Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 09:46 pm GMT

PDB ID	:	1W1Z
Title	:	Structure of the plant like 5-Aminolaevulinic Acid Dehydratase from Chlorobium vibrioforme
Authors	:	Coates, L.; Beaven, G.; Erskine, P.T.; Beale, S.I.; Avissar, Y.J.; Gill, R.; Mohammed, F.; Wood, S.P.; Shoolingin-Jordan, P.; Cooper, J.B.
Deposited on	:	2004-06-24
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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 (i)) were used in the production of this report:

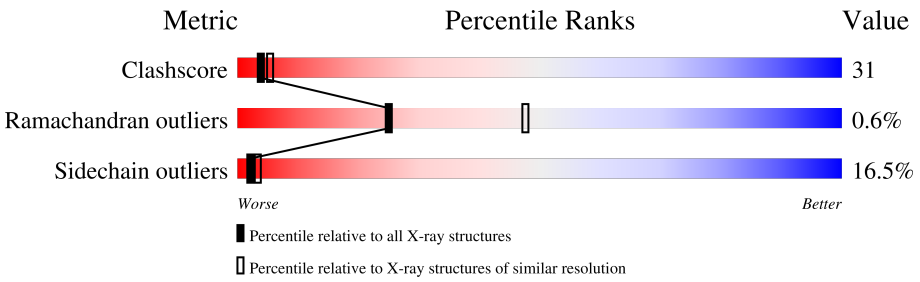
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	328	45% 42% 10% •
1	B	328	45% 42% 11% •

2 Entry composition (i)

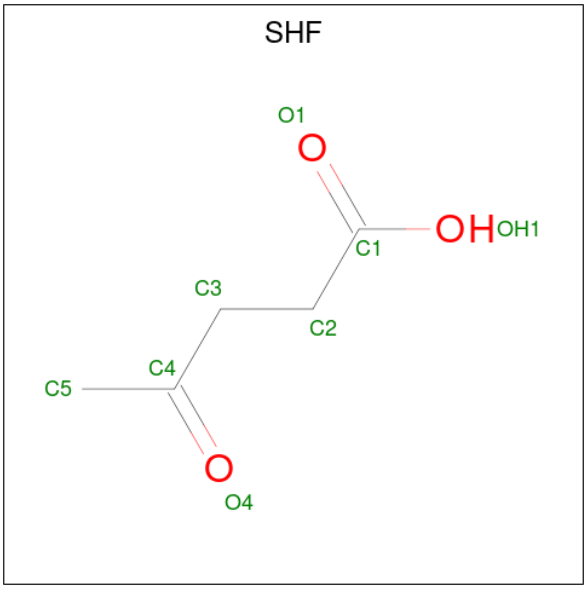
There are 4 unique types of molecules in this entry. The entry contains 5303 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DELTA-AMINOLEVULINIC ACID DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	2481	1569	418	478	16	0	0	0
1	B	319	2481	1569	418	478	16	0	0	0

- Molecule 2 is LAEVULINIC ACID (three-letter code: SHF) (formula: $C_5H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	7	5	2	0	0
2	B	1	7	5	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
			Total	Mg		
3	B	1	1	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	153	153	153	0	0
			Total	O		
4	B	172	172	172	0	0

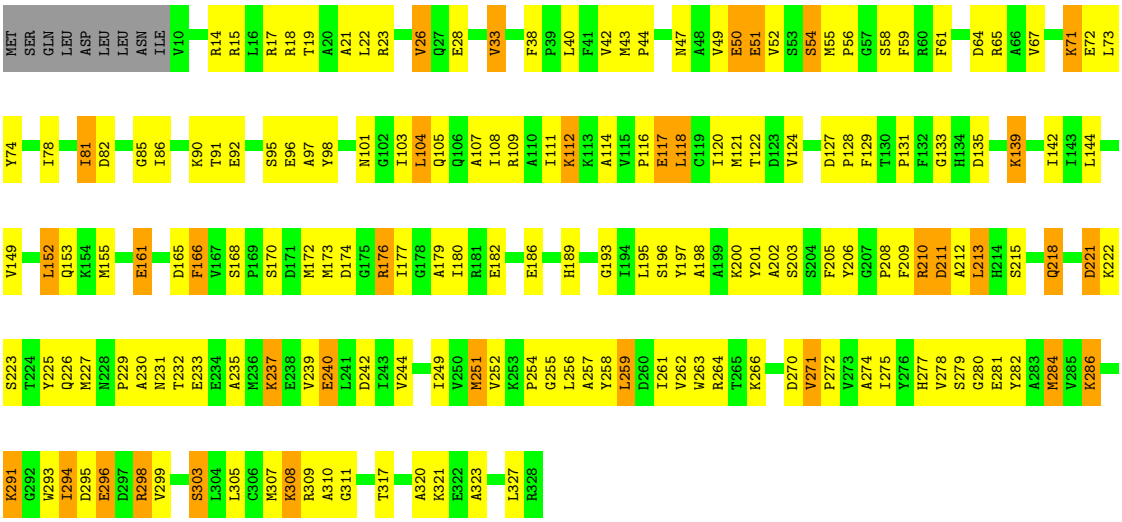
3 Residue-property plots (i)

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. 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. 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.

