1.40	1.51
3	A	500	HEM	C3D-C4D	-8.35	1.40	1.51
3	C	500	HEM	C3D-C4D	-8.25	1.41	1.51
3	D	500	HEM	C3D-C4D	-8.21	1.41	1.51
3	B	500	HEM	C2C-C1C	-7.67	1.38	1.52
3	A	500	HEM	C2C-C1C	-7.56	1.38	1.52
3	A	500	HEM	C3C-CAC	-7.49	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	500	HEM	C2C-C1C	-7.44	1.38	1.52
3	D	500	HEM	C2C-C1C	-7.39	1.38	1.52
3	D	500	HEM	C3C-CAC	-7.16	1.37	1.51
3	C	500	HEM	C3C-CAC	-7.13	1.37	1.51
3	B	500	HEM	C3C-CAC	-6.90	1.38	1.51
3	A	500	HEM	C2D-C3D	-6.16	1.36	1.54
3	D	500	HEM	C2D-C3D	-5.99	1.36	1.54
3	C	500	HEM	C2D-C3D	-5.77	1.37	1.54
3	B	500	HEM	C2D-C3D	-5.70	1.37	1.54
3	C	500	HEM	C3B-CAB	-4.37	1.43	1.51
3	B	500	HEM	C3B-CAB	-4.08	1.43	1.51
3	A	500	HEM	C3B-CAB	-4.00	1.43	1.51
3	D	500	HEM	C3B-CAB	-3.96	1.43	1.51
3	D	500	HEM	C2D-C1D	-3.60	1.40	1.51
3	C	500	HEM	C2D-C1D	-3.55	1.40	1.51
3	B	500	HEM	C2D-C1D	-3.54	1.40	1.51
3	A	500	HEM	C2D-C1D	-3.52	1.40	1.51
4	B	501	D4G	C4-S_1	-3.20	1.73	1.78
3	C	500	HEM	C2B-C1B	-3.15	1.41	1.51
4	A	501	D4G	C4-S_1	-2.93	1.73	1.78
3	D	500	HEM	C1C-NC	-2.85	1.32	1.36
3	D	500	HEM	C2B-C1B	-2.84	1.42	1.51
3	B	500	HEM	C2B-C1B	-2.84	1.42	1.51
3	A	500	HEM	C2B-C1B	-2.75	1.42	1.51
3	B	500	HEM	C1C-NC	-2.65	1.32	1.36
4	C	501	D4G	C4-S_1	-2.28	1.74	1.78
3	C	500	HEM	C1C-NC	-2.27	1.33	1.36
4	D	501	D4G	C4-S_1	-2.16	1.74	1.78
4	C	501	D4G	C3-C4	2.00	1.43	1.39
4	A	501	D4G	C7-C8	2.05	1.42	1.38
4	C	501	D4G	C7-C8	2.11	1.42	1.38
3	A	500	HEM	CBC-CAC	2.13	1.41	1.29
3	B	500	HEM	CBC-CAC	2.15	1.41	1.29
4	B	501	D4G	C3-C4	2.15	1.43	1.39
4	D	501	D4G	C3-C4	2.17	1.43	1.39
4	D	501	D4G	C5-C4	2.20	1.43	1.39
3	D	500	HEM	CBC-CAC	2.22	1.42	1.29
3	B	500	HEM	FE-NC	2.22	2.04	1.95
4	B	501	D4G	C7-C8	2.23	1.43	1.38
3	C	500	HEM	CBC-CAC	2.24	1.42	1.29
4	A	501	D4G	C10-C6	2.29	1.43	1.39
4	C	501	D4G	C5-C4	2.31	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	D4G	C5-C1	2.32	1.43	1.38
4	D	501	D4G	C10-C6	2.34	1.44	1.39
4	A	501	D4G	C5-C4	2.37	1.44	1.39
3	D	500	HEM	FE-NC	2.39	2.05	1.95
4	B	501	D4G	C10-C6	2.40	1.44	1.39
4	C	501	D4G	C10-C6	2.43	1.44	1.39
3	C	500	HEM	FE-NC	2.57	2.05	1.95
4	A	501	D4G	C5-C1	2.60	1.43	1.38
4	A	501	D4G	C7-C6	2.65	1.44	1.39
4	D	501	D4G	C7-C6	2.75	1.44	1.39
4	D	501	D4G	C5-C1	2.79	1.44	1.38
4	C	501	D4G	C7-C6	2.80	1.44	1.39
4	B	501	D4G	C7-C6	2.83	1.45	1.39
