W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 03:25 PM GMT

PDB ID   :   2IAA
Title   :   Crystal Structure of an Electron Transfer Complex Between Aromatic Amine
            Dephydrogenase and Azurin from Alcaligenes Faecalis (Form 2)
Authors   :   Sukumar, N.; Chen, Z.; Leys, D.; Scrutton, N.S.; Ferrati, D.; Merli, A.; Rossi,
              G.L.; Bellamy, H.D.; Chistoserdov, A.; Davidson, V.L.; Mathews, F.S.
Deposited on   :   2006-09-07
Resolution   :   1.95 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 1.95 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.206
Clashscore		12
Ramachandran outliers		0.4%
Sidechain outliers		1.8%
RSRZ outliers		8.9%

Worse ▮ Percentile relative to all X-ray structures *Better*

▯ Percentile relative to X-ray structures of similar resolution
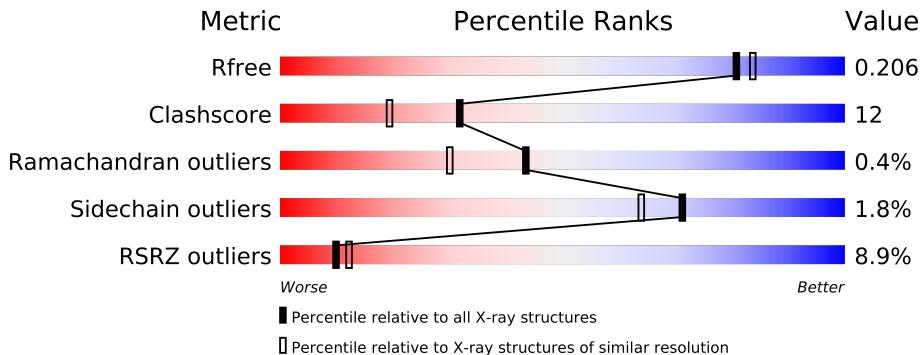
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	390	
1	D	390	
2	B	135	
2	E	135	
3	C	128	
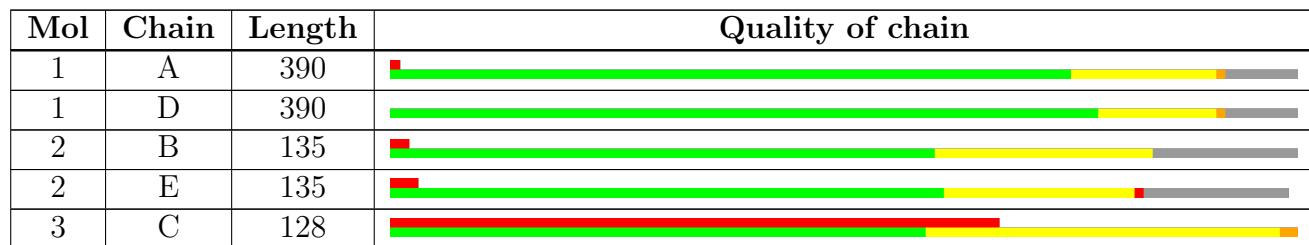
2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 9307 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Aromatic Amine Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	1	0
			2813	1775	490	534	14			
1	D	359	Total	C	N	O	S	0	1	0
			2813	1775	490	534	14			

- Molecule 2 is a protein called Aromatic Amine Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	113	Total	C	N	O	S	0	0	0
			867	528	152	172	15			
2	E	113	Total	C	N	O	S	0	0	0
			867	528	152	172	15			

- Molecule 3 is a protein called Azurin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	128	Total	C	N	O	S	0	0	0
			957	596	160	194	7			

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cu	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	374	Total	O	0	0
			374	374		
5	B	97	Total	O	0	0
			97	97		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	25	Total 25	O 25	0	0
5	D	393	Total 393	O 393	0	0
5	E	100	Total 100	O 100	0	0

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: Aromatic Amine Dehydrogenase

Chain A:
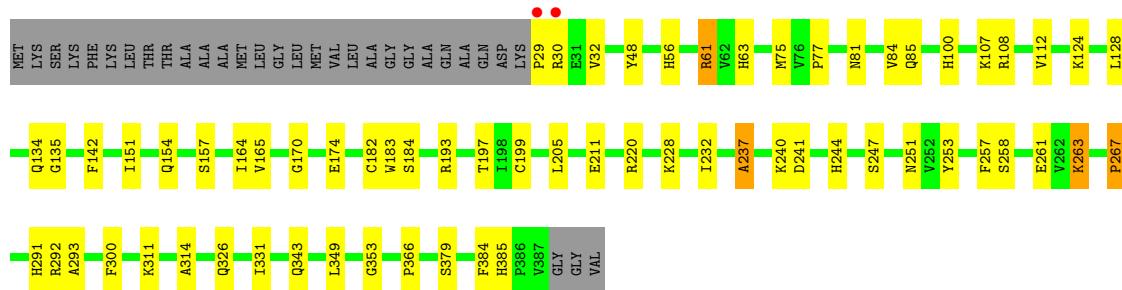
• Molecule 1: Aromatic Amine Dehydrogenase

