



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 01:57 PM EDT

PDB ID : 5WIO
Title : TraE protein in complex with 4-(1H-pyrrol-1-yl)pyridine-2-carboxylic acid
Authors : Casu, B.; Arya, T.; Bessette, B.; Baron, C.
Deposited on : 2017-07-19
Resolution : 2.52 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

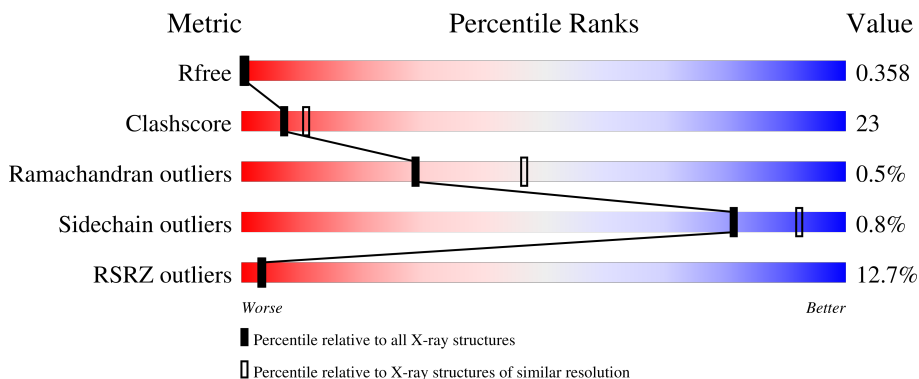
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 $\leq 5\%$. 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	163	 4% 63% 25% 12%
1	B	163	 4% 60% 27% 13%
1	C	163	 16% 44% 40% 15%
1	D	163	 19% 44% 37% 18%

2 Entry composition [i](#)

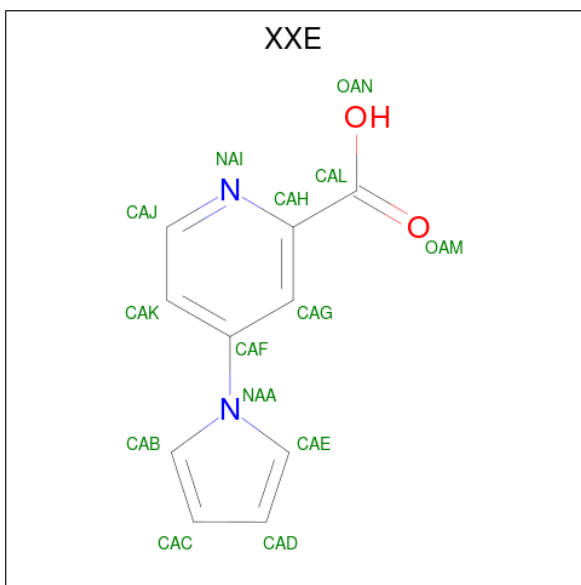
There are 3 unique types of molecules in this entry. The entry contains 4472 atoms, of which 7 are hydrogens and 0 are deuteriums.

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 Conjugal transfer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	143	Total	C	N	O	S	0	0	0
			1167	736	206	222	3			
1	B	142	Total	C	N	O	S	0	0	0
			1155	729	202	221	3			
1	C	139	Total	C	N	O	S	0	0	0
			1106	700	191	212	3			
1	D	134	Total	C	N	O	S	0	0	0
			1013	633	177	200	3			

- Molecule 2 is 4-(1H-pyrrol-1-yl)pyridine-2-carboxylic acid (three-letter code: XXE) (formula: C₁₀H₈N₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	Total	C	H	N	O	0	0
			21	10	7	2	2		

