



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:28 PM GMT

PDB ID : 5C2V
Title : Kuenenia stuttgartiensis Hydrazine Synthase
Authors : Dietl, A.; Ferousi, C.; Maalcke, W.J.; Menzel, A.; de Vries, S.; Keltjens, J.T.;
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Deposited on : 2015-06-16
Resolution : 2.70 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

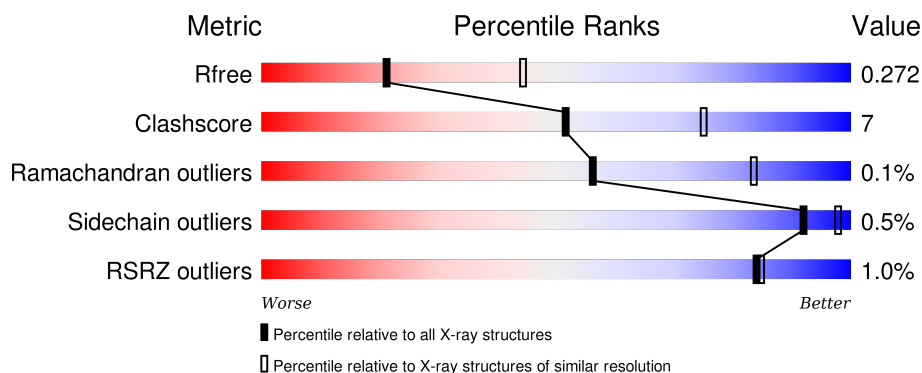
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 $\leq 5\%$. 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	782	<div> <div>85%</div> <div>13%</div> <div>•</div> </div>
1	D	782	<div> <div>2%</div> <div>85%</div> <div>14%</div> <div>•</div> </div>
2	B	352	<div> <div>79%</div> <div>21%</div> </div>
2	E	352	<div> <div>2%</div> <div>78%</div> <div>22%</div> </div>
3	C	314	<div> <div>2%</div> <div>84%</div> <div>15%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	314	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	901[A]	-	-	-	X
4	CL	A	901[B]	-	-	-	X
8	BET	A	907	-	-	-	X
8	BET	A	909	-	-	-	X
8	BET	D	907	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 23385 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 HYDRAZINE SYNTHASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	768	Total	C	N	O	S	0	0	0
			6081	3867	1045	1144	25			
1	D	770	Total	C	N	O	S	0	0	0
			6087	3871	1044	1147	25			

- Molecule 2 is a protein called HYDRAZINE SYNTHASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	0	1	0
			2706	1697	464	531	14			
2	E	352	Total	C	N	O	S	0	1	0
			2692	1688	459	531	14			

- Molecule 3 is a protein called HYDRAZINE SYNTHASE GAMMA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	314	Total	C	N	O	S	0	0	0
			2457	1543	432	472	10			
3	F	314	Total	C	N	O	S	0	0	0
			2443	1534	427	472	10			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	1
			2	2		
4	D	1	Total	Cl	0	0
			1	1		

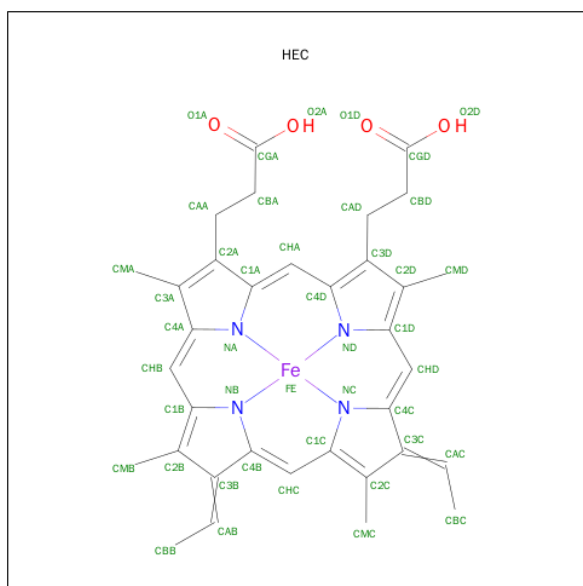
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	2	Total Ca 2 2	0	0
5	E	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0
5	C	3	Total Ca 3 3	0	0
5	A	2	Total Ca 2 2	0	0
5	F	3	Total Ca 3 3	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0
6	D	1	Total Zn 1 1	0	0

- Molecule 7 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



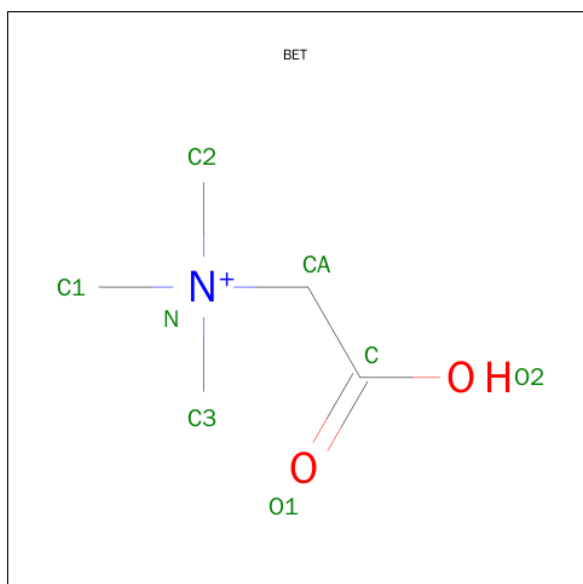
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C Fe N O 43 34 1 4 4	0	0
7	A	1	Total C Fe N O 43 34 1 4 4	0	0

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

- Molecule 8 is TRIMETHYL GLYCINE (three-letter code: BET) (formula: $C_5H_{12}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O		
			8	5	1	2		
8	A	1	Total	C	N	O		
			8	5	1	2		
8	A	1	Total	C	N	O		
			8	5	1	2		
8	B	1	Total	C	N	O		
			8	5	1	2		
8	C	1	Total	C	N	O		
			8	5	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	N	O	0	0
			8	5	1	2		
8	E	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		
9	E	1	Total	Mg	0	0
			1	1		

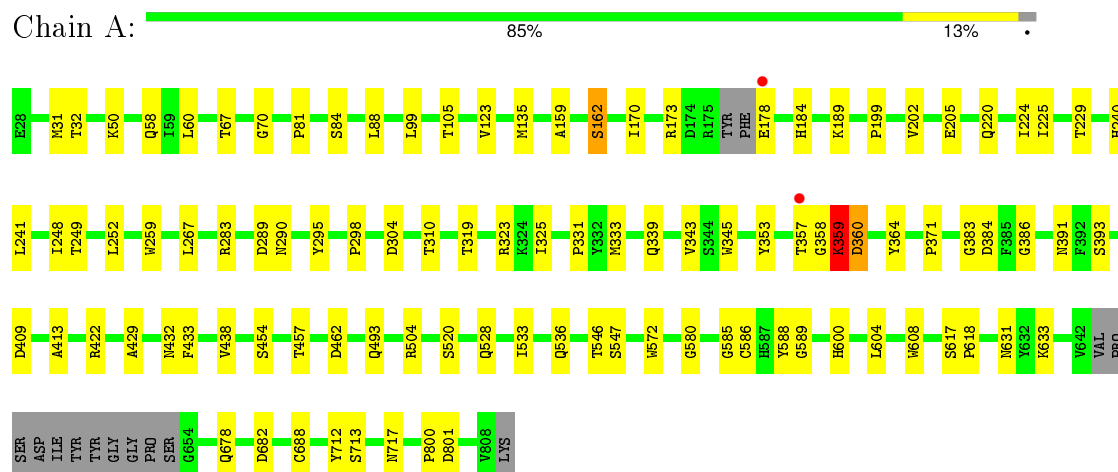
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	168	Total	O	0	0
			168	168		
10	B	60	Total	O	0	0
			60	60		
10	C	84	Total	O	0	0
			84	84		
10	D	112	Total	O	0	0
			112	112		
10	E	30	Total	O	0	0
			30	30		
10	F	46	Total	O	0	0
			46	46		

