Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:26 PM GMT

PDB ID	:	1AR1
Title	:	Structure at 2.7 Angstrom Resolution of the Paracoccus Denitrificans two-subunit Cytochrome C Oxidase Complexed with an Antibody Fv Fragment
Authors	:	Ostermeier, C.; Harrenga, A.; Ermler, U.; Michel, H.
Deposited on	:	1997-08-08
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:

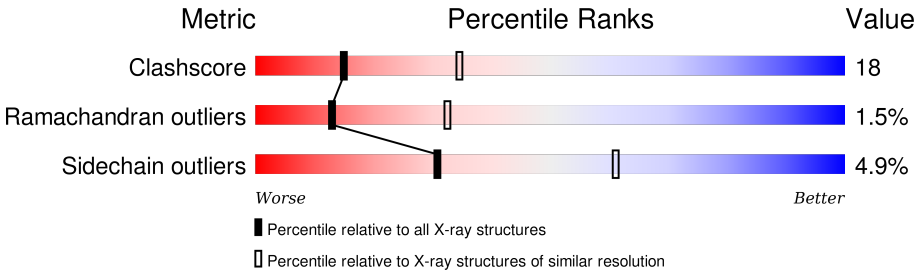
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	558	56% 36% • 5%
2	B	298	54% 29% • 15%
3	C	127	66% 25% • 7%
4	D	120	63% 24% •• 10%

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
8	HEA	A	562	X	-	-	-
8	HEA	A	563	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8243 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4183	2807	654	689	33			

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	0	0
			1976	1295	319	354	8			

- Molecule 3 is a protein called ANTIBODY FV FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	118	Total	C	N	O	S	0	0	0
			932	586	156	184	6			

- Molecule 4 is a protein called ANTIBODY FV FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	108	Total	C	N	O	S	0	0	0
			831	530	135	164	2			

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cu	0	0
			2	2		
5	A	1	Total	Cu	0	0
			1	1		

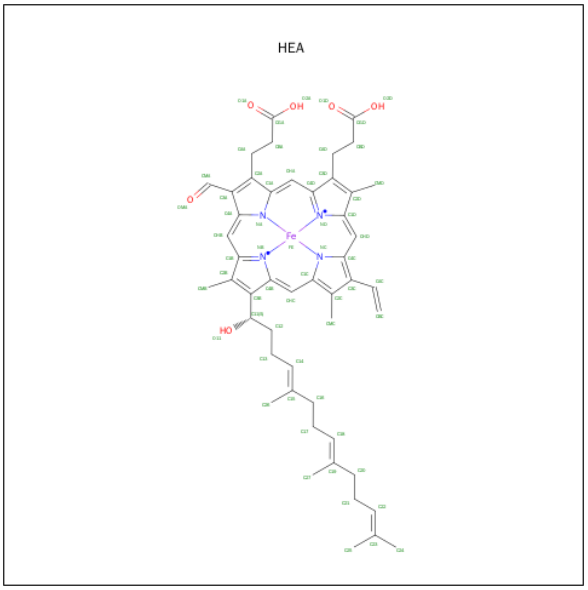
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

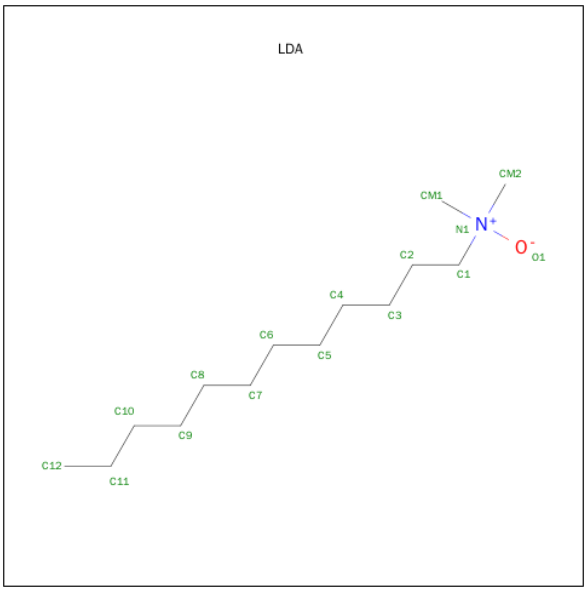
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0

- Molecule 8 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C Fe N O 60 49 1 4 6	0	0
8	A	1	Total C Fe N O 60 49 1 4 6	0	0

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O 16 14 1 1	0	0
9	B	1	Total C N O 16 14 1 1	0	0
9	A	1	Total C N O 16 14 1 1	0	0
9	A	1	Total C N O 16 14 1 1	0	0
9	A	1	Total C N O 16 14 1 1	0	0
9	A	1	Total C N O 16 14 1 1	0	0
9	A	1	Total C N O 16 14 1 1	0	0
9	B	1	Total C N O 16 14 1 1	0	0
9	A	1	Total C N O 16 14 1 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	21	Total O 21 21	0	0
10	B	21	Total O 21 21	0	0
10	C	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	5	Total O 5 5	0	0

