



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:00 AM GMT

PDB ID : 2VJQ
Title : FORMYL-COA TRANSFERASE MUTANT VARIANT W48Q
Authors : Toyota, C.G.; Berthold, C.L.; Gruez, A.; Jonsson, S.; Lindqvist, Y.; Cambillau, C.; Richards, N.G.J.
Deposited on : 2007-12-11
Resolution : 1.80 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

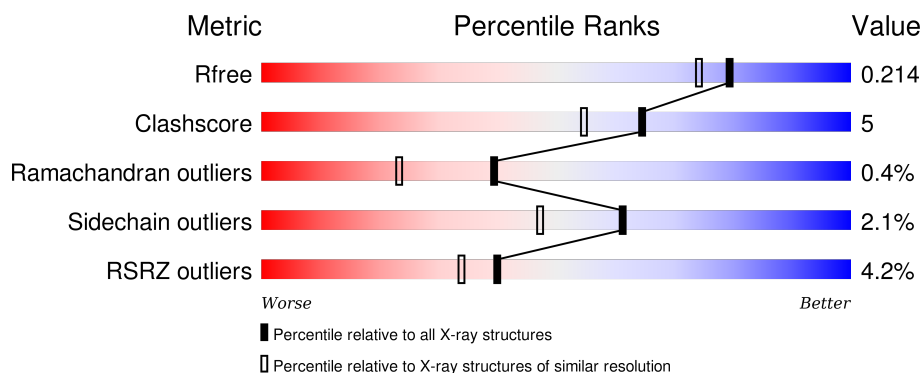
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	428	<div> <div>7%</div> <div>91%</div> <div>7%</div> </div>
1	B	428	<div> <div>7%</div> <div>89%</div> <div>11%</div> </div>
1	C	428	<div> <div>%</div> <div>88%</div> <div>11%</div> </div>
1	D	428	<div> <div>8%</div> <div>90%</div> <div>9%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14791 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.

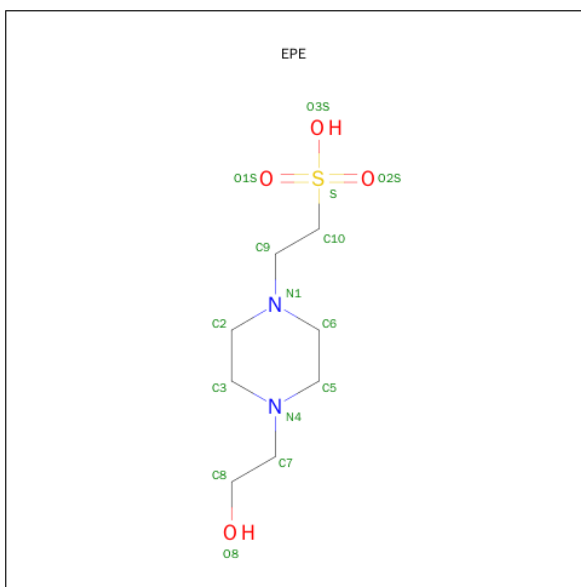
- Molecule 1 is a protein called FORMYL-COENZYME A TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	6	0
			3337	2111	571	631	24			
1	B	427	Total	C	N	O	S	0	6	0
			3341	2114	572	631	24			
1	C	427	Total	C	N	O	S	0	12	0
			3369	2132	576	637	24			
1	D	427	Total	C	N	O	S	0	5	0
			3335	2109	571	630	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLN	TRP	ENGINEERED MUTATION	UNP O06644
A	186	ILE	MET	SEE REMARK 999	UNP O06644
B	48	GLN	TRP	ENGINEERED MUTATION	UNP O06644
B	186	ILE	MET	SEE REMARK 999	UNP O06644
C	48	GLN	TRP	ENGINEERED MUTATION	UNP O06644
C	186	ILE	MET	SEE REMARK 999	UNP O06644
D	48	GLN	TRP	ENGINEERED MUTATION	UNP O06644
D	186	ILE	MET	SEE REMARK 999	UNP O06644

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

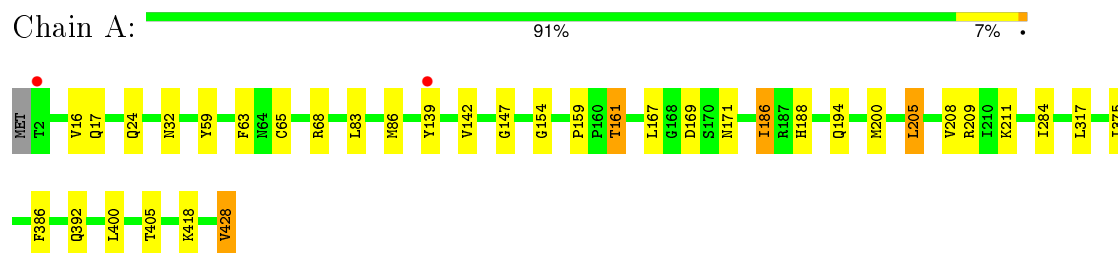
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	396	Total	O	0	0
			396	396		
3	B	322	Total	O	0	0
			322	322		
3	C	390	Total	O	0	0
			390	390		
3	D	271	Total	O	0	0
			271	271		

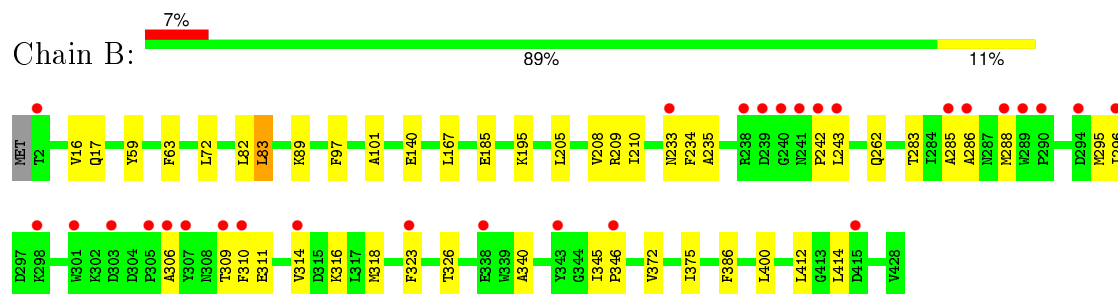
3 Residue-property plots

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.