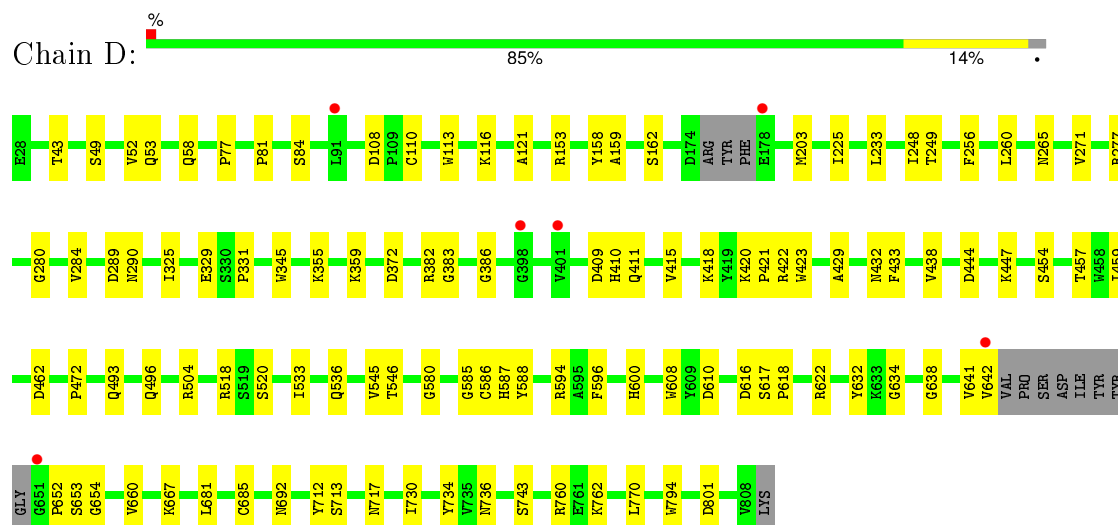
3 Residue-property plots

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.

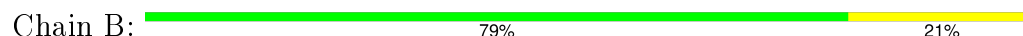
• Molecule 1: HYDRAZINE SYNTHASE ALPHA SUBUNIT

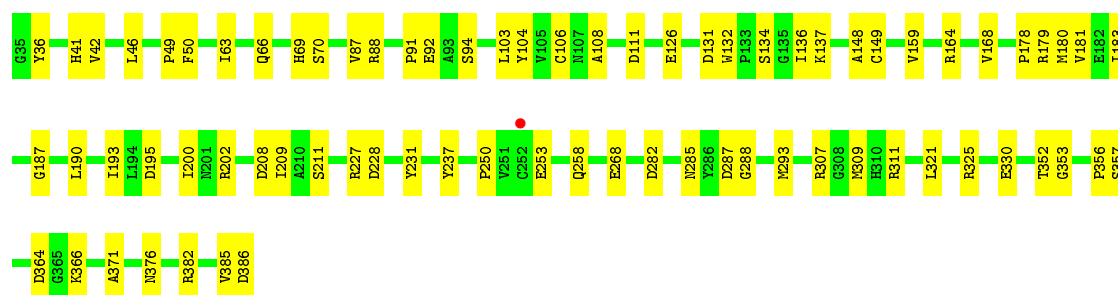


• Molecule 1: HYDRAZINE SYNTHASE ALPHA SUBUNIT

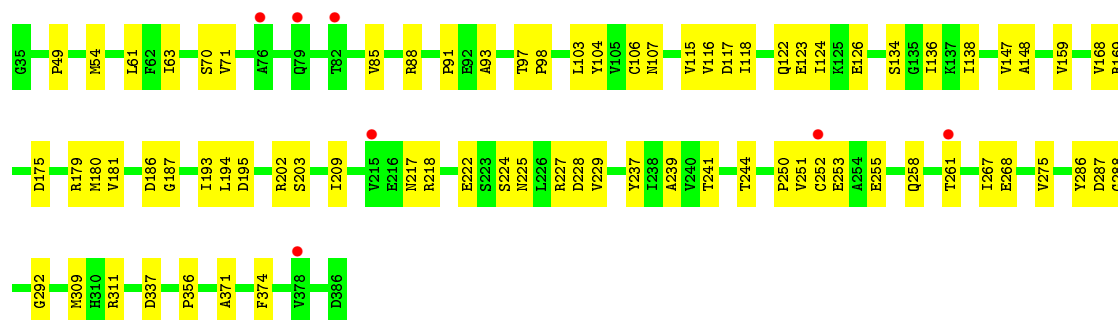
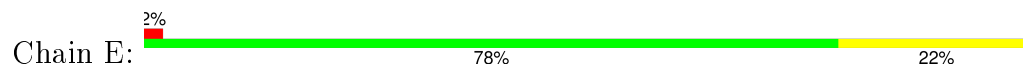


• Molecule 2: HYDRAZINE SYNTHASE BETA SUBUNIT

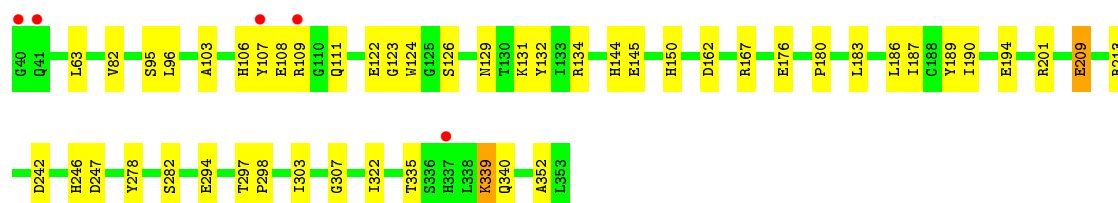
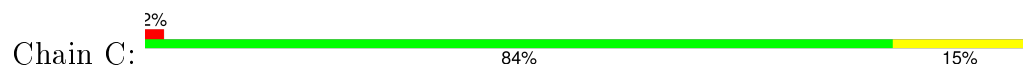