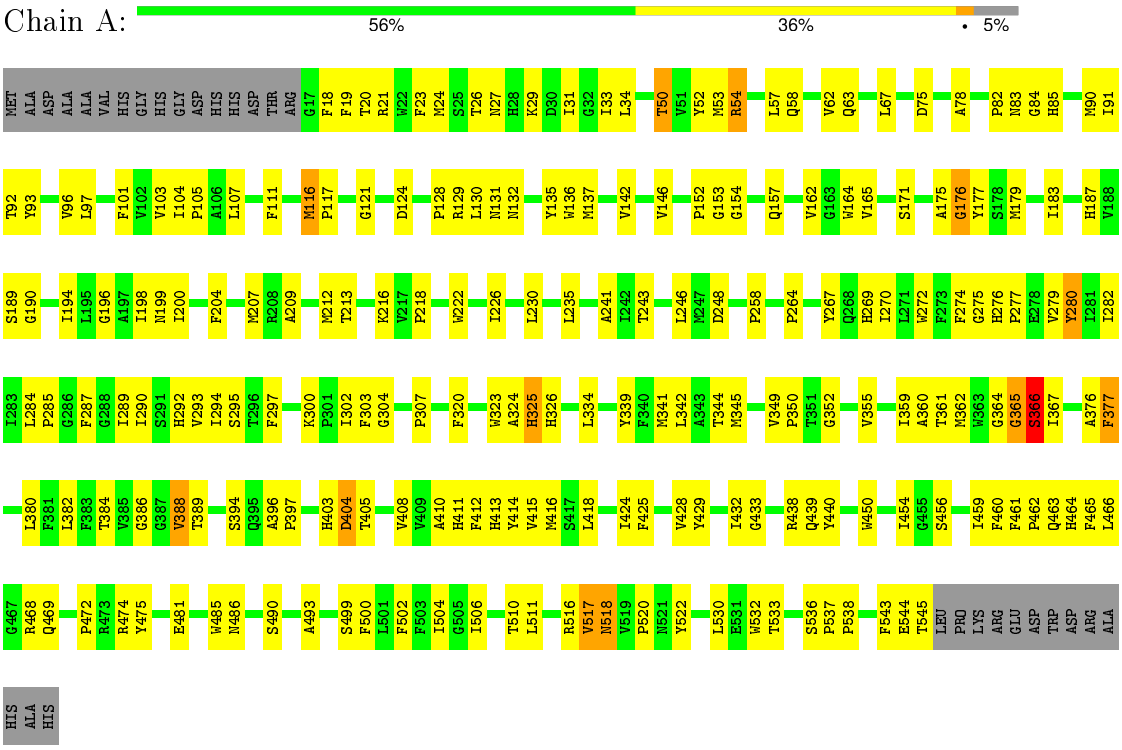
3 Residue-property plots (i)

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

Note EDS was not executed.

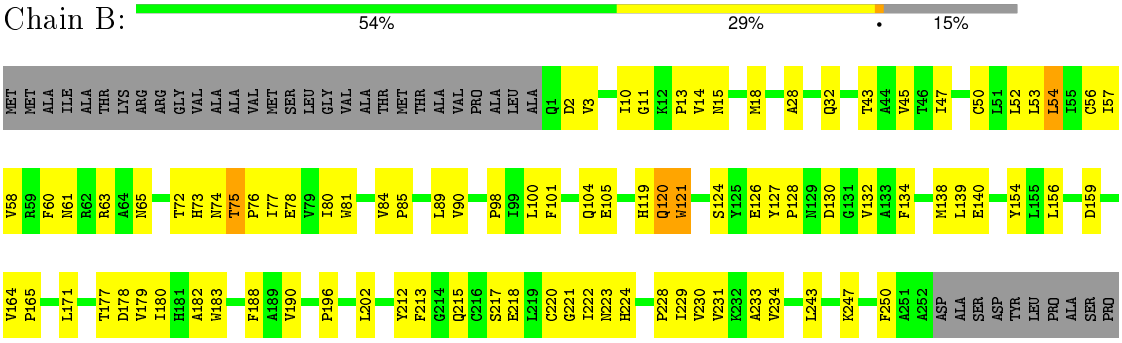
- Molecule 1: CYTOCHROME C OXIDASE

Chain A:



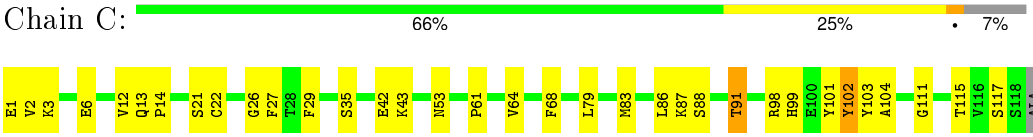
- Molecule 2: CYTOCHROME C OXIDASE

Chain B:



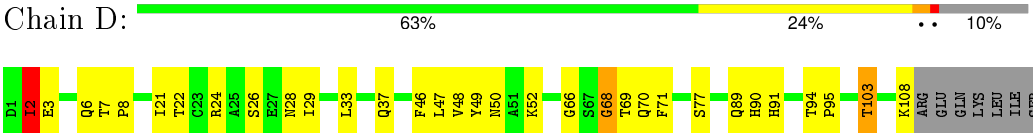
• Molecule 3: ANTIBODY FV FRAGMENT

Chain C:



• Molecule 4: ANTIBODY FV FRAGMENT

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.50Å 151.00Å 156.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	93.1 (30.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.207 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8243	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, LDA, CA, CU, HEA

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	0.51	0/4339	0.64	0/5923
2	B	0.52	0/2033	0.69	0/2787
3	C	0.47	0/954	0.65	0/1291
4	D	0.48	0/852	0.62	0/1156
All	All	0.51	0/8178	0.66	0/11157

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	TYR	Sidechain
1	A	339	TYR	Sidechain

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	4183	0	4103	182	0
2	B	1976	0	1963	67	0
3	C	932	0	889	23	0
4	D	831	0	807	23	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	120	0	108	20	0
9	A	96	0	186	4	0
9	B	48	0	93	5	0
10	A	21	0	0	2	0
10	B	21	0	0	1	0
10	C	5	0	0	1	0
10	D	5	0	0	0	0
All	All	8243	0	8149	287	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 18.