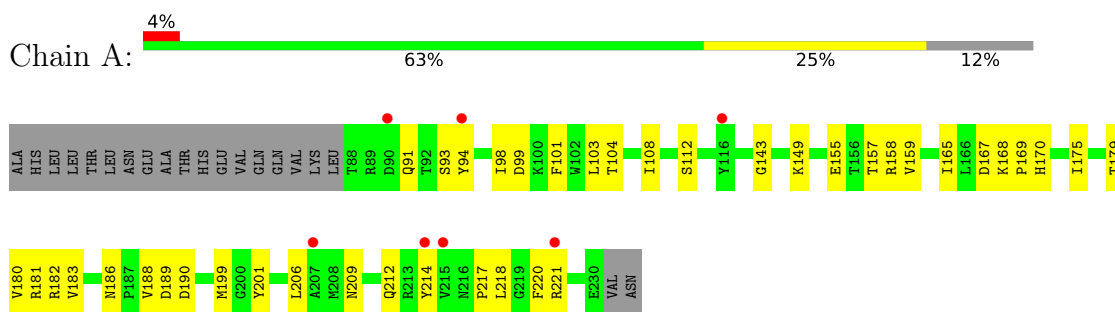
- Molecule 3 is water.

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

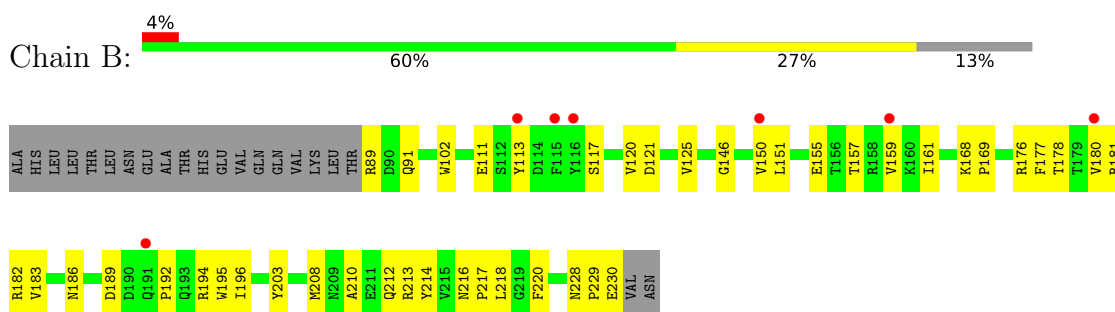
3 Residue-property plots [i](#)

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 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.