3	C	500	HEM	CMA-C3A	3.02	1.57	1.51
3	A	500	HEM	CMA-C3A	3.02	1.57	1.51
3	B	500	HEM	CMA-C3A	3.13	1.58	1.51
3	C	500	HEM	CBB-CAB	3.26	1.48	1.29
3	A	500	HEM	CBB-CAB	3.27	1.48	1.29
3	B	500	HEM	CBB-CAB	3.40	1.48	1.29
3	D	500	HEM	CBB-CAB	3.47	1.49	1.29
3	D	500	HEM	CMA-C3A	3.53	1.58	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	D4G	C5-C1-N_1	-3.08	118.28	123.64
4	C	501	D4G	C5-C1-N_1	-2.93	118.54	123.64
4	D	501	D4G	C5-C1-N_1	-2.79	118.77	123.64
4	A	501	D4G	C10-C9-N_2	-2.79	118.78	123.64
4	C	501	D4G	C10-C9-N_2	-2.77	118.81	123.64
4	D	501	D4G	C7-C8-N_2	-2.77	118.82	123.64
4	B	501	D4G	C5-C1-N_1	-2.75	118.84	123.64
4	B	501	D4G	C10-C9-N_2	-2.72	118.91	123.64
4	D	501	D4G	C10-C9-N_2	-2.71	118.92	123.64
4	A	501	D4G	C7-C8-N_2	-2.70	118.94	123.64
4	C	501	D4G	C7-C8-N_2	-2.69	118.95	123.64
4	B	501	D4G	C3-C2-N_1	-2.66	119.00	123.64
4	B	501	D4G	C7-C8-N_2	-2.63	119.05	123.64
4	C	501	D4G	C3-C2-N_1	-2.45	119.38	123.64
4	D	501	D4G	C3-C2-N_1	-2.41	119.44	123.64
4	A	501	D4G	C3-C2-N_1	-2.26	119.71	123.64
4	B	501	D4G	C5-C4-C3	2.04	122.53	118.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	500	HEM	CAA-CBA-CGA	2.17	116.73	112.75
3	D	500	HEM	CAA-CBA-CGA	2.23	116.83	112.75
4	D	501	D4G	C6-S_2-S_1	2.25	109.06	104.92
4	A	501	D4G	C6-S_2-S_1	2.42	109.38	104.92
3	B	500	HEM	C1D-CHD-C4C	2.48	129.96	125.82
3	A	500	HEM	CMD-C2D-C3D	2.48	125.31	114.35
3	A	500	HEM	C1D-CHD-C4C	2.54	130.07	125.82
3	D	500	HEM	CMD-C2D-C3D	2.56	125.67	114.35
3	C	500	HEM	CMD-C2D-C3D	2.58	125.75	114.35
3	B	500	HEM	CMD-C2D-C3D	2.61	125.87	114.35
3	C	500	HEM	C1D-CHD-C4C	2.67	130.28	125.82
3	D	500	HEM	C1D-CHD-C4C	2.98	130.80	125.82
4	B	501	D4G	C6-S_2-S_1	3.04	110.53	104.92
3	B	500	HEM	C3C-CAC-CBC	3.15	129.28	124.46
3	C	500	HEM	C4B-CHC-C1C	3.24	131.24	125.82
4	C	501	D4G	C6-S_2-S_1	3.25	110.91	104.92
3	B	500	HEM	C4B-CHC-C1C	3.35	131.42	125.82
4	D	501	D4G	C1-N_1-C2	3.35	124.93	116.83
3	A	500	HEM	C3C-CAC-CBC	3.36	129.61	124.46
3	A	500	HEM	C4B-CHC-C1C	3.38	131.47	125.82
3	D	500	HEM	C3C-CAC-CBC	3.38	129.65	124.46
4	B	501	D4G	C9-N_2-C8	3.39	125.03	116.83
4	A	501	D4G	C1-N_1-C2	3.43	125.12	116.83
4	C	501	D4G	C1-N_1-C2	3.43	125.13	116.83
4	C	501	D4G	C9-N_2-C8	3.48	125.24	116.83
4	A	501	D4G	C9-N_2-C8	3.48	125.25	116.83