All (287) 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:153:GLY:HA2	1:A:176:GLY:H	1.23	1.03
1:A:23:PHE:HB3	1:A:136:TRP:HZ2	1.35	0.91
8:A:562:HEA:HMC1	8:A:562:HEA:HBC1	1.56	0.88
4:D:50:ASN:H	4:D:91:HIS:HE1	1.24	0.86
1:A:300:LYS:HD2	1:A:364:GLY:HA3	1.57	0.85
4:D:50:ASN:H	4:D:91:HIS:CE1	1.99	0.81
1:A:334:LEU:HD13	2:B:104:GLN:HB3	1.63	0.81
1:A:23:PHE:HB3	1:A:136:TRP:CZ2	2.16	0.80
1:A:20:THR:HA	1:A:24:MET:HB2	1.64	0.78
1:A:365:GLY:HA3	2:B:65:ASN:ND2	2.00	0.77
1:A:276:HIS:NE2	1:A:280:TYR:HE2	1.82	0.77
1:A:62:VAL:HG21	1:A:82:PRO:HB3	1.67	0.76
1:A:276:HIS:O	1:A:279:VAL:HG22	1.87	0.75
1:A:153:GLY:HA2	1:A:176:GLY:N	2.00	0.75
1:A:516:ARG:NH2	1:A:518:ASN:HB3	2.02	0.74
1:A:50:THR:HG21	8:A:562:HEA:O11	1.87	0.74
1:A:349:VAL:HB	1:A:350:PRO:HD3	1.69	0.73
1:A:432:ILE:HD13	1:A:510:THR:HG21	1.70	0.73
4:D:24:ARG:HB3	4:D:24:ARG:CZ	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLU:HG2	2:B:13:PRO:O	1.88	0.73
2:B:54:LEU:O	2:B:58:VAL:HG22	1.88	0.73
1:A:469:GLN:HE22	2:B:14:VAL:H	1.34	0.73
2:B:43:THR:O	2:B:47:ILE:HG12	1.89	0.73
3:C:88:SER:O	3:C:91:THR:HG23	1.89	0.72
1:A:300:LYS:HD2	1:A:364:GLY:CA	2.19	0.72
1:A:433:GLY:HA2	1:A:438:ARG:O	1.89	0.72
1:A:464:HIS:O	1:A:468:ARG:HG3	1.90	0.71
2:B:126:GLU:O	2:B:128:PRO:HD3	1.91	0.71
1:A:258:PRO:HG3	2:B:196:PRO:HB2	1.74	0.70
1:A:62:VAL:HG11	1:A:82:PRO:HA	1.74	0.69
1:A:183:ILE:HG21	1:A:246:LEU:HD22	1.75	0.69
1:A:412:PHE:CD2	8:A:563:HEA:HAD1	2.28	0.69
1:A:103:VAL:HG11	1:A:282:ILE:HG23	1.74	0.68
2:B:84:VAL:HB	2:B:85:PRO:HD3	1.75	0.67
1:A:382:LEU:HD13	1:A:418:LEU:HD23	1.76	0.67
1:A:412:PHE:HA	1:A:415:VAL:HG22	1.77	0.67
1:A:325:HIS:CD2	1:A:326:HIS:CD2	2.83	0.67
2:B:75:THR:HA	2:B:78:GLU:HB2	1.77	0.66
1:A:341:MET:O	1:A:345:MET:HG3	1.96	0.66
1:A:289:ILE:O	1:A:293:VAL:HG23	1.95	0.65
4:D:8:PRO:O	4:D:103:THR:HB	1.95	0.65
2:B:56:CYS:HA	2:B:60:PHE:HD2	1.61	0.64
2:B:180:ILE:HG22	2:B:218:GLU:HG2	1.80	0.63
3:C:6:GLU:HA	3:C:21:SER:O	1.99	0.63
1:A:362:MET:SD	1:A:377:PHE:CE1	2.92	0.63
1:A:468:ARG:HD3	2:B:18:MET:O	1.99	0.63
4:D:2:ILE:HG12	4:D:3:GLU:N	2.14	0.62
4:D:66:GLY:HA3	4:D:71:PHE:HA	1.79	0.62
1:A:75:ASP:HB3	1:A:78:ALA:HB3	1.82	0.62
1:A:284:LEU:HB2	1:A:285:PRO:HD3	1.81	0.62
1:A:121:GLY:HA3	1:A:209:ALA:HB2	1.81	0.62
1:A:530:LEU:O	1:A:533:THR:HB	2.00	0.62
1:A:276:HIS:NE2	1:A:280:TYR:CE2	2.66	0.62
2:B:243:LEU:O	2:B:247:LYS:HG3	2.00	0.62
1:A:410:ALA:HB2	1:A:463:GLN:HB2	1.84	0.60
1:A:116:MET:HE3	1:A:200:ILE:HG23	1.83	0.60
1:A:365:GLY:HA2	2:B:60:PHE:HB3	1.82	0.60
2:B:119:HIS:O	2:B:121:TRP:N	2.35	0.59
1:A:230:LEU:HD22	1:A:320:PHE:HE1	1.65	0.59
2:B:139:LEU:HD21	2:B:159:ASP:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ASN:HB2	1:A:199:ASN:HD21	1.68	0.59
1:A:116:MET:HE1	1:A:204:PHE:HB2	1.86	0.58
1:A:276:HIS:CD2	1:A:280:TYR:HE2	2.21	0.58
1:A:412:PHE:CE1	1:A:413:HIS:CE1	2.91	0.58
2:B:98:PRO:HD3	9:B:274:LDA:HM11	1.86	0.58
1:A:544:GLU:HG3	1:A:545:THR:H	1.69	0.57
1:A:53:MET:HE2	1:A:91:ILE:HG22	1.86	0.57
2:B:72:THR:O	2:B:73:HIS:HB3	2.05	0.57
1:A:342:LEU:HA	1:A:345:MET:CE	2.34	0.57
1:A:196:GLY:O	1:A:200:ILE:HG12	2.05	0.57
1:A:121:GLY:HA2	1:A:543:PHE:CE2	2.40	0.56
1:A:459:ILE:HD11	1:A:493:ALA:HA	1.87	0.56
1:A:325:HIS:HD2	1:A:326:HIS:CD2	2.23	0.56