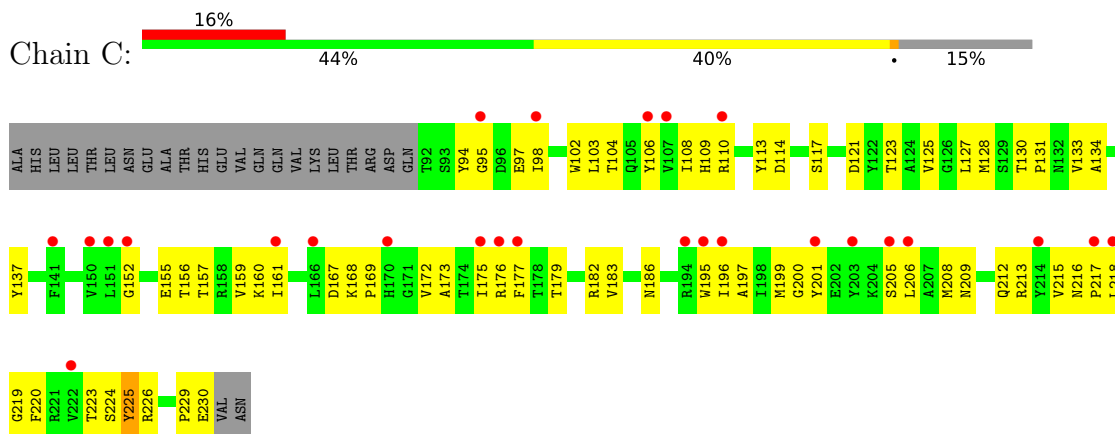
- Molecule 1: Conjugal transfer protein



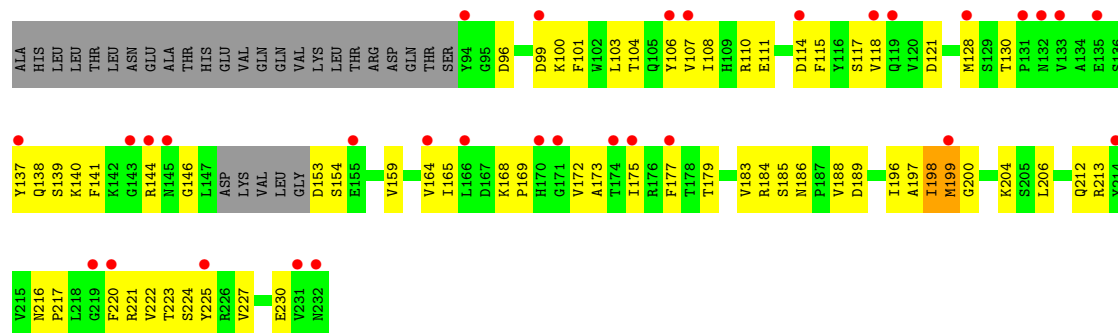
- Molecule 1: Conjugal transfer protein



- Molecule 1: Conjugal transfer protein



- Molecule 1: Conjugal transfer protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	112.91Å 125.53Å 110.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.48 – 2.52 39.48 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.48-2.52) 99.7 (39.48-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.300 , 0.356 0.308 , 0.358	Depositor DCC
R_{free} test set	1622 reflections (6.06%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtrriage
Anisotropy	0.550	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4472	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: XXE

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	0.33	0/1193	0.42	0/1618
1	B	0.29	0/1181	0.44	0/1602
1	C	0.34	0/1132	0.43	0/1539
1	D	0.25	0/1032	0.49	0/1407
All	All	0.31	0/4538	0.44	0/6166

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1167	0	1136	33	0
1	B	1155	0	1121	42	0
1	C	1106	0	1045	64	0
1	D	1013	0	920	64	0
2	A	14	7	0	2	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
All	All	4465	7	4222	198	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 23.