4	B	501	D4G	C1-N_1-C2	3.50	125.29	116.83
4	D	501	D4G	C9-N_2-C8	3.56	125.43	116.83
3	D	500	HEM	C4B-CHC-C1C	3.56	131.77	125.82
3	C	500	HEM	C3C-CAC-CBC	3.67	130.08	124.46
3	C	500	HEM	CAD-C3D-C4D	4.02	126.65	112.47
3	B	500	HEM	CAD-C3D-C4D	4.15	127.12	112.47
3	D	500	HEM	CAD-C3D-C4D	4.26	127.49	112.47
3	D	500	HEM	CMC-C2C-C3C	4.39	127.48	116.53
3	A	500	HEM	CAD-C3D-C4D	4.39	127.94	112.47
3	A	500	HEM	CMC-C2C-C3C	4.41	127.53	116.53
3	B	500	HEM	CMC-C2C-C3C	4.45	127.64	116.53
3	C	500	HEM	C3B-CAB-CBB	4.46	131.30	124.46
3	A	500	HEM	C3B-CAB-CBB	4.53	131.41	124.46
3	C	500	HEM	CMC-C2C-C3C	4.54	127.86	116.53
3	D	500	HEM	C3B-CAB-CBB	4.67	131.62	124.46
3	B	500	HEM	C3B-CAB-CBB	4.75	131.75	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	HEM	CAD-C3D-C2D	5.05	127.72	113.22
3	D	500	HEM	CAD-C3D-C2D	5.20	128.16	113.22
3	B	500	HEM	CAD-C3D-C2D	5.29	128.44	113.22
3	A	500	HEM	CMB-C2B-C3B	5.35	129.89	116.53
3	C	500	HEM	CAD-C3D-C2D	5.47	128.96	113.22
3	C	500	HEM	CMB-C2B-C3B	5.63	130.58	116.53
3	D	500	HEM	CMB-C2B-C3B	5.67	130.69	116.53
3	B	500	HEM	CMB-C2B-C3B	5.71	130.78	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	HEM	3	0
4	A	501	D4G	4	0
3	B	500	HEM	2	0
4	B	501	D4G	1	0
3	C	500	HEM	4	0
4	C	501	D4G	1	0
3	D	500	HEM	4	0
4	D	501	D4G	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	465/476 (97%)	1.10	46 (9%) 9 15	14, 26, 44, 64	0
1	B	464/476 (97%)	1.30	82 (17%) 2 3	16, 33, 51, 71	0
1	C	464/476 (97%)	1.07	50 (10%) 8 12	13, 25, 42, 51	0
1	D	464/476 (97%)	1.20	80 (17%) 2 3	14, 27, 54, 68	0
All	All	1857/1904 (97%)	1.17	258 (13%) 4 6	13, 28, 48, 71	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	495	HIS	8.7
1	B	193	TYR	6.1
1	A	61	ILE	6.0
1	D	261	PRO	5.8
1	D	264	PRO	5.4
1	D	143	ARG	5.2
1	B	323	VAL	4.7
1	A	30	LYS	4.6
1	C	417	LEU	4.3
1	B	189	ASP	4.3
1	D	138	PHE	4.2
1	B	384	PHE	4.2
1	D	355	VAL	4.2
1	D	276	GLN	4.1
1	D	144	GLY	4.1
1	B	325	ALA	4.0
1	A	249	ALA	3.9
1	A	268	ILE	3.9
1	D	334	VAL	3.9
1	A	32	LYS	3.9
1	D	273	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	417	LEU	3.8
1	C	391	VAL	3.7
1	D	78	VAL	3.7
1	D	140	VAL	3.7
1	C	31	GLY	3.7
1	B	405	PHE	3.6
1	D	141	GLY	3.6
1	C	451	LEU	3.6
1	B	379	LYS	3.6
1	D	379	LYS	3.6
1	C	384	PHE	3.5
1	A	384	PHE	3.5
1	B	33	LEU	3.5
1	B	143	ARG	3.4
