

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	5MNV
Title	:	Structural and functional characterization of OleP in complex with 6DEB in
		PEG
Authors	:	Parisi, G.; Savino, C.; Montemiglio, L.C.
Deposited on	:	2016-12-13
Resolution	:	2.97 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.97 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R _{free}	130704	2754 (3.00-2.96)		
Clashscore	141614	3103 (3.00-2.96)		
Ramachandran outliers	138981	2993 (3.00-2.96)		
Sidechain outliers	138945	2996 (3.00-2.96)		
RSRZ outliers	127900	2644 (3.00-2.96)		

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	А	407	.% 7 0%	25%	•••		
1	В	407	71%	23%	•••		
1	С	407	69%	27%	•••		
1	D	407	% 74%	20%	•••		
1	Е	407	^{2%} 72%	21%	•••		



Mol	Chain	Length	Quality of chain		
1	F	407	78%	18%	•••
1	G	407	7%	17%	7%
1	Н	407	.% • 75%	20%	••
1	Ι	407	17% 49% 19% •	30%	



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2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27464 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace	
1	Δ	307	Total	С	Ν	0	\mathbf{S}	0	0	0	
1	Л	591	3091	1944	554	580	13	0	0	0	
1	В	304	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0	
1	D	394	3072	1934	551	574	13	0	0	0	
1	С	306	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0	
1	U	550	3086	1941	553	579	13	0	0	U	
1	П	30/	Total	\mathbf{C}	N O S	0	Ο	0			
1	D	094	3073	1934	551	575	13	0	0	0	
1	F	E	300	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
T	Ľ	550	3034	1913	546	562	13	0	0	0	
1	F	305	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0	
1	Ľ		3078	1937	552	576	13	0	0	0	
1	G	380	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0	
1	u	300	2961	1868	530	550	13	0	0	0	
1	н	305	Total	\mathbf{C}	Ν	0	\mathbf{S}	0	0	0	
	11	000	3078	1937	552	576	13	0	0	0	
1	T	286	Total	C	Ν	0	S	0	0	0	
	L	280	2250	1414	404	420	12	0	0		

• Molecule 1 is a protein called Cytochrome P-450.

• 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	
9	Λ	1	Total	С	Fe	Ν	Ο	0	0
	Л	1	43	34	1	4	4	0	0
9	В	1	Total	С	Fe	Ν	Ο	0	0
2	D	T	43	34	1	4	4	0	0
2	С	1	Total	С	Fe	Ν	Ο	0	0
2	U	1	43	34	1	4	4	0	0
2	Л	1	Total	С	Fe	Ν	Ο	0	0
2	D	T	43	34	1	4	4	0	0
2	E	1	Total	С	Fe	Ν	Ο	0	0
2	Ľ	T	43	34	1	4	4	0	0
2	F	1	Total	С	Fe	Ν	Ο	0	0
2	Ľ	1	43	34	1	4	4	0	0
2	G	1	Total	С	Fe	Ν	Ο	0	0
2	ŭ	1	43	34	1	4	4	0	0
2	н	1	Total	С	Fe	Ν	Ο	0	0
	11	1	43	34	1	4	4	0	U
2	T	1	Total	С	Fe	Ν	Ο	0	0
	L	1	43	34	1	4	4		0

• Molecule 3 is 6-DEOXYERYTHRONOLIDE B (three-letter code: DEB) (formula: $C_{21}H_{38}O_6$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C O 27 21 6	0	0
3	В	1	Total C O 27 21 6	0	0
3	С	1	Total C O 27 21 6	0	0
3	D	1	Total C O 27 21 6	0	0
3	Е	1	Total C O 27 21 6	0	0
3	F	1	Total C O 27 21 6	0	0
3	G	1	Total C O 27 21 6	0	0
3	Н	1	Total C O 27 21 6	0	0
3	Ι	1	Total C O 27 21 6	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	26	TotalO2626	0	0
4	В	7	Total O 7 7	0	0
4	С	13	Total O 13 13	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	28	TotalO2828	0	0
4	Е	7	Total O 7 7	0	0
4	F	15	Total O 15 15	0	0
4	G	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	0	0
4	Н	10	Total O 10 10	0	0



Chain C:

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.



69%

• Molecule 1: Cytochrome P-450



27%





H340 H354 H157 H354 H157 H357 L179 L360 L179 L361 L160 L362 L179 L363 L179 L361 L179 L362 L186 L363 L186 L382 L186 A383 L184 A383 L184 A385 A186 A385 A186 A385 A186 A386 A186 A386 A186 A386 A186 A386 A186 A386 A186 A386 A186 A395 A186 A386 A186 A386 A386 A407 M237 A407 M237 A407 M236 A407 M237 A407 M237 A407 M236 A407 M247 <t









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	112.50Å 116.70Å 123.30Å	Deperitor
a, b, c, α , β , γ	103.90° 104.30° 114.70°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	39.97 - 2.97	Depositor
Resolution (A)	39.97 - 2.97	EDS
% Data completeness	97.1 (39.97-2.97)	Depositor
(in resolution range)	97.1 (39.97-2.97)	EDS
R_{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.06 (at 2.95 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
P. P.	0.238 , 0.311	Depositor
Λ, Λ_{free}	0.239 , 0.307	DCC
R_{free} test set	5097 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	54.4	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.27, 44.3	EDS
L-test for $twinning^2$	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.010 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	27464	wwPDB-VP
Average B, all atoms $(Å^2)$	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.86% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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).

Mal	Chain	Bond	lengths	Bond angles		
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.45	0/3158	0.69	2/4302~(0.0%)	
1	В	0.37	0/3139	0.62	0/4276	
1	С	0.47	0/3153	0.63	0/4295	
1	D	0.38	0/3140	0.62	0/4277	
1	Ε	0.37	0/3099	0.63	3/4217~(0.1%)	
1	F	0.36	0/3145	0.62	3/4284~(0.1%)	
1	G	0.38	0/3025	0.55	0/4117	
1	Н	0.38	0/3145	0.61	0/4284	
1	Ι	0.39	0/2281	0.55	0/3081	
All	All	0.40	0/27285	0.62	8/37133~(0.0%)	

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	F	187	ALA	N-CA-C	-7.33	91.20	111.00
1	Е	81	PRO	CB-CA-C	-7.26	93.84	112.00
1	F	186	ALA	CB-CA-C	-7.10	99.45	110.10
1	F	186	ALA	N-CA-C	6.92	129.68	111.00
1	Е	81	PRO	N-CA-C	6.27	128.41	112.10



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	163	VAL	C-N-CD	5.91	140.81	128.40
1	Е	82	ARG	N-CA-CB	-5.87	100.03	110.60
1	А	14	VAL	C-N-CD	5.57	140.10	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	293	ALA	Peptide
1	D	295	SER	Peptide

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	А	3091	0	3065	67	0
1	В	3072	0	3048	56	0
1	С	3086	0	3060	82	0
1	D	3073	0	3051	46	0
1	Ε	3034	0	3012	52	0
1	F	3078	0	3056	55	0
1	G	2961	0	2944	43	0
1	Н	3078	0	3057	58	0
1	Ι	2250	0	2257	117	0
2	А	43	0	30	5	0
2	В	43	0	30	3	0
2	С	43	0	30	3	0
2	D	43	0	30	3	0
2	Е	43	0	30	5	0
2	F	43	0	30	4	0
2	G	43	0	30	4	0
2	Н	43	0	30	10	0
2	Ι	43	0	30	8	0
3	А	27	0	38	1	0
3	В	27	0	38	0	0
3	С	27	0	38	0	0
3	D	27	0	38	6	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Е	27	0	38	2	0
3	F	27	0	38	1	0
3	G	27	0	38	1	0
3	Н	27	0	38	1	0
3	Ι	27	0	38	0	0
4	А	26	0	0	0	0
4	В	7	0	0	0	0
4	С	13	0	0	0	0
4	D	28	0	0	1	0
4	Е	7	0	0	0	0
4	F	15	0	0	1	0
4	G	5	0	0	0	0
4	Н	10	0	0	2	0
All	All	27464	0	27162	608	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 (608) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:I:263:GLU:HB3	1:I:266:ARG:CD	1.64	1.27
1:G:359:ALA:O	1:G:363:ARG:HG3	1.38	1.23
1:F:184:LEU:O	1:F:189:ILE:CG1	1.86	1.21
1:I:251:ASN:O	1:I:255:ASN:OD1	1.55	1.21
1:I:62:ARG:NH2	1:I:63:ILE:HG12	1.57	1.17
1:F:184:LEU:O	1:F:189:ILE:HG13	1.40	1.14
1:I:62:ARG:HH21	1:I:63:ILE:CG1	1.63	1.11
1:D:185:THR:HG22	1:D:188:GLU:HB2	1.33	1.09
1:A:175:SER:HB3	1:A:246:HIS:CE1	1.88	1.08
1:I:62:ARG:NH2	1:I:63:ILE:CG1	2.15	1.08
1:I:327:ASP:HB3	1:I:330:VAL:HB	1.31	1.08
1:C:92:GLY:HA2	1:C:236:ASN:ND2	1.69	1.08
1:D:175:SER:HB3	1:D:246:HIS:ND1	1.69	1.04
1:I:328:GLU:N	1:I:328:GLU:OE1	1.88	1.04
1:I:263:GLU:O	1:I:266:ARG:HG2	1.58	1.03
1:I:263:GLU:CB	1:I:266:ARG:HD3	1.89	1.03
1:I:62:ARG:HH21	1:I:63:ILE:HG12	0.88	1.00
1:I:327:ASP:HB3	1:I:330:VAL:CB	1.91	1.00
1:I:259:LEU:HB2	1:I:284:MET:HE3	1.46	0.97
1:I:283:GLU:O	1:I:286:ARG:HG3	1.65	0.96



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:I:266:ARG:O	1:I:270:LEU:HD13	1.68	0.94
1:F:187:ALA:HA	1:F:190:GLN:NE2	1.82	0.93
1:I:263:GLU:HB3	1:I:266:ARG:HD3	0.95	0.93
1:C:157:ILE:HD11	1:C:161:LEU:HD13	1.48	0.93
1:E:259:LEU:O	1:E:266:ARG:NH1	2.03	0.91
1:F:184:LEU:O	1:F:189:ILE:CD1	2.19	0.91
1:I:327:ASP:HB3	1:I:330:VAL:CG2	2.05	0.87
1:I:258:HIS:O	1:I:262:THR:HG22	1.76	0.86
1:I:259:LEU:HB2	1:I:284:MET:CE	2.04	0.86
1:I:266:ARG:O	1:I:269:SER:OG	1.93	0.85
1:G:42:ARG:NH1	1:G:53:TRP:CE2	2.45	0.84
1:H:331:PHE:HZ	1:H:345:PRO:O	1.60	0.84
1:B:168:ARG:HA	1:B:171:PHE:CE2	2.13	0.84
1:H:331:PHE:CZ	1:H:345:PRO:O	2.30	0.84
1:C:251:ASN:ND2	1:C:399:GLY:HA3	1.94	0.82
1:D:175:SER:HB3	1:D:246:HIS:CE1	2.16	0.81
1:A:256:LEU:HD22	1:A:284:MET:HB3	1.62	0.81
1:G:359:ALA:O	1:G:363:ARG:CG	2.28	0.80
1:B:157:ILE:HG21	1:B:245:GLY:HA3	1.62	0.80
1:B:165:LEU:O	1:B:167:ASP:N	2.15	0.80
1:H:28:ASP:OD1	1:H:29:PRO:HD2	1.81	0.79
1:E:175:SER:HB3	1:E:246:HIS:ND1	1.98	0.79
1:E:107:LEU:HD22	1:E:229:LEU:HG	1.65	0.78
1:I:257:VAL:HG13	1:I:403:GLN:HE22	1.47	0.78
1:G:154:VAL:HB	1:G:246:HIS:HE1	1.48	0.78
1:C:140:SER:HB3	1:C:141:PRO:HD3	1.65	0.78
1:G:117:VAL:HG12	1:G:364:LEU:HD13	1.64	0.78
1:I:263:GLU:CB	1:I:266:ARG:CD	2.57	0.77
1:B:167:ASP:OD2	1:B:199:TYR:OH	2.01	0.77
1:C:259:LEU:O	1:C:266:ARG:NH1	2.17	0.77
1:I:330:VAL:HG12	1:I:331:PHE:CD2	2.19	0.77
1:B:183:ARG:NH2	1:B:393:GLN:O	2.17	0.77
1:G:42:ARG:NH1	1:G:53:TRP:NE1	2.32	0.77
1:D:256:LEU:HD22	1:D:284:MET:HB3	1.67	0.76
1:F:394:GLY:C	1:F:395:MET:HG2	2.05	0.76
1:E:17:TYR:CE1	1:E:31:TYR:OH	2.38	0.76
1:I:327:ASP:O	1:I:330:VAL:HB	1.86	0.76
1:C:191:ARG:O	1:C:195:ASP:OD1	2.03	0.76
1:F:184:LEU:O	1:F:189:ILE:HD11	1.84	0.76
1:G:154:VAL:HB	1:G:246:HIS:CE1	2.20	0.76
1:A:383:ALA:HB3	1:A:404:ILE:HG22	1.67	0.75