All (198) 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:C:113:TYR:OH	1:C:152:GLY:O	1.56	1.22
1:D:173:ALA:O	1:D:198:ILE:HG23	1.50	1.10
1:C:113:TYR:OH	1:C:152:GLY:HA2	1.61	0.99
1:C:113:TYR:OH	1:C:152:GLY:CA	2.15	0.94
1:C:113:TYR:OH	1:C:152:GLY:C	2.07	0.92
1:D:204:LYS:NZ	1:D:206:LEU:CD1	2.33	0.91
1:D:204:LYS:HZ1	1:D:206:LEU:HD11	1.35	0.91
1:D:204:LYS:NZ	1:D:206:LEU:HD11	1.86	0.90
1:D:173:ALA:O	1:D:198:ILE:CG2	2.23	0.87
1:D:164:VAL:O	1:D:165:ILE:HD13	1.75	0.86
1:D:204:LYS:HZ1	1:D:206:LEU:CD1	1.88	0.85
1:A:158:ARG:HH21	1:A:180:VAL:HG11	1.44	0.83
1:C:155:GLU:HB3	1:C:183:VAL:HG22	1.62	0.79
1:D:204:LYS:NZ	1:D:206:LEU:HD12	2.01	0.74
1:D:197:ALA:HB2	1:D:227:VAL:HG22	1.70	0.74
1:D:114:ASP:O	1:D:118:VAL:HB	1.87	0.74
1:B:182:ARG:HB3	1:B:189:ASP:HA	1.70	0.73
1:C:130:THR:HB	1:C:131:PRO:HD2	1.70	0.72
1:D:115:PHE:CZ	1:D:153:ASP:HA	2.26	0.71
1:B:182:ARG:NH2	1:B:186:ASN:O	2.24	0.70
1:D:204:LYS:HZ2	1:D:206:LEU:CD1	2.03	0.70
1:D:103:LEU:HB3	1:D:175:ILE:HD11	1.74	0.69
1:C:113:TYR:H	1:C:157:THR:HB	1.58	0.69
1:D:159:VAL:HG22	1:D:179:THR:HG22	1.74	0.69
1:D:196:ILE:HD11	1:D:230:GLU:HG3	1.75	0.69
1:B:117:SER:O	1:B:120:VAL:N	2.27	0.68
1:A:188:VAL:HG22	1:A:189:ASP:H	1.59	0.68
1:A:93:SER:OG	1:A:168:LYS:NZ	2.25	0.67
1:D:153:ASP:O	1:D:184:ARG:NE	2.26	0.67
1:A:157:THR:O	2:A:301:XXE:CAC	2.42	0.67
1:D:225:TYR:CE2	1:D:227:VAL:HG23	2.30	0.67
1:B:168:LYS:HB2	1:B:169:PRO:HD3	1.75	0.67
1:B:196:ILE:HD11	1:B:230:GLU:HG3	1.76	0.67
1:C:168:LYS:HB2	1:C:169:PRO:HD3	1.76	0.67
1:D:138:GLN:O	1:D:140:LYS:N	2.28	0.66
1:A:168:LYS:HB2	1:A:169:PRO:HD3	1.76	0.66
1:C:160:LYS:O	1:C:177:PHE:HB2	1.96	0.66
1:D:197:ALA:CB	1:D:227:VAL:HG22	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HD21	1:A:221:ARG:CZ	2.27	0.65
1:D:117:SER:O	1:D:121:ASP:N	2.27	0.65
1:B:102:TRP:HH2	1:B:217:PRO:HD2	1.62	0.65
1:C:108:ILE:HG12	1:C:159:VAL:HG11	1.78	0.64
1:B:113:TYR:HE2	1:B:155:GLU:O	1.81	0.64
1:C:110:ARG:HG3	1:C:137:TYR:CD1	2.33	0.64
1:C:229:PRO:O	1:C:230:GLU:HB2	1.96	0.64
1:D:204:LYS:HZ2	1:D:206:LEU:HD12	1.60	0.64
1:D:110:ARG:HG3	1:D:137:TYR:CD1	2.33	0.64
1:B:157:THR:HA	1:B:181:ARG:HB2	1.80	0.63
1:D:114:ASP:HB3	1:D:117:SER:HB3	1.78	0.63
1:C:216:ASN:OD1	1:C:219:GLY:N	2.31	0.63
1:B:113:TYR:CE2	1:B:155:GLU:O	2.53	0.62
1:A:181:ARG:HG2	1:A:182:ARG:N	2.14	0.62
1:D:115:PHE:O	1:D:118:VAL:HG12	1.99	0.61
1:C:94:TYR:CD2	1:C:218:LEU:HD13	2.36	0.61
1:C:183:VAL:HB	1:C:186:ASN:ND2	2.15	0.61
1:B:89:ARG:NH1	1:B:91:GLN:OE1	2.32	0.60
1:C:167:ASP:HB3	1:C:172:VAL:HB	1.84	0.60
1:D:130:THR:HG22	1:D:221:ARG:CZ	2.31	0.60
1:B:180:VAL:HG22	1:B:180:VAL:O	2.00	0.60
1:D:212:GLN:HB3	1:D:216:ASN:O	2.01	0.60
1:B:214:TYR:CZ	1:C:95:GLY:HA2	2.36	0.59
1:A:104:THR:O	1:A:108:ILE:HG13	2.03	0.58
1:C:229:PRO:O	1:C:230:GLU:CB	2.51	0.58
1:C:108:ILE:HG12	1:C:159:VAL:CG1	2.35	0.57
1:C:155:GLU:HA	1:C:183:VAL:HA	1.86	0.57
1:B:102:TRP:NE1	1:B:218:LEU:HD12	2.20	0.57
1:C:104:THR:O	1:C:108:ILE:HG13	2.05	0.57
1:D:100:LYS:HG2	1:D:164:VAL:HG11	1.85	0.57