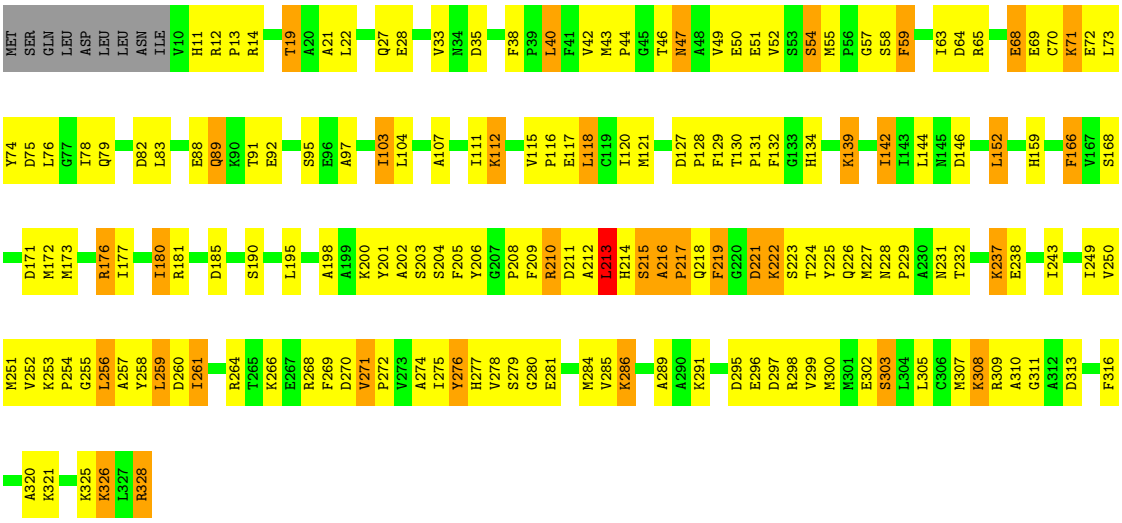
• Molecule 1: DELTA-AMINOLEVULINIC ACID DEHYDRATASE

Chain A: 45% 42% 10% •



• Molecule 1: DELTA-AMINOLEVULINIC ACID DEHYDRATASE

Chain B: 45% 42% 11% •



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	125.23Å 125.23Å 164.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	93.9 (8.00-2.60)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELX	Depositor
R, R_{free}	0.296 , 0.382	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5303	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

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: MG, SHF

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	0.21	0/2528	0.40	0/3421
1	B	0.24	0/2528	0.44	1/3421 (0.0%)
All	All	0.23	0/5056	0.42	1/6842 (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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	213	LEU	C-N-CA	-5.26	108.54	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	216	ALA	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2481	0	2448	160	0
1	B	2481	0	2448	158	0
2	A	7	0	7	0	0
2	B	7	0	7	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	153	0	0	16	1
4	B	172	0	0	9	1
All	All	5303	0	4910	304	1

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 31.