1:A:279:VAL:HB	8:A:563:HEA:CAC	2.35	0.56
2:B:179:VAL:CG1	2:B:180:ILE:N	2.68	0.56
1:A:31:ILE:HD12	1:A:132:ASN:HA	1.88	0.56
1:A:53:MET:CE	1:A:91:ILE:HG22	2.35	0.55
2:B:220:CYS:SG	2:B:224:HIS:HA	2.47	0.55
3:C:35:SER:OG	3:C:99:HIS:HE1	1.90	0.55
3:C:3:LYS:HG2	10:C:131:HOH:O	2.06	0.55
1:A:269:HIS:HD2	1:A:323:TRP:HE1	1.54	0.55
1:A:362:MET:HB3	1:A:367:ILE:HD11	1.89	0.54
1:A:284:LEU:O	1:A:287:PHE:HB2	2.08	0.54
1:A:469:GLN:NE2	2:B:14:VAL:H	2.05	0.54
1:A:91:ILE:HG13	1:A:92:THR:N	2.22	0.54
1:A:325:HIS:HD1	1:A:344:THR:HG21	1.72	0.54
2:B:119:HIS:HD2	2:B:177:THR:OG1	1.89	0.54
1:A:152:PRO:O	1:A:176:GLY:HA3	2.07	0.53
1:A:279:VAL:HB	8:A:563:HEA:C3C	2.38	0.53
2:B:10:ILE:HB	2:B:212:TYR:CE1	2.44	0.53
1:A:131:ASN:HB2	1:A:199:ASN:ND2	2.23	0.53
1:A:466:LEU:HD21	1:A:485:TRP:HB2	1.90	0.53
8:A:563:HEA:HMC1	8:A:563:HEA:HBC1	1.91	0.53
1:A:418:LEU:HD11	1:A:456:SER:HB3	1.91	0.53
2:B:188:PHE:HB2	2:B:190:VAL:HG22	1.91	0.53
8:A:562:HEA:HMC1	8:A:562:HEA:CBC	2.35	0.53
1:A:129:ARG:HG3	1:A:130:LEU:N	2.24	0.52
2:B:138:MET:HB2	2:B:228:PRO:HD2	1.90	0.52
1:A:500:PHE:HB2	8:A:562:HEA:H261	1.91	0.52
1:A:342:LEU:HA	1:A:345:MET:HE2	1.92	0.52
3:C:27:PHE:CE2	3:C:29:PHE:HA	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ALA:HB2	1:A:270:ILE:CG2	2.40	0.52
1:A:396:ALA:HB3	1:A:397:PRO:HD3	1.93	0.51
2:B:56:CYS:HA	2:B:60:PHE:CD2	2.43	0.51
1:A:413:HIS:CG	1:A:460:PHE:CE1	2.99	0.51
2:B:179:VAL:HG13	2:B:180:ILE:H	1.75	0.51
1:A:325:HIS:HD1	1:A:344:THR:CG2	2.24	0.51
1:A:412:PHE:HE1	1:A:413:HIS:CE1	2.29	0.51
3:C:91:THR:HB	3:C:115:THR:HA	1.93	0.51
3:C:12:VAL:HG12	3:C:13:GLN:N	2.26	0.51
1:A:179:MET:O	1:A:183:ILE:HG13	2.10	0.50
1:A:101:PHE:CE1	1:A:189:SER:HB2	2.46	0.50
1:A:103:VAL:CG1	1:A:282:ILE:HG23	2.41	0.50
2:B:165:PRO:HA	2:B:234:VAL:O	2.12	0.50
1:A:276:HIS:HB3	1:A:277:PRO:HD3	1.93	0.50
2:B:53:LEU:O	2:B:57:ILE:HG13	2.11	0.50
3:C:99:HIS:HD2	3:C:104:ALA:O	1.94	0.50
1:A:91:ILE:CD1	1:A:474:ARG:HG2	2.42	0.50
3:C:53:ASN:H	3:C:53:ASN:ND2	2.10	0.50
1:A:52:TYR:HD2	1:A:90:MET:CE	2.25	0.50
1:A:300:LYS:HD3	1:A:361:THR:O	2.12	0.50
8:A:563:HEA:C26	8:A:563:HEA:H273	2.41	0.50
1:A:355:VAL:O	1:A:359:ILE:HG12	2.12	0.50
1:A:276:HIS:CE1	1:A:280:TYR:CE2	3.00	0.50
1:A:432:ILE:CD1	1:A:510:THR:HG21	2.41	0.50
1:A:101:PHE:HE1	1:A:189:SER:HB2	1.76	0.50
1:A:57:LEU:O	1:A:486:ASN:HB3	2.11	0.50
4:D:46:PHE:HZ	4:D:49:TYR:HB3	1.76	0.50
2:B:220:CYS:H	2:B:224:HIS:HB2	1.77	0.49
2:B:28:ALA:O	2:B:32:GLN:HG3	2.11	0.49
1:A:405:THR:HA	1:A:472:PRO:HA	1.93	0.49
2:B:182:ALA:HB3	2:B:217:SER:C	2.32	0.49
1:A:142:VAL:O	1:A:146:VAL:HG23	2.12	0.49
3:C:42:GLU:O	3:C:43:LYS:HB2	2.12	0.49
1:A:26:THR:HB	1:A:128:PRO:HB3	1.93	0.49
4:D:24:ARG:HB3	4:D:24:ARG:NH1	2.27	0.49
4:D:46:PHE:CZ	4:D:49:TYR:HB3	2.47	0.49
1:A:26:THR:HB	1:A:128:PRO:CB	2.43	0.49
2:B:121:TRP:HZ2	2:B:221:GLY:HA3	1.78	0.49
1:A:276:HIS:CE1	1:A:280:TYR:HE2	2.30	0.49
1:A:475:TYR:OH	2:B:215:GLN:HB3	2.12	0.49
3:C:14:PRO:HD3	3:C:117:SER:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:MET:HE2	3:C:86:LEU:HD21	1.95	0.49
4:D:89:GLN:HG2	4:D:90:HIS:N	2.28	0.49
4:D:2:ILE:HG12	4:D:3:GLU:H	1.78	0.48
1:A:362:MET:SD	1:A:377:PHE:HE1	2.36	0.48
1:A:93:TYR:O	1:A:97:LEU:HG	2.13	0.48