Chain D:
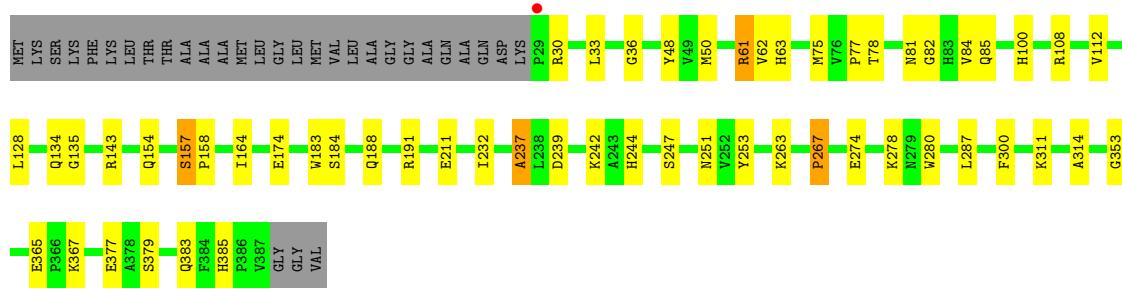
• Molecule 2: Aromatic Amine Dehydrogenase

Chain B:

• Molecule 2: Aromatic Amine Dehydrogenase

Chain E:

ALA GLY GLY GLY GLY SER SER SER GLY ALA ASP HIS ILE LEU SER LEU ASN PRO ASP LEU ALA ASN E22 D23 E24 V25 N26 Y30 H33 C34 F39 C51 S55 T56 P57 S58 S61 W62 Y79 K85 G89 R90 T95 G102 H108 N109 D110 V111 N112

W113 N117 S120 A133 K134 ASN
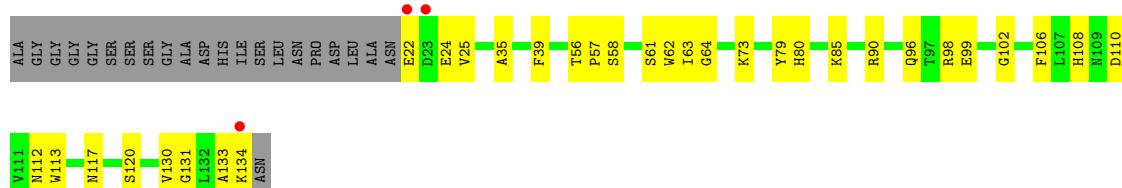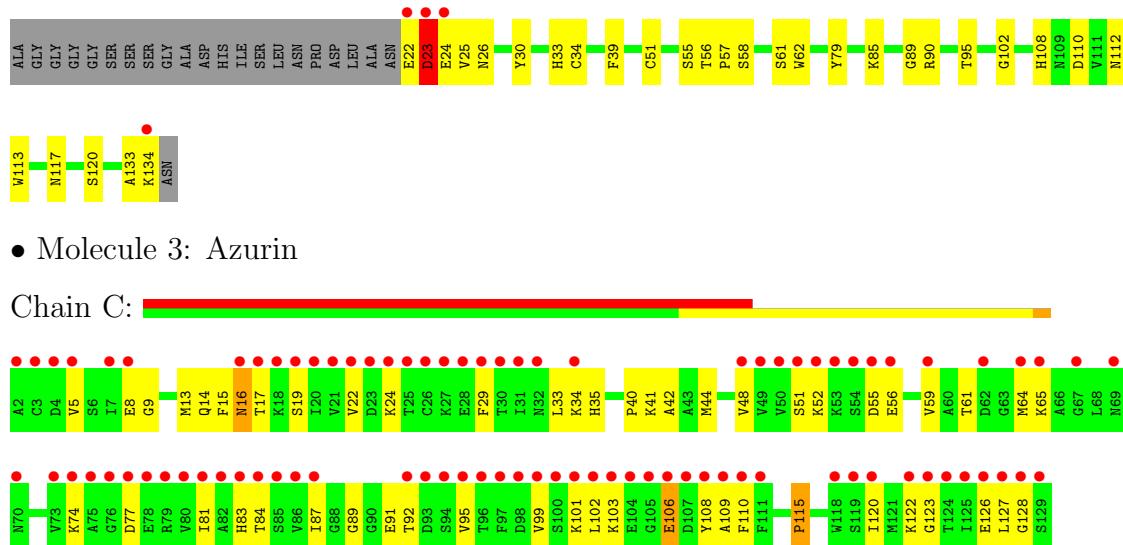
• Molecule 3: Azurin