1:C:200:GLY:O	1:C:223:THR:N	2.36	0.56
1:D:103:LEU:HD23	1:D:220:PHE:HZ	1.69	0.56
1:C:110:ARG:HH12	1:C:133:VAL:HG12	1.69	0.56
1:D:213:ARG:HA	1:D:217:PRO:HB3	1.88	0.56
1:A:91:GLN:NE2	1:A:93:SER:O	2.37	0.56
1:C:208:MET:HA	1:C:212:GLN:OE1	2.06	0.56
1:A:155:GLU:HB2	1:A:182:ARG:O	2.06	0.56
1:C:108:ILE:HA	1:C:159:VAL:HG11	1.88	0.55
1:B:102:TRP:CH2	1:B:217:PRO:HD2	2.40	0.55
1:C:94:TYR:O	1:C:98:ILE:HD12	2.06	0.55
1:C:205:SER:O	1:C:206:LEU:HD22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ARG:HG2	1:B:196:ILE:HG12	1.89	0.55
1:B:180:VAL:HG23	1:B:192:PRO:HG3	1.88	0.55
1:B:182:ARG:HD2	1:B:189:ASP:HA	1.89	0.55
1:D:138:GLN:C	1:D:140:LYS:H	2.09	0.55
1:D:106:TYR:CD1	1:D:199:MET:HE1	2.41	0.55
1:D:130:THR:HG22	1:D:221:ARG:NH1	2.22	0.54
1:D:111:GLU:HG3	1:D:177:PHE:CZ	2.43	0.54
1:C:114:ASP:HB3	1:C:117:SER:HB3	1.88	0.54
1:B:178:THR:OG1	1:B:194:ARG:HG2	2.08	0.54
1:B:177:PHE:CZ	1:B:195:TRP:HB2	2.44	0.53
1:C:209:ASN:OD1	1:C:212:GLN:HG2	2.09	0.53
1:D:115:PHE:CE1	1:D:153:ASP:HA	2.43	0.53
1:B:203:TYR:CE2	1:B:220:PHE:HB2	2.44	0.53
1:D:154:SER:O	1:D:184:ARG:HG2	2.09	0.53
1:D:96:ASP:HB3	1:D:100:LYS:HE3	1.91	0.53
1:A:190:ASP:OD1	1:A:190:ASP:N	2.33	0.53
1:A:103:LEU:HB3	1:A:175:ILE:HD11	1.91	0.52
1:D:141:PHE:HA	1:D:146:GLY:HA2	1.91	0.52
1:D:110:ARG:HE	1:D:137:TYR:HB2	1.72	0.52
1:A:181:ARG:HG2	1:A:182:ARG:H	1.73	0.52
1:C:155:GLU:CB	1:C:183:VAL:HG22	2.37	0.51
1:D:183:VAL:HG22	1:D:185:SER:H	1.74	0.51
1:B:102:TRP:HE1	1:B:218:LEU:HD12	1.74	0.51
1:B:155:GLU:OE1	1:B:183:VAL:HG12	2.11	0.51
1:C:113:TYR:CZ	1:C:152:GLY:O	2.59	0.51
1:A:188:VAL:HG22	1:A:189:ASP:N	2.25	0.51
1:D:110:ARG:NE	1:D:137:TYR:HB2	2.25	0.51
1:A:182:ARG:NH2	1:A:186:ASN:O	2.44	0.50
1:A:209:ASN:ND2	1:A:212:GLN:CD	2.65	0.50
1:D:138:GLN:C	1:D:140:LYS:N	2.64	0.50
1:C:104:THR:HB	1:C:161:ILE:HG13	1.94	0.50
1:D:172:VAL:HG12	1:D:173:ALA:N	2.27	0.50
1:D:154:SER:C	1:D:184:ARG:HG2	2.33	0.49
1:A:159:VAL:HG22	1:A:179:THR:HG22	1.93	0.49
1:C:121:ASP:O	1:C:125:VAL:HG23	2.12	0.49
1:D:96:ASP:O	1:D:100:LYS:HG3	2.13	0.49
1:B:216:ASN:ND2	1:B:220:PHE:O	2.44	0.49
1:C:109:HIS:O	1:C:121:ASP:HB3	2.14	0.48
1:C:175:ILE:HD12	1:C:175:ILE:N	2.28	0.48
1:A:175:ILE:HD12	1:A:199:MET:SD	2.53	0.48
1:A:94:TYR:CZ	1:A:218:LEU:HD22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TYR:O	1:A:98:ILE:HD12	2.14	0.47
1:D:164:VAL:C	1:D:165:ILE:HD13	2.33	0.47
1:C:199:MET:HA	1:C:224:SER:O	2.15	0.47
1:B:91:GLN:HE22	1:C:213:ARG:HD3	1.80	0.47
1:A:168:LYS:NZ	1:A:168:LYS:HB3	2.30	0.47
1:D:104:THR:O	1:D:108:ILE:HG13	2.15	0.47
1:C:106:TYR:CD1	1:C:128:MET:HB2	2.50	0.47
1:D:168:LYS:CB	1:D:169:PRO:HD3	2.44	0.47
1:C:103:LEU:HD23	1:C:220:PHE:HZ	1.79	0.47
1:D:103:LEU:HD13	1:D:173:ALA:CB	2.45	0.46
1:B:180:VAL:CG2	1:B:192:PRO:HG3	2.44	0.46
1:B:208:MET:SD	1:B:213:ARG:HA	2.55	0.46
1:B:121:ASP:O	1:B:125:VAL:HG23	2.16	0.46
1:A:103:LEU:HD23	1:A:220:PHE:HZ	1.81	0.46
1:B:155:GLU:HB3	1:B:183:VAL:HG12	1.96	0.46
1:C:176:ARG:HG2	1:C:196:ILE:CD1	2.46	0.46
1:C:197:ALA:HA	1:C:226:ARG:O	2.16	0.46