All (304) 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:54:SER:HB2	1:A:208:PRO:HB3	1.50	0.92
1:B:38:PHE:HD2	1:B:320:ALA:HB3	1.42	0.84
1:B:54:SER:HB2	1:B:208:PRO:HB3	1.61	0.82
1:B:68:GLU:HA	1:B:71:LYS:HD3	1.63	0.81
1:A:232:THR:HG22	1:A:264:ARG:HH11	1.42	0.80
1:A:182:GLU:O	1:A:186:GLU:HG3	1.83	0.78
1:A:65:ARG:HD2	4:A:2043:HOH:O	1.83	0.78
1:A:22:LEU:O	1:A:26:VAL:HG22	1.86	0.76
1:B:266:LYS:HD3	1:B:311:GLY:O	1.86	0.76
1:A:112:LYS:HG2	1:A:120:ILE:HD12	1.68	0.76
1:B:69:GLU:OE2	1:B:321:LYS:HE2	1.87	0.74
1:A:28:GLU:H	1:B:231:ASN:ND2	1.89	0.71
1:B:266:LYS:HB3	4:B:2153:HOH:O	1.91	0.71
1:A:107:ALA:O	1:A:111:ILE:HG13	1.90	0.70
1:A:153:GLN:OE1	1:A:179:ALA:HB1	1.91	0.70
1:A:38:PHE:HD2	1:A:320:ALA:HB3	1.55	0.70
1:A:108:ILE:HD11	1:A:122:THR:HG21	1.73	0.70
1:B:278:VAL:HG22	1:B:281:GLU:OE1	1.92	0.70
1:B:139:LYS:HB2	1:B:144:LEU:HD21	1.72	0.69
1:A:74:TYR:CZ	1:A:117:GLU:HB2	2.29	0.68
1:A:38:PHE:O	1:A:81:ILE:HB	1.94	0.68
1:A:168:SER:HA	1:A:195:LEU:O	1.92	0.68
1:A:112:LYS:HZ3	1:A:112:LYS:HA	1.60	0.67
1:B:328:ARG:HG3	4:B:2169:HOH:O	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASP:OD1	4:A:2089:HOH:O	2.12	0.67
1:B:70:CYS:SG	1:B:111:ILE:HD13	2.35	0.67
1:A:82:ASP:HA	1:A:121:MET:O	1.95	0.67
1:B:232:THR:HG23	1:B:261:ILE:HD12	1.76	0.67
1:A:213:LEU:HD12	1:A:213:LEU:H	1.61	0.66
1:B:232:THR:HG22	1:B:264:ARG:HH11	1.60	0.66
1:A:74:TYR:OH	1:A:117:GLU:HB2	1.95	0.66
1:A:90:LYS:HE3	1:A:128:PRO:O	1.95	0.66
1:A:235:ALA:O	1:A:239:VAL:HG23	1.94	0.66
1:A:33:VAL:HG22	4:A:2023:HOH:O	1.96	0.66
1:A:280:GLY:O	1:A:284:MET:HB2	1.95	0.66
1:A:266:LYS:HE2	1:A:311:GLY:O	1.94	0.66
1:A:218:GLN:HB3	4:A:2070:HOH:O	1.96	0.65
1:A:282:TYR:HB2	4:A:2135:HOH:O	1.94	0.65
1:A:271:VAL:HG22	1:A:272:PRO:HD2	1.78	0.65
1:B:206:TYR:HE1	1:B:278:VAL:HG11	1.59	0.65
1:A:275:ILE:HD13	1:A:307:MET:HG2	1.78	0.65
1:A:51:GLU:HG2	1:A:59:PHE:CE2	2.32	0.65
1:B:168:SER:HA	1:B:195:LEU:O	1.97	0.65
1:B:121:MET:HG2	1:B:166:PHE:HB3	1.79	0.64
1:B:277:HIS:HE1	4:B:2158:HOH:O	1.80	0.64
1:A:112:LYS:HA	1:A:112:LYS:NZ	2.13	0.64
1:A:121:MET:HG2	1:A:166:PHE:HB2	1.79	0.63
1:B:232:THR:HG21	4:B:2150:HOH:O	1.98	0.63
1:A:201:TYR:CE2	1:A:227:MET:HE2	2.34	0.63
1:B:209:PHE:CZ	1:B:213:LEU:HD21	2.34	0.62
1:A:51:GLU:HG3	4:A:2035:HOH:O	1.98	0.61
1:B:254:PRO:HD2	1:B:258:TYR:CE1	2.35	0.61
1:A:67:VAL:HG12	1:A:71:LYS:NZ	2.16	0.61
1:A:291:LYS:HD2	4:A:2140:HOH:O	2.00	0.61
1:B:280:GLY:O	1:B:284:MET:HG3	2.00	0.61
1:B:146:ASP:HB2	4:B:2099:HOH:O	1.99	0.61
1:A:19:THR:HG23	1:A:21:ALA:N	2.16	0.61
1:A:86:ILE:HD11	1:A:213:LEU:HA	1.82	0.61
1:A:242:ASP:OD1	4:A:2120:HOH:O	2.16	0.60
1:B:115:VAL:HG12	1:B:118:LEU:HB2	1.81	0.60