8:A:563:HEA:H253	2:B:45:VAL:HG21	1.94	0.48
2:B:74:ASN:O	2:B:77:ILE:HG22	2.13	0.48
3:C:22:CYS:HB3	3:C:79:LEU:HB3	1.95	0.48
1:A:544:GLU:HG3	1:A:545:THR:N	2.29	0.48
3:C:2:VAL:HG13	3:C:27:PHE:CD1	2.48	0.48
2:B:183:TRP:CD1	2:B:229:ILE:HD13	2.49	0.48
1:A:290:ILE:O	1:A:294:ILE:HG12	2.14	0.48
4:D:21:ILE:HG23	4:D:103:THR:HG21	1.95	0.47
2:B:120:GLN:HG3	2:B:121:TRP:CE2	2.48	0.47
1:A:425:PHE:O	1:A:429:TYR:HD2	1.97	0.47
1:A:465:PHE:HE1	9:B:272:LDA:H82	1.78	0.47
1:A:342:LEU:HD23	1:A:345:MET:CE	2.44	0.47
1:A:389:THR:CG2	1:A:411:HIS:HB2	2.44	0.47
2:B:61:ASN:ND2	2:B:63:ARG:HB3	2.29	0.47
1:A:439:GLN:OE1	1:A:439:GLN:HA	2.14	0.47
2:B:18:MET:CE	9:B:273:LDA:H51	2.44	0.47
1:A:500:PHE:O	1:A:504:ILE:HG12	2.15	0.47
1:A:469:GLN:NE2	2:B:14:VAL:O	2.48	0.47
2:B:156:LEU:O	2:B:228:PRO:HB2	2.15	0.47
9:A:569:LDA:HM13	9:B:272:LDA:HM22	1.97	0.47
4:D:37:GLN:HB2	4:D:47:LEU:HD11	1.97	0.47
2:B:164:VAL:O	2:B:233:ALA:HA	2.14	0.47
4:D:29:ILE:HD11	4:D:71:PHE:CE1	2.50	0.47
1:A:293:VAL:O	1:A:297:PHE:HD1	1.98	0.47
1:A:359:ILE:HA	1:A:362:MET:HE2	1.97	0.46
1:A:241:ALA:HB2	1:A:270:ILE:HG22	1.98	0.46
1:A:190:GLY:HA2	1:A:235:LEU:HD13	1.95	0.46
2:B:101:PHE:O	2:B:105:GLU:HB2	2.16	0.46
1:A:27:ASN:HA	1:A:124:ASP:OD2	2.14	0.46
1:A:412:PHE:HA	1:A:415:VAL:CG2	2.46	0.46
1:A:243:THR:O	1:A:246:LEU:HD23	2.15	0.46
4:D:24:ARG:HD2	4:D:70:GLN:NE2	2.30	0.46
1:A:386:GLY:HA3	1:A:414:TYR:HB3	1.96	0.46
3:C:68:PHE:N	3:C:68:PHE:CD1	2.82	0.46
1:A:54:ARG:HD3	1:A:490:SER:OG	2.15	0.46
8:A:563:HEA:HMC1	8:A:563:HEA:CBC	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:TYR:CD1	1:A:440:TYR:C	2.89	0.46
2:B:179:VAL:HG13	2:B:180:ILE:N	2.31	0.46
1:A:536:SER:HA	1:A:537:PRO:HA	1.86	0.46
3:C:61:PRO:HD2	3:C:64:VAL:HG22	1.98	0.46
1:A:304:GLY:C	1:A:307:PRO:HD2	2.35	0.46
8:A:563:HEA:H271	8:A:563:HEA:H212	1.64	0.45
1:A:485:TRP:CE3	1:A:485:TRP:HA	2.51	0.45
2:B:90:VAL:HA	9:B:274:LDA:H71	1.98	0.45
9:A:565:LDA:H112	2:B:52:LEU:HD13	1.98	0.45
2:B:220:CYS:SG	2:B:224:HIS:HB2	2.56	0.45
1:A:34:LEU:HB3	1:A:135:TYR:CE1	2.50	0.45
1:A:58:GLN:HG3	1:A:490:SER:HB2	1.98	0.45
2:B:202:LEU:C	2:B:202:LEU:HD12	2.36	0.45
2:B:76:PRO:O	2:B:80:ILE:HG12	2.17	0.45
1:A:213:THR:OG1	1:A:216:LYS:HB2	2.16	0.45
1:A:152:PRO:HD2	1:A:177:TYR:CE1	2.52	0.45
1:A:50:THR:HG23	8:A:562:HEA:HMB3	1.99	0.45
4:D:33:LEU:HD22	4:D:71:PHE:CB	2.47	0.45
2:B:127:TYR:HB2	2:B:132:VAL:HB	1.99	0.45
2:B:134:PHE:HB3	2:B:250:PHE:CD1	2.52	0.45
2:B:171:LEU:HD12	2:B:202:LEU:O	2.15	0.45
1:A:290:ILE:HD12	1:A:376:ALA:HA	1.99	0.45
2:B:229:ILE:HA	10:B:279:HOH:O	2.17	0.44
4:D:24:ARG:HD2	4:D:70:GLN:HE21	1.82	0.44
1:A:116:MET:HB3	1:A:117:PRO:HD3	1.99	0.44
1:A:27:ASN:ND2	1:A:29:LYS:HB2	2.32	0.44
1:A:384:THR:O	1:A:388:VAL:HB	2.16	0.44
1:A:209:ALA:HB3	1:A:212:MET:HB2	2.00	0.44
1:A:276:HIS:CE1	1:A:325:HIS:CE1	3.05	0.44
2:B:130:ASP:O	2:B:247:LYS:HE3	2.17	0.44
1:A:162:VAL:HG11	1:A:171:SER:HA	1.99	0.44
1:A:341:MET:HG3	1:A:394:SER:O	2.17	0.44
4:D:6:GLN:NE2	4:D:103:THR:HG23	2.32	0.44
1:A:91:ILE:HD12	1:A:474:ARG:HG2	2.00	0.44
3:C:103:TYR:HB2	4:D:91:HIS:O	2.18	0.43
2:B:121:TRP:CG	2:B:223:ASN:HB2	2.53	0.43
1:A:416:MET:HG2	8:A:563:HEA:CBC	2.49	0.43
3:C:53:ASN:H	3:C:53:ASN:HD22	1.66	0.43