1:A:112:SER:HB3	2:A:301:XXE:CAB	2.46	0.46
1:C:103:LEU:HD21	1:C:201:TYR:CD2	2.50	0.46
1:C:113:TYR:N	1:C:157:THR:HB	2.27	0.46
1:D:223:THR:HG23	1:D:224:SER:H	1.81	0.45
1:B:161:ILE:HD13	1:B:177:PHE:HB3	1.97	0.45
1:B:228:ASN:HB3	1:B:229:PRO:CD	2.46	0.45
1:A:201:TYR:HB2	1:A:220:PHE:CE1	2.51	0.45
1:B:146:GLY:O	1:B:150:VAL:HG23	2.17	0.45
1:C:94:TYR:CE2	1:C:218:LEU:HD22	2.52	0.45
1:D:188:VAL:HG22	1:D:189:ASP:N	2.31	0.45
1:A:182:ARG:HD2	1:A:183:VAL:H	1.82	0.45
1:C:110:ARG:HD3	1:C:225:TYR:CE2	2.52	0.45
1:D:144:ARG:HD2	1:D:144:ARG:H	1.81	0.45
1:C:173:ALA:HB2	1:C:201:TYR:HE2	1.82	0.45
1:D:99:ASP:O	1:D:103:LEU:HG	2.17	0.44
1:B:196:ILE:HG13	1:B:230:GLU:HB2	1.99	0.44
1:C:167:ASP:N	1:C:172:VAL:O	2.48	0.44
1:D:183:VAL:HG13	1:D:186:ASN:H	1.83	0.44
1:D:223:THR:HG23	1:D:224:SER:N	2.32	0.44
1:A:206:LEU:HD21	1:A:221:ARG:NH1	2.32	0.44
1:D:107:VAL:HG11	1:D:177:PHE:CD1	2.53	0.44
1:A:167:ASP:CG	1:A:170:HIS:HD1	2.21	0.44
1:B:210:ALA:O	1:B:214:TYR:HB2	2.17	0.43
1:C:102:TRP:HE1	1:C:218:LEU:HD12	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ASN:HB3	1:B:229:PRO:HD2	2.00	0.43
1:B:217:PRO:HG2	1:C:98:ILE:HD13	2.00	0.43
1:C:97:GLU:OE2	1:C:97:GLU:HA	2.18	0.43
1:D:128:MET:O	1:D:222:VAL:N	2.48	0.43
1:B:208:MET:HG3	1:B:212:GLN:HB2	2.00	0.43
1:B:208:MET:CG	1:B:212:GLN:HB2	2.48	0.43
1:A:101:PHE:HB2	1:D:101:PHE:CE1	2.53	0.43
1:C:182:ARG:NH1	1:C:186:ASN:O	2.52	0.43
1:C:103:LEU:HD23	1:C:220:PHE:CZ	2.53	0.43
1:D:154:SER:HA	1:D:184:ARG:HG2	2.01	0.43
1:D:200:GLY:O	1:D:222:VAL:HA	2.19	0.43
1:A:99:ASP:O	1:A:103:LEU:HG	2.20	0.42
1:A:158:ARG:HE	1:A:180:VAL:HB	1.84	0.42
1:A:143:GLY:O	1:A:149:LYS:HD2	2.19	0.42
1:C:176:ARG:HG2	1:C:196:ILE:HD12	2.00	0.42
1:C:156:THR:N	1:C:182:ARG:O	2.42	0.42
1:B:113:TYR:OH	1:B:151:LEU:HB2	2.20	0.42
1:B:155:GLU:CB	1:B:183:VAL:HG12	2.49	0.42
1:A:165:ILE:HG12	3:A:404:HOH:O	2.18	0.42
1:C:123:THR:O	1:C:127:LEU:HG	2.20	0.42
1:C:127:LEU:HD12	1:C:215:VAL:HG11	2.00	0.42
1:C:159:VAL:HG22	1:C:160:LYS:N	2.34	0.42
1:D:216:ASN:HD21	1:D:220:PHE:N	2.18	0.42
1:C:130:THR:O	1:C:134:ALA:N	2.51	0.41
1:C:108:ILE:HG23	1:C:159:VAL:CG1	2.50	0.41
1:D:172:VAL:HG12	1:D:173:ALA:H	1.84	0.41
1:A:158:ARG:HH21	1:A:180:VAL:CG1	2.22	0.41
1:C:94:TYR:CE2	1:C:218:LEU:HB3	2.56	0.41
1:C:197:ALA:HB1	1:C:225:TYR:HE1	1.85	0.41
1:D:200:GLY:HA3	1:D:223:THR:HG23	2.03	0.41
1:B:217:PRO:HG2	1:C:98:ILE:CD1	2.51	0.41
1:B:182:ARG:CB	1:B:189:ASP:HA	2.47	0.41
1:D:130:THR:HG23	1:D:222:VAL:O	2.22	0.40
1:B:111:GLU:HB2	1:B:159:VAL:HG21	2.03	0.40
1:C:179:THR:HG1	1:C:195:TRP:HZ3	1.68	0.40
1:D:137:TYR:O	1:D:140:LYS:HG2	2.22	0.40
1:C:201:TYR:CD1	1:C:201:TYR:C	2.94	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	141/163 (86%)	137 (97%)	3 (2%)	1 (1%)	22	37
1	B	140/163 (86%)	137 (98%)	3 (2%)	0	100	100
1	C	137/163 (84%)	133 (97%)	3 (2%)	1 (1%)	22	37
1	D	130/163 (80%)	126 (97%)	3 (2%)	1 (1%)	19	33
All	All	548/652 (84%)	533 (97%)	12 (2%)	3 (0%)	29	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	217	PRO
1	D	139	SER
1	A	217	PRO