1:A:222:LYS:HD2	1:A:225:TYR:OH	2.00	0.60
1:A:222:LYS:HB3	1:A:225:TYR:CZ	2.35	0.60
1:B:251:MET:HA	1:B:274:ALA:O	2.02	0.60
1:B:121:MET:HG2	1:B:166:PHE:CB	2.32	0.60
1:A:209:PHE:CZ	1:A:213:LEU:HD21	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:HG2	1:B:224:THR:O	2.02	0.60
1:B:232:THR:HG23	1:B:261:ILE:CD1	2.32	0.60
1:A:91:THR:O	1:A:131:PRO:HD3	2.02	0.60
1:B:131:PRO:O	1:B:217:PRO:HD2	2.02	0.59
1:B:209:PHE:CE1	1:B:213:LEU:HD21	2.38	0.59
1:A:19:THR:CG2	1:A:22:LEU:H	2.16	0.59
1:B:259:LEU:HG	1:B:310:ALA:HB2	1.85	0.59
1:B:232:THR:CG2	1:B:264:ARG:HH11	2.16	0.58
1:A:209:PHE:CE1	1:A:213:LEU:HD21	2.38	0.58
1:A:225:TYR:HB3	1:B:14:ARG:NE	2.18	0.58
1:A:259:LEU:HG	1:A:310:ALA:HB2	1.85	0.58
1:B:172:MET:HE1	1:B:227:MET:HG3	1.85	0.58
1:B:176:ARG:HG2	1:B:177:ILE:N	2.19	0.58
1:A:139:LYS:HB2	1:A:144:LEU:HD21	1.85	0.58
1:B:103:ILE:HD11	4:B:2044:HOH:O	2.02	0.58
1:B:52:VAL:HG23	1:B:58:SER:O	2.04	0.58
1:A:251:MET:HA	1:A:274:ALA:O	2.04	0.57
1:A:240:GLU:O	1:A:244:VAL:HG23	2.04	0.57
1:B:222:LYS:HB3	1:B:225:TYR:CZ	2.39	0.57
1:B:213:LEU:HD12	1:B:213:LEU:H	1.68	0.57
1:A:232:THR:OG1	1:B:309:ARG:HG2	2.05	0.57
1:B:131:PRO:O	1:B:216:ALA:HB1	2.05	0.57
1:A:67:VAL:O	1:A:71:LYS:HD3	2.05	0.56
1:A:28:GLU:H	1:B:231:ASN:HD21	1.53	0.56
1:A:92:GLU:HG2	4:A:2072:HOH:O	2.05	0.56
1:B:289:ALA:CB	1:B:296:GLU:HB2	2.36	0.56
1:A:232:THR:HG23	1:A:261:ILE:CD1	2.36	0.56
1:B:112:LYS:NZ	1:B:112:LYS:HA	2.21	0.56
1:A:161:GLU:HA	1:A:161:GLU:OE1	2.05	0.56
1:A:232:THR:HG21	4:A:2129:HOH:O	2.06	0.56
4:A:2089:HOH:O	1:B:13:PRO:HD2	2.05	0.56
1:A:295:ASP:HB3	1:A:298:ARG:HB2	1.88	0.55
1:B:76:LEU:HD23	1:B:328:ARG:HD3	1.88	0.55
1:B:271:VAL:HG22	1:B:272:PRO:HD2	1.88	0.55
1:B:321:LYS:O	1:B:325:LYS:HG3	2.07	0.54
1:A:293:TRP:O	1:A:294:ILE:HG23	2.08	0.54
1:B:51:GLU:HG3	1:B:59:PHE:CE2	2.43	0.54
1:A:172:MET:CG	1:A:200:LYS:HB3	2.37	0.54
1:A:28:GLU:OE2	1:B:231:ASN:HB3	2.08	0.54
1:B:55:MET:O	1:B:58:SER:HB2	2.07	0.54
1:B:201:TYR:CE2	1:B:227:MET:HE2	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASP:O	1:B:172:MET:HB2	2.08	0.53
1:A:170:SER:HB3	1:A:197:TYR:CE1	2.44	0.53
1:B:270:ASP:O	1:B:270:ASP:OD2	2.26	0.53
1:B:127:ASP:HA	1:B:134:HIS:O	2.08	0.53
1:B:214:HIS:O	1:B:215:SER:O	2.27	0.53
1:B:127:ASP:HB3	4:B:2092:HOH:O	2.09	0.52
1:B:209:PHE:HB2	2:B:1253:SHF:O1	2.09	0.52
1:A:270:ASP:O	1:A:270:ASP:OD2	2.27	0.52
1:B:208:PRO:O	1:B:211:ASP:OD1	2.28	0.52
1:A:298:ARG:HG2	1:A:298:ARG:HH11	1.75	0.52
1:A:67:VAL:HG12	1:A:71:LYS:HZ3	1.75	0.52
1:A:166:PHE:CZ	1:A:193:GLY:HA3	2.44	0.52
1:B:221:ASP:OD2	1:B:223:SER:HB3	2.09	0.52
1:A:42:VAL:HA	1:A:61:PHE:O	2.09	0.52
1:A:73:LEU:HD22	1:A:78:ILE:HD13	1.92	0.52
1:B:172:MET:CE	1:B:227:MET:HG3	2.39	0.51