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:I:127:LEU:HD21	1:I:155:ALA:HB3	1.69	0.75
1:I:283:GLU:O	1:I:286:ARG:CG	2.35	0.74
1:F:184:LEU:O	1:F:184:LEU:HG	1.84	0.74
1:B:190:GLN:O	1:B:194:GLN:HG3	1.87	0.74
1:G:363:ARG:O	1:G:367:GLN:HG3	1.88	0.74
1:H:284:MET:O	1:H:288:THR:OG1	2.03	0.74
1:I:260:LEU:HA	1:I:266:ARG:HG3	1.68	0.74
3:D:502:DEB:H72	3:D:502:DEB:H11	1.70	0.74
1:A:82:ARG:NH2	1:A:87:PRO:HG3	2.03	0.74
1:A:175:SER:HB3	1:A:246:HIS:ND1	2.03	0.74
1:F:185:THR:HA	1:F:189:ILE:HG13	1.69	0.74
1:I:62:ARG:NE	1:I:63:ILE:HG13	2.03	0.74
1:C:217:GLY:O	1:C:221:LEU:HD13	1.88	0.73
1:F:81:PRO:O	1:F:297:VAL:HG21	1.89	0.72
1:I:259:LEU:HD23	1:I:259:LEU:N	2.02	0.72
1:F:187:ALA:HA	1:F:190:GLN:HE22	1.53	0.72
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.72	0.71
1:E:45:LEU:HD22	1:E:81:PRO:HB2	1.72	0.71
1:I:259:LEU:CB	1:I:284:MET:HE3	2.19	0.71
1:F:184:LEU:O	1:F:184:LEU:CG	2.38	0.70
1:H:105:ARG:NH2	1:H:355:HIS:O	2.24	0.70
1:A:175:SER:CB	1:A:246:HIS:CE1	2.71	0.70
1:I:128:VAL:CG2	1:I:152:PHE:CE1	2.75	0.70
3:G:502:DEB:H222	3:G:502:DEB:H201	1.72	0.70
2:H:501:HEM:HMB2	2:H:501:HEM:HBB2	1.73	0.70
1:C:93:VAL:HG21	1:C:237:MET:SD	2.31	0.70
1:E:17:TYR:CD1	1:E:18:PRO:HA	2.26	0.70
1:I:328:GLU:OE2	1:I:329:GLU:HG2	1.91	0.70
1:I:254:THR:O	1:I:257:VAL:HG12	1.91	0.69
1:C:168:ARG:HA	1:C:171:PHE:CE2	2.28	0.69
1:E:40:VAL:HG12	1:E:53:TRP:CE3	2.26	0.69
1:F:185:THR:HA	1:F:189:ILE:CG1	2.23	0.69
1:C:246:HIS:O	1:C:247:GLU:C	2.31	0.69
1:I:62:ARG:CZ	1:I:63:ILE:HG13	2.24	0.68
1:I:264:ARG:NH1	1:I:268:GLU:OE2	2.27	0.68
1:D:283:GLU:HG3	1:D:337:LEU:CD2	2.23	0.67
1:F:185:THR:HA	1:F:189:ILE:CD1	2.25	0.67
1:I:263:GLU:O	1:I:266:ARG:CG	2.39	0.67
1:A:175:SER:HB3	1:A:246:HIS:HE1	1.54	0.67
3:A:502:DEB:H222	3:A:502:DEB:H201	1.77	0.67
1:H:175:SER:HB3	1:H:246:HIS:CE1	2.29	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:I:258:HIS:CE1	1:I:391:TRP:HZ2	2.13	0.67
1:G:117:VAL:HG12	1:G:364:LEU:CD1	2.24	0.67
1:E:175:SER:HB3	1:E:246:HIS:CE1	2.30	0.66
1:C:252:GLN:HA	1:C:252:GLN:OE1	1.94	0.66
1:H:185:THR:O	1:H:189:ILE:HG12	1.96	0.66
1:H:185:THR:O	1:H:189:ILE:CG1	2.44	0.66
3:D:502:DEB:H232	3:D:502:DEB:H221	1.77	0.65
2:E:501:HEM:HMB1	2:E:501:HEM:HBB2	1.77	0.65
1:G:384:GLU:OE1	1:G:402:ARG:NH1	2.30	0.65
1:I:259:LEU:HG	1:I:284:MET:HE2	1.78	0.65
3:F:502:DEB:H222	3:F:502:DEB:H201	1.78	0.65
1:I:328:GLU:CD	1:I:329:GLU:H	1.98	0.65
1:F:394:GLY:O	1:F:395:MET:HG2	1.97	0.65
1:A:295:SER:HB2	1:A:319:VAL:N	2.12	0.64
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.78	0.64
1:G:297:VAL:HG12	1:G:318:VAL:HG22	1.79	0.64
1:B:284:MET:O	1:B:288:THR:HG23	1.98	0.64
1:H:357:ILE:HD12	2:H:501:HEM:HMD2	1.80	0.64
1:C:179:LEU:HD22	1:C:397:ILE:CD1	2.26	0.64
1:I:327:ASP:CB	1:I:330:VAL:HB	2.19	0.64
2:E:501:HEM:HBC2	2:E:501:HEM:HMC2	1.79	0.63
1:I:40:VAL:HG23	1:I:55:VAL:HG22	1.80	0.63
1:A:105:ARG:NH2	1:A:355:HIS:O	2.32	0.63
1:G:132:LEU:O	1:G:136:VAL:HG23	1.98	0.63
1:I:264:ARG:HG3	1:I:268:GLU:HG2	1.80	0.63
1:I:259:LEU:HD12	1:I:284:MET:CE	2.29	0.62
1:I:62:ARG:NH2	1:I:63:ILE:HG13	2.10	0.62
1:D:55:VAL:HG21	1:D:64:VAL:HG21	1.82	0.62
1:A:307:SER:C	1:A:308:THR:HG23	2.20	0.62
1:D:175:SER:CB	1:D:246:HIS:CE1	2.82	0.62
1:I:62:ARG:CZ	1:I:63:ILE:CG1	2.78	0.62
1:I:62:ARG:HE	1:I:63:ILE:HG13	1.64	0.62
2:I:501:HEM:HMB1	2:I:501:HEM:HBB2	1.81	0.62
1:A:175:SER:CB	1:A:246:HIS:HE1	2.12	0.62
1:I:145:VAL:HA	1:I:149:ALA:HB3	1.82	0.62
1:D:185:THR:HB	1:D:189:ILE:HG23	1.82	0.61
1:E:34:LEU:HD22	1:E:38:GLU:HB3	1.82	0.61
1:B:259:LEU:O	1:B:266:ARG:NH1	2.33	0.61
1:G:145:VAL:HG22	1:G:254:THR:HG21	1.82	0.61
2:G:501:HEM:HMC2	2:G:501:HEM:HBC2	1.81	0.61
1:E:17:TYR:HE1	1:E:31:TYR:OH	1.84	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:55:VAL:HG21	1:E:64:VAL:HG21	1.82	0.61
1:A:332:ASP:O	1:A:333:HIS:C	2.38	0.61
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.81	0.61
2:G:501:HEM:HMB2	2:G:501:HEM:HBB2	1.82	0.60
1:H:347:ILE:O	1:H:347:ILE:HG13	2.00	0.60
1:I:256:LEU:HD11	1:I:366:LEU:HD13	1.82	0.60
1:D:104:LEU:O	1:D:108:VAL:HG12	2.00	0.60
1:H:290:LEU:HD12	1:H:397:ILE:HG23	1.83	0.60
1:B:145:VAL:HA	1:B:149:ALA:HB3	1.84	0.60
1:A:308:THR:O	1:A:309:VAL:HG23	2.01	0.60
1:I:259:LEU:CB	1:I:284:MET:CE	2.78	0.60
2:F:501:HEM:HMC2	2:F:501:HEM:HBC2	1.82	0.60
1:G:42:ARG:HH12	1:G:53:TRP:HE1	1.50	0.60
1:I:357:ILE:HD11	2:I:501:HEM:CBD	2.31	0.60
1:C:179:LEU:HD22	1:C:397:ILE:HD12	1.84	0.60
1:C:251:ASN:HD22	1:C:398:ARG:C	2.05	0.60
1:A:13:ALA:O	1:A:14:VAL:HG23	2.01	0.60
2:F:501:HEM:HMB1	2:F:501:HEM:HBB2	1.83	0.60
1:F:184:LEU:O	1:F:189:ILE:HG12	1.98	0.59
2:H:501:HEM:HMC2	2:H:501:HEM:HBC2	1.84	0.59
1:I:263:GLU:HB3	1:I:266:ARG:HD2	1.74	0.59
1:I:328:GLU:HG2	1:I:329:GLU:OE1	2.02	0.59
1:A:252:GLN:HE21	1:A:285:LEU:HD23	1.68	0.59
1:B:157:ILE:HD12	1:B:242:LEU:HD12	1.83	0.59
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.85	0.59
1:E:40:VAL:HG12	1:E:53:TRP:HE3	1.66	0.59
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.85	0.59
1:H:94:LEU:HD12	1:H:354:HIS:ND1	2.18	0.59
1:H:358:GLY:HA3	2:H:501:HEM:C3C	2.38	0.59
1:G:53:TRP:HB2	1:G:317:CYS:SG	2.43	0.59
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.83	0.58
1:F:185:THR:HA	1:F:189:ILE:HD12	1.85	0.58
1:C:202:GLY:O	1:C:206:GLN:HG3	2.02	0.58
1:I:337:LEU:HD23	1:I:338:ASP:N	2.18	0.58
1:I:128:VAL:HG22	1:I:152:PHE:CE1	2.39	0.58
1:G:117:VAL:CG1	1:G:364:LEU:HD13	2.33	0.58
1:I:259:LEU:CG	1:I:284:MET:CE	2.82	0.58
2:I:501:HEM:HMC2	2:I:501:HEM:HBC2	1.85	0.58
3:H:502:DEB:H201	3:H:502:DEB:H222	1.86	0.58
1:A:150:VAL:HB	1:A:151:PRO:HD3	1.85	0.58
1:C:145:VAL:HA	1:C:149:ALA:HB3	1.86	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:197:MET:CE	1:C:235:VAL:HG12	2.34	0.57
1:F:263:GLU:HB3	1:F:266:ARG:HD2	1.86	0.57
1:C:197:MET:HE1	1:C:235:VAL:HG12	1.85	0.57
1:C:284:MET:O	1:C:288:THR:HG22	2.04	0.57
1:E:77:ASP:O	1:E:80:THR:OG1	2.20	0.57
1:F:184:LEU:C	1:F:189:ILE:HG13	2.22	0.57
1:H:28:ASP:CG	1:H:29:PRO:HD2	2.24	0.57
1:H:286:ARG:NH2	1:H:336:GLU:O	2.37	0.57
1:F:264:ARG:NH1	1:F:380:LEU:O	2.32	0.57
1:A:84:PHE:HB2	1:A:85:PRO:HD2	1.86	0.57
1:A:105:ARG:NH1	1:A:357:ILE:HG12	2.19	0.57
1:I:291:VAL:O	1:I:292:SER:HB2	2.04	0.57
1:D:361:LEU:O	1:D:365:GLU:HB2	2.05	0.57
1:H:283:GLU:OE1	1:H:341:ARG:NE	2.38	0.57
1:A:195:ASP:O	1:A:198:VAL:HG12	2.03	0.57
1:A:295:SER:HB2	1:A:319:VAL:H	1.69	0.57
1:B:132:LEU:HD13	1:B:148:LEU:HD13	1.87	0.57
1:C:228:HIS:N	1:C:228:HIS:CD2	2.73	0.57
1:C:55:VAL:HG21	1:C:64:VAL:HG21	1.87	0.56
1:F:48:GLY:HA3	1:F:81:PRO:HA	1.86	0.56
1:B:165:LEU:O	1:B:166:GLU:HG2	2.06	0.56
1:D:185:THR:HG22	1:D:188:GLU:CB	2.21	0.56
1:D:283:GLU:HG3	1:D:337:LEU:HD22	1.87	0.56
1:H:356:CYS:HB3	1:H:359:ALA:HB2	1.88	0.56
1:I:259:LEU:CG	1:I:284:MET:HE2	2.36	0.56
1:A:121:ARG:HB3	1:A:122:PRO:CD	2.35	0.56
1:F:184:LEU:O	1:F:184:LEU:HD23	2.05	0.56
1:D:17:TYR:HA	1:D:18:PRO:C	2.26	0.56
1:D:129:ASP:OD1	1:D:375:ARG:NH2	2.34	0.56
1:F:145:VAL:HA	1:F:149:ALA:HB3	1.87	0.56
1:E:263:GLU:O	1:E:266:ARG:HG3	2.06	0.56
1:I:252:GLN:O	1:I:256:LEU:HG	2.05	0.56
1:A:157:ILE:HD13	1:A:242:LEU:HA	1.88	0.56
1:B:183:ARG:HB3	1:B:184:LEU:HD13	1.87	0.55
1:E:81:PRO:O	1:E:297:VAL:HG21	2.06	0.55
1:I:259:LEU:HD12	1:I:284:MET:HE3	1.88	0.55
1:E:84:PHE:CZ	3:E:502:DEB:H182	2.41	0.55
1:G:42:ARG:NH1	1:G:53:TRP:CZ2	2.71	0.55
1:G:175:SER:HB3	1:G:246:HIS:CE1	2.41	0.55
1:I:128:VAL:HG22	1:I:152:PHE:CD1	2.41	0.55
1:C:284:MET:O	1:C:288:THR:CG2	2.55	0.55