Chain C:

A2 C3 D4 V5 S6 I7 E8 G9 M13 Q14 F15 N16 T17 K18 S19 I20 V21 V22 D23 K24 T25 C26 K27 E28 F29 T30 I31 N32 L33 K34 H35 P40 K41 A42 A43 M44 V48 V49 V50 S51 K52 K53 S54 D55 E56 V59 A60 T61 D62 G63 M64 K65 A66 G67 L68 N69

N70 V73 K74 A75 G76 D77 E78 R79 V80 I81 A82 H83 T84 S85 V86 I87 G88 G89 G90 E91 T92 D93 S94 V95 T96 F97 D98 V99 S100 K101 L102 K103 E104 G105 E106 D107 Y108 A109 F110 F111 P115 W118 S119 I120 M121 K122 G123 T124 I125 E126 L127 G128 S129

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.22Å　　131.72Å　　133.20Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	47.04　–　1.95 47.04　–　1.95	Depositor EDS
% Data completeness (in resolution range)	89.5 (47.04-1.95) 89.6 (47.04-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.67 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.174　,　0.205 0.176　,　0.206	Depositor DCC
R_{free} test set	3893 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.8	EDS
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
L-test for twinning	$<\lvert L\rvert> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	0 of 80127 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9307	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

5   Model quality (i)

5.1   Standard geometry (i)

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

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	0.31	0/2878	0.67	1/3900 (0.0%)
1	D	0.32	0/2878	0.67	1/3900 (0.0%)
2	B	0.32	0/873	0.67	0/1187
2	E	0.31	0/873	0.67	0/1187
3	C	0.28	0/972	0.49	0/1307
All	All	0.31	0/8474	0.65	2/11481 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ALA	N-CA-C	-6.06	94.65	111.00
1	D	237	ALA	N-CA-C	-5.60	95.88	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2   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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2813	0	2757	50	0
1	D	2813	0	2757	45	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	867	0	760	30	0
2	E	867	0	760	27	0
3	C	957	0	932	58	0
4	C	1	0	0	0	0
5	A	374	0	0	7	0
5	B	97	0	0	2	0
5	C	25	0	0	1	0
5	D	393	0	0	3	0
5	E	100	0	0	2	0
All	All	9307	0	7966	188	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (188) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:85:LYS:HD3	1:D:75[B]:MET:HE2	1.43	0.98
2:B:62:TRQ:HB2	2:B:113:TRP:NE1	1.81	0.94
1:A:75[B]:MET:HE2	2:E:85:LYS:HD3	1.48	0.94
2:E:62:TRQ:HB2	2:E:113:TRP:NE1	1.86	0.90
2:E:133:ALA:O	2:E:134:LYS:HG2	1.77	0.85
1:D:278:LYS:HE2	1:D:280:TRP:HE1	1.45	0.82
2:E:62:TRQ:HB2	2:E:113:TRP:HE1	1.44	0.81
2:B:62:TRQ:HB2	2:B:113:TRP:HE1	1.41	0.81
2:B:133:ALA:O	2:B:134:LYS:HG3	1.82	0.79
3:C:102:LEU:HD12	3:C:127:LEU:HD22	1.65	0.76