1:A:517:VAL:O	1:A:536:SER:HB2	2.18	0.43
2:B:77:ILE:CG2	2:B:78:GLU:N	2.82	0.43
1:A:164:TRP:CE2	1:A:165:VAL:HG13	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:PRO:HB3	1:A:292:HIS:HE1	1.84	0.43
1:A:522:TYR:CE1	1:A:532:TRP:HZ3	2.36	0.43
1:A:272:TRP:CE3	1:A:275:GLY:HA3	2.53	0.43
1:A:481:GLU:O	2:B:15:ASN:HA	2.18	0.43
1:A:31:ILE:CD1	1:A:132:ASN:HA	2.48	0.43
3:C:1:GLU:O	3:C:26:GLY:HA3	2.18	0.43
1:A:518:ASN:ND2	1:A:518:ASN:H	2.15	0.43
1:A:342:LEU:HA	1:A:345:MET:HE3	1.99	0.43
1:A:104:ILE:HB	1:A:105:PRO:HD3	2.01	0.43
3:C:101:TYR:HB3	4:D:49:TYR:CD2	2.53	0.43
1:A:511:LEU:HD21	9:A:566:LDA:H42	2.01	0.43
1:A:83:ASN:HD21	1:A:157:GLN:HE22	1.67	0.43
1:A:29:LYS:HE2	1:A:538:PRO:HB2	2.01	0.42
1:A:304:GLY:O	1:A:307:PRO:HD2	2.18	0.42
1:A:33:ILE:HD13	9:A:566:LDA:H32	2.01	0.42
1:A:359:ILE:HA	1:A:362:MET:CE	2.49	0.42
1:A:516:ARG:HH21	1:A:518:ASN:HB3	1.83	0.42
2:B:119:HIS:CE1	2:B:124:SER:HB3	2.55	0.42
1:A:403:HIS:HD2	1:A:404:ASP:HB2	1.83	0.42
1:A:450:TRP:O	1:A:454:ILE:HD13	2.19	0.42
4:D:94:THR:HA	4:D:95:PRO:HD3	1.90	0.42
1:A:31:ILE:HG13	1:A:131:ASN:ND2	2.34	0.42
1:A:107:LEU:HD21	1:A:424:ILE:HG13	2.00	0.42
1:A:502:PHE:CE2	1:A:506:ILE:HD11	2.54	0.42
1:A:352:GLY:HA2	8:A:563:HEA:H272	2.01	0.42
3:C:6:GLU:CD	3:C:111:GLY:H	2.23	0.42
1:A:461:PHE:N	1:A:462:PRO:CD	2.83	0.42
1:A:320:PHE:HA	10:A:587:HOH:O	2.20	0.42
3:C:101:TYR:O	3:C:102:TYR:HB2	2.20	0.42
1:A:303:PHE:CD2	1:A:360:ALA:HB1	2.55	0.42
1:A:412:PHE:HB2	8:A:563:HEA:HMD3	2.02	0.41
1:A:440:TYR:HA	1:A:510:THR:OG1	2.19	0.41
1:A:190:GLY:O	1:A:194:ILE:HG13	2.20	0.41
1:A:84:GLY:HA3	2:B:222:ILE:O	2.20	0.41
1:A:366:SER:H	2:B:65:ASN:HB3	1.85	0.41
1:A:364:GLY:O	1:A:365:GLY:O	2.39	0.41
1:A:416:MET:HG2	8:A:563:HEA:HBC2	2.02	0.41
1:A:389:THR:HG22	1:A:411:HIS:HB2	2.03	0.41
8:A:562:HEA:HMB1	8:A:562:HEA:O11	2.20	0.41
1:A:300:LYS:HE2	1:A:300:LYS:HB3	1.81	0.41
1:A:264:PRO:O	1:A:267:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:THR:O	1:A:96:VAL:HG23	2.20	0.41
1:A:164:TRP:HD1	8:A:562:HEA:O1D	2.03	0.41
1:A:295:SER:HB2	1:A:300:LYS:O	2.21	0.41
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.74	0.41
1:A:396:ALA:HB3	2:B:100:LEU:HD13	2.02	0.41
1:A:386:GLY:HA2	10:A:573:HOH:O	2.21	0.41
1:A:222:TRP:O	1:A:226:ILE:HG13	2.21	0.41
2:B:213:PHE:CD1	2:B:230:VAL:HG22	2.56	0.41
4:D:50:ASN:N	4:D:91:HIS:HE1	2.03	0.41
1:A:67:LEU:HA	1:A:67:LEU:HD12	1.85	0.41
1:A:19:PHE:HA	1:A:23:PHE:HD2	1.86	0.40
8:A:563:HEA:H241	2:B:89:LEU:HD21	2.02	0.40
3:C:68:PHE:N	3:C:68:PHE:HD1	2.19	0.40
4:D:28:ASN:HA	4:D:68:GLY:O	2.21	0.40
1:A:520:PRO:O	1:A:532:TRP:HA	2.21	0.40
1:A:111:PHE:HZ	1:A:428:VAL:HG23	1.85	0.40
2:B:77:ILE:HG23	2:B:78:GLU:N	2.37	0.40
1:A:52:TYR:HD2	1:A:90:MET:HE3	1.86	0.40
1:A:85:HIS:CE1	1:A:154:GLY:HA3	2.56	0.40
1:A:324:ALA:C	1:A:326:HIS:H	2.24	0.40
1:A:294:ILE:HD11	1:A:376:ALA:HB1	2.04	0.40
2:B:80:ILE:HD13	2:B:80:ILE:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	527/558 (94%)	478 (91%)	43 (8%)	6 (1%)	17 42
2	B	250/298 (84%)	223 (89%)	22 (9%)	5 (2%)	9 24
3	C	116/127 (91%)	111 (96%)	4 (3%)	1 (1%)	21 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	106/120 (88%)	96 (91%)	7 (7%)	3 (3%)	6 15
All	All	999/1103 (91%)	908 (91%)	76 (8%)	15 (2%)	13 32