	A t and D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:H:290:LEU:O	1:H:397:ILE:HG23	2.06	0.55
1:I:251:ASN:O	1:I:254:THR:OG1	2.24	0.55
1:I:357:ILE:HD11	2:I:501:HEM:HBD2	1.88	0.55
1:F:228:HIS:HD2	1:F:229:LEU:O	1.89	0.55
1:I:128:VAL:HG23	1:I:152:PHE:CE1	2.42	0.55
1:D:121:ARG:HB3	1:D:122:PRO:CD	2.36	0.55
1:E:17:TYR:CZ	1:E:31:TYR:OH	2.59	0.54
1:F:182:THR:OG1	1:F:184:LEU:CD2	2.56	0.54
1:C:197:MET:HE3	1:C:235:VAL:CG1	2.37	0.54
1:F:393:GLN:OE1	1:F:393:GLN:HA	2.08	0.54
1:C:92:GLY:HA2	1:C:236:ASN:HD21	1.67	0.54
1:C:283:GLU:HG3	1:C:337:LEU:HD22	1.90	0.54
1:C:157:ILE:HD11	1:C:161:LEU:CD1	2.32	0.54
1:A:295:SER:CB	1:A:319:VAL:H	2.21	0.54
1:C:252:GLN:HB3	1:C:366:LEU:HD21	1.90	0.54
1:A:40:VAL:HG12	1:A:53:TRP:CE3	2.43	0.54
1:C:384:GLU:OE1	1:C:402:ARG:NH1	2.40	0.54
1:D:256:LEU:HD11	1:D:366:LEU:HD13	1.89	0.54
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	1.89	0.53
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.89	0.53
1:H:163:VAL:HG21	1:H:171:PHE:CZ	2.42	0.53
1:I:127:LEU:HD21	1:I:155:ALA:CB	2.37	0.53
1:I:248:THR:HG21	2:I:501:HEM:C4B	2.44	0.53
1:I:268:GLU:O	1:I:271:VAL:HG22	2.07	0.53
1:I:327:ASP:HB3	1:I:330:VAL:HG21	1.89	0.53
1:A:13:ALA:C	1:A:14:VAL:HG23	2.29	0.53
1:A:283:GLU:HG3	1:A:338:ASP:O	2.09	0.53
1:A:59:SER:HB2	1:C:271:VAL:CG2	2.39	0.53
1:C:139:GLY:O	1:C:407:TRP:CZ2	2.61	0.53
1:F:17:TYR:HA	1:F:18:PRO:C	2.29	0.53
1:I:255:ASN:OD1	1:I:255:ASN:N	2.33	0.53
1:A:326:ARG:HA	1:A:334:ALA:HB1	1.90	0.53
1:C:197:MET:CE	1:C:235:VAL:CG1	2.87	0.53
1:F:184:LEU:O	1:F:184:LEU:CD2	2.57	0.53
1:I:117:VAL:HG11	1:I:360:GLN:HB2	1.90	0.53
1:G:175:SER:CB	1:G:246:HIS:CE1	2.92	0.53
1:B:167:ASP:O	1:B:170:LEU:N	2.40	0.52
1:E:24:ALA:HB3	1:E:391:TRP:CD2	2.43	0.52
1:I:252:GLN:OE1	1:I:255:ASN:ND2	2.43	0.52
1:B:165:LEU:C	1:B:167:ASP:H	2.11	0.52
1:D:294:GLY:HA3	1:D:318:VAL:HG22	1.91	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:F:266:ARG:O	1:F:269:SER:OG	2.26	0.52
1:H:255:ASN:HB3	1:H:288:THR:HG21	1.90	0.52
1:A:379:THR:OG1	1:A:407:TRP:O	2.25	0.52
1:C:207:ARG:NH1	1:C:216:LEU:HD23	2.24	0.52
1:G:256:LEU:HD22	1:G:284:MET:HB3	1.90	0.52
1:C:228:HIS:CD2	1:C:228:HIS:H	2.28	0.52
1:I:328:GLU:CG	1:I:329:GLU:N	2.73	0.52
1:B:196:PHE:O	1:B:199:TYR:HB3	2.10	0.52
1:B:220:ALA:O	1:B:223:THR:HG22	2.10	0.52
1:H:290:LEU:HD12	1:H:397:ILE:CG2	2.40	0.52
1:F:185:THR:HG23	4:F:615:HOH:O	2.09	0.52
1:H:286:ARG:HD3	1:H:344:ASN:HD22	1.75	0.52
1:A:31:TYR:CE1	1:A:320:HIS:CD2	2.98	0.51
1:F:30:HIS:CE1	1:F:34:LEU:HD11	2.46	0.51
1:C:161:LEU:HG	1:C:216:LEU:HD13	1.91	0.51
3:D:502:DEB:H232	3:D:502:DEB:C22	2.40	0.51
1:E:189:ILE:HD12	1:E:189:ILE:N	2.24	0.51
1:C:274:PRO:O	1:C:277:VAL:HG23	2.11	0.51
1:D:232:GLY:O	1:D:236:ASN:ND2	2.43	0.51
1:H:283:GLU:OE1	1:H:286:ARG:NE	2.43	0.51
1:I:357:ILE:HD11	2:I:501:HEM:HBD1	1.93	0.51
1:A:307:SER:O	1:A:308:THR:OG1	2.16	0.51
1:I:329:GLU:OE2	1:I:329:GLU:HA	2.09	0.51
1:C:152:PHE:HB3	1:C:153:PRO:HD3	1.93	0.51
1:H:286:ARG:HG3	1:H:325:ASN:HB3	1.93	0.51
1:H:357:ILE:HD12	2:H:501:HEM:CMD	2.40	0.51
1:F:337:LEU:HD21	1:F:339:PHE:CE1	2.46	0.50
1:I:204:VAL:HG21	1:I:235:VAL:HG22	1.92	0.50
1:C:179:LEU:HD13	1:C:397:ILE:HD12	1.92	0.50
1:E:354:HIS:HA	2:E:501:HEM:O2D	2.11	0.50
1:H:64:VAL:HG12	1:H:64:VAL:O	2.10	0.50
1:C:230:THR:O	1:C:233:GLU:N	2.43	0.50
1:F:332:ASP:O	1:F:341:ARG:NH1	2.44	0.50
1:C:108:VAL:CG2	1:C:215:LEU:HD13	2.42	0.50
1:E:377:PHE:HB3	1:E:380:LEU:HB2	1.93	0.50
1:G:152:PHE:HB3	1:G:153:PRO:HD3	1.93	0.50
1:H:328:GLU:OE2	1:H:328:GLU:N	2.42	0.50
1:B:133:ASP:OD1	1:B:376:ARG:NH2	2.38	0.50
1:I:62:ARG:NH2	1:I:63:ILE:CD1	2.74	0.49
1:I:256:LEU:N	1:I:256:LEU:HD23	2.27	0.49
1:I:270:LEU:N	1:I:270:LEU:CD1	2.74	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:246:HIS:HD2	1:E:250:VAL:CG2	2.25	0.49
1:B:165:LEU:C	1:B:167:ASP:N	2.65	0.49
1:D:14:VAL:HB	1:D:15:PRO:HD3	1.94	0.49
1:F:94:LEU:HD12	1:F:354:HIS:CD2	2.47	0.49
1:B:150:VAL:HB	1:B:151:PRO:HD3	1.94	0.49
1:B:287:TYR:CG	1:B:337:LEU:HD23	2.48	0.49
1:C:149:ALA:O	1:C:153:PRO:CD	2.60	0.49
1:D:264:ARG:NH2	1:D:380:LEU:O	2.45	0.49
1:F:287:TYR:O	1:F:326:ARG:NH1	2.46	0.49
1:D:224:ASP:OD1	1:D:225:ASN:N	2.45	0.49
1:C:176:ASP:OD1	1:C:247:GLU:OE2	2.30	0.49
1:D:244:ALA:HA	3:D:502:DEB:C22	2.42	0.49
1:I:40:VAL:CG2	1:I:55:VAL:HG22	2.42	0.49
1:A:300:ALA:HB1	1:A:302:GLU:O	2.12	0.49
1:C:251:ASN:ND2	1:C:399:GLY:CA	2.72	0.49
1:E:17:TYR:OH	1:E:31:TYR:OH	2.22	0.49
1:I:252:GLN:HG2	1:I:366:LEU:HD11	1.94	0.49
1:B:165:LEU:HB2	1:B:166:GLU:OE1	2.13	0.49
1:C:384:GLU:CD	1:C:402:ARG:NH1	2.66	0.49
1:I:246:HIS:CE1	1:I:247:GLU:HG2	2.48	0.49
1:A:42:ARG:HA	1:A:52:ALA:O	2.13	0.49
1:B:152:PHE:HB3	1:B:153:PRO:HD3	1.94	0.49
1:C:220:ALA:O	1:C:223:THR:OG1	2.30	0.49
1:G:260:LEU:HD11	1:G:284:MET:HE1	1.93	0.49
1:A:104:LEU:O	1:A:108:VAL:HG12	2.13	0.48
1:B:93:VAL:HG11	1:B:237:MET:SD	2.52	0.48
1:C:292:SER:HA	1:C:398:ARG:HE	1.78	0.48
1:D:252:GLN:HE21	1:D:285:LEU:HD23	1.78	0.48
1:A:227:ASP:HB3	1:H:227:ASP:HB2	1.94	0.48
1:F:153:PRO:O	1:F:157:ILE:HG13	2.13	0.48
1:G:105:ARG:NH2	1:G:355:HIS:O	2.46	0.48
1:H:185:THR:O	1:H:189:ILE:HG13	2.12	0.48
1:H:290:LEU:CD1	1:H:397:ILE:CG2	2.92	0.48
1:A:82:ARG:CZ	1:A:87:PRO:HG3	2.42	0.48
1:B:196:PHE:O	1:B:196:PHE:HD1	1.95	0.48
1:F:264:ARG:O	1:F:268:GLU:HG3	2.13	0.48
1:F:354:HIS:HD2	2:F:501:HEM:O1D	1.95	0.48
1:A:283:GLU:HA	1:A:283:GLU:OE1	2.13	0.48
1:C:179:LEU:HD22	1:C:397:ILE:HD11	1.96	0.48
1:A:133:ASP:OD1	1:A:376:ARG:NH2	2.47	0.48
1:C:260:LEU:HG	1:C:284:MET:HE1	1.96	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:I:357:ILE:N	1:I:357:ILE:HD13	2.29	0.48
1:B:168:ARG:O	1:B:172:ARG:HG3	2.14	0.48
1:H:290:LEU:CD1	1:H:397:ILE:HG23	2.43	0.48
1:H:129:ASP:OD1	1:H:376:ARG:NH1	2.47	0.48
1:I:327:ASP:CB	1:I:330:VAL:HG21	2.44	0.48
1:B:215:LEU:O	1:B:219:LEU:N	2.45	0.48
1:C:402:ARG:O	1:C:402:ARG:HG3	2.13	0.48
1:G:286:ARG:HB2	1:G:346:HIS:HB3	1.96	0.48
1:I:34:LEU:HD23	1:I:41:SER:OG	2.13	0.48
1:B:176:ASP:OD1	1:B:247:GLU:OE2	2.32	0.47
1:E:30:HIS:HA	1:E:33:GLU:OE1	2.14	0.47
1:B:67:ASP:OD2	1:B:69:ARG:NH2	2.47	0.47
1:I:263:GLU:HG2	1:I:266:ARG:HD2	1.95	0.47
1:I:291:VAL:O	1:I:291:VAL:HG13	2.14	0.47
1:D:84:PHE:HB3	1:D:396:LEU:HD21	1.97	0.47
1:I:255:ASN:O	1:I:258:HIS:HB3	2.14	0.47
1:I:40:VAL:HG22	1:I:41:SER:N	2.29	0.47
1:I:360:GLN:N	1:I:360:GLN:OE1	2.48	0.47
1:D:121:ARG:HB3	1:D:122:PRO:HD3	1.96	0.47
1:B:277:VAL:HB	1:B:278:PRO:HD3	1.97	0.47
1:F:267:TYR:O	1:F:271:VAL:HG23	2.14	0.47
1:G:295:SER:N	1:G:319:VAL:O	2.48	0.47
1:I:264:ARG:O	1:I:268:GLU:HB2	2.15	0.47
1:A:121:ARG:CZ	1:A:364:LEU:HD23	2.45	0.47
1:C:96:GLN:HA	1:C:96:GLN:HE21	1.80	0.47
1:C:384:GLU:CD	1:C:389:LEU:HD23	2.35	0.47
2:E:501:HEM:HBB2	2:E:501:HEM:CMB	2.43	0.47
1:G:54:LEU:HG	1:G:55:VAL:N	2.29	0.47
1:D:244:ALA:HA	3:D:502:DEB:H222	1.96	0.47
1:D:267:TYR:OH	1:D:373:LEU:O	2.33	0.47
1:F:55:VAL:HG12	1:F:56:THR:N	2.30	0.47
1:H:245:GLY:HA3	2:H:501:HEM:C2C	2.49	0.47
1:I:258:HIS:CE1	1:I:391:TRP:CZ2	3.00	0.47
1:G:297:VAL:HG12	1:G:318:VAL:CG2	2.44	0.47
1:H:277:VAL:HA	1:H:280:ALA:HB3	1.96	0.47
1:A:163:VAL:HG21	1:A:171:PHE:CZ	2.50	0.47
1:E:347:ILE:HG22	1:E:350:GLY:O	2.14	0.47
1:H:30:HIS:CE1	4:H:604:HOH:O	2.67	0.47
1:I:357:ILE:HG12	2:I:501:HEM:C2D	2.49	0.47
1:A:283:GLU:CG	1:A:338:ASP:O	2.63	0.46
1:C:34:LEU:HD22	1:C:41:SER:OG	2.15	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:121:ARG:HB3	1:C:122:PRO:HD3	1.97	0.46
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.45	0.46
1:A:128:VAL:HG13	1:A:152:PHE:CZ	2.51	0.46
1:B:93:VAL:HG12	1:B:104:LEU:HD13	1.96	0.46
1:B:271:VAL:HA	1:B:374:VAL:HG13	1.97	0.46
1:H:128:VAL:HG13	1:H:152:PHE:CE1	2.50	0.46
1:I:327:ASP:CB	1:I:330:VAL:CG2	2.85	0.46
1:B:105:ARG:NH2	1:B:355:HIS:O	2.47	0.46
1:E:82:ARG:HG3	1:E:84:PHE:O	2.15	0.46
1:F:264:ARG:O	1:F:265:LYS:C	2.54	0.46
1:H:175:SER:O	1:H:179:LEU:HD23	2.15	0.46
1:B:256:LEU:HD11	1:B:366:LEU:HD12	1.97	0.46
1:D:177:ALA:HA	1:D:182:THR:CG2	2.46	0.46
1:D:302:GLU:HA	1:D:313:ALA:HB2	1.96	0.46
1:E:386:VAL:HG13	1:E:389:LEU:HD12	1.97	0.46
1:A:357:ILE:HG13	2:A:501:HEM:HBD2	1.97	0.46
1:B:157:ILE:HG21	1:B:245:GLY:CA	2.42	0.46
1:C:200:MET:HG3	1:C:239:VAL:HG22	1.97	0.46
1:G:48:GLY:HA3	1:G:81:PRO:HA	1.98	0.46
1:I:284:MET:O	1:I:288:THR:OG1	2.33	0.46
1:A:402:ARG:CD	1:A:404:ILE:CD1	2.94	0.46
1:B:383:ALA:HB3	1:B:404:ILE:HG22	1.97	0.46
1:C:242:LEU:O	1:C:246:HIS:HD2	1.99	0.46
1:H:31:TYR:CE1	1:H:320:HIS:CD2	3.04	0.46
1:H:45:LEU:HD21	1:H:318:VAL:HG21	1.98	0.46
1:B:139:GLY:O	1:B:407:TRP:CZ2	2.68	0.46
1:E:152:PHE:HB3	1:E:153:PRO:HD3	1.98	0.46
1:B:48:GLY:HA3	1:B:81:PRO:HA	1.98	0.46
1:E:259:LEU:C	1:E:266:ARG:NH1	2.69	0.46
1:A:355:HIS:O	1:A:356:CYS:C	2.53	0.46
1:F:183:ARG:HH11	1:F:183:ARG:HB2	1.80	0.46
1:E:246:HIS:HD2	1:E:250:VAL:HG23	1.80	0.45
1:F:14:VAL:HB	1:F:15:PRO:HD2	1.97	0.45
1:F:188:GLU:H	1:F:188:GLU:HG3	1.53	0.45
1:A:42:ARG:NH2	1:A:51:THR:OG1	2.47	0.45
3:D:502:DEB:H221	3:D:502:DEB:C23	2.45	0.45
1:B:31:TYR:CZ	1:B:320:HIS:CD2	3.05	0.45
1:D:349:PHE:HB3	1:D:356:CYS:HB3	1.98	0.45
2:A:501:HEM:HBB2	2:A:501:HEM:CMB	2.41	0.45
1:I:328:GLU:HG2	1:I:329:GLU:CD	2.36	0.45
1:B:165:LEU:C	1:B:166:GLU:CG	2.85	0.45