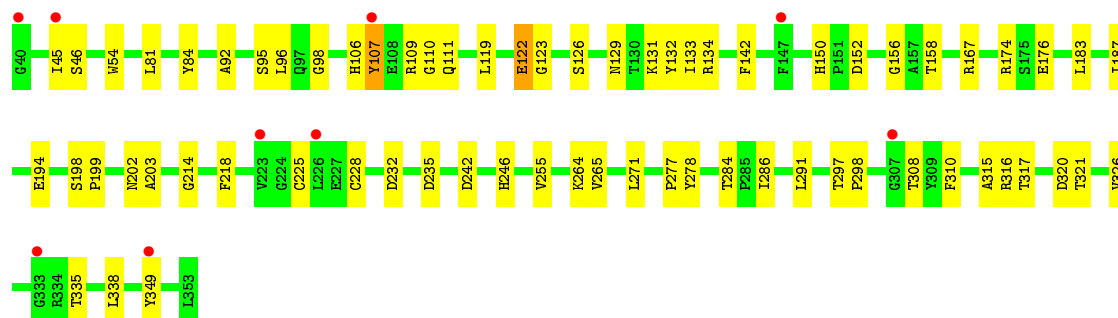
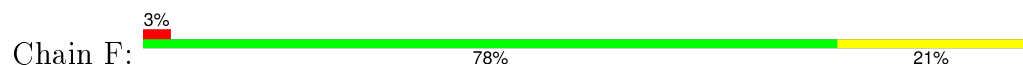
• Molecule 2: HYDRAZINE SYNTHASE BETA SUBUNIT



• Molecule 3: HYDRAZINE SYNTHASE GAMMA SUBUNIT



• Molecule 3: HYDRAZINE SYNTHASE GAMMA SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	464.54Å 464.54Å 145.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 48.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.70) 99.8 (48.98-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.234 , 0.271 0.241 , 0.272	Depositor DCC
R_{free} test set	8145 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 162815 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23385	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, CL, CA, ZN, HEC, BET

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	0.23	0/6259	0.44	0/8503
1	D	0.22	0/6266	0.43	0/8514
2	B	0.24	0/2758	0.49	0/3752
2	E	0.23	0/2744	0.49	0/3737
3	C	0.26	0/2522	0.46	0/3421
3	F	0.24	0/2508	0.45	0/3406
All	All	0.23	0/23057	0.45	0/31333

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	LYS	Peptide
1	A	360	ASP	Peptide
3	C	339	LYS	Peptide

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	6081	0	5783	72	0
1	D	6087	0	5784	72	0
2	B	2706	0	2675	49	0
2	E	2692	0	2642	52	0
3	C	2457	0	2324	41	0
3	F	2443	0	2291	45	0
4	A	2	0	0	2	0
4	D	1	0	0	1	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	F	3	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	86	0	61	10	0
7	C	86	0	59	6	0
7	D	86	0	60	7	0
7	F	86	0	59	4	0
8	A	24	0	33	0	0
8	B	8	0	11	0	0
8	C	8	0	11	0	0
8	D	8	0	11	0	0
8	E	8	0	11	0	0
9	B	1	0	0	0	0
9	E	1	0	0	0	0
10	A	168	0	0	1	0
10	B	60	0	0	1	0
10	C	84	0	0	3	0
10	D	112	0	0	4	0
10	E	30	0	0	1	0
10	F	46	0	0	2	0
All	All	23385	0	21815	303	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 7.