1:A:323:ALA:O	1:A:327:LEU:HD12	2.09	0.51
1:B:89:GLN:OE1	1:B:89:GLN:HA	2.11	0.51
1:B:266:LYS:HE2	1:B:313:ASP:OD2	2.11	0.51
1:A:124:VAL:CG1	1:A:152:LEU:HG	2.40	0.51
1:A:210:ARG:HG3	1:A:215:SER:OG	2.11	0.51
1:A:127:ASP:HB3	1:A:128:PRO:HD3	1.93	0.51
1:A:19:THR:HG23	1:A:21:ALA:H	1.75	0.51
1:B:210:ARG:O	1:B:213:LEU:HD12	2.11	0.50
1:A:252:VAL:HG21	1:A:261:ILE:HG22	1.93	0.50
1:A:176:ARG:O	1:A:180:ILE:HG13	2.11	0.50
1:A:208:PRO:O	1:A:211:ASP:OD1	2.30	0.50
1:B:259:LEU:HG	1:B:310:ALA:CB	2.41	0.50
1:B:279:SER:OG	2:B:1253:SHF:O1	2.22	0.50
1:B:289:ALA:HB1	1:B:296:GLU:HB2	1.94	0.49
1:B:42:VAL:HG12	1:B:103:ILE:HG23	1.94	0.49
1:A:85:GLY:CA	1:A:104:LEU:HD23	2.42	0.49
1:A:251:MET:HG3	1:A:252:VAL:N	2.27	0.49
1:A:55:MET:HB2	1:A:58:SER:HB2	1.95	0.49
1:B:68:GLU:HG2	1:B:69:GLU:N	2.28	0.49
1:A:52:VAL:HG11	1:A:55:MET:HG3	1.94	0.49
1:A:174:ASP:OD1	1:B:14:ARG:HG3	2.11	0.49
1:A:211:ASP:OD1	1:A:212:ALA:N	2.46	0.49
1:B:107:ALA:O	1:B:111:ILE:HG13	2.12	0.49
1:B:222:LYS:O	1:B:226:GLN:HB2	2.13	0.49
1:A:286:LYS:HE2	1:A:296:GLU:OE1	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:THR:HG22	1:B:22:LEU:H	1.78	0.49
1:B:201:TYR:CZ	1:B:227:MET:HE2	2.48	0.49
1:B:200:LYS:HG3	1:B:253:LYS:HD3	1.95	0.49
1:B:51:GLU:HG3	1:B:59:PHE:CD2	2.47	0.49
1:A:230:ALA:O	1:B:309:ARG:HG3	2.13	0.48
1:A:249:ILE:HG12	1:A:272:PRO:HB2	1.94	0.48
1:A:74:TYR:CD2	1:A:118:LEU:HG	2.49	0.48
1:B:142:ILE:HG22	1:B:144:LEU:HD23	1.95	0.48
1:B:216:ALA:HB1	1:B:217:PRO:HD2	1.96	0.48
1:B:291:LYS:HB3	1:B:291:LYS:HE2	1.59	0.48
1:B:47:ASN:H	1:B:64:ASP:CG	2.16	0.48
1:A:72:GLU:HG2	1:A:321:LYS:NZ	2.28	0.48
1:B:115:VAL:HG12	1:B:115:VAL:O	2.14	0.48
1:A:72:GLU:HG2	1:A:321:LYS:HZ1	1.78	0.47
1:A:299:VAL:O	1:A:303:SER:OG	2.27	0.47
1:B:198:ALA:HA	4:B:2141:HOH:O	2.14	0.47
1:A:218:GLN:H	1:A:218:GLN:HG3	1.35	0.47
1:A:210:ARG:NE	4:A:2105:HOH:O	2.47	0.47
1:A:308:LYS:HD2	1:A:308:LYS:HA	1.55	0.47
1:A:50:GLU:O	1:A:59:PHE:HA	2.15	0.47
1:A:52:VAL:CG1	1:A:55:MET:HG3	2.44	0.47
1:B:111:ILE:HG22	1:B:120:ILE:HD11	1.97	0.47
1:A:18:ARG:HH11	1:A:18:ARG:HG2	1.78	0.47
1:A:105:GLN:O	1:A:108:ILE:HB	2.15	0.47
1:A:254:PRO:HD2	1:A:258:TYR:CE1	2.49	0.47
1:A:317:THR:HG23	1:A:320:ALA:N	2.29	0.47
1:B:112:LYS:HE2	1:B:120:ILE:HG13	1.97	0.47
1:A:233:GLU:OE2	1:A:264:ARG:NH2	2.47	0.47
1:B:252:VAL:HG21	1:B:261:ILE:HG22	1.96	0.47
1:A:231:ASN:ND2	1:B:28:GLU:H	2.13	0.46
1:B:35:ASP:OD2	1:B:308:LYS:NZ	2.48	0.46
1:B:104:LEU:HD12	1:B:159:HIS:NE2	2.30	0.46
1:A:86:ILE:CD1	1:A:213:LEU:HA	2.44	0.46
1:A:104:LEU:HD22	1:A:104:LEU:HA	1.77	0.46
1:A:251:MET:HE2	1:A:275:ILE:N	2.30	0.46
1:B:171:ASP:OD2	1:B:173:MET:HB2	2.15	0.46