	A L	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:150:VAL:HB	1:D:151:PRO:HD3	1.98	0.45
1:B:17:TYR:HA	1:B:18:PRO:C	2.37	0.45
1:E:292:SER:HA	1:E:398:ARG:HE	1.82	0.45
2:H:501:HEM:HBB2	2:H:501:HEM:CMB	2.44	0.45
1:A:208:ARG:NH2	1:H:100:ASP:OD1	2.50	0.45
1:I:360:GLN:OE1	1:I:363:ARG:NH1	2.49	0.45
1:A:248:THR:O	1:A:252:GLN:HB2	2.17	0.45
1:B:344:ASN:OD1	1:B:344:ASN:O	2.34	0.45
1:G:150:VAL:HB	1:G:151:PRO:HD3	1.98	0.45
1:H:264:ARG:HH11	1:H:268:GLU:HG3	1.82	0.45
1:D:247:GLU:O	1:D:251:ASN:ND2	2.49	0.45
1:B:141:PRO:HA	1:B:405:VAL:O	2.17	0.44
1:G:283:GLU:OE1	1:G:341:ARG:NE	2.50	0.44
1:I:259:LEU:CD1	1:I:284:MET:CE	2.95	0.44
1:A:322:ALA:O	1:A:326:ARG:HG2	2.16	0.44
1:B:266:ARG:HD3	1:B:337:LEU:HD12	2.00	0.44
1:F:184:LEU:HG	1:F:189:ILE:HG12	1.99	0.44
1:C:246:HIS:CG	1:C:247:GLU:N	2.85	0.44
1:E:14:VAL:HG12	1:E:44:ARG:HB2	1.99	0.44
1:H:145:VAL:HA	1:H:149:ALA:HB3	1.99	0.44
1:H:245:GLY:CA	2:H:501:HEM:C2C	3.00	0.44
1:A:121:ARG:CB	1:A:122:PRO:CD	2.94	0.44
1:B:274:PRO:O	1:B:277:VAL:HG23	2.17 0.44	
1:A:55:VAL:HG21	1:A:64:VAL:HG21	2.00	0.44
1:A:128:VAL:HG13	1:A:152:PHE:CE1	2.53	0.44
1:C:283:GLU:HG3	1:C:337:LEU:CD2	2.48	0.44
1:F:260:LEU:HD21	1:F:284:MET:HE3	2.00	0.44
1:A:129:ASP:OD1	1:A:375:ARG:NH2	2.50	0.44
1:B:124:VAL:HG13	1:B:152:PHE:CE1	2.53	0.44
1:C:248:THR:O	1:C:252:GLN:HB2	2.17	0.44
1:D:94:LEU:HD12	1:D:354:HIS:CD2	2.51	0.44
1:E:175:SER:CB	1:E:246:HIS:CE1	2.98	0.44
2:E:501:HEM:HBC2	2:E:501:HEM:CMC	2.48	0.44
1:F:383:ALA:HB3	1:F:404:ILE:HG22	2.00	0.44
1:A:128:VAL:O	1:A:132:LEU:HD13	2.18	0.44
1:I:145:VAL:HG12	1:I:150:VAL:HG23	1.98	0.44
1:B:259:LEU:HD11	1:B:288:THR:HG22	2.00	0.43
1:B:261:LEU:HD11	1:B:380:LEU:HD23	1.99	0.43
1:G:175:SER:HB3	1:G:246:HIS:ND1	2.33	0.43
1:C:183:ARG:HB2	1:C:394:GLY:O	2.19	0.43
1:F:237:MET:HE1	1:F:357:ILE:HD13	1.99	0.43