All (303) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:CYS:SG	7:A:906:HEC:CAC	2.16	1.32
1:A:688:CYS:SG	7:A:906:HEC:HBC1	1.83	1.07
1:A:688:CYS:CB	7:A:906:HEC:HBC2	1.84	1.06
1:A:688:CYS:SG	7:A:906:HEC:HBC2	0.51	1.04
1:A:688:CYS:SG	7:A:906:HEC:CBC	1.04	1.03
3:C:339:LYS:HG3	3:C:340:GLN:H	1.34	0.93
1:A:688:CYS:HG	7:A:906:HEC:HBC3	1.18	0.91
1:A:688:CYS:SG	7:A:906:HEC:C3C	2.61	0.88
1:D:520:SER:O	1:D:712:TYR:OH	2.01	0.78
2:B:288:GLY:H	2:B:309:MET:HG2	1.49	0.76
3:F:122:GLU:OE2	3:F:126:SER:OG	2.03	0.76
3:F:123:GLY:O	3:F:126:SER:OG	2.03	0.75
1:D:429:ALA:HB3	1:D:433:PHE:HB3	1.67	0.75
2:E:288:GLY:H	2:E:309:MET:HG2	1.53	0.74
1:A:688:CYS:SG	7:A:906:HEC:HBC3	1.32	0.73
3:C:122:GLU:OE2	10:C:501:HOH:O	2.06	0.73
2:E:122:GLN:NE2	2:E:123:GLU:O	2.24	0.71
3:C:339:LYS:HG3	3:C:340:GLN:N	2.06	0.71
1:D:642:VAL:HG12	1:D:652:PRO:HG3	1.71	0.70
1:D:608:TRP:NE1	1:D:610:ASP:O	2.24	0.70
1:D:438:VAL:O	3:F:167:ARG:NH2	2.24	0.69
3:F:129:ASN:ND2	10:F:501:HOH:O	2.26	0.69
1:A:422:ARG:NH1	3:C:95:SER:O	2.26	0.68
3:C:129:ASN:ND2	10:C:504:HOH:O	2.27	0.67
1:D:280:GLY:O	1:D:518:ARG:NH1	2.26	0.67
1:A:386:GLY:HA2	1:A:409:ASP:HB2	1.77	0.67
1:A:429:ALA:HB3	1:A:433:PHE:HB3	1.76	0.67
2:E:195:ASP:OD1	2:E:202:ARG:NH1	2.27	0.66
1:A:589:GLY:N	4:A:901[B]:CL:CL	2.66	0.66
2:B:250:PRO:O	2:B:258:GLN:NE2	2.29	0.66
3:C:307:GLY:O	10:C:502:HOH:O	2.12	0.65
1:A:32:THR:OG1	2:B:309:MET:O	2.12	0.64
1:D:418:LYS:NZ	10:D:1002:HOH:O	2.30	0.64
2:B:36:TYR:H	2:B:69:HIS:HE2	1.44	0.64
2:E:252:CYS:H	2:E:258:GLN:HE22	1.45	0.64
1:D:496:GLN:NE2	10:D:1003:HOH:O	2.31	0.64
1:D:622:ARG:NH2	1:D:667:LYS:O	2.31	0.63
1:A:422:ARG:HB2	3:C:176:GLU:HB2	1.80	0.62
1:D:386:GLY:HA2	1:D:409:ASP:HB2	1.80	0.62
1:D:248:ILE:HG13	1:D:249:THR:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:98:PRO:HD3	2:E:138:ILE:HD11	1.81	0.61
1:D:203:MET:O	1:D:496:GLN:NE2	2.33	0.61
3:C:322:ILE:HG23	3:C:335:THR:HG21	1.82	0.61
2:B:195:ASP:OD1	2:B:202:ARG:NH1	2.33	0.61
1:D:108:ASP:OD1	1:D:411:GLN:NE2	2.33	0.61
1:D:622:ARG:HD2	1:D:638:GLY:HA3	1.83	0.60
3:C:106:HIS:CD2	7:C:404:HEC:NB	2.70	0.60
2:B:227:ARG:NH2	3:C:107:TYR:HE1	2.00	0.60
1:D:422:ARG:HB3	3:F:176:GLU:HB2	1.84	0.59
1:D:760:ARG:NE	1:D:762:LYS:O	2.24	0.59
1:A:438:VAL:O	3:C:167:ARG:NH2	2.36	0.59
2:E:228:ASP:HB2	2:E:292:GLY:HA2	1.85	0.58
2:E:287:ASP:OD1	2:E:311:ARG:NH2	2.31	0.58
3:C:297:THR:HG22	7:C:405:HEC:HMD3	1.85	0.58
2:E:218:ARG:NH1	2:E:268:GLU:O	2.37	0.57
2:B:228:ASP:HB3	2:B:293:MET:HE2	1.85	0.57
1:A:162:SER:HB3	1:A:189:LYS:HB3	1.86	0.56
2:B:159:VAL:HG23	2:B:168:VAL:HB	1.87	0.56
1:A:432:ASN:ND2	1:A:454:SER:OG	2.34	0.56
3:F:106:HIS:CD2	7:F:404:HEC:NB	2.74	0.56
1:D:504:ARG:NH2	1:D:801:ASP:O	2.38	0.56
1:D:457:THR:O	1:D:580:GLY:HA2	2.06	0.55
1:A:248:ILE:HG13	1:A:249:THR:HG23	1.88	0.55
2:B:183:ILE:HG12	2:B:190:LEU:HD23	1.88	0.55
3:C:111:GLN:HB3	3:C:132:TYR:CE1	2.42	0.55
2:E:70:SER:OG	2:E:71:VAL:N	2.39	0.55
1:A:588:TYR:HB3	4:A:901[A]:CL:CL	2.45	0.54
3:F:142:PHE:HB2	3:F:158:THR:HB	1.88	0.54
1:A:283:ARG:NH2	1:A:304:ASP:OD1	2.40	0.54
1:A:162:SER:CB	1:A:189:LYS:HB3	2.38	0.54
1:A:462:ASP:O	1:A:585:GLY:HA2	2.08	0.54
3:F:315:ALA:HB2	3:F:326:VAL:HG21	1.90	0.54
1:D:770:LEU:HD21	7:D:906:HEC:HBC2	1.90	0.54
2:B:287:ASP:OD1	2:B:311:ARG:NH2	2.35	0.54
2:B:111:ASP:OD2	2:B:131:ASP:HA	2.07	0.54
1:A:631:ASN:ND2	10:A:1007:HOH:O	2.40	0.54
3:F:335:THR:HA	3:F:338:LEU:HD13	1.88	0.54
1:D:159:ALA:HB1	1:D:162:SER:O	2.07	0.54
3:C:145:GLU:OE1	3:C:150:HIS:NE2	2.32	0.53
1:D:359:LYS:NZ	10:D:1005:HOH:O	2.35	0.53
3:C:82:VAL:HG23	3:C:189:TYR:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:148:ALA:HB2	2:E:181:VAL:HG13	1.89	0.53
1:A:170:ILE:HB	1:A:184:HIS:O	2.09	0.52
1:A:520:SER:O	1:A:712:TYR:OH	2.22	0.52
3:F:132:TYR:CE2	3:F:134:ARG:HB2	2.44	0.52
3:C:144:HIS:ND1	7:C:404:HEC:O2D	2.34	0.52
3:C:132:TYR:CE2	3:C:134:ARG:HB2	2.45	0.52
7:D:906:HEC:HHA	7:D:906:HEC:HBD2	1.91	0.52
2:B:42:VAL:HG11	3:C:82:VAL:HG11	1.92	0.51
1:A:159:ALA:HB1	1:A:162:SER:O	2.10	0.51
1:D:493:GLN:HB2	1:D:533:ILE:HG13	1.93	0.51
1:D:325:ILE:HD11	1:D:345:TRP:HE3	1.75	0.51
3:C:63:LEU:HD21	3:C:180:PRO:HG3	1.92	0.51
1:D:462:ASP:O	1:D:585:GLY:HA2	2.11	0.51
3:F:202:ASN:OD1	3:F:203:ALA:N	2.43	0.51
2:B:70:SER:HA	2:B:87:VAL:HG22	1.92	0.51
2:B:307:ARG:HE	2:B:357:SER:HB3	1.75	0.51
2:B:88:ARG:NE	2:B:126:GLU:OE2	2.44	0.51
1:D:265:ASN:OD1	1:D:290:ASN:ND2	2.44	0.51
1:D:713:SER:O	1:D:717:ASN:ND2	2.39	0.51
1:D:422:ARG:NH1	3:F:95:SER:O	2.43	0.50
1:A:678:GLN:NE2	1:A:682:ASP:OD1	2.44	0.50
3:F:81:LEU:HA	3:F:84:TYR:HD2	1.76	0.50
1:D:608:TRP:CE3	3:F:123:GLY:HA2	2.47	0.50