2:B:58:SER:HA	2:B:117:ASN:HD21	1.51	0.76
2:E:23:ASP:HA	2:E:26:ASN:HB2	1.69	0.75
3:C:109:ALA:HB1	3:C:122:LYS:HE2	1.69	0.74
3:C:22:VAL:HG22	3:C:127:LEU:HA	1.73	0.69
2:B:22:GLU:O	2:B:25:VAL:HG22	1.94	0.67
1:D:48:TYR:OH	1:D:385:HIS:HD2	1.78	0.67
2:E:58:SER:HA	2:E:117:ASN:HD21	1.59	0.67
3:C:51:SER:HA	3:C:81:ILE:HD13	1.76	0.67
1:D:61:ARG:HH11	1:D:63:HIS:HE1	1.43	0.66
3:C:56:GLU:OE1	3:C:122:LYS:HG3	1.96	0.66
3:C:24:LYS:HG3	3:C:128:GLY:HA2	1.78	0.66
2:B:130:VAL:O	1:D:30:ARG:HB2	1.97	0.65
3:C:52:LYS:HD2	3:C:106:GLU:OE1	1.97	0.64
1:D:81:ASN:HD21	1:D:135:GLY:H	1.46	0.63
1:D:134:GLN:HE22	2:E:120:SER:HB2	1.63	0.63
2:B:108:HIS:NE2	2:B:110:ASP:HB2	2.14	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:251:ASN:HB3	1:D:267:PRO:HB2	1.81	0.62
1:D:278:LYS:CE	1:D:280:TRP:HE1	2.11	0.62
1:A:251:ASN:HB3	1:A:267:PRO:HB2	1.81	0.61
1:A:134:GLN:HE22	2:B:120:SER:HB2	1.65	0.61
3:C:101:LYS:O	3:C:101:LYS:HG3	2.02	0.60
1:A:75[B]:MET:CE	1:A:77:PRO:HD3	2.31	0.60
1:A:61:ARG:HH11	1:A:63:HIS:HE1	1.48	0.60
1:A:29:PRO:HB3	5:A:609:HOH:O	2.01	0.60
1:A:48:TYR:OH	1:A:385:HIS:HD2	1.85	0.60
1:D:75[B]:MET:CE	1:D:77:PRO:HD3	2.32	0.59
3:C:33:LEU:HD22	3:C:48:VAL:HG23	1.83	0.59
3:C:102:LEU:HD13	3:C:127:LEU:HB2	1.84	0.59
2:B:131:GLY:HA2	1:D:30:ARG:HH11	1.67	0.59
1:A:326:GLN:HG2	5:A:605:HOH:O	2.01	0.59
3:C:52:LYS:HE3	3:C:55:ASP:OD2	2.03	0.59
3:C:61:THR:HG22	3:C:65:LYS:NZ	2.17	0.59
1:A:134:GLN:NE2	2:B:112:ASN:HD22	2.01	0.58
3:C:22:VAL:HG12	3:C:29:PHE:CE1	2.38	0.58
2:E:133:ALA:O	2:E:134:LYS:CG	2.50	0.58
1:A:300:PHE:HB3	1:A:314:ALA:HB2	1.85	0.57
1:D:100:HIS:CE1	1:D:108:ARG:HB2	2.40	0.57
1:D:278:LYS:HE2	1:D:280:TRP:NE1	2.19	0.56
2:B:85:LYS:HD3	1:D:75[B]:MET:CE	2.27	0.56
1:D:164:ILE:HB	1:D:174:GLU:HB3	1.87	0.56
1:A:81:ASN:HD21	1:A:135:GLY:H	1.54	0.56
1:D:253:TYR:CZ	1:D:267:PRO:HB3	2.41	0.56
1:A:253:TYR:CZ	1:A:267:PRO:HB3	2.41	0.56
3:C:22:VAL:HG23	3:C:127:LEU:HD12	1.88	0.55
3:C:122:LYS:HD3	3:C:123:GLY:N	2.21	0.55
3:C:34:LYS:HA	3:C:92:THR:HG22	1.89	0.55
3:C:55:ASP:O	3:C:59:VAL:HG23	2.06	0.55
2:E:90:ARG:HG3	2:E:90:ARG:HH11	1.73	0.54
1:A:228:LYS:HG2	5:A:730:HOH:O	2.08	0.54
1:D:134:GLN:NE2	2:E:112:ASN:HD22	2.06	0.54
3:C:17:THR:HG22	3:C:19:SER:H	1.73	0.53
3:C:81:ILE:N	3:C:81:ILE:HD12	2.24	0.53
3:C:110:PHE:CE1	3:C:123:GLY:HA3	2.44	0.53
1:A:261:GLU:HB2	1:A:263:LYS:HE3	1.92	0.52
2:B:106:PHE:CZ	3:C:13:MET:HE1	2.43	0.52
3:C:16:ASN:HD22	3:C:16:ASN:N	2.05	0.52
1:A:107:LYS:HE2	5:A:585:HOH:O	2.08	0.52
1:D:75[B]:MET:HE3	1:D:77:PRO:HD3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:61:SER:HB2	2:B:79:TYR:O	2.10	0.52
1:A:75[B]:MET:HE3	1:A:77:PRO:HD3	1.90	0.51
1:D:61:ARG:HH11	1:D:63:HIS:CE1	2.27	0.51