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	128/147 (87%)	127 (99%)	1 (1%)	81	92
1	B	127/147 (86%)	127 (100%)	0	100	100
1	C	117/147 (80%)	116 (99%)	1 (1%)	78	91
1	D	102/147 (69%)	100 (98%)	2 (2%)	55	78
All	All	474/588 (81%)	470 (99%)	4 (1%)	81	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	TYR
1	C	225	TYR
1	D	198	ILE
1	D	199	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	C	186	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	XXE	A	301	-	15,15,15	1.05	0	19,20,20	1.57	5 (26%)

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	XXE	A	301	-	-	4/8/8/8	0/2/2/2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	XXE	CAK-CAJ-NAI	-3.30	119.86	123.96
2	A	301	XXE	CAJ-CAK-CAF	2.58	120.01	117.42
2	A	301	XXE	CAG-CAH-NAI	-2.49	120.06	123.19
2	A	301	XXE	CAJ-NAI-CAH	2.45	120.11	116.93
2	A	301	XXE	OAN-CAL-CAH	2.36	120.05	114.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	XXE	NAI-CAH-CAL-OAN
2	A	301	XXE	CAG-CAH-CAL-OAM
2	A	301	XXE	NAI-CAH-CAL-OAM
2	A	301	XXE	CAG-CAH-CAL-OAN