1:D:329:GLU:OE2	1:D:355:LYS:NZ	2.31	0.50
3:F:317:THR:OG1	3:F:320:ASP:OD2	2.26	0.50
2:B:49:PRO:HB3	2:B:63:ILE:CG2	2.41	0.50
3:C:186:LEU:HD21	7:C:404:HEC:HMB1	1.94	0.50
2:E:251:VAL:HG12	10:F:518:HOH:O	2.10	0.50
2:E:71:VAL:HG23	2:E:85:VAL:HB	1.92	0.50
2:B:94:SER:HB2	2:B:103:LEU:HD11	1.94	0.50
1:A:339:GLN:HB3	1:A:357:THR:O	2.12	0.50
2:E:168:VAL:HG12	2:E:169:ARG:HG3	1.94	0.50
2:E:91:PRO:HA	2:E:106:CYS:O	2.11	0.49
3:F:109:ARG:HH11	3:F:109:ARG:HG2	1.77	0.49
1:D:536:GLN:HG2	1:D:546:THR:HB	1.93	0.49
3:F:284:THR:HG21	3:F:308:THR:HG21	1.93	0.49
3:C:242:ASP:OD2	3:C:246:HIS:NE2	2.41	0.49
1:A:604:LEU:HD13	2:B:250:PRO:HG3	1.93	0.49
1:D:225:ILE:HG13	1:D:233:LEU:HB2	1.94	0.49
1:A:504:ARG:NH1	1:A:801:ASP:O	2.40	0.49
2:E:88:ARG:NE	2:E:126:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LYS:HE3	1:A:360:ASP:H	1.77	0.49
2:E:202:ARG:HD2	2:E:224:SER:HA	1.93	0.49
1:A:713:SER:O	1:A:717:ASN:ND2	2.35	0.49
2:E:225:ASN:HA	2:E:227:ARG:NH2	2.28	0.48
3:F:228:CYS:HA	3:F:242:ASP:HB2	1.94	0.48
1:D:432:ASN:HD22	1:D:454:SER:HB3	1.76	0.48
3:F:255:VAL:HA	3:F:264:LYS:HG3	1.95	0.48
2:B:92:GLU:OE1	2:B:132:TRP:NE1	2.42	0.48
1:A:608:TRP:CE3	3:C:123:GLY:HA2	2.49	0.48
1:A:58:GLN:HB3	1:A:88:LEU:HD11	1.95	0.48
2:E:203:SER:HB3	2:E:217:ASN:OD1	2.13	0.48
3:F:277:PRO:HA	3:F:286:ILE:HD11	1.95	0.48
2:B:46:LEU:HD13	2:B:376:ASN:HD21	1.78	0.48
1:D:444:ASP:OD1	1:D:447:LYS:N	2.46	0.48
1:A:81:PRO:HB2	1:A:84:SER:OG	2.14	0.48
1:A:383:GLY:HA3	1:D:383:GLY:HA3	1.96	0.48
2:B:91:PRO:HA	2:B:106:CYS:O	2.14	0.48
1:D:736:ASN:HD22	1:D:743:SER:HA	1.79	0.47
2:E:97:THR:HA	2:E:138:ILE:HD11	1.96	0.47
2:B:352:THR:HG22	2:B:353:GLY:H	1.79	0.47
3:C:131:LYS:HB3	7:C:404:HEC:HBA1	1.97	0.47
2:B:382:ARG:NH1	2:B:385:VAL:O	2.41	0.47
2:E:356:PRO:HA	2:E:371:ALA:O	2.15	0.47
3:F:111:GLN:HB3	3:F:132:TYR:CE1	2.50	0.47
3:C:107:TYR:CG	3:C:108:GLU:N	2.83	0.47
1:A:325:ILE:HD11	1:A:345:TRP:HE3	1.78	0.46
3:F:92:ALA:O	3:F:98:GLY:HA2	2.15	0.46
2:E:159:VAL:HG22	2:E:169:ARG:H	1.79	0.46
3:F:119:LEU:HB2	3:F:122:GLU:OE1	2.15	0.46
2:E:93:ALA:HB3	2:E:106:CYS:HB2	1.98	0.46
2:B:208:ASP:HB3	2:B:211:SER:HB3	1.97	0.46
1:D:260:LEU:HD13	1:D:421:PRO:HG2	1.97	0.46
1:D:81:PRO:HB2	1:D:84:SER:OG	2.16	0.46
1:D:110:CYS:SG	10:D:1002:HOH:O	2.61	0.46
1:D:382:ARG:HD3	1:D:382:ARG:HA	1.42	0.46
1:D:472:PRO:HB2	1:D:730:ILE:HD13	1.97	0.46
1:A:31:MET:O	2:B:311:ARG:NH1	2.46	0.46
3:F:45:ILE:HG23	3:F:46:SER:H	1.80	0.46
3:F:214:GLY:HA3	3:F:349:TYR:HB2	1.98	0.46
1:A:173:ARG:HH21	1:A:178:GLU:HG3	1.81	0.46
2:B:50:PHE:HB2	2:B:66:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:ARG:NH2	3:C:107:TYR:CE1	2.82	0.46
1:A:391:ASN:OD1	1:A:393:SER:OG	2.27	0.46
2:E:186:ASP:OD1	2:E:187:GLY:N	2.48	0.46
1:A:310:THR:O	1:A:333:MET:HG3	2.16	0.46
2:E:116:VAL:HG22	2:E:123:GLU:HA	1.97	0.45
1:D:653:SER:OG	1:D:654:GLY:N	2.48	0.45
1:A:60:LEU:O	1:A:413:ALA:N	2.43	0.45
1:A:240:HIS:CD2	1:A:241:LEU:HG	2.51	0.45
2:B:108:ALA:HB1	2:B:132:TRP:CE2	2.51	0.45
1:A:225:ILE:O	1:A:229:THR:OG1	2.18	0.45
1:D:432:ASN:HA	1:D:454:SER:HB3	1.99	0.45
2:E:49:PRO:HB3	2:E:63:ILE:CG2	2.47	0.45
1:A:586:CYS:SG	7:A:905:HEC:HHD	2.57	0.45
1:A:319:THR:O	1:A:323:ARG:HA	2.16	0.45
1:A:331:PRO:HB2	1:D:331:PRO:HB3	1.98	0.45
2:B:200:ILE:HD12	3:C:282:SER:O	2.17	0.45
1:A:504:ARG:HD3	1:A:800:PRO:HB3	1.99	0.45
2:B:187:GLY:O	2:B:209:ILE:HD12	2.17	0.45
3:F:150:HIS:CD2	3:F:156:GLY:H	2.34	0.45
2:E:253[B]:GLU:HA	3:F:174:ARG:HG3	1.98	0.45
3:C:209:GLU:O	3:C:213:ARG:HB2	2.16	0.45
1:D:77:PRO:HB3	1:D:256:PHE:CG	2.52	0.45
1:A:99:LEU:HB3	1:A:135:MET:HE1	1.99	0.45
2:B:227:ARG:NH2	10:B:507:HOH:O	2.50	0.44
1:A:536:GLN:HG2	1:A:546:THR:HB	1.97	0.44
1:D:271:VAL:HG22	1:D:284:VAL:HG22	1.99	0.44
2:E:267:ILE:HG12	2:E:275:VAL:HG13	1.98	0.44
3:C:303:ILE:HG12	7:C:405:HEC:HMA3	2.00	0.44
3:F:134:ARG:NH1	3:F:194:GLU:O	2.44	0.44
2:E:88:ARG:HB2	2:E:107:ASN:CG	2.38	0.44
3:C:183:LEU:O	3:C:187:ILE:HG12	2.17	0.44
2:E:103:LEU:HD23	2:E:104:TYR:N	2.32	0.44
2:E:286:TYR:O	2:E:311:ARG:NH2	2.50	0.44
2:B:149:CYS:O	2:B:178:PRO:HD2	2.18	0.44
1:D:681:LEU:O	1:D:685:CYS:HB2	2.17	0.44
1:A:493:GLN:HB2	1:A:533:ILE:HG13	1.99	0.44
2:B:250:PRO:HB3	3:C:124:TRP:CZ3	2.52	0.44
2:B:227:ARG:NH1	3:C:108:GLU:OE2	2.51	0.44
3:F:297:THR:HA	3:F:298:PRO:HD3	1.80	0.44
2:B:104:TYR:HB3	2:B:136:ILE:HD13	2.00	0.44
3:F:131:LYS:HB3	7:F:404:HEC:HBA1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:586:CYS:SG	7:D:905:HEC:HHD	2.58	0.44
1:A:633:LYS:HD2	1:A:633:LYS:HA	1.73	0.44
1:D:641:VAL:HA	1:D:660:VAL:O	2.17	0.44
1:D:113:TRP:CG	1:D:420:LYS:HE2	2.53	0.43