2:B:63:ILE:HD13	3:C:120:ILE:HD11	1.93	0.51
2:B:35:ALA:HB3	2:B:79:TYR:CE1	2.46	0.51
3:C:8:GLU:H	3:C:16:ASN:ND2	2.07	0.50
1:D:143:ARG:HH22	1:D:383:GLN:NE2	2.07	0.50
3:C:61:THR:HG22	3:C:65:LYS:HZ2	1.76	0.50
1:A:232:ILE:HA	1:A:247:SER:HA	1.93	0.50
1:D:242:LYS:HD2	5:D:491:HOH:O	2.11	0.50
3:C:109:ALA:CB	3:C:122:LYS:HE2	2.40	0.50
1:A:56:HIS:NE2	1:D:377:GLU:OE2	2.40	0.50
1:D:300:PHE:HB3	1:D:314:ALA:HB2	1.92	0.50
1:A:220:ARG:NH2	3:C:64:MET:HE1	2.26	0.50
3:C:84:THR:HG22	3:C:95:VAL:CG2	2.41	0.50
3:C:16:ASN:H	3:C:16:ASN:ND2	2.10	0.49
3:C:103:LYS:HD3	3:C:106:GLU:OE1	2.12	0.49
1:D:154:GLN:NE2	1:D:184:SER:H	2.11	0.49
2:E:108:HIS:NE2	2:E:110:ASP:HB2	2.27	0.49
1:D:311:LYS:HZ3	2:E:110:ASP:CG	2.16	0.49
2:E:108:HIS:CE1	2:E:110:ASP:HB2	2.48	0.48
3:C:99:VAL:O	3:C:99:VAL:HG12	2.14	0.48
1:A:183:TRP:CD1	2:B:102:GLY:HA3	2.49	0.48
1:A:311:LYS:HD2	2:B:96:GLN:CD	2.35	0.47
1:D:36:GLY:HA2	5:D:624:HOH:O	2.13	0.47
2:E:34:CYS:O	2:E:95:THR:HG22	2.13	0.47
2:B:62:TRQ:CB	2:B:113:TRP:NE1	2.68	0.47
1:D:183:TRP:CD1	2:E:102:GLY:HA3	2.50	0.47
3:C:40:PRO:HB2	5:C:826:HOH:O	2.15	0.47
3:C:16:ASN:N	3:C:16:ASN:ND2	2.63	0.47
3:C:99:VAL:CG1	3:C:102:LEU:HD11	2.46	0.46
2:B:99:GLU:OE2	2:B:108:HIS:HD2	1.97	0.46
2:B:22:GLU:C	2:B:24:GLU:H	2.19	0.46
3:C:8:GLU:O	3:C:15:PHE:HA	2.15	0.46
1:A:164:ILE:HB	1:A:174:GLU:HB3	1.98	0.46
1:A:291:HIS:CE1	1:A:293:ALA:HB3	2.51	0.46
1:A:75[B]:MET:CE	2:E:85:LYS:HD3	2.35	0.46
5:A:513:HOH:O	2:B:108:HIS:HE1	1.99	0.46
3:C:122:LYS:HD3	3:C:122:LYS:C	2.36	0.46
3:C:84:THR:HG22	3:C:95:VAL:HG23	1.97	0.46
1:D:84:VAL:HG22	1:D:85:GLN:N	2.31	0.46
1:A:193:ARG:NH2	1:A:211:GLU:HG3	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:34:LYS:HG2	3:C:92:THR:CG2	2.45	0.46
1:A:220:ARG:HH21	3:C:64:MET:HE1	1.81	0.46
2:E:51:CYS:HB3	2:E:55:SER:OG	2.16	0.46
1:D:154:GLN:HE21	1:D:184:SER:H	1.62	0.46
1:A:154:GLN:NE2	1:A:184:SER:H	2.14	0.46
1:A:311:LYS:HZ3	2:B:110:ASP:CG	2.20	0.45
2:E:25:VAL:HG13	5:E:204:HOH:O	2.16	0.45
1:A:75[B]:MET:HE1	1:A:77:PRO:HD3	1.99	0.45
1:D:278:LYS:NZ	5:D:740:HOH:O	2.49	0.45
1:A:237:ALA:HB3	1:A:244:HIS:HB2	1.99	0.45
1:A:182:CYS:HA	1:A:199:CYS:HA	1.99	0.45
1:A:100:HIS:CE1	1:A:108:ARG:HB2	2.51	0.45
3:C:52:LYS:HB2	3:C:55:ASP:OD2	2.17	0.45
1:A:100:HIS:HD2	5:A:536:HOH:O	2.00	0.45
1:A:85:GLN:HG2	1:A:142:PHE:CE2	2.52	0.45
3:C:5:VAL:CG2	3:C:29:PHE:HZ	2.29	0.44
1:A:151:ILE:HB	1:A:165:VAL:HB	1.99	0.44
1:A:84:VAL:HG22	1:A:85:GLN:N	2.32	0.44
3:C:44:MET:O	3:C:44:MET:HG3	2.17	0.44
2:B:80:HIS:HB2	1:D:33:LEU:HD22	1.99	0.44
1:D:75[B]:MET:HE1	1:D:77:PRO:HD3	2.00	0.44
3:C:81:ILE:HG23	3:C:101:LYS:HD2	1.99	0.44
3:C:24:LYS:HE3	3:C:128:GLY:CA	2.48	0.44
2:E:24:GLU:HB3	5:E:204:HOH:O	2.18	0.44
1:D:112:VAL:HG23	1:D:128:LEU:HD11	1.99	0.44