	A (D	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:286:ARG:O	1:A:325:ASN:HB3	2.19	0.43	
1:E:42:ARG:HA	1:E:52:ALA:O	2.18	0.43	
1:G:283:GLU:HG3	1:G:338:ASP:O	2.18	0.43	
1:D:187:ALA:O	1:D:190:GLN:HB2	2.18	0.43	
1:E:39:PRO:HB3	1:E:57:ARG:HD3	2.01	0.43	
1:A:383:ALA:HB2	1:A:406:SER:HB3	1.99	0.43	
1:B:39:PRO:HD2	1:B:308:THR:HG21	2.00	0.43	
1:B:252:GLN:HE21	1:B:285:LEU:HD23	1.84	0.43	
2:C:501:HEM:HBC2	2:C:501:HEM:CMC	2.46	0.43	
1:A:96:GLN:HB3	1:A:101:HIS:HB2	1.99	0.43	
1:C:105:ARG:CZ	1:C:357:ILE:CG2	2.96	0.43	
2:G:501:HEM:HBC2	2:G:501:HEM:CMC	2.48	0.43	
1:H:354:HIS:ND1	2:H:501:HEM:O1D	2.52	0.43	
1:C:256:LEU:HD22	1:C:284:MET:CB	2.49	0.43	
1:A:402:ARG:HD3	1:A:404:ILE:CD1	2.48	0.43	
1:D:123:ARG:O	1:D:127:LEU:HD23	2.19	0.43	
1:G:383:ALA:HB3	1:G:404:ILE:HG22	2.01	0.43	
1:C:61:ALA:O	1:C:65:LEU:HG	2.19	0.43	
1:C:230:THR:O	1:C:231:LYS:C	2.54	0.43	
1:F:94:LEU:HA	1:F:354:HIS:CD2	2.53	0.43	
1:F:160:LEU:HD22	1:F:361:LEU:HD22	2.01	0.43	
1:G:292:SER:HB3	1:G:398:ARG:CG	2.48	0.43	
1:H:175:SER:HB3	1:H:246:HIS:ND1	2.34	0.43	
1:H:400:LEU:HD22	1:H:402:ARG:O	2.19	0.43	
1:I:328:GLU:O	1:I:331:PHE:O	2.37	0.43	
1:D:208:ARG:NH1	1:D:220:ALA:O	2.52	0.42	
1:E:267:TYR:O	1:E:271:VAL:HG23	2.19	0.42	
1:G:292:SER:HB3	1:G:398:ARG:HG3	2.00	0.42	
1:E:189:ILE:N	1:E:189:ILE:CD1	2.82	0.42	
1:A:312:ARG:HD2	1:B:23:HIS:CE1	2.55	0.42	
1:F:267:TYR:CE2	1:F:380:LEU:HB3	2.54	0.42	
1:G:157:ILE:HG21	1:G:242:LEU:HD13	2.01	0.42	
1:I:259:LEU:HG	1:I:284:MET:CE	2.45	0.42	
1:E:391:TRP:CZ3	1:E:400:LEU:HG	2.54	0.42	
1:H:143:ASP:HA	1:H:404:ILE:HA	2.01	0.42	
1:C:256:LEU:O	1:C:257:VAL:C	2.58	0.42	
1:C:37:ASP:O	1:C:39:PRO:HD3	2.19	0.42	
1:C:251:ASN:ND2	1:C:398:ARG:C	2.72	0.42	
1:D:17:TYR:O	1:D:46:PRO:HD3	2.19	0.42	
2:F:501:HEM:HBB2	2:F:501:HEM:CMB	2.47	0.42	
2:G:501:HEM:HBB2	2:G:501:HEM:CMB	2.48	0.42	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:I:327:ASP:OD2	1:I:330:VAL:HG23	2.19	0.42
1:E:384:GLU:CD	1:E:402:ARG:NH1	2.73	0.42
1:G:286:ARG:NH2	1:G:336:GLU:O	2.52	0.42
1:I:371:SER:HA	1:I:374:VAL:HG12	2.00	0.42
1:C:69:ARG:HD2	1:C:302:GLU:HB3	2.02	0.42
1:C:141:PRO:HA	1:C:405:VAL:O	2.19	0.42
1:E:188:GLU:O	1:E:191:ARG:HG2	2.20	0.42
1:E:199:TYR:O	1:E:203:LEU:N	2.50	0.42
1:E:370:LEU:O	1:E:374:VAL:HG23	2.20	0.42
1:E:396:LEU:HD23	3:E:502:DEB:H202	2.00	0.42
1:C:268:GLU:O	1:C:271:VAL:HG22	2.20	0.42
1:I:259:LEU:HD23	1:I:259:LEU:H	1.80	0.42
1:A:245:GLY:HA3	2:A:501:HEM:C2C	2.55	0.42
1:C:256:LEU:O	1:C:259:LEU:N	2.53	0.42
1:G:277:VAL:O	1:G:281:VAL:HG23	2.20	0.42
1:H:264:ARG:NH2	1:H:380:LEU:O	2.53	0.42
1:E:123:ARG:O	1:E:127:LEU:HG	2.20	0.41
1:G:17:TYR:CE2	1:G:54:LEU:HD22	2.55	0.41
1:G:284:MET:HE1	1:G:370:LEU:HD11	2.02	0.41
1:H:17:TYR:HA	1:H:18:PRO:C	2.40	0.41
1:I:34:LEU:O	1:I:38:GLU:O	2.38	0.41
1:I:263:GLU:CG	1:I:266:ARG:HD2	2.50	0.41
1:C:157:ILE:HG13	1:C:161:LEU:HB2	2.02	0.41
1:D:160:LEU:HD22	1:D:361:LEU:HD22	2.01	0.41
1:H:94:LEU:HA	1:H:354:HIS:CE1	2.55	0.41
1:D:152:PHE:HB3	1:D:153:PRO:HD3	2.01	0.41
1:E:373:LEU:HD22	1:E:380:LEU:HG	2.02	0.41
1:I:335:ASP:OD1	1:I:336:GLU:HG2	2.20	0.41
1:C:197:MET:HE1	1:C:235:VAL:CG1	2.50	0.41
1:C:273:ASP:O	1:C:276:LEU:HB2	2.20	0.41
1:C:282:GLU:OE2	1:C:363:ARG:NE	2.47	0.41
1:F:190:GLN:HE21	1:F:190:GLN:HB3	1.64	0.41
1:F:384:GLU:HG3	1:F:404:ILE:HB	2.02	0.41
1:H:348:ALA:O	2:H:501:HEM:HMA1	2.21	0.41
1:I:157:ILE:HD12	1:I:242:LEU:HD12	2.03	0.41
1:I:257:VAL:HG13	1:I:403:GLN:NE2	2.26	0.41
1:A:149:ALA:O	1:A:153:PRO:CD	2.69	0.41
1:C:242:LEU:O	1:C:246:HIS:CD2	2.73	0.41
1:D:152:PHE:O	1:D:156:VAL:HG23	2.20	0.41
1:E:246:HIS:CD2	1:E:250:VAL:CG2	3.02	0.41
1:E:364:LEU:HD23	1:E:368:GLU:HG2	2.02	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:H:320:HIS:CD2	1:H:323:SER:HB2	2.55	0.41
1:A:134:ASP:O	1:A:137:ALA:HB3	2.20	0.41
1:C:221:LEU:N	1:C:221:LEU:HD12	2.36	0.41
1:H:403:GLN:O	1:H:405:VAL:HG13	2.20	0.41
1:A:228:HIS:HD2	1:A:229:LEU:O	2.04	0.41
1:B:283:GLU:OE1	1:B:283:GLU:HA	2.20	0.41
1:C:128:VAL:O	1:C:132:LEU:HD22	2.20	0.41
1:C:148:LEU:O	1:C:151:PRO:HD2	2.21	0.41
1:C:149:ALA:O	1:C:153:PRO:HD2	2.21	0.41
1:C:384:GLU:CD	1:C:402:ARG:HH12	2.23	0.41
1:E:258:HIS:CE1	1:E:262:THR:HG21	2.54	0.41
1:I:153:PRO:HG2	1:I:250:VAL:HG22	2.03	0.41
1:A:70:PHE:CE2	1:A:304:VAL:HG11	2.55	0.41
1:H:159:GLU:OE2	1:H:168:ARG:NH2	2.41	0.41
1:I:337:LEU:HD23	1:I:338:ASP:C	2.41	0.41
1:E:84:PHE:CD1	1:E:84:PHE:N	2.89	0.41
1:E:377:PHE:CB	1:E:380:LEU:HB2	2.51	0.41
1:F:53:TRP:NE1	1:F:315:GLU:OE2	2.50	0.41
1:F:55:VAL:HG21	1:F:64:VAL:HG21	2.02	0.41
1:G:129:ASP:HA	1:G:376:ARG:HH12	1.85	0.41
1:H:117:VAL:HG11	1:H:360:GLN:O	2.21	0.41
1:H:228:HIS:ND1	1:H:229:LEU:O	2.46 0.41	
1:H:384:GLU:HG3	4:H:607:HOH:O	2.19 0.41	
1:I:124:VAL:HG13	1:I:152:PHE:CE1	2.56	0.41
1:I:157:ILE:HG21	1:I:245:GLY:HA3	2.02	0.41
1:I:259:LEU:HA	1:I:262:THR:CG2	2.51	0.41
1:I:328:GLU:HG2	1:I:329:GLU:N	2.35	0.41
1:A:200:MET:CE	1:A:203:LEU:HD23	2.51	0.41
1:A:227:ASP:OD1	1:A:227:ASP:N	2.52	0.41
1:B:168:ARG:CD	1:B:168:ARG:C	2.89	0.41
1:E:134:ASP:O	1:E:137:ALA:N	2.54	0.41
1:I:156:VAL:HG21	1:I:365:GLU:OE1	2.21	0.41
1:I:260:LEU:HG	1:I:284:MET:HE1	2.03	0.41
1:B:168:ARG:O	1:B:172:ARG:CG	2.69	0.40
1:C:290:LEU:CD1	1:C:397:ILE:HG23	2.51	0.40
1:D:132:LEU:HG	1:D:377:PHE:HE2	1.86	0.40
1:D:376:ARG:O	1:D:377:PHE:CD1	2.74	0.40
1:E:117:VAL:CG1	1:E:364:LEU:HD12	2.51	0.40
1:I:270:LEU:N	1:I:270:LEU:HD12	2.35	0.40
1:C:246:HIS:O	1:C:250:VAL:HG23	2.21	0.40
1:D:88:PRO:HA	4:D:622:HOH:O	2.20	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:195:ASP:HA	1:D:198:VAL:HG12	2.02	0.40
1:B:165:LEU:O	1:B:166:GLU:CG	2.70	0.40
1:D:355:HIS:O	1:D:356:CYS:C	2.60	0.40
1:F:185:THR:CA	1:F:189:ILE:HG13	2.46	0.40
1:G:105:ARG:NH1	1:G:357:ILE:HG12	2.35	0.40
1:C:358:GLY:O	1:C:361:LEU:N	2.54	0.40
1:G:135:MET:HG2	1:G:407:TRP:CH2	2.57	0.40
1:H:124:VAL:HG21	1:H:364:LEU:HD12	2.04	0.40
1:I:59:SER:HA	1:I:62:ARG:HG2	2.03	0.40
2:I:501:HEM:HBC2	2:I:501:HEM:CMC	2.51	0.40
1:A:193:GLN:HE21	1:A:193:GLN:HB3	1.73	0.40
1:B:348:ALA:O	2:B:501:HEM:HMA1	2.22	0.40
1:D:112:PHE:O	1:D:112:PHE:CD1	2.75	0.40
1:I:97:ASP:HB3	1:I:98:PRO:HD2	2.02	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	Perce	ntiles
1	А	395/407~(97%)	374 (95%)	21 (5%)	0	100	100
1	В	392/407~(96%)	367 (94%)	25~(6%)	0	100	100
1	С	394/407~(97%)	358 (91%)	36 (9%)	0	100	100
1	D	392/407~(96%)	364 (93%)	28 (7%)	0	100	100
1	Ε	384/407~(94%)	361 (94%)	23~(6%)	0	100	100
1	F	393/407~(97%)	360 (92%)	33 (8%)	0	100	100
1	G	374/407~(92%)	342 (91%)	32 (9%)	0	100	100
1	Н	393/407~(97%)	354 (90%)	38 (10%)	1 (0%)	41	74
1	Ι	268/407~(66%)	255~(95%)	13 (5%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3385/3663~(92%)	3135 (93%)	249 (7%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Η	345	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	entiles
1	А	332/341~(97%)	299~(90%)	33 (10%)	8	28
1	В	330/341~(97%)	292 (88%)	38 (12%)	5	22
1	С	332/341~(97%)	301 (91%)	31 (9%)	9	31
1	D	331/341~(97%)	302 (91%)	29 (9%)	10	34
1	Ε	324/341~(95%)	290 (90%)	34 (10%)	7	25
1	F	331/341~(97%)	307~(93%)	24 (7%)	14	42
1	G	318/341~(93%)	298 (94%)	20 (6%)	18	49
1	Н	331/341~(97%)	305~(92%)	26 (8%)	12	39
1	Ι	243/341 (71%)	214 (88%)	29 (12%)	5	21
All	All	2872/3069~(94%)	2608 (91%)	264 (9%)	9	32

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	14	VAL
1	А	45	LEU
1	А	59	SER
1	А	72	THR
1	А	86	THR
1	А	96	GLN
1	А	106	ARG



Mol	Chain	Res	Type
1	А	112	PHE
1	А	130	SER
1	А	166	GLU
1	А	172	ARG
1	А	183	ARG
1	А	193	GLN
1	А	197	MET
1	А	223	THR
1	А	226	ASP
1	А	240	SER
1	А	264	ARG
1	А	265	LYS
1	А	283	GLU
1	А	292	SER
1	А	295	SER
1	А	301	THR
1	А	310	THR
1	А	311	VAL
1	А	337	LEU
1	А	364	LEU
1	А	371	SER
1	А	376	ARG
1	А	380	LEU
1	А	390	LYS
1	А	395	MET
1	А	402	ARG
1	В	41	SER
1	В	100	ASP
1	В	106	ARG
1	В	108	VAL
1	В	116	ARG
1	В	129	ASP
1	В	132	LEU
1	В	165	LEU
1	В	166	GLU
1	В	168	ARG
1	В	169	ASP
1	В	176	ASP
1	В	178	MET
1	В	183	ARG
1	В	184	LEU
1	В	185	THR