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	GLY
2	B	120	GLN
1	A	175	ALA
1	A	207	MET
2	B	154	TYR
4	D	77	SER
1	A	366	SER
2	B	121	TRP
4	D	2	ILE
2	B	75	THR
3	C	102	TYR
1	A	176	GLY
4	D	68	GLY
2	B	11	GLY
1	A	517	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	432/454 (95%)	411 (95%)	21 (5%)	31 61
2	B	211/243 (87%)	203 (96%)	8 (4%)	40 71
3	C	101/107 (94%)	98 (97%)	3 (3%)	48 79
4	D	92/104 (88%)	83 (90%)	9 (10%)	10 23
All	All	836/908 (92%)	795 (95%)	41 (5%)	31 61

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	PHE
1	A	21	ARG
1	A	50	THR
1	A	54	ARG
1	A	63	GLN
1	A	116	MET
1	A	137	MET
1	A	187	HIS
1	A	198	ILE
1	A	248	ASP
1	A	274	PHE
1	A	302	ILE
1	A	325	HIS
1	A	366	SER
1	A	377	PHE
1	A	380	LEU
1	A	388	VAL
1	A	404	ASP
1	A	408	VAL
1	A	499	SER
1	A	518	ASN
2	B	2	ASP
2	B	3	VAL
2	B	50	CYS
2	B	54	LEU
2	B	81	TRP
2	B	140	GLU
2	B	178	ASP
2	B	231	VAL
3	C	87	LYS
3	C	91	THR
3	C	98	ARG
4	D	2	ILE
4	D	7	THR
4	D	22	THR
4	D	26	SER
4	D	48	VAL
4	D	52	LYS
4	D	69	THR
4	D	103	THR
4	D	108	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	131	ASN
1	A	157	GLN
1	A	269	HIS
1	A	469	GLN
1	A	486	ASN
1	A	518	ASN
2	B	21	GLN
2	B	65	ASN
2	B	119	HIS
2	B	160	ASN
2	B	208	GLN
2	B	215	GLN
3	C	99	HIS
4	D	91	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 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	$\#\|Z\|>2$
8	HEA	A	562	1	40,67,67	1.48	6 (15%)	41,103,103	1.15	4 (9%)
8	HEA	A	563	1	40,67,67	1.51	7 (17%)	41,103,103	1.04	3 (7%)
9	LDA	A	564	-	15,15,15	4.29	2 (13%)	16,17,17	0.81	1 (6%)
9	LDA	A	565	-	15,15,15	4.75	2 (13%)	16,17,17	0.53	0
9	LDA	A	566	-	15,15,15	4.46	2 (13%)	16,17,17	0.47	0
9	LDA	A	567	-	15,15,15	4.49	1 (6%)	16,17,17	0.40	0
9	LDA	A	568	-	15,15,15	3.29	1 (6%)	16,17,17	0.80	0
9	LDA	A	569	-	15,15,15	4.27	3 (20%)	16,17,17	0.83	0
9	LDA	B	272	-	15,15,15	4.29	1 (6%)	16,17,17	0.58	0
9	LDA	B	273	-	15,15,15	3.86	2 (13%)	16,17,17	0.76	1 (6%)
9	LDA	B	274	-	15,15,15	3.51	1 (6%)	16,17,17	0.72	0