1:B:249:ILE:HG23	1:B:272:PRO:HB2	1.96	0.46
1:B:127:ASP:HB3	1:B:128:PRO:HD3	1.96	0.46
1:A:127:ASP:HB2	1:A:135:ASP:OD1	2.16	0.46
1:A:198:ALA:HA	4:A:2119:HOH:O	2.15	0.46
1:A:133:GLY:HA2	4:A:2069:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:THR:HG23	1:A:261:ILE:HD13	1.98	0.46
1:B:52:VAL:HB	1:B:55:MET:HB2	1.97	0.46
1:B:286:LYS:HE3	1:B:296:GLU:OE2	2.16	0.46
1:B:299:VAL:O	1:B:303:SER:OG	2.28	0.46
1:A:203:SER:OG	1:A:205:PHE:HD1	1.98	0.46
1:A:255:GLY:CA	1:A:275:ILE:HD11	2.45	0.46
1:B:103:ILE:HD12	1:B:103:ILE:HA	1.77	0.46
1:B:68:GLU:O	1:B:71:LYS:HB2	2.16	0.46
1:A:47:ASN:O	1:A:47:ASN:ND2	2.50	0.45
1:A:202:ALA:HA	1:A:226:GLN:OE1	2.15	0.45
1:B:91:THR:O	1:B:131:PRO:HD3	2.16	0.45
1:B:284:MET:HB3	1:B:284:MET:HE3	1.82	0.45
1:A:262:VAL:HG21	1:A:275:ILE:HD12	1.97	0.45
1:A:72:GLU:OE2	1:A:72:GLU:O	2.34	0.45
1:A:263:TRP:HA	1:A:310:ALA:O	2.16	0.45
1:A:15:ARG:NH2	4:A:2005:HOH:O	2.50	0.45
1:B:27:GLN:NE2	4:B:2028:HOH:O	2.48	0.45
1:A:56:PRO:HB2	1:A:286:LYS:HG2	1.98	0.45
1:B:54:SER:OG	1:B:211:ASP:OD2	2.31	0.45
1:B:209:PHE:O	1:B:212:ALA:HB3	2.15	0.45
1:A:201:TYR:CD2	1:A:229:PRO:HA	2.52	0.45
1:B:152:LEU:HB3	1:B:180:ILE:HD11	1.99	0.45
1:B:219:PHE:O	1:B:219:PHE:CG	2.70	0.45
1:B:229:PRO:HB3	1:B:258:TYR:OH	2.16	0.45
1:B:112:LYS:HD3	1:B:116:PRO:HA	1.99	0.45
1:B:260:ASP:OD2	1:B:261:ILE:HD13	2.17	0.45
1:B:285:VAL:HG11	1:B:300:MET:HG2	1.98	0.45
1:A:161:GLU:OE1	1:A:189:HIS:NE2	2.50	0.45
1:B:97:ALA:HA	1:B:129:PHE:CE1	2.51	0.45
1:B:254:PRO:HB3	1:B:278:VAL:CG2	2.47	0.45
1:B:251:MET:HE1	1:B:316:PHE:CG	2.51	0.45
1:B:11:HIS:O	1:B:12:ARG:HG3	2.17	0.44
1:A:17:ARG:O	1:A:23:ARG:NH1	2.50	0.44
1:B:43:MET:HB2	1:B:44:PRO:HD2	1.99	0.44
1:B:222:LYS:H	1:B:222:LYS:HG2	1.60	0.44
1:A:257:ALA:CB	1:B:256:LEU:HD22	2.48	0.44
1:B:203:SER:OG	1:B:205:PHE:HB2	2.18	0.44
1:B:286:LYS:HE3	1:B:296:GLU:CD	2.37	0.44
1:B:298:ARG:HG2	1:B:298:ARG:HH11	1.81	0.44
1:A:177:ILE:HG12	1:A:242:ASP:OD1	2.18	0.44
1:A:208:PRO:HB2	1:A:279:SER:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:VAL:HG23	1:B:281:GLU:HG3	1.99	0.44
1:A:49:VAL:CG1	1:A:59:PHE:HB3	2.47	0.44
1:B:303:SER:O	1:B:307:MET:HG3	2.18	0.44
1:A:96:GLU:HB3	1:A:129:PHE:HD1	1.83	0.44
1:A:173:MET:O	1:A:176:ARG:HD2	2.17	0.44
1:A:237:LYS:HB3	1:A:237:LYS:HE2	1.68	0.44
1:A:277:HIS:HA	1:A:281:GLU:OE2	2.18	0.44
1:B:115:VAL:CG1	1:B:118:LEU:HB2	2.47	0.44
1:B:237:LYS:HE2	1:B:237:LYS:HB3	1.33	0.44
1:A:43:MET:HB2	1:A:44:PRO:HD2	2.00	0.43
1:A:54:SER:HB2	1:A:208:PRO:CB	2.33	0.43
1:A:133:GLY:O	1:A:210:ARG:NH2	2.50	0.43
1:A:149:VAL:HA	1:A:152:LEU:HB2	2.00	0.43
1:A:291:LYS:HE2	1:A:291:LYS:HB3	1.48	0.43
1:A:298:ARG:HG2	1:A:298:ARG:NH1	2.32	0.43
1:B:74:TYR:CZ	1:B:117:GLU:HB2	2.53	0.43