Mol	Chain	Res	Type
1	В	191	ARG
1	В	195	ASP
1	В	196	PHE
1	В	197	MET
1	В	200	MET
1	В	207	ARG
1	В	209	ASP
1	В	224	ASP
1	В	229	LEU
1	В	263	GLU
1	В	265	LYS
1	В	276	LEU
1	В	288	THR
1	В	299	VAL
1	В	312	ARG
1	В	342	GLU
1	В	345	PRO
1	В	364	LEU
1	В	366	LEU
1	В	384	GLU
1	В	393	GLN
1	В	402	ARG
1	С	58	MET
1	С	80	THR
1	С	96	GLN
1	С	97	ASP
1	С	100	ASP
1	С	120	MET
1	С	127	LEU
1	С	132	LEU
1	С	173	THR
1	С	178	MET
1	С	185	THR
1	С	196	PHE
1	С	197	MET
1	С	200	MET
1	С	216	LEU
1	С	219	LEU
1	С	229	LEU
1	С	252	GLN
1	С	263	GLU
1	С	265	LYS



Mol	Chain	Res	Type
1	С	276	LEU
1	С	288	THR
1	С	292	SER
1	С	297	VAL
1	С	298	ARG
1	С	305	GLU
1	С	318	VAL
1	С	330	VAL
1	С	364	LEU
1	С	374	VAL
1	С	395	MET
1	D	34	LEU
1	D	43	VAL
1	D	44	ARG
1	D	80	THR
1	D	105	ARG
1	D	106	ARG
1	D	107	LEU
1	D	112	PHE
1	D	125	ARG
1	D	128	VAL
1	D	129	ASP
1	D	132	LEU
1	D	182	THR
1	D	185	THR
1	D	191	ARG
1	D	201	ASP
1	D	254	THR
1	D	264	ARG
1	D	265	LYS
1	D	269	SER
1	D	292	SER
1	D	301	THR
1	D	310	THR
1	D	337	LEU
1	D	364	LEU
1	D	371	SER
1	D	380	LEU
1	D	382	LEU
1	D	396	LEU
1	E	19	PHE
1	Е	41	SER



Mol	Chain	Res	Type	
1	Е	44	ARG	
1	Е	57	ARG	
1	Е	67	ASP	
1	Е	80	THR	
1	Е	83	MET	
1	Е	107	LEU	
1	Е	110	LYS	
1	Е	112	PHE	
1	Е	116	ARG	
1	Е	121	ARG	
1	Е	125	ARG	
1	Е	129	ASP	
1	Е	151	PRO	
1	Е	173	THR	
1	Е	176	ASP	
1	E	180	SER	
1	Е	183	ARG	
1	Е	243	ILE	
1	Е	256	LEU	
1	Е	264	ARG	
1	Е	265	LYS	
1	Е	284	MET	
1	Ε	298	ARG	
1	E	301	THR	
1	Е	343	ARG	
1	Е	364	LEU	
1	Е	370	LEU	
1	Е	376	ARG	
1	E	382	LEU	
1	E	393	GLN	
1	Е	395	MET	
1	Е	402	ARG	
1	F	36	ARG	
1	F	37	ASP	
1	F	42	ARG	
1	F	44	ARG	
1	F	96	GLN	
1	F	97	ASP	
1	F	112	PHE	
1	F	125	ARG	
1	F	128	VAL	
1	F	129	ASP	



Mol	Chain	Res	Type	
1	F	132	LEU	
1	F	154	VAL	
1	F	179	LEU	
1	F	183	ARG	
1	F	188	GLU	
1	F	190	GLN	
1	F	191	ARG	
1	F	240	SER	
1	F	263	GLU	
1	F	291	VAL	
1	F	292	SER	
1	F	335	ASP	
1	F	382	LEU	
1	F	398	ARG	
1	G	86	THR	
1	G	103	ARG	
1	G	106	ARG	
1	G	112	PHE	
1	G	113	THR	
1	G	115	ARG	
1	G	116	ARG	
1	G	173	THR	
1	G	191	ARG	
1	G	194	GLN	
1	G	209	ASP	
1	G	264	ARG	
1	G	265	LYS	
1	G	312	ARG	
1	G	317	CYS	
1	G	332	ASP	
1	G	343	ARG	
1	G	360	GLN	
1	G	380	LEU	
1	G	402	ARG	
1	Н	41	SER	
1	Н	43	VAL	
1	Н	83	MET	
1	Н	96	GLN	
1	Н	107	LEU	
1	Н	112	PHE	
1	Н	123	ARG	
1	Н	128	VAL	


Mol	Chain	Res	Type
1	Н	132	LEU
1	Н	182	THR
1	Н	183	ARG
1	Н	198	VAL
1	Н	201	ASP
1	Н	221	LEU
1	Н	225	ASN
1	Н	237	MET
1	Н	256	LEU
1	Н	264	ARG
1	Н	265	LYS
1	Н	283	GLU
1	Н	288	THR
1	Н	297	VAL
1	Н	344	ASN
1	Н	380	LEU
1	Н	382	LEU
1	Н	400	LEU
1	Ι	36	ARG
1	Ι	38	GLU
1	Ι	42	ARG
1	Ι	58	MET
1	Ι	62	ARG
1	Ι	93	VAL
1	Ι	103	ARG
1	Ι	105	ARG
1	Ι	106	ARG
1	Ι	107	LEU
1	Ι	140	SER
1	Ι	160	LEU
1	I	168	ARG
1	Ι	169	ASP
1	Ι	203	LEU
1	Ι	207	ARG
1	Ι	209	ASP
1	Ι	224	ASP
1	Ι	241	LEU
1	Ι	255	ASN
1	Ι	259	LEU
1	Ι	266	ARG
1	I	284	MET
1	Ι	286	ARG



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Mol	Chain	Res	Type
1	Ι	288	THR
1	Ι	292	SER
1	Ι	327	ASP
1	Ι	338	ASP
1	Ι	363	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	228	HIS
1	А	246	HIS
1	А	320	HIS
1	В	193	GLN
1	В	246	HIS
1	В	320	HIS
1	В	344	ASN
1	В	393	GLN
1	С	96	GLN
1	С	193	GLN
1	С	228	HIS
1	С	236	ASN
1	С	246	HIS
1	С	320	HIS
1	С	351	HIS
1	D	194	GLN
1	D	228	HIS
1	D	236	ASN
1	D	246	HIS
1	D	354	HIS
1	Е	190	GLN
1	Е	246	HIS
1	Е	320	HIS
1	F	30	HIS
1	F	190	GLN
1	F	228	HIS
1	F	236	ASN
1	F	354	HIS
1	G	206	GLN
1	G	246	HIS
1	Н	194	GLN
1	Н	246	HIS
1	Н	320	HIS



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Mol	Chain	Res	Type
1	Н	344	ASN
1	Ι	255	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

18 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).

Mal	Turne	Chain	Dec	Tink	Bo	Bond lengths			ond ang	gles
WIOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DEB	Ι	502	-	$27,\!27,\!27$	1.08	1 (3%)	$35,\!39,\!39$	1.19	4 (11%)
2	HEM	В	501	1	$41,\!50,\!50$	1.32	4 (9%)	45,82,82	1.89	12 (26%)
3	DEB	А	502	-	27,27,27	1.11	2 (7%)	35,39,39	1.02	2 (5%)
2	HEM	G	501	1	41,50,50	1.31	5 (12%)	45,82,82	1.74	9 (20%)
3	DEB	F	502	-	27,27,27	1.10	1 (3%)	35,39,39	1.38	5 (14%)
3	DEB	Е	502	-	$27,\!27,\!27$	1.12	1 (3%)	35,39,39	1.36	3 (8%)
3	DEB	Н	502	-	$27,\!27,\!27$	1.07	1 (3%)	$35,\!39,\!39$	1.17	2 (5%)
2	HEM	А	501	1,4	41,50,50	1.32	5 (12%)	45,82,82	1.79	11 (24%)
2	HEM	Ι	501	-	41,50,50	1.34	5 (12%)	45,82,82	1.80	10 (22%)



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm sths}$	B	ond ang	gles
INIOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	HEM	Н	501	1,4	41,50,50	1.31	6 (14%)	45,82,82	1.76	7 (15%)
3	DEB	В	502	-	27,27,27	1.10	1 (3%)	35,39,39	1.19	3 (8%)
3	DEB	G	502	-	27,27,27	1.12	1 (3%)	35,39,39	1.11	1 (2%)
2	HEM	F	501	1,4	41,50,50	1.30	5 (12%)	45,82,82	1.85	9 (20%)
3	DEB	С	502	-	27,27,27	1.12	1 (3%)	35,39,39	1.19	3 (8%)
2	HEM	Е	501	1	41,50,50	1.35	6 (14%)	45,82,82	1.72	9 (20%)
2	HEM	D	501	-	41,50,50	1.31	6 (14%)	45,82,82	1.80	10 (22%)
2	HEM	С	501	1	41,50,50	1.39	5 (12%)	45,82,82	1.85	8 (17%)
3	DEB	D	502	-	27,27,27	1.12	1 (3%)	35,39,39	1.32	7 (20%)

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
3	DEB	Ι	502	-	-	8/50/50/50	0/1/1/1
2	HEM	В	501	1	-	0/12/54/54	-
3	DEB	А	502	-	-	1/50/50/50	0/1/1/1
2	HEM	G	501	1	-	0/12/54/54	-
3	DEB	F	502	-	-	13/50/50/50	0/1/1/1
3	DEB	Е	502	-	-	15/50/50/50	0/1/1/1
3	DEB	Н	502	-	-	8/50/50/50	0/1/1/1
2	HEM	А	501	1,4	-	0/12/54/54	-
2	HEM	Ι	501	-	-	4/12/54/54	-
2	HEM	Н	501	1,4	-	2/12/54/54	-
3	DEB	В	502	-	-	12/50/50/50	0/1/1/1
3	DEB	G	502	-	-	4/50/50/50	0/1/1/1
2	HEM	F	501	1,4	-	0/12/54/54	-
3	DEB	С	502	-	-	8/50/50/50	0/1/1/1
2	HEM	Е	501	1	-	4/12/54/54	-
2	HEM	D	501	-	-	3/12/54/54	-
2	HEM	С	501	1	-	2/12/54/54	-
3	DEB	D	502	-	-	9/50/50/50	0/1/1/1

All (57) bond length outliers are listed below:



5M]	N	V
OWL	LN	v

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
3	Ε	502	DEB	O16-C1	5.52	1.47	1.34
3	G	502	DEB	O16-C1	5.38	1.46	1.34
3	В	502	DEB	O16-C1	5.21	1.46	1.34
3	Ι	502	DEB	O16-C1	5.15	1.46	1.34
3	С	502	DEB	O16-C1	5.12	1.46	1.34
3	Н	502	DEB	O16-C1	5.08	1.46	1.34
3	F	502	DEB	O16-C1	5.02	1.46	1.34
3	D	502	DEB	O16-C1	4.96	1.45	1.34
3	А	502	DEB	O16-C1	4.79	1.45	1.34
2	В	501	HEM	C1B-NB	-4.01	1.33	1.40
2	D	501	HEM	C1B-NB	-3.88	1.33	1.40
2	С	501	HEM	C1B-NB	-3.83	1.33	1.40
2	А	501	HEM	C1B-NB	-3.69	1.33	1.40
2	С	501	HEM	C4D-ND	-3.65	1.34	1.40
2	Е	501	HEM	C1B-NB	-3.63	1.34	1.40
2	F	501	HEM	C1B-NB	-3.61	1.34	1.40
2	Н	501	HEM	C1B-NB	-3.49	1.34	1.40
2	Ι	501	HEM	C1B-NB	-3.43	1.34	1.40
2	G	501	HEM	C1B-NB	-3.40	1.34	1.40
2	Ι	501	HEM	FE-NB	3.03	2.11	1.96
2	Ι	501	HEM	C4D-ND	-3.02	1.35	1.40
2	F	501	HEM	C4D-ND	-2.93	1.35	1.40
2	Н	501	HEM	FE-NB	2.87	2.11	1.96
2	G	501	HEM	C4D-ND	-2.85	1.35	1.40
2	А	501	HEM	C4D-ND	-2.84	1.35	1.40
2	F	501	HEM	FE-NB	2.84	2.10	1.96
2	В	501	HEM	C4D-ND	-2.84	1.35	1.40
2	G	501	HEM	FE-NB	2.79	2.10	1.96
2	Е	501	HEM	FE-NB	2.76	2.10	1.96
2	Ε	501	HEM	C4D-ND	-2.76	1.35	1.40
2	С	501	HEM	FE-NB	2.73	2.10	1.96
2	А	501	HEM	FE-NB	2.68	2.10	1.96
2	D	501	HEM	C4B-NB	-2.68	1.33	1.38
2	В	501	HEM	FE-NB	2.66	2.10	1.96
2	Н	501	HEM	C4D-ND	-2.64	1.35	1.40
2	В	501	HEM	CHB-C1B	2.47	1.41	1.35
2	Н	501	HEM	CHB-C1B	2.45	1.41	1.35
2	A	501	HEM	CHB-C1B	2.43	1.41	1.35
2	A	501	HEM	C4B-NB	-2.40	1.33	1.38
2	F	501	HEM	CHB-C1B	2.39	1.41	1.35
2	Ε	501	HEM	C3B-C4B	2.39	1.49	1.44
2	С	501	HEM	CHB-C1B	2.38	1.41	1.35
2	D	501	HEM	FE-NB	2.35	2.08	1.96