1:A:349:LEU:HG	1:A:384:PHE:CZ	2.53	0.44
1:D:263:LYS:HA	1:D:263:LYS:HE2	2.00	0.44
1:D:232:ILE:HA	1:D:247:SER:HA	2.00	0.44
3:C:48:VAL:O	3:C:83:HIS:HA	2.18	0.44
3:C:52:LYS:HG2	3:C:108:TYR:CE1	2.53	0.43
2:B:108:HIS:CE1	2:B:110:ASP:HB2	2.52	0.43
2:B:56:THR:HA	2:B:57:PRO:HD3	1.87	0.43
1:A:197:THR:HG22	1:A:205:LEU:HB3	2.01	0.43
1:D:81:ASN:HD21	1:D:135:GLY:N	2.11	0.43
1:A:30:ARG:HH21	1:A:30:ARG:HG2	1.82	0.43
2:E:134:LYS:HA	2:E:134:LYS:HD2	1.81	0.43
1:D:78:THR:HB	1:D:82:GLY:HA3	2.00	0.43
2:E:90:ARG:HG3	2:E:90:ARG:NH1	2.32	0.43
1:D:237:ALA:HB3	1:D:244:HIS:HB2	2.00	0.43
1:A:241:ASP:HA	1:A:257:PHE:CE1	2.54	0.43
3:C:102:LEU:CD1	3:C:127:LEU:HD22	2.45	0.43
1:A:112:VAL:HG23	1:A:128:LEU:HD11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:22:GLU:C	2:E:24:GLU:H	2.23	0.42
3:C:9:GLY:HA2	3:C:14:GLN:O	2.19	0.42
1:D:50:MET:SD	1:D:62:VAL:HG22	2.59	0.42
1:A:100:HIS:HA	1:A:107:LYS:O	2.20	0.42
2:E:30:TYR:HB3	2:E:33:HIS:CD2	2.54	0.42
3:C:35:HIS:ND1	3:C:89:GLY:HA2	2.34	0.42
2:B:64:GLY:HA2	5:B:181:HOH:O	2.20	0.42
3:C:51:SER:HA	3:C:81:ILE:CD1	2.49	0.42
1:A:292:ARG:H	1:A:343:GLN:HE22	1.67	0.42
2:E:61:SER:HB2	2:E:79:TYR:O	2.19	0.42
1:D:239:ASP:HB3	1:D:242:LYS:HG2	2.02	0.41
3:C:41:LYS:HG3	3:C:42:ALA:N	2.35	0.41
2:E:62:TRQ:CB	2:E:113:TRP:NE1	2.71	0.41
3:C:24:LYS:HE3	3:C:128:GLY:HA3	2.02	0.41
1:A:124:LYS:HE2	1:A:170:GLY:HA3	2.02	0.41
2:E:39:PHE:CE2	2:E:89:GLY:HA2	2.55	0.41
2:E:56:THR:HA	2:E:57:PRO:HD3	1.89	0.41
1:D:157:SER:N	1:D:158:PRO:CA	2.83	0.41
2:B:39:PHE:HB3	2:B:90:ARG:O	2.20	0.41
1:A:124:LYS:CE	1:A:170:GLY:HA3	2.49	0.41
1:D:157:SER:N	1:D:158:PRO:HA	2.36	0.41
3:C:74:LYS:O	3:C:77:ASP:HB2	2.20	0.41
1:D:353:GLY:HA2	1:D:379:SER:O	2.21	0.41
1:A:240:LYS:HD3	5:A:533:HOH:O	2.19	0.41
1:A:353:GLY:HA2	1:A:379:SER:O	2.20	0.41
3:C:87:ILE:HB	3:C:91:GLU:HB2	2.02	0.41
2:B:73:LYS:NZ	5:B:146:HOH:O	2.53	0.41
3:C:102:LEU:CD1	3:C:127:LEU:HB2	2.51	0.41
1:A:311:LYS:NZ	2:B:96:GLN:NE2	2.69	0.41
3:C:84:THR:HA	3:C:95:VAL:CG2	2.51	0.41
1:A:331:ILE:HD13	1:A:366:PRO:HB2	2.03	0.41
3:C:22:VAL:HG12	3:C:29:PHE:CD1	2.56	0.41
1:D:367:LYS:C	1:D:367:LYS:HD3	2.40	0.41
1:A:241:ASP:OD2	1:A:258:SER:HB3	2.20	0.40
3:C:87:ILE:HD12	3:C:91:GLU:O	2.21	0.40
1:D:188:GLN:NE2	1:D:191:ARG:HH11	2.19	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	358/390 (92%)	340 (95%)	17 (5%)	1 (0%)	50	38
1	D	358/390 (92%)	343 (96%)	14 (4%)	1 (0%)	50	38
2	B	110/135 (82%)	101 (92%)	9 (8%)	0	100	100
2	E	110/135 (82%)	101 (92%)	8 (7%)	1 (1%)	25	11
3	C	126/128 (98%)	116 (92%)	9 (7%)	1 (1%)	27	12
All	All	1062/1178 (90%)	1001 (94%)	57 (5%)	4 (0%)	43	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	115	PRO
1	A	157	SER
2	E	23	ASP
1	D	157	SER