1:A:259:LEU:HD23	1:B:257:ALA:O	2.18	0.43
1:A:121:MET:HG2	1:A:166:PHE:CB	2.47	0.43
1:B:73:LEU:HD22	1:B:78:ILE:HD13	2.01	0.43
1:B:185:ASP:OD1	1:B:190:SER:HA	2.19	0.43
1:A:284:MET:HB3	1:A:284:MET:HE2	1.72	0.43
1:B:91:THR:O	1:B:130:THR:HA	2.19	0.43
1:A:19:THR:HG22	1:A:22:LEU:H	1.84	0.43
1:A:221:ASP:OD1	1:A:221:ASP:N	2.50	0.43
1:B:201:TYR:CD2	1:B:229:PRO:HA	2.54	0.43
1:B:112:LYS:HA	1:B:112:LYS:HZ3	1.83	0.42
1:A:206:TYR:HE1	1:A:278:VAL:HG11	1.84	0.42
1:B:40:LEU:HD22	1:B:40:LEU:HA	1.87	0.42
1:A:112:LYS:HG2	1:A:120:ILE:CD1	2.41	0.42
1:A:203:SER:OG	1:B:302:GLU:OE2	2.27	0.42
1:B:38:PHE:CD2	1:B:320:ALA:HB3	2.35	0.42
1:A:97:ALA:HB1	1:A:155:MET:SD	2.60	0.42
1:B:216:ALA:O	1:B:218:GLN:N	2.53	0.42
1:B:64:ASP:OD2	1:B:65:ARG:N	2.50	0.42
1:B:255:GLY:CA	1:B:275:ILE:HD11	2.49	0.42
1:A:309:ARG:O	1:A:309:ARG:HG2	2.19	0.42
1:B:79:GLN:O	1:B:118:LEU:HD23	2.19	0.42
1:A:19:THR:O	1:A:23:ARG:HG3	2.20	0.42
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.83	0.42
1:B:203:SER:HG	1:B:205:PHE:HD1	1.66	0.42
1:A:277:HIS:HE1	4:A:2136:HOH:O	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:HD12	1:B:152:LEU:HA	1.82	0.41
1:B:202:ALA:HA	1:B:226:GLN:OE1	2.19	0.41
1:B:228:ASN:OD1	1:B:229:PRO:HD2	2.20	0.41
1:A:298:ARG:HB3	1:B:204:SER:CB	2.50	0.41
1:A:95:SER:HA	1:A:98:TYR:CE2	2.55	0.41
1:A:251:MET:HB2	1:A:274:ALA:HB3	2.01	0.41
1:B:54:SER:HB2	1:B:208:PRO:CB	2.42	0.41
1:B:249:ILE:HG22	1:B:250:VAL:N	2.34	0.41
1:A:49:VAL:HG12	1:A:59:PHE:CD2	2.56	0.41
1:B:254:PRO:HB3	1:B:278:VAL:HG21	2.02	0.41
1:B:275:ILE:HG12	1:B:276:TYR:N	2.36	0.41
1:A:114:ALA:C	1:A:116:PRO:HD3	2.40	0.41
1:A:205:PHE:HB3	1:A:278:VAL:HG21	2.02	0.41
1:B:55:MET:HB3	1:B:58:SER:HB2	2.02	0.41
1:A:209:PHE:O	1:A:212:ALA:HB3	2.21	0.41
1:A:177:ILE:CD1	1:A:196:SER:HB2	2.51	0.41
1:B:83:LEU:HB3	1:B:104:LEU:HD21	2.03	0.41
1:B:243:ILE:CD1	1:B:269:PHE:HB3	2.50	0.41
1:B:259:LEU:HA	1:B:259:LEU:HD12	1.84	0.41
1:B:295:ASP:HB3	1:B:298:ARG:HB2	2.03	0.41
1:B:42:VAL:CG1	1:B:103:ILE:HG23	2.51	0.41
1:B:308:LYS:HA	1:B:308:LYS:HD2	1.51	0.41
1:A:74:TYR:HD2	1:A:118:LEU:HG	1.86	0.40
1:B:19:THR:CG2	1:B:21:ALA:HB3	2.51	0.40
1:A:38:PHE:CD1	1:A:73:LEU:HD11	2.56	0.40
1:B:112:LYS:HE2	1:B:120:ILE:CD1	2.51	0.40
1:B:297:ASP:HB3	1:B:326:LYS:HE3	2.03	0.40
1:A:17:ARG:NH2	1:B:238:GLU:OE2	2.50	0.40
1:A:232:THR:HG22	1:A:264:ARG:NH1	2.24	0.40
1:A:172:MET:CE	1:A:227:MET:HG3	2.52	0.40
1:B:57:GLY:O	1:B:59:PHE:CE1	2.75	0.40
1:B:82:ASP:HA	1:B:121:MET:O	2.21	0.40
1:B:92:GLU:OE1	1:B:132:PHE:HZ	2.05	0.40
1:A:295:ASP:OD2	1:A:298:ARG:HD3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2127:HOH:O	4:B:2007:HOH:O[3_555]	2.14	0.06