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C4D-ND	-2.35	1.36	1.40
2	G	501	HEM	C4B-NB	-2.33	1.34	1.38
3	А	502	DEB	O16-C13	-2.29	1.42	1.46
2	Н	501	HEM	C3B-C4B	2.24	1.49	1.44
2	Ι	501	HEM	CHB-C1B	2.23	1.40	1.35
2	Е	501	HEM	C4B-NB	-2.23	1.34	1.38
2	D	501	HEM	C3B-C4B	2.22	1.49	1.44
2	Н	501	HEM	C4B-NB	-2.17	1.34	1.38
2	Е	501	HEM	CHB-C1B	2.16	1.40	1.35
2	G	501	HEM	CHB-C1B	2.15	1.40	1.35
2	С	501	HEM	C4B-NB	-2.10	1.34	1.38
2	F	501	HEM	C4B-NB	-2.08	1.34	1.38
2	D	501	HEM	CHB-C1B	2.07	1.40	1.35
2	Ι	501	HEM	C3B-C4B	2.06	1.49	1.44

1: 1 0

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	В	501	HEM	C1B-NB-C4B	5.07	110.31	105.07
2	С	501	HEM	CHC-C4B-NB	4.96	129.82	124.43
2	D	501	HEM	C1B-NB-C4B	4.88	110.12	105.07
2	В	501	HEM	CHC-C4B-NB	4.88	129.73	124.43
2	F	501	HEM	CHD-C1D-ND	4.83	129.68	124.43
2	С	501	HEM	C1B-NB-C4B	4.82	110.06	105.07
2	А	501	HEM	C1B-NB-C4B	4.82	110.05	105.07
2	F	501	HEM	CHC-C4B-NB	4.71	129.55	124.43
2	Ι	501	HEM	CHC-C4B-NB	4.60	129.42	124.43
2	F	501	HEM	C1B-NB-C4B	4.59	109.82	105.07
2	G	501	HEM	CHC-C4B-NB	4.57	129.40	124.43
2	G	501	HEM	C1B-NB-C4B	4.50	109.72	105.07
2	Н	501	HEM	C1B-NB-C4B	4.47	109.69	105.07
2	А	501	HEM	CHC-C4B-NB	4.33	129.13	124.43
2	Ι	501	HEM	CHD-C1D-ND	4.32	129.12	124.43
2	Е	501	HEM	C1B-NB-C4B	4.32	109.53	105.07
3	С	502	DEB	O16-C1-C2	4.27	120.94	111.56
2	В	501	HEM	CHD-C1D-ND	4.21	129.00	124.43
2	Н	501	HEM	CHD-C1D-ND	4.20	129.00	124.43
2	D	501	HEM	CHC-C4B-NB	4.18	128.97	124.43
2	Н	501	HEM	CHC-C4B-NB	4.11	128.89	124.43
3	В	502	DEB	O16-C1-C2	4.10	120.55	111.56
2	G	501	HEM	CHD-C1D-ND	4.04	128.82	124.43
2	Е	501	HEM	CHD-C1D-ND	4.04	128.81	124.43



5N	1N	V
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Н	501	HEM	CHA-C4D-ND	4.02	129.34	124.38
2	Е	501	HEM	CHC-C4B-NB	4.01	128.79	124.43
2	А	501	HEM	CHD-C1D-ND	3.88	128.64	124.43
2	С	501	HEM	CHD-C1D-ND	3.87	128.64	124.43
3	Е	502	DEB	O16-C1-C2	3.83	119.96	111.56
2	D	501	HEM	CHD-C1D-ND	3.79	128.55	124.43
3	Ι	502	DEB	O16-C1-C2	3.78	119.86	111.56
3	Е	502	DEB	C6-C5-C4	-3.78	110.41	116.27
2	Ι	501	HEM	C1B-NB-C4B	3.73	108.92	105.07
2	F	501	HEM	CHA-C4D-ND	3.70	128.96	124.38
2	G	501	HEM	CHA-C4D-ND	3.58	128.81	124.38
3	G	502	DEB	O16-C1-C2	3.49	119.22	111.56
2	Ι	501	HEM	CHA-C4D-ND	3.47	128.66	124.38
2	D	501	HEM	CHA-C4D-ND	3.38	128.56	124.38
2	F	501	HEM	CHD-C1D-C2D	-3.29	119.83	124.98
2	Е	501	HEM	CHA-C4D-ND	3.27	128.42	124.38
2	С	501	HEM	CHA-C4D-ND	3.24	128.39	124.38
2	D	501	HEM	CHD-C1D-C2D	-3.24	119.91	124.98
3	Н	502	DEB	O16-C1-C2	3.21	118.61	111.56
2	В	501	HEM	CHA-C4D-ND	3.17	128.30	124.38
2	А	501	HEM	CHD-C1D-C2D	-3.12	120.10	124.98
2	Е	501	HEM	CHD-C1D-C2D	-3.07	120.18	124.98
3	D	502	DEB	C23-C8-C7	3.02	117.91	111.55
2	Н	501	HEM	CHA-C4D-C3D	-3.01	119.67	125.33
2	С	501	HEM	CAD-CBD-CGD	-3.00	107.14	113.60
2	А	501	HEM	CHA-C4D-ND	3.00	128.09	124.38
2	С	501	HEM	CHD-C1D-C2D	-2.92	120.41	124.98
2	В	501	HEM	CHD-C1D-C2D	-2.91	120.43	124.98
2	Е	501	HEM	CMD-C2D-C1D	2.88	129.42	125.04
2	Ι	501	HEM	CHD-C1D-C2D	-2.77	120.65	124.98
2	D	501	HEM	CHA-C4D-C3D	-2.74	120.19	125.33
3	D	502	DEB	O16-C13-C12	2.74	112.65	107.78
2	В	501	HEM	C4B-C3B-C2B	-2.73	104.95	107.11
2	А	501	HEM	CHB-C1B-NB	2.71	127.73	124.38
2	Н	501	HEM	CHD-C1D-C2D	-2.68	120.79	124.98
2	G	501	HEM	CHD-C1D-C2D	-2.68	120.80	124.98
2	В	501	HEM	CMD-C2D-C1D	2.63	129.05	125.04
2	C	501	HEM	C4B-C3B-C2B	-2.60	105.05	107.11
2	D	501	HEM	CHB-C1B-NB	2.57	127.56	124.38
3	D	502	DEB	C11-C10-C9	2.57	115.00	110.36
2	G	501	HEM	CHA-C4D-C3D	-2.56	120.52	125.33
3	D	502	DEB	O16-C1-C2	2.55	117.16	111.56



5M	NV	-
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	$Ideal(^{o})$
2	Ι	501	HEM	CBA-CAA-C2A	2.53	116.94	112.62
3	F	502	DEB	O16-C1-C2	2.52	117.10	111.56
3	Ι	502	DEB	C13-O16-C1	-2.52	114.12	117.89
2	А	501	HEM	CAD-C3D-C4D	2.50	129.02	124.66
2	F	501	HEM	CHA-C4D-C3D	-2.45	120.72	125.33
2	А	501	HEM	CMD-C2D-C1D	2.44	128.76	125.04
2	Е	501	HEM	CAD-C3D-C4D	2.42	128.88	124.66
2	Е	501	HEM	CHA-C4D-C3D	-2.41	120.80	125.33
2	А	501	HEM	CHA-C4D-C3D	-2.41	120.80	125.33
2	Ι	501	HEM	CHA-C4D-C3D	-2.35	120.92	125.33
2	С	501	HEM	CHA-C4D-C3D	-2.35	120.92	125.33
2	В	501	HEM	CAD-CBD-CGD	-2.33	108.59	113.60
2	Ι	501	HEM	C4B-C3B-C2B	-2.33	105.27	107.11
2	В	501	HEM	CAD-C3D-C4D	2.32	128.71	124.66
2	G	501	HEM	CHB-C1B-NB	2.31	127.24	124.38
2	А	501	HEM	CMA-C3A-C4A	-2.31	124.92	128.46
2	Ε	501	HEM	CHB-C1B-NB	2.31	127.23	124.38
3	А	502	DEB	O16-C13-C12	2.28	111.85	107.78
3	В	502	DEB	O16-C1-O17	-2.27	119.70	123.94
3	Ι	502	DEB	O16-C1-O17	-2.25	119.74	123.94
3	F	502	DEB	C5-C4-C3	-2.24	108.03	112.54
2	G	501	HEM	CMD-C2D-C1D	2.23	128.44	125.04
3	В	502	DEB	C22-C6-C5	-2.23	107.40	111.54
2	F	501	HEM	CAD-CBD-CGD	-2.23	108.81	113.60
3	Η	502	DEB	C25-C10-C9	2.23	111.94	108.08
3	С	502	DEB	C13-O16-C1	-2.21	114.58	117.89
3	Ε	502	DEB	C18-C2-C3	-2.21	108.69	112.37
3	F	502	DEB	O21-C5-C6	-2.20	105.69	109.83
2	D	501	HEM	C4B-CHC-C1C	2.20	125.45	122.56
3	D	502	DEB	O26-C11-C10	2.20	113.92	108.82
2	H	501	HEM	CMD-C2D-C1D	2.19	128.37	125.04
3	I	502	DEB	O16-C13-C14	2.17	110.39	106.92
2	D	501	HEM	CBA-CAA-C2A	2.16	116.31	112.62
3	А	502	DEB	O16-C1-C2	2.15	116.27	111.56
2	I	501	HEM	CMD-C2D-C1D	2.14	128.30	125.04
2	F	501	HEM	C4B-C3B-C2B	-2.12	105.43	107.11
2	В	501	HEM	CHB-C1B-NB	2.12	127.00	124.38
2	А	501	HEM	C4B-C3B-C2B	-2.11	105.44	107.11
2	F	501	HEM	CMD-C2D-C1D	2.11	128.26	125.04
3	F	502	DEB	C7-C8-C9	-2.09	105.93	110.85
2	В	501	HEM	CHA-C4D-C3D	-2.08	121.41	125.33
3	D	502	DEB	C22-C6-C7	2.08	113.80	110.69



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	F	502	DEB	C6-C5-C4	2.07	119.48	116.27
2	G	501	HEM	O2D-CGD-O1D	-2.06	118.16	123.30
3	С	502	DEB	O17-C1-C2	-2.04	118.61	124.08
3	D	502	DEB	C22-C6-C5	-2.04	107.75	111.54
2	В	501	HEM	CMC-C2C-C3C	2.03	128.47	124.68
2	D	501	HEM	O2A-CGA-CBA	2.02	120.53	114.03
2	Ι	501	HEM	CAD-C3D-C4D	2.01	128.16	124.66

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
2	С	501	HEM	C2D-C3D-CAD-CBD
2	Ι	501	HEM	C1A-C2A-CAA-CBA
2	Ι	501	HEM	C3A-C2A-CAA-CBA
3	D	502	DEB	C4-C5-C6-C7
3	D	502	DEB	O21-C5-C6-C7
3	D	502	DEB	O21-C5-C6-C22
3	D	502	DEB	C22-C6-C7-C8
3	D	502	DEB	C11-C10-C9-C8
3	D	502	DEB	C11-C10-C9-O24
3	Е	502	DEB	C5-C6-C7-C8
3	F	502	DEB	C9-C10-C11-O26
3	F	502	DEB	C11-C12-C13-O16
3	F	502	DEB	C27-C12-C13-O16
3	G	502	DEB	C1-C2-C3-C4
3	Н	502	DEB	C11-C12-C13-O16
3	Н	502	DEB	C27-C12-C13-O16
2	С	501	HEM	C4D-C3D-CAD-CBD
3	Ι	502	DEB	C2-C1-O16-C13
3	Ι	502	DEB	O17-C1-O16-C13
3	В	502	DEB	C3-C4-C5-O21
3	F	502	DEB	O19-C3-C4-C5
3	F	502	DEB	O19-C3-C4-C20
3	С	502	DEB	C18-C2-C3-C4
3	С	502	DEB	C3-C4-C5-O21
3	В	502	DEB	C2-C1-O16-C13
3	Е	502	DEB	C3-C4-C5-O21
3	F	502	DEB	C2-C3-C4-C5
3	F	502	DEB	C9-C10-C11-C12
3	В	502	DEB	C20-C4-C5-O21
3	С	502	DEB	C20-C4-C5-O21