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
8	HEA	A	562	1	3/3/7/16	0/24/76/76	0/0/8/8
8	HEA	A	563	1	3/3/7/16	0/24/76/76	0/0/8/8
9	LDA	A	564	-	-	0/13/13/13	0/0/0/0
9	LDA	A	565	-	-	0/13/13/13	0/0/0/0
9	LDA	A	566	-	-	0/13/13/13	0/0/0/0
9	LDA	A	567	-	-	0/13/13/13	0/0/0/0
9	LDA	A	568	-	-	0/13/13/13	0/0/0/0
9	LDA	A	569	-	-	0/13/13/13	0/0/0/0
9	LDA	B	272	-	-	0/13/13/13	0/0/0/0
9	LDA	B	273	-	-	0/13/13/13	0/0/0/0
9	LDA	B	274	-	-	0/13/13/13	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	565	LDA	O1-N1	-18.15	1.22	1.39
9	A	567	LDA	O1-N1	-17.26	1.23	1.39
9	A	566	LDA	O1-N1	-16.90	1.23	1.39
9	B	272	LDA	O1-N1	-16.30	1.24	1.39
9	A	564	LDA	O1-N1	-16.28	1.24	1.39
9	A	569	LDA	O1-N1	-15.98	1.24	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	273	LDA	O1-N1	-14.54	1.25	1.39
9	B	274	LDA	O1-N1	-13.48	1.26	1.39
9	A	568	LDA	O1-N1	-12.52	1.27	1.39
8	A	563	HEA	C3A-C2A	-4.75	1.34	1.40
8	A	562	HEA	C3A-C2A	-4.71	1.34	1.40
8	A	562	HEA	C3C-CAC	-3.85	1.39	1.47
8	A	563	HEA	C3C-CAC	-3.22	1.41	1.47
8	A	562	HEA	C3C-C2C	-2.94	1.36	1.40
8	A	563	HEA	C3C-C2C	-2.86	1.36	1.40
9	B	273	LDA	CM1-N1	-2.42	1.45	1.49
9	A	566	LDA	CM2-N1	-2.31	1.45	1.49
9	A	569	LDA	CM1-N1	-2.27	1.46	1.49
9	A	564	LDA	C1-N1	-2.17	1.47	1.51
8	A	563	HEA	C3B-C2B	-2.16	1.33	1.41
9	A	565	LDA	C1-N1	-2.13	1.47	1.51
8	A	563	HEA	C22-C23	2.19	1.39	1.32
9	A	569	LDA	C1-N1	2.27	1.55	1.51
8	A	562	HEA	C3A-CMA	2.63	1.52	1.46
8	A	562	HEA	C18-C19	2.74	1.38	1.33
8	A	563	HEA	C18-C19	2.83	1.38	1.33
8	A	563	HEA	C14-C15	2.84	1.38	1.33
8	A	562	HEA	C14-C15	3.17	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	562	HEA	C17-C18-C19	-3.09	121.03	127.76
8	A	562	HEA	C13-C14-C15	-2.59	122.13	127.76
9	B	273	LDA	CM2-N1-CM1	-2.57	105.93	108.83
8	A	563	HEA	C17-C18-C19	-2.43	122.48	127.76
8	A	563	HEA	C13-C14-C15	-2.36	122.64	127.76
8	A	562	HEA	C4B-C3B-C11	-2.04	124.79	127.01
8	A	562	HEA	C3C-C4C-NC	2.17	112.02	109.21
9	A	564	LDA	C12-C11-C10	2.42	132.42	113.44
8	A	563	HEA	C3C-C4C-NC	2.79	112.81	109.21

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	563	HEA	ND
8	A	563	HEA	NA
8	A	563	HEA	NB

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Mol	Chain	Res	Type	Atom
8	A	562	HEA	ND
8	A	562	HEA	NA
8	A	562	HEA	NB

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	562	HEA	7	0
8	A	563	HEA	13	0
9	A	565	LDA	1	0
9	A	566	LDA	2	0
9	A	569	LDA	1	0
9	B	272	LDA	2	0
9	B	273	LDA	1	0
9	B	274	LDA	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.