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	306/325 (94%)	302 (99%)	4 (1%)	80	76
1	D	306/325 (94%)	300 (98%)	6 (2%)	68	59
2	B	98/112 (88%)	97 (99%)	1 (1%)	85	84
2	E	98/112 (88%)	97 (99%)	1 (1%)	85	84
3	C	106/106 (100%)	102 (96%)	4 (4%)	44	29
All	All	914/980 (93%)	898 (98%)	16 (2%)	71	64

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	61	ARG
1	A	263	LYS
1	A	267	PRO
2	B	98	ARG
3	C	16	ASN
3	C	106	GLU
3	C	115	PRO
3	C	126	GLU
1	D	61	ARG
1	D	211	GLU
1	D	267	PRO
1	D	274	GLU
1	D	287	LEU
1	D	365	GLU
2	E	23	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	63	HIS
1	A	81	ASN
1	A	85	GLN
1	A	100	HIS
1	A	134	GLN
1	A	137	ASN
1	A	144	GLN
1	A	154	GLN
1	A	188	GLN
1	A	223	GLN
1	A	343	GLN
1	A	344	GLN
1	A	381	GLN
1	A	383	GLN
1	A	385	HIS
2	B	92	GLN
2	B	96	GLN
2	B	108	HIS
2	B	117	ASN
3	C	16	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	43	GLN
1	D	63	HIS
1	D	81	ASN
1	D	85	GLN
1	D	100	HIS
1	D	134	GLN
1	D	137	ASN
1	D	144	GLN
1	D	154	GLN
1	D	188	GLN
1	D	223	GLN
1	D	326	GLN
1	D	343	GLN
1	D	363	GLN
1	D	381	GLN
1	D	383	GLN
1	D	385	HIS
2	E	92	GLN
2	E	96	GLN
2	E	108	HIS
2	E	117	ASN