All (93) torsion outliers are listed below:



5MNV	
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Mol	Chain	Res	Type	Atoms
3	Е	502	DEB	C20-C4-C5-O21
3	B	502	DEB	C18-C2-C3-C4
3	F	502	DEB	C25-C10-C11-C12
3	Ι	502	DEB	C18-C2-C3-C4
3	В	502	DEB	O17-C1-O16-C13
3	Е	502	DEB	C11-C10-C9-O24
3	F	502	DEB	C2-C3-C4-C20
3	D	502	DEB	C5-C6-C7-C8
3	В	502	DEB	C18-C2-C3-O19
3	С	502	DEB	C18-C2-C3-O19
3	Ι	502	DEB	C18-C2-C3-O19
3	Е	502	DEB	C11-C10-C9-C8
3	G	502	DEB	C18-C2-C3-C4
3	F	502	DEB	C27-C12-C13-C14
3	Ι	502	DEB	C3-C4-C5-O21
2	Е	501	HEM	C2A-CAA-CBA-CGA
3	В	502	DEB	C3-C4-C5-C6
3	F	502	DEB	C11-C12-C13-C14
3	Н	502	DEB	C11-C12-C13-C14
3	E	502	DEB	C18-C2-C3-C4
3	F	502	DEB	C18-C2-C3-C4
3	E	502	DEB	C25-C10-C9-O24
3	D	502	DEB	C3-C4-C5-O21
2	D	501	HEM	C2A-CAA-CBA-CGA
3	В	502	DEB	C1-C2-C3-C4
3	В	502	DEB	C1-C2-C3-O19
3	С	502	DEB	C1-C2-C3-C4
3	С	502	DEB	C1-C2-C3-O19
3	Ι	502	DEB	C1-C2-C3-C4
3	Ι	502	DEB	C1-C2-C3-O19
3	H	502	DEB	C9-C10-C11-O26
2	E	501	HEM	C3D-CAD-CBD-CGD
3	D	502	DEB	C18-C2-C3-C4
3	Н	502	DEB	C9-C10-C11-C12
3	E	502	DEB	C4-C5-C6-C22
3	B	502	DEB	C20-C4-C5-C6
3	I	502	DEB	C20-C4-C5-O21
3	E	502	DEB	C22-C6-C7-C8
2	D	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O1A
3	B	502	DEB	O21-C5-C6-C7
3	E	502	DEB	C20-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	Ι	501	HEM	CAA-CBA-CGA-O1A
3	Е	502	DEB	O21-C5-C6-C22
2	Ι	501	HEM	CAA-CBA-CGA-O2A
2	Н	501	HEM	CAD-CBD-CGD-O2D
3	С	502	DEB	C3-C4-C5-C6
3	Ε	502	DEB	C3-C4-C5-C6
3	Н	502	DEB	C27-C12-C13-C14
2	Н	501	HEM	CAD-CBD-CGD-O1D
3	Е	502	DEB	C10-C11-C12-C27
3	Е	502	DEB	C25-C10-C9-C8
3	G	502	DEB	C11-C10-C9-O24
2	Ε	501	HEM	CAA-CBA-CGA-O2A
3	С	502	DEB	C20-C4-C5-C6
3	В	502	DEB	C11-C12-C13-O16
2	Ε	501	HEM	CAA-CBA-CGA-O1A
3	А	502	DEB	C11-C10-C9-C8
3	F	502	DEB	C11-C10-C9-C8
3	G	502	DEB	C11-C10-C9-C8
3	Н	502	DEB	C11-C10-C9-C8
3	Н	502	DEB	C11-C10-C9-O24
3	Е	502	DEB	C4-C5-C6-C7

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There are no ring outliers.

15 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	501	HEM	3	0
3	А	502	DEB	1	0
2	G	501	HEM	4	0
3	F	502	DEB	1	0
3	Е	502	DEB	2	0
3	Н	502	DEB	1	0
2	А	501	HEM	5	0
2	Ι	501	HEM	8	0
2	Н	501	HEM	10	0
3	G	502	DEB	1	0
2	F	501	HEM	4	0
2	Ε	501	HEM	5	0
2	D	501	HEM	3	0
2	С	501	HEM	3	0
3	D	502	DEB	6	0



5MNV

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

















































































5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	А	397/407~(97%)	-0.48	5 (1%) 77 59	23, 43, 96, 128	0
1	В	394/407~(96%)	-0.36	0 100 100	33,67,97,113	0
1	С	396/407~(97%)	-0.49	1 (0%) 94 87	19, 54, 82, 116	0
1	D	394/407~(96%)	-0.44	4 (1%) 82 66	28, 50, 96, 125	0
1	Е	390/407~(95%)	-0.07	8 (2%) 63 43	34, 80, 117, 130	0
1	F	395/407~(97%)	-0.37	2 (0%) 91 80	30,64,98,117	0
1	G	380/407~(93%)	0.26	30 (7%) 12 6	45, 96, 140, 168	0
1	Н	395/407~(97%)	-0.15	6 (1%) 73 54	37, 71, 108, 148	0
1	Ι	286/407~(70%)	1.15	68~(23%) 0 0	88, 121, 148, 182	0
All	All	3427/3663~(93%)	-0.15	124 (3%) 42 26	19, 67, 126, 182	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ι	204	VAL	8.5
1	Ι	39	PRO	7.9
1	Н	185	THR	6.7
1	Ι	177	ALA	6.5
1	Ι	59	SER	5.7
1	G	194	GLN	5.2
1	Ι	203	LEU	5.1
1	Ι	122	PRO	5.1
1	Ι	330	VAL	4.8
1	G	213	GLU	4.8
1	Ι	223	THR	4.6
1	Ι	331	PHE	4.5
1	Ι	36	ARG	4.5
1	D	184	LEU	4.4
1	G	199	TYR	4.4



Mol	Chain	Res	Type	RSRZ
1	G	191	ARG	4.2
1	Ι	225	ASN	4.0
1	Ι	40	VAL	3.9
1	Ι	272	ALA	3.9
1	Ι	334	ALA	3.8
1	Ι	57	ARG	3.8
1	G	211	PRO	3.8
1	G	196	PHE	3.8
1	Ι	163	VAL	3.7
1	G	106	ARG	3.7
1	Ι	287	TYR	3.6
1	Ι	205	ALA	3.6
1	Ι	193	GLN	3.4
1	Ι	202	GLY	3.4
1	Ι	166	GLU	3.4
1	G	204	VAL	3.4
1	Ι	56	THR	3.4
1	G	308	THR	3.3
1	Ι	100	ASP	3.2
1	D	188	GLU	3.2
1	G	49	GLU	3.2
1	G	208	ARG	3.2
1	G	222	ALA	3.2
1	G	209	ASP	3.1
1	F	185	THR	3.1
1	G	221	LEU	3.1
1	Ι	234	ILE	3.1
1	Ι	393	GLN	3.1
1	Ι	165	LEU	3.1
1	Ι	41	SER	3.1
1	Е	13	ALA	3.0
1	G	195	ASP	3.0
1	Ι	30	HIS	3.0
1	Ι	209	ASP	3.0
1	G	200	MET	2.9
1	Ι	358	GLY	2.9
1	G	53	TRP	2.9
1	Ι	112	PHE	2.9
1	Н	224	ASP	2.9
1	Ι	61	ALA	2.9
1	Ι	222	ALA	2.9
1	Ι	206	GLN	2.9



Mol	Chain	Res	Type	RSRZ	
1	Ι	95	ALA	2.8	
1	Ι	187	ALA	2.8	
1	D	183	ARG	2.8	
1	Ι	335	ASP	2.8	
1	А	185	THR	2.8	
1	Е	226	ASP	2.8	
1	Ι	385	PRO	2.7	
1	Ι	201	ASP	2.7	
1	Ι	230	THR	2.7	
1	Ι	208	ARG	2.7	
1	G	202	GLY	2.7	
1	Ι	231	LYS	2.7	
1	Н	184	LEU	2.7	
1	Ι	329	GLU	2.6	
1	Ι	113	THR	2.6	
1	А	12	ASP	2.6	
1	Ι	337	LEU	2.6	
1	G	174	PHE	2.6	
1	Ι	195	ASP	2.6	
1	Ι	106	ARG	2.6	
1	Ι	399	GLY	2.5	
1	Ι	103	ARG	2.5	
1	Н	225	ASN	2.5	
1	Ι	236	ASN	2.5	
1	Ι	98	PRO	2.5	
1	Ι	333	HIS	2.5	
1	Е	206	GLN	2.5	
1	G	230	THR	2.5	
1	Ι	167	ASP	2.5	
1	Ι	224	ASP	2.5	
1	Ι	38	GLU	2.4	
1	Ι	35	ARG	2.4	
1	Е	303	ASP	2.4	
1	Ι	126	SER	2.4	
1	G	210	ALA	2.4	
1	Ι	269	SER	2.4	
1	Ι	274	PRO	2.3	
1	А	187	ALA	2.3	
1	G	224	ASP	2.3	
1	D	225	ASN	2.3	
1	G	30	HIS	2.3	
1	С	36	ARG	2.3	



Mol	Chain	Res	Type	RSRZ	
1	А	13	ALA	2.3	
1	Н	63	ILE	2.2	
1	F	50	GLY	2.2	
1	Ι	97	ASP	2.2	
1	Ι	211	PRO	2.2	
1	G	218	ALA	2.2	
1	G	231	LYS	2.2	
1	G	36	ARG	2.2	
1	Е	203	LEU	2.2	
1	А	186	ALA	2.2	
1	Е	227	ASP	2.1	
1	Ι	332	ASP	2.1	
1	Ι	261	LEU	2.1	
1	Ι	336	GLU	2.1	
1	G	41	SER	2.1	
1	G	201	ASP	2.1	
1	Н	348	ALA	2.1	
1	Ι	96	GLN	2.0	
1	Ι	129	ASP	2.0	
1	Ι	200	MET	2.0	
1	G	242	LEU	2.0	
1	Ι	174	PHE	2.0	
1	Е	209	ASP	2.0	
1	G	238	GLY	2.0	
1	Е	81	PRO	2.0	

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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 monosaccharides 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. 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	$B-factors(Å^2)$	Q<0.9
3	DEB	G	502	27/27	0.84	0.33	101,112,116,118	0
3	DEB	F	502	27/27	0.88	0.25	55,58,62,64	0
3	DEB	Ι	502	27/27	0.88	0.31	116,128,135,139	0
3	DEB	Н	502	27/27	0.89	0.22	60,65,68,71	0
2	HEM	Ι	501	43/43	0.89	0.21	107,135,141,146	0
3	DEB	А	502	27/27	0.93	0.19	$41,\!46,\!53,\!56$	0
3	DEB	D	502	27/27	0.94	0.20	$41,\!44,\!51,\!52$	0
3	DEB	Е	502	27/27	0.94	0.23	72,77,82,85	0
2	HEM	F	501	43/43	0.94	0.22	65,81,84,89	0
2	HEM	В	501	43/43	0.96	0.21	54,60,71,80	0
2	HEM	G	501	43/43	0.96	0.24	77,84,97,98	0
2	HEM	Н	501	43/43	0.96	0.22	63,84,89,94	0
2	HEM	D	501	43/43	0.96	0.18	31,35,41,44	0
2	HEM	Е	501	43/43	0.96	0.27	61,68,81,86	0
3	DEB	В	502	27/27	0.96	0.18	$51,\!53,\!56,\!62$	0
2	HEM	С	501	43/43	0.97	0.20	43,46,52,57	0
3	DEB	С	502	27/27	0.97	0.17	42,45,47,50	0
2	HEM	А	501	43/43	0.98	0.16	26,35,38,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.








































































6.5 Other polymers (i)

There are no such residues in this entry.