1:D:53:GLN:NE2	1:D:372:ASP:OD1	2.51	0.43
3:C:297:THR:HA	3:C:298:PRO:HD3	1.80	0.43
1:A:50:LYS:HG2	1:A:371:PRO:O	2.18	0.43
3:C:247:ASP:HB2	3:C:294:GLU:HG2	2.01	0.43
2:E:374:PHE:HB3	3:F:54:TRP:CZ3	2.53	0.43
3:F:232:ASP:HB3	3:F:235:ASP:HB2	2.00	0.43
3:C:103:ALA:O	3:C:107:TYR:HA	2.18	0.43
1:D:289:ASP:OD1	1:D:290:ASN:N	2.51	0.43
3:C:187:ILE:HA	3:C:190:ILE:HD12	2.00	0.43
2:E:244:THR:HB	2:E:261:THR:OG1	2.19	0.43
1:D:43:THR:O	1:D:422:ARG:NH2	2.46	0.43
1:A:547:SER:OG	1:A:617:SER:OG	2.32	0.43
2:E:134:SER:OG	2:E:179:ARG:O	2.36	0.43
1:D:734:TYR:HE1	7:D:906:HEC:HBA2	1.84	0.43
1:A:358:GLY:C	1:A:359:LYS:HG3	2.39	0.43
1:A:298:PRO:HD3	7:A:905:HEC:HMA2	1.99	0.43
1:A:457:THR:O	1:A:580:GLY:HA2	2.19	0.43
1:A:289:ASP:OD1	1:A:290:ASN:N	2.52	0.43
2:E:180:MET:HB3	2:E:193:ILE:HD11	2.01	0.43
2:E:237:TYR:CE1	2:E:268:GLU:HG2	2.54	0.43
1:A:259:TRP:N	1:A:267:LEU:O	2.50	0.42
1:D:121:ALA:HB2	1:D:153:ARG:HA	2.00	0.42
3:C:107:TYR:HE2	3:C:109:ARG:CG	2.33	0.42
3:F:242:ASP:OD2	3:F:246:HIS:NE2	2.42	0.42
2:B:41:HIS:CD2	3:C:194:GLU:HG3	2.55	0.42
2:E:237:TYR:HE1	2:E:268:GLU:HG2	1.84	0.42
1:D:587:HIS:HB2	7:D:905:HEC:C1D	2.49	0.42
1:D:158:TYR:OH	1:D:423:TRP:HA	2.20	0.42
1:D:617:SER:HA	1:D:618:PRO:HD3	1.90	0.42
1:D:459:ILE:HB	1:D:545:VAL:HG23	2.01	0.42
1:D:712:TYR:HD1	1:D:794:TRP:CG	2.38	0.42
1:A:81:PRO:HB2	1:A:84:SER:HG	1.85	0.42
1:A:343:VAL:HG12	1:A:353:TYR:HA	2.01	0.42
3:C:201:ARG:HD3	3:C:352:ALA:HB1	2.01	0.42
3:F:265:VAL:HB	3:F:271:LEU:HD12	2.02	0.42
3:F:111:GLN:O	3:F:132:TYR:HA	2.19	0.42
1:D:277:ARG:HG3	7:D:905:HEC:O1D	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ARG:HH11	2:B:164:ARG:HG2	1.84	0.42
1:A:357:THR:HG21	1:A:364:TYR:CE2	2.55	0.42
2:B:136:ILE:O	2:B:137:LYS:HG3	2.20	0.42
3:F:310:PHE:N	7:F:405:HEC:O1A	2.53	0.42
1:A:67:THR:HB	1:A:70:GLY:H	1.85	0.42
1:D:49:SER:HA	1:D:52:VAL:HG12	2.02	0.42
1:D:588:TYR:HB3	4:D:901:CL:CL	2.57	0.41
1:D:632:TYR:CZ	1:D:634:GLY:HA2	2.55	0.41
2:E:228:ASP:CB	2:E:292:GLY:HA2	2.50	0.41
2:B:364:ASP:CG	2:B:366:LYS:HG3	2.41	0.41
2:B:180:MET:HB3	2:B:193:ILE:HD11	2.02	0.41
2:E:288:GLY:H	2:E:309:MET:CG	2.27	0.41
2:E:115:VAL:O	2:E:124:ILE:N	2.50	0.41
2:E:117:ASP:OD1	2:E:118:ILE:N	2.53	0.41
2:B:325:ARG:HD3	1:D:692:ASN:HA	2.02	0.41
2:E:136:ILE:HG22	2:E:147:VAL:HG22	2.03	0.41
3:F:218:PHE:O	3:F:225:CYS:HB2	2.21	0.41
2:B:386:ASP:N	2:B:386:ASP:OD1	2.54	0.41
2:E:175:ASP:H	2:E:194:LEU:HD13	1.85	0.41
3:F:183:LEU:O	3:F:187:ILE:HG12	2.20	0.41
1:A:173:ARG:NH2	1:A:178:GLU:OE2	2.54	0.41
2:E:54:MET:HE2	2:E:61:LEU:HD21	2.02	0.41
1:A:252:LEU:HD12	1:A:572:TRP:CZ2	2.55	0.41
1:D:600:HIS:HB3	3:F:278:TYR:O	2.21	0.41
1:D:596:PHE:HB2	2:E:258:GLN:HA	2.02	0.41
2:E:179:ARG:NH1	3:F:107:TYR:OH	2.54	0.41
3:F:321:THR:HG21	7:F:405:HEC:HMA2	2.02	0.41
3:F:198:SER:HA	3:F:199:PRO:HD3	1.85	0.41
1:D:410:HIS:CD2	1:D:411:GLN:HG3	2.56	0.41
3:C:123:GLY:O	3:C:126:SER:OG	2.32	0.41
2:E:255:GLU:OE1	2:E:255:GLU:N	2.54	0.41
1:A:205:GLU:HA	1:A:528:GLN:NE2	2.35	0.41
1:D:116:LYS:HA	1:D:116:LYS:HD3	1.89	0.41
3:F:122:GLU:O	3:F:291:LEU:HD22	2.20	0.41
1:D:58:GLN:O	1:D:415:VAL:HG22	2.20	0.41
2:E:229:VAL:HA	2:E:239:ALA:O	2.21	0.41
2:B:237:TYR:CE1	2:B:268:GLU:HG2	2.55	0.41
2:E:253[A]:GLU:HB3	2:E:255:GLU:OE1	2.20	0.41
1:A:617:SER:HA	1:A:618:PRO:HD3	1.93	0.41
2:B:148:ALA:HB2	2:B:181:VAL:HG13	2.03	0.41
1:D:594:ARG:NH2	2:E:337:ASP:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:SER:OG	2:B:179:ARG:O	2.19	0.41
2:B:356:PRO:HA	2:B:371:ALA:O	2.21	0.41
2:B:282:ASP:N	2:B:285:ASN:O	2.50	0.41
1:A:600:HIS:HB3	3:C:278:TYR:O	2.21	0.41
2:E:250:PRO:O	2:E:258:GLN:NE2	2.54	0.41
2:E:222:GLU:OE2	10:E:501:HOH:O	2.22	0.41
2:E:187:GLY:O	2:E:209:ILE:HD12	2.21	0.40
1:A:105:THR:HB	1:A:123:VAL:HG12	2.02	0.40
1:A:199:PRO:HG2	1:A:202:VAL:HG21	2.03	0.40
1:A:295:TYR:CE1	2:B:253[A]:GLU:HG3	2.56	0.40
3:C:131:LYS:HE2	3:C:144:HIS:CE1	2.57	0.40
3:F:110:GLY:HA2	3:F:133:ILE:HD11	2.03	0.40
3:F:308:THR:HG23	3:F:316:ARG:HA	2.03	0.40
1:D:608:TRP:HD1	1:D:616:ASP:OD2	2.05	0.40
1:D:277:ARG:NH1	7:D:905:HEC:O2D	2.55	0.40
2:B:321:LEU:O	2:B:325:ARG:HG3	2.22	0.40
1:A:220:GLN:HB2	1:A:224:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	762/782 (97%)	731 (96%)	31 (4%)	0	100	100
1	D	764/782 (98%)	739 (97%)	25 (3%)	0	100	100
2	B	351/352 (100%)	343 (98%)	8 (2%)	0	100	100
2	E	351/352 (100%)	342 (97%)	9 (3%)	0	100	100
3	C	312/314 (99%)	295 (95%)	16 (5%)	1 (0%)	46	75
3	F	312/314 (99%)	298 (96%)	13 (4%)	1 (0%)	46	75
All	All	2852/2896 (98%)	2748 (96%)	102 (4%)	2 (0%)	56	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	96	LEU
3	F	96	LEU