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	XXE	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	143/163 (87%)	0.55	7 (4%) 29 32	39, 56, 84, 96	0
1	B	142/163 (87%)	0.58	7 (4%) 29 32	40, 61, 82, 87	0
1	C	139/163 (85%)	1.07	26 (18%) 1 1	64, 87, 101, 108	0
1	D	134/163 (82%)	1.34	31 (23%) 0 0	70, 94, 111, 132	0
All	All	558/652 (85%)	0.88	71 (12%) 3 3	39, 75, 104, 132	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	195	TRP	5.7
1	D	137	TYR	5.2
1	D	225	TYR	5.1
1	A	215	VAL	4.8
1	D	143	GLY	4.4
1	D	219	GLY	4.3
1	A	207	ALA	4.3
1	D	164	VAL	4.1
1	C	175	ILE	4.1
1	C	203	TYR	3.8
1	D	94	TYR	3.8
1	D	145	ASN	3.8
1	C	217	PRO	3.8
1	C	170	HIS	3.8
1	D	175	ILE	3.7
1	C	161	ILE	3.6
1	B	116	TYR	3.5
1	D	144	ARG	3.5
1	D	131	PRO	3.4
1	B	159	VAL	3.4
1	C	95	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	199	MET	3.4
1	D	231	VAL	3.4
1	D	170	HIS	3.3
1	C	151	LEU	3.3
1	D	174	THR	3.2
1	C	150	VAL	3.2
1	D	171	GLY	3.1
1	C	107	VAL	3.1
1	C	218	LEU	3.0
1	C	196	ILE	3.0
1	D	220	PHE	3.0
1	D	177	PHE	3.0
1	D	132	ASN	2.9
1	C	206	LEU	2.8
1	C	222	VAL	2.8
1	C	152	GLY	2.8
1	D	106	TYR	2.7
1	C	177	PHE	2.7
1	A	90	ASP	2.6
1	D	135	GLU	2.6
1	C	194	ARG	2.6
1	D	155	GLU	2.6
1	C	201	TYR	2.5
1	C	214	TYR	2.5
1	B	115	PHE	2.5
1	D	232	ASN	2.5
1	A	214	TYR	2.4
1	D	214	TYR	2.4
1	D	118	VAL	2.4
1	D	166	LEU	2.4
1	A	116	TYR	2.3
1	C	176	ARG	2.3
1	D	128	MET	2.3
1	C	110	ARG	2.3
1	B	191	GLN	2.3
1	D	99	ASP	2.2
1	A	221	ARG	2.2
1	A	94	TYR	2.2
1	C	166	LEU	2.1
1	C	98	ILE	2.1
1	D	119	GLN	2.1
1	B	113	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	114	ASP	2.1
1	C	141	PHE	2.1
1	C	205	SER	2.1
1	B	180	VAL	2.0
1	D	107	VAL	2.0
1	C	106	TYR	2.0
1	D	133	VAL	2.0
1	B	150	VAL	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
2	XXE	A	301	14/14	0.87	0.29	60,69,82,83	2

6.5 Other polymers [i](#)

There are no such residues in this entry.