1	C	327	VAL	3.4
1	D	31	GLY	3.3
1	B	482	THR	3.3
1	A	33	LEU	3.3
1	D	280	LYS	3.3
1	C	149	ILE	3.3
1	D	456	VAL	3.2
1	C	420	LYS	3.2
1	B	259	LEU	3.2
1	B	411	PHE	3.2
1	A	379	LYS	3.2
1	D	277	GLU	3.2
1	A	287	TYR	3.1
1	B	194	LYS	3.1
1	D	331	ILE	3.1
1	B	469	LYS	3.1
1	D	336	GLY	3.1
1	B	380	PHE	3.1
1	D	139	GLY	3.1
1	D	335	ILE	3.1
1	A	155	PHE	3.1
1	D	274	ARG	3.0
1	A	230	LEU	3.0
1	D	302	GLY	3.0
1	B	480	PHE	3.0
1	C	365	VAL	3.0
1	D	492	LEU	3.0
1	B	494	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	359	ILE	2.9
1	D	194	LYS	2.9
1	B	336	GLY	2.9
1	B	483	ILE	2.9
1	C	418	ASN	2.9
1	A	483	ILE	2.9
1	D	279	GLU	2.9
1	D	135	LEU	2.8
1	D	259	LEU	2.8
1	B	70	THR	2.8
1	A	383	PHE	2.8
1	B	257	ARG	2.8
1	B	64	ARG	2.8
1	D	136	ARG	2.8
1	A	465	SER	2.8
1	C	370	LEU	2.7
1	D	278	GLU	2.7
1	D	445	ALA	2.7
1	A	238	PHE	2.7
1	D	460	PHE	2.7
1	A	291	LEU	2.7
1	D	430	VAL	2.7
1	D	284	THR	2.7
1	B	343	PHE	2.7
1	B	465	SER	2.6
1	A	306	VAL	2.6
1	A	258	THR	2.6
1	B	464	SER	2.6
1	D	288	LEU	2.6
1	B	292	VAL	2.6
1	B	374	VAL	2.6
1	B	61	ILE	2.6
1	C	138	PHE	2.6
1	D	370	LEU	2.6
1	B	473	VAL	2.6
1	D	339	ARG	2.6
1	C	273	ILE	2.6
1	B	467	SER	2.6
1	C	409	GLN	2.6
1	B	196	LYS	2.5
1	D	115	GLY	2.5
1	B	53	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	491	PHE	2.5
1	D	198	PHE	2.5
1	B	493	PRO	2.5
1	B	312	TYR	2.5
1	D	450	PHE	2.5
1	B	479	GLY	2.5
1	A	282	PRO	2.5
1	C	105	ALA	2.5
1	C	445	ALA	2.5
1	A	219	LEU	2.5
1	B	383	PHE	2.5
1	D	452	PHE	2.5
1	D	129	ARG	2.5
1	D	420	LYS	2.5
1	A	382	ASP	2.5
1	C	472	ASP	2.5
1	B	478	VAL	2.4
1	B	471	ILE	2.4
1	A	272	LEU	2.4
1	D	444	LEU	2.4
1	B	419	GLU	2.4
1	B	125	LYS	2.4
1	C	287	TYR	2.4
1	B	256	GLN	2.4
1	B	276	GLN	2.4
1	B	382	ASP	2.4
1	B	461	ARG	2.4
1	B	209	PHE	2.4
1	C	178	VAL	2.4
1	C	306	VAL	2.4
1	D	92	VAL	2.4
1	C	262	ASN	2.4
1	D	325	ALA	2.4
1	D	185	ILE	2.4
1	C	369	SER	2.4
1	D	252	VAL	2.4
1	C	481	ALA	2.4
1	A	70	THR	2.4
1	C	300	ILE	2.4
1	D	145	ILE	2.4
1	D	257	ARG	2.4
1	B	287	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	246	ASP	2.4
1	C	431	PRO	2.4
1	D	327	VAL	2.4
1	D	423	PHE	2.4
1	B	208	ILE	2.3
1	C	298	LEU	2.3
1	D	81	LEU	2.3
1	C	350	PRO	2.3
1	D	468	PRO	2.3
1	C	334	VAL	2.3
1	C	398	VAL	2.3
1	B	314	PHE	2.3
1	B	484	PRO	2.3
1	D	350	PRO	2.3
1	D	178	VAL	2.3
1	A	463	LYS	2.3
1	D	142	LYS	2.3