5.3.2 Protein sidechains ⓘ

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	641/653 (98%)	638 (100%)	3 (0%)	92	98
1	D	642/653 (98%)	642 (100%)	0	100	100
2	B	303/302 (100%)	301 (99%)	2 (1%)	88	96
2	E	300/302 (99%)	299 (100%)	1 (0%)	94	99
3	C	262/264 (99%)	260 (99%)	2 (1%)	86	96
3	F	259/264 (98%)	256 (99%)	3 (1%)	78	93
All	All	2407/2438 (99%)	2396 (100%)	11 (0%)	92	98

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	SER
1	A	359	LYS
1	A	384	ASP
2	B	231	TYR
2	B	330	GLU
3	C	162	ASP
3	C	209	GLU
2	E	241	THR
3	F	107	TYR
3	F	122	GLU
3	F	152	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	41	HIS
3	C	340	GLN
3	C	344	GLN
1	D	184	HIS
1	D	290	ASN
1	D	432	ASN
1	D	468	GLN
1	D	496	GLN
1	D	606	ASN
2	E	90	GLN
2	E	122	GLN
3	F	150	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 19 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	HEC	A	905	1,6	24,50,50	2.52	4 (16%)	19,82,82	2.88	3 (15%)
7	HEC	A	906	1	24,50,50	2.42	3 (12%)	19,82,82	2.79	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BET	A	907	-	4,7,7	0.82	0	7,10,10	1.93	1 (14%)
8	BET	A	908	-	4,7,7	0.81	0	7,10,10	2.05	1 (14%)
8	BET	A	909	-	4,7,7	0.78	0	7,10,10	2.07	1 (14%)
8	BET	B	403	-	4,7,7	0.77	0	7,10,10	2.03	1 (14%)
7	HEC	C	404	10,3	24,50,50	2.41	4 (16%)	19,82,82	2.83	5 (26%)
7	HEC	C	405	3	24,50,50	2.41	4 (16%)	19,82,82	2.84	4 (21%)
8	BET	C	406	-	4,7,7	0.82	0	7,10,10	1.88	1 (14%)
7	HEC	D	905	1,6	24,50,50	2.51	4 (16%)	19,82,82	2.90	3 (15%)
7	HEC	D	906	1	24,50,50	2.44	5 (20%)	19,82,82	2.81	3 (15%)
8	BET	D	907	-	4,7,7	0.78	0	7,10,10	2.07	1 (14%)
8	BET	E	403	-	4,7,7	0.80	0	7,10,10	2.06	1 (14%)
7	HEC	F	404	10,3	24,50,50	2.42	4 (16%)	19,82,82	2.84	3 (15%)
7	HEC	F	405	3	24,50,50	2.44	4 (16%)	19,82,82	2.85	4 (21%)

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
7	HEC	A	905	1,6	-	0/6/54/54	0/0/8/8
7	HEC	A	906	1	-	0/6/54/54	0/0/8/8
8	BET	A	907	-	-	0/3/5/5	0/0/0/0
8	BET	A	908	-	-	0/3/5/5	0/0/0/0
8	BET	A	909	-	-	0/3/5/5	0/0/0/0
8	BET	B	403	-	-	0/3/5/5	0/0/0/0
7	HEC	C	404	10,3	-	0/6/54/54	0/0/8/8
7	HEC	C	405	3	-	0/6/54/54	0/0/8/8
8	BET	C	406	-	-	0/3/5/5	0/0/0/0
7	HEC	D	905	1,6	-	0/6/54/54	0/0/8/8
7	HEC	D	906	1	-	0/6/54/54	0/0/8/8
8	BET	D	907	-	-	0/3/5/5	0/0/0/0
8	BET	E	403	-	-	0/3/5/5	0/0/0/0
7	HEC	F	404	10,3	-	0/6/54/54	0/0/8/8
7	HEC	F	405	3	-	0/6/54/54	0/0/8/8