5.3.3   RNA ⓘ

There are no RNA chains in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
2	TRQ	B	62	2	17,17,18	5.50	6 (35%)	20,24,26	2.80	3 (15%)
2	TRQ	E	62	2	17,17,18	5.65	6 (35%)	20,24,26	2.71	4 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRQ	B	62	2	-	0/4/19/21	0/0/2/2
2	TRQ	E	62	2	-	0/4/19/21	0/0/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	62	TRQ	O-C	18.55	1.24	1.11
2	B	62	TRQ	O-C	17.84	1.23	1.11
2	B	62	TRQ	CE2-CZ2	-11.55	1.40	1.50
2	E	62	TRQ	CE2-CZ2	-11.50	1.40	1.50
2	B	62	TRQ	CH2-CZ2	-5.57	1.37	1.54
2	E	62	TRQ	CH2-CZ2	-5.55	1.37	1.54
2	E	62	TRQ	CZ3-CE3	3.27	1.40	1.34
2	E	62	TRQ	CA-C	3.19	1.54	1.48
2	B	62	TRQ	CZ3-CE3	3.14	1.39	1.34
2	B	62	TRQ	CA-C	2.85	1.53	1.48
2	E	62	TRQ	CD2-CG	2.61	1.46	1.41
2	B	62	TRQ	CD2-CG	2.38	1.45	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	62	TRQ	C-CA-N	-10.78	103.07	113.83
2	E	62	TRQ	C-CA-N	-9.60	104.24	113.83
2	E	62	TRQ	O7-CZ2-CH2	4.31	124.33	119.09
2	B	62	TRQ	CD1-CG-CD2	3.21	106.51	104.97
2	E	62	TRQ	CD1-CG-CD2	3.14	106.47	104.97
2	E	62	TRQ	CG-CD2-CE3	2.60	136.87	127.38
2	B	62	TRQ	CG-CD2-CE3	2.49	136.46	127.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	359/390 (92%)	-0.15	2 (0%) 86	92	13, 21, 35, 60	0
1	D	359/390 (92%)	-0.16	1 (0%) 91	95	13, 20, 32, 53	0
2	B	113/135 (83%)	-0.04	3 (2%) 52	60	16, 20, 33, 73	0
2	E	113/135 (83%)	-0.05	4 (3%) 42	48	13, 19, 29, 75	0
3	C	128/128 (100%)	3.62	86 (67%) 0	0	38, 63, 82, 87	0
All	All	1072/1178 (91%)	0.32	96 (8%) 10	12	13, 21, 68, 87	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	127	LEU	13.1
3	C	97	PHE	8.5
3	C	22	VAL	8.5
1	A	29	PRO	8.4
3	C	20	ILE	7.9
3	C	3	CYS	7.9
3	C	128	GLY	7.9
3	C	102	LEU	7.8
3	C	21	VAL	7.7
3	C	129	SER	7.6
3	C	106	GLU	7.4
3	C	31	ILE	7.4
3	C	103	LYS	7.4
2	E	23	ASP	7.4
3	C	101	LYS	7.3
3	C	27	LYS	6.9
3	C	24	LYS	6.8
3	C	25	THR	6.8
3	C	76	GLY	6.7
3	C	29	PHE	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	23	ASP	6.5
3	C	98	ASP	6.5
3	C	95	VAL	6.5
3	C	2	ALA	6.5
3	C	81	ILE	6.3
2	E	22	GLU	6.3
3	C	7	ILE	6.2
3	C	26	CYS	6.1
3	C	5	VAL	6.1
3	C	99	VAL	6.1
3	C	104	GLU	5.7
3	C	108	TYR	5.5
3	C	126	GLU	5.4
3	C	118	TRP	5.4
3	C	124	THR	5.3
3	C	75	ALA	5.3
3	C	100	SER	5.2
2	B	22	GLU	5.1
3	C	4	ASP	5.0
2	B	134	LYS	5.0
3	C	54	SER	5.0
3	C	82	ALA	5.0
3	C	120	ILE	4.7
3	C	34	LYS	4.7
3	C	110	PHE	4.7
3	C	80	VAL	4.6
3	C	18	LYS	4.5
3	C	28	GLU	4.5
3	C	59	VAL	4.5
3	C	48	VAL	4.4
3	C	94	SER	4.4
3	C	78	GLU	4.4
3	C	109	ALA	4.4
3	C	122	LYS	4.1
3	C	111	PHE	4.1
3	C	17	THR	4.1
3	C	107	ASP	4.0
3	C	30	THR	4.0
3	C	55	ASP	3.8
3	C	123	GLY	3.8
3	C	96	THR	3.8
3	C	19	SER	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	125	ILE	3.7
3	C	73	VAL	3.6
3	C	87	ILE	3.5
3	C	86	VAL	3.5
3	C	105	GLY	3.5
1	D	29	PRO	3.4
3	C	32	ASN	3.4
3	C	74	LYS	3.3
3	C	51	SER	3.2
3	C	53	LYS	3.2
3	C	119	SER	3.1
3	C	50	VAL	3.0
3	C	49	VAL	3.0
3	C	92	THR	3.0
3	C	93	ASP	3.0
3	C	56	GLU	2.9
2	B	23	ASP	2.8
3	C	83	HIS	2.7
2	E	134	LYS	2.6
2	E	24	GLU	2.6
3	C	52	LYS	2.5
3	C	65	LYS	2.4
3	C	64	MET	2.4
3	C	69	ASN	2.3
3	C	16	ASN	2.3
3	C	70	ASN	2.2
1	A	30	ARG	2.2
3	C	77	ASP	2.2
3	C	84	THR	2.2
3	C	79	ARG	2.2
3	C	62	ASP	2.1
3	C	85	SER	2.1
3	C	8	GLU	2.1
3	C	67	GLY	2.0

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

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	TRQ	E	62	16/17	0.10	0.25	12,15,20,20	0
2	TRQ	B	62	16/17	0.10	0.08	15,18,23,27	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CU	C	130	1/1	0.08	-2.76	53,53,53,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.