1	A	31	GLY	2.3
1	A	336	GLY	2.3
1	D	271	PHE	2.3
1	D	286	PHE	2.3
1	A	335	ILE	2.3
1	A	330	GLU	2.3
1	A	467	SER	2.3
1	D	308	THR	2.3
1	A	462	LEU	2.2
1	D	417	LEU	2.2
1	D	332	ASP	2.2
1	D	35	PRO	2.2
1	C	194	LYS	2.2
1	B	421	GLY	2.2
1	A	69	PHE	2.2
1	B	491	PHE	2.2
1	D	196	LYS	2.2
1	B	212	THR	2.2
1	B	69	PHE	2.2
1	C	107	PHE	2.2
1	A	366	ILE	2.2
1	B	300	ILE	2.2
1	B	170	PRO	2.2
1	C	259	LEU	2.2
1	C	395	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	366	ILE	2.2
1	C	462	LEU	2.2
1	A	378	THR	2.2
1	D	109	TRP	2.2
1	D	371	ALA	2.2
1	A	376	LYS	2.2
1	D	424	LYS	2.2
1	B	407	ASN	2.2
1	A	434	ILE	2.2
1	B	315	LEU	2.2
1	B	492	LEU	2.2
1	D	391	VAL	2.2
1	C	261	PRO	2.1
1	B	98	PHE	2.1
1	C	69	PHE	2.1
1	A	373	ARG	2.1
1	B	335	ILE	2.1
1	C	61	ILE	2.1
1	A	60	LYS	2.1
1	B	213	SER	2.1
1	C	219	LEU	2.1
1	C	272	LEU	2.1
1	D	283	ASN	2.1
1	B	337	LYS	2.1
1	B	476	LYS	2.1
1	B	107	PHE	2.1
1	C	209	PHE	2.1
1	D	268	ILE	2.1
1	C	241	LEU	2.1
1	B	423	PHE	2.1
1	D	187	PHE	2.1
1	D	384	PHE	2.1
1	C	366	ILE	2.1
1	B	439	CYS	2.1
1	D	254	HIS	2.1
1	A	91	LEU	2.1
1	D	199	LEU	2.1
1	A	365	VAL	2.1
1	C	333	ARG	2.1
1	C	454	THR	2.1
1	A	261	PRO	2.1
1	B	413	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	185	ILE	2.1
1	B	73	LEU	2.1
1	C	444	LEU	2.1
1	D	418	ASN	2.1
1	B	215	SER	2.1
1	B	355	VAL	2.1
1	A	93	ASP	2.1
1	B	60	LYS	2.0
1	B	356	ILE	2.0
1	A	55	TYR	2.0
1	D	462	LEU	2.0
1	A	430	VAL	2.0
1	A	473	VAL	2.0
1	B	226	VAL	2.0
1	B	456	VAL	2.0
1	C	134	THR	2.0
1	D	275	MET	2.0
1	B	168	ILE	2.0
1	B	366	ILE	2.0
1	D	453	PHE	2.0
1	D	310	LEU	2.0
1	B	378	THR	2.0
1	A	257	ARG	2.0
1	B	341	PRO	2.0
1	C	342	LYS	2.0
1	C	436	LYS	2.0
1	B	182	ILE	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	D4G	A	501	14/14	0.75	0.25	3.71	28,42,52,52	0
4	D4G	D	501	14/14	0.75	0.29	3.50	35,43,48,50	0
3	HEM	D	500	43/43	0.94	0.21	1.00	18,21,23,25	0
3	HEM	C	500	43/43	0.94	0.21	0.71	15,19,22,26	0
4	D4G	C	501	14/14	0.81	0.20	0.68	28,42,46,49	0
4	D4G	B	501	14/14	0.81	0.19	0.50	26,40,46,48	0
3	HEM	A	500	43/43	0.95	0.17	0.17	12,17,20,22	0
3	HEM	B	500	43/43	0.94	0.16	-0.05	16,20,24,28	0
2	SO4	A	2503	5/5	0.96	0.13	-3.06	31,33,33,34	0
2	SO4	B	2504	5/5	0.87	0.13	-	63,64,64,64	0
2	SO4	A	2502	5/5	0.78	0.21	-	66,66,66,67	0

6.5 Other polymers (i)

There are no such residues in this entry.