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	905	HEC	C3B-C2B	-6.67	1.33	1.40
7	A	905	HEC	C3B-C2B	-6.66	1.33	1.40
7	D	905	HEC	C3C-C2C	-6.53	1.34	1.40
7	A	905	HEC	C3C-C2C	-6.53	1.34	1.40
7	F	405	HEC	C3C-C2C	-6.26	1.34	1.40
7	D	906	HEC	C3B-C2B	-6.24	1.34	1.40
7	F	405	HEC	C3B-C2B	-6.24	1.34	1.40
7	A	906	HEC	C3B-C2B	-6.24	1.34	1.40
7	C	405	HEC	C3C-C2C	-6.21	1.34	1.40
7	F	404	HEC	C3B-C2B	-6.20	1.34	1.40
7	C	404	HEC	C3B-C2B	-6.16	1.34	1.40
7	D	906	HEC	C3C-C2C	-6.12	1.34	1.40
7	C	404	HEC	C3C-C2C	-6.10	1.34	1.40
7	A	906	HEC	C3C-C2C	-6.06	1.34	1.40
7	F	404	HEC	C3C-C2C	-6.00	1.34	1.40
7	C	405	HEC	C3B-C2B	-6.00	1.34	1.40
7	F	405	HEC	CAA-C2A	2.02	1.54	1.52
7	D	906	HEC	CAA-C2A	2.02	1.54	1.52
7	D	905	HEC	CAA-C2A	2.04	1.54	1.52
7	C	405	HEC	CAA-C2A	2.06	1.54	1.52
7	A	905	HEC	CAA-C2A	2.12	1.55	1.52
7	D	906	HEC	CAD-C3D	2.14	1.55	1.52
7	F	404	HEC	CAA-C2A	2.39	1.55	1.52
7	C	404	HEC	CAA-C2A	2.44	1.55	1.52
7	D	905	HEC	C3D-C2D	5.41	1.53	1.37
7	A	905	HEC	C3D-C2D	5.44	1.53	1.37
7	C	404	HEC	C3D-C2D	5.48	1.53	1.37
7	D	906	HEC	C3D-C2D	5.48	1.53	1.37
7	F	405	HEC	C3D-C2D	5.49	1.53	1.37
7	A	906	HEC	C3D-C2D	5.50	1.54	1.37
7	F	404	HEC	C3D-C2D	5.50	1.54	1.37
7	C	405	HEC	C3D-C2D	5.53	1.54	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	905	HEC	CBC-CAC-C3C	-8.20	109.42	127.34
7	A	905	HEC	CBB-CAB-C3B	-8.15	109.52	127.34
7	A	905	HEC	CBC-CAC-C3C	-8.04	109.77	127.34
7	D	905	HEC	CBB-CAB-C3B	-8.01	109.82	127.34
7	A	906	HEC	CBB-CAB-C3B	-7.98	109.91	127.34
7	F	404	HEC	CBC-CAC-C3C	-7.96	109.95	127.34
7	D	906	HEC	CBB-CAB-C3B	-7.92	110.02	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	404	HEC	CBC-CAC-C3C	-7.81	110.27	127.34
7	F	405	HEC	CBB-CAB-C3B	-7.80	110.29	127.34
7	C	405	HEC	CBB-CAB-C3B	-7.77	110.36	127.34
7	C	405	HEC	CBC-CAC-C3C	-7.63	110.66	127.34
7	F	405	HEC	CBC-CAC-C3C	-7.54	110.86	127.34
7	C	404	HEC	CBB-CAB-C3B	-7.51	110.91	127.34
7	F	404	HEC	CBB-CAB-C3B	-7.50	110.94	127.34
7	D	906	HEC	CBC-CAC-C3C	-7.43	111.09	127.34
7	A	906	HEC	CBC-CAC-C3C	-7.05	111.94	127.34
8	D	907	BET	C-CA-N	-5.31	109.67	115.26
8	A	909	BET	C-CA-N	-5.30	109.68	115.26
8	E	403	BET	C-CA-N	-5.25	109.73	115.26
8	A	908	BET	C-CA-N	-5.23	109.75	115.26
8	B	403	BET	C-CA-N	-5.18	109.80	115.26
8	A	907	BET	C-CA-N	-4.96	110.04	115.26
8	C	406	BET	C-CA-N	-4.82	110.19	115.26
7	F	404	HEC	CMC-C2C-C1C	-2.73	123.67	128.31
7	D	906	HEC	CMC-C2C-C1C	-2.63	123.84	128.31
7	C	404	HEC	CMC-C2C-C1C	-2.61	123.87	128.31
7	F	405	HEC	CMC-C2C-C1C	-2.53	124.01	128.31
7	F	405	HEC	CBA-CAA-C2A	-2.50	108.09	112.47
7	C	405	HEC	CMC-C2C-C1C	-2.30	124.40	128.31
7	C	404	HEC	CBD-CAD-C3D	-2.27	108.50	112.49
7	D	905	HEC	CBD-CAD-C3D	-2.16	108.69	112.49
7	A	906	HEC	CMC-C2C-C1C	-2.13	124.69	128.31
7	C	404	HEC	CMB-C2B-C1B	-2.04	124.84	128.31
7	A	906	HEC	CBD-CAD-C3D	-2.02	108.93	112.49
7	A	905	HEC	CAD-CBD-CGD	-2.02	108.85	112.78
7	C	405	HEC	CMB-C2B-C1B	-2.01	124.89	128.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	905	HEC	2	0
7	A	906	HEC	8	0
7	C	404	HEC	4	0
7	C	405	HEC	2	0
7	D	905	HEC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	906	HEC	3	0
7	F	404	HEC	2	0
7	F	405	HEC	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	768/782 (98%)	-0.23	2 (0%) 94 95	32, 54, 77, 111	0
1	D	770/782 (98%)	-0.03	6 (0%) 87 88	37, 61, 83, 119	0
2	B	352/352 (100%)	0.01	1 (0%) 94 95	38, 60, 80, 96	0
2	E	352/352 (100%)	0.29	7 (1%) 68 69	46, 77, 99, 113	0
3	C	314/314 (100%)	-0.03	5 (1%) 74 75	36, 57, 79, 97	0
3	F	314/314 (100%)	0.35	9 (2%) 55 55	46, 74, 91, 103	0
All	All	2870/2896 (99%)	0.00	30 (1%) 84 85	32, 62, 87, 119	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	107	TYR	4.1
3	F	107	TYR	4.1
3	F	223	VAL	3.3
3	F	333	GLY	3.0
1	D	178	GLU	2.9
3	C	109	ARG	2.8
2	E	76	ALA	2.7
2	E	378	VAL	2.7
3	C	337	HIS	2.6
1	D	91	LEU	2.5
2	B	252	CYS	2.4
1	A	357	THR	2.3
3	F	40	GLY	2.3
3	F	226	LEU	2.3
1	D	651	GLY	2.3
3	C	40	GLY	2.3
2	E	252	CYS	2.3
3	F	307	GLY	2.3
1	D	401	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	79	GLN	2.2
2	E	82	THR	2.2
3	F	147	PHE	2.2
2	E	215	VAL	2.2
3	C	41	GLN	2.2
1	D	642	VAL	2.1
3	F	349	TYR	2.1
2	E	261	THR	2.1
1	A	178	GLU	2.1
1	D	398	GLY	2.1
3	F	45	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, 95th 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	CL	A	901[A]	1/1	0.91	0.40	5.82	14,14,14,14	1
4	CL	A	901[B]	1/1	0.91	0.40	4.60	40,40,40,40	1
8	BET	A	909	8/8	0.94	0.38	3.93	72,80,84,89	0
8	BET	D	907	8/8	0.92	0.32	3.36	64,72,84,86	0
8	BET	A	907	8/8	0.84	0.25	2.26	62,75,83,86	0
8	BET	E	403	8/8	0.95	0.20	1.37	63,66,71,74	0
8	BET	B	403	8/8	0.95	0.21	1.21	52,58,69,69	0
8	BET	A	908	8/8	0.95	0.20	0.87	62,69,72,77	0
5	CA	C	403	1/1	0.57	0.20	0.57	48,48,48,48	0
9	MG	E	401	1/1	0.90	0.29	0.24	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	HEC	F	404	43/43	0.95	0.21	-0.07	47,62,77,82	0
9	MG	B	401	1/1	0.80	0.27	-0.14	33,33,33,33	0
7	HEC	C	405	43/43	0.97	0.17	-0.17	42,61,70,75	0
7	HEC	A	906	43/43	0.97	0.16	-0.17	37,55,69,94	0
7	HEC	D	905	43/43	0.97	0.18	-0.27	38,53,67,71	0
7	HEC	D	906	43/43	0.97	0.15	-0.28	36,46,58,74	0
7	HEC	F	405	43/43	0.96	0.19	-0.41	64,77,87,93	0
7	HEC	A	905	43/43	0.97	0.16	-0.42	23,37,49,54	0
7	HEC	C	404	43/43	0.97	0.18	-0.43	26,44,61,66	0
5	CA	F	401	1/1	0.35	0.18	-1.38	79,79,79,79	0
5	CA	C	402	1/1	0.85	0.09	-1.47	59,59,59,59	0
5	CA	F	402	1/1	0.96	0.13	-1.71	70,70,70,70	0
5	CA	A	903	1/1	0.89	0.09	-1.83	68,68,68,68	0
5	CA	F	403	1/1	0.83	0.12	-2.28	88,88,88,88	0
4	CL	D	901	1/1	0.91	0.11	-2.33	60,60,60,60	0
5	CA	E	402	1/1	0.85	0.06	-2.57	76,76,76,76	0
5	CA	D	902	1/1	0.94	0.05	-2.71	68,68,68,68	0
5	CA	C	401	1/1	0.70	0.15	-2.90	54,54,54,54	0
5	CA	A	902	1/1	0.97	0.04	-4.63	59,59,59,59	0
5	CA	D	903	1/1	0.94	0.06	-4.75	65,65,65,65	0
6	ZN	D	904	1/1	0.94	0.18	-	53,53,53,53	0
5	CA	B	402	1/1	0.85	0.13	-	68,68,68,68	0
8	BET	C	406	8/8	0.90	0.33	-	65,74,80,81	0
6	ZN	A	904	1/1	0.98	0.18	-	46,46,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.