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	317/328 (97%)	299 (94%)	18 (6%)	0	100	100
1	B	317/328 (97%)	298 (94%)	15 (5%)	4 (1%)	12	24
All	All	634/656 (97%)	597 (94%)	33 (5%)	4 (1%)	25	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	215	SER
1	B	219	PHE
1	B	217	PRO
1	B	47	ASN

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	263/272 (97%)	219 (83%)	44 (17%)	2	3
1	B	263/272 (97%)	220 (84%)	43 (16%)	2	3
All	All	526/544 (97%)	439 (84%)	87 (16%)	2	3

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	33	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	40	LEU
1	A	50	GLU
1	A	51	GLU
1	A	54	SER
1	A	64	ASP
1	A	71	LYS
1	A	81	ILE
1	A	101	ASN
1	A	103	ILE
1	A	104	LEU
1	A	109	ARG
1	A	112	LYS
1	A	117	GLU
1	A	118	LEU
1	A	139	LYS
1	A	142	ILE
1	A	152	LEU
1	A	161	GLU
1	A	165	ASP
1	A	166	PHE
1	A	176	ARG
1	A	210	ARG
1	A	211	ASP
1	A	213	LEU
1	A	218	GLN
1	A	221	ASP
1	A	223	SER
1	A	237	LYS
1	A	240	GLU
1	A	251	MET
1	A	256	LEU
1	A	259	LEU
1	A	271	VAL
1	A	284	MET
1	A	286	LYS
1	A	291	LYS
1	A	294	ILE
1	A	296	GLU
1	A	298	ARG
1	A	303	SER
1	A	305	LEU
1	A	308	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	19	THR
1	B	33	VAL
1	B	40	LEU
1	B	46	THR
1	B	49	VAL
1	B	50	GLU
1	B	54	SER
1	B	59	PHE
1	B	63	ILE
1	B	68	GLU
1	B	71	LYS
1	B	72	GLU
1	B	75	ASP
1	B	88	GLU
1	B	89	GLN
1	B	95	SER
1	B	103	ILE
1	B	112	LYS
1	B	118	LEU
1	B	139	LYS
1	B	142	ILE
1	B	152	LEU
1	B	166	PHE
1	B	176	ARG
1	B	180	ILE
1	B	181	ARG
1	B	210	ARG
1	B	213	LEU
1	B	221	ASP
1	B	222	LYS
1	B	237	LYS
1	B	256	LEU
1	B	259	LEU
1	B	261	ILE
1	B	268	ARG
1	B	271	VAL
1	B	276	TYR
1	B	286	LYS
1	B	303	SER
1	B	305	LEU
1	B	308	LYS
1	B	326	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	328	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	99	ASN
1	A	106	GLN
1	A	231	ASN
1	A	277	HIS
1	B	27	GLN
1	B	79	GLN
1	B	99	ASN
1	B	106	GLN
1	B	231	ASN
1	B	277	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	SHF	A	1253	1	6,6,7	0.83	0	6,6,8	1.00	0
2	SHF	B	1253	1	6,6,7	0.83	0	6,6,8	1.00	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
2	SHF	A	1253	1	-	1/4/4/5	-
2	SHF	B	1253	1	-	3/4/4/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1253	SHF	C2-C3-C4-C5
2	B	1253	SHF	C2-C3-C4-C5
2	B	1253	SHF	OH1-C1-C2-C3
2	B	1253	SHF	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1253	SHF	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.