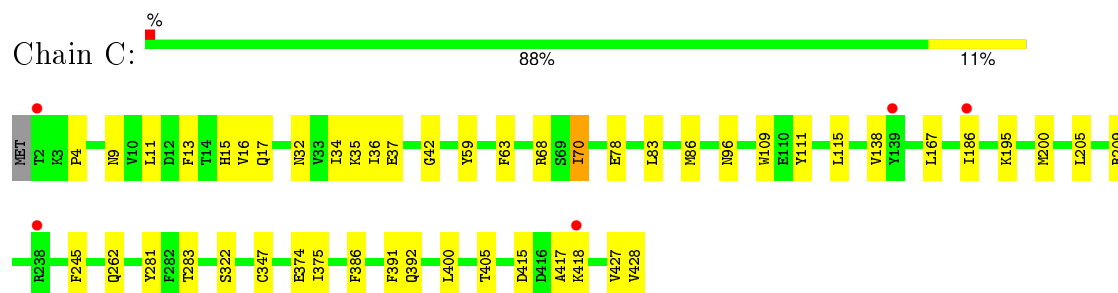
• Molecule 1: FORMYL-COENZYME A TRANSFERASE



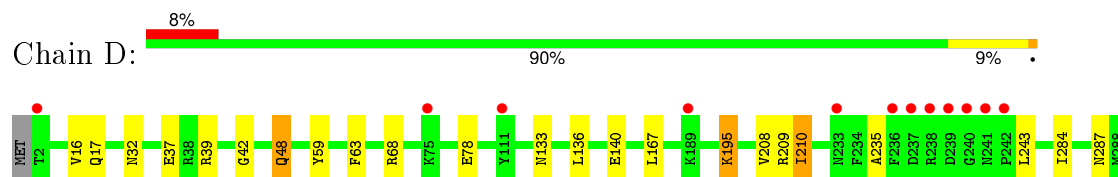
• Molecule 1: FORMYL-COENZYME A TRANSFERASE

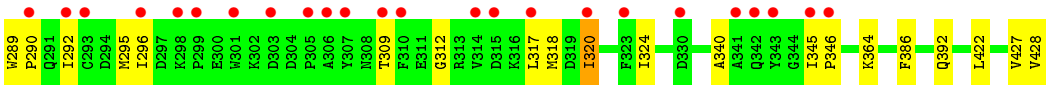


• Molecule 1: FORMYL-COENZYME A TRANSFERASE



• Molecule 1: FORMYL-COENZYME A TRANSFERASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.16 Å 98.92 Å 152.53 Å 90.00° 135.27° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 55.83 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.8 (30.00-1.80) 91.8 (55.83-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.80 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.212 0.184 , 0.214	Depositor DCC
R_{free} test set	9536 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.8	EDS
Estimated twinning fraction	0.156 for -h-2*k,h+1 0.022 for h,-k,-h-l 0.024 for h+2*k,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 190051 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14791	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.43	0/3428	0.57	0/4634
1	B	0.41	0/3432	0.55	0/4640
1	C	0.42	0/3478	0.58	0/4701
1	D	0.40	0/3423	0.54	0/4626
All	All	0.42	0/13761	0.56	0/18601

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	3337	0	3290	38	0
1	B	3341	0	3295	40	0
1	C	3369	0	3335	36	0
1	D	3335	0	3285	39	0
2	B	15	0	17	0	0
2	D	15	0	17	0	0
3	A	396	0	0	1	0
3	B	322	0	0	1	0
3	C	390	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	271	0	0	4	0
All	All	14791	0	13239	135	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 5.

All (135) 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:D:295:MET:HE3	1:D:345:ILE:HD12	1.24	1.12
1:A:167:LEU:HD21	1:B:167:LEU:HD21	1.24	1.11
1:C:167:LEU:HD21	1:D:167:LEU:HD21	1.25	1.08
1:D:295:MET:CE	1:D:345:ILE:HD12	1.93	0.99
1:B:295:MET:CE	1:B:345:ILE:HD12	1.97	0.94
1:A:167:LEU:HD21	1:B:167:LEU:CD2	1.99	0.92
1:A:405:THR:HG21	1:A:428:VAL:HG13	1.53	0.91
1:C:167:LEU:CD2	1:D:167:LEU:HD21	2.01	0.91
1:C:11:LEU:HD11	1:C:36:ILE:HD11	1.55	0.89
1:A:161:THR:HG21	3:A:2064:HOH:O	1.79	0.82
1:D:295:MET:HE3	1:D:345:ILE:CD1	2.09	0.82
1:D:422:LEU:HD22	1:D:427:VAL:HG21	1.61	0.82
1:D:317:LEU:O	1:D:320:ILE:HG22	1.80	0.81
1:B:295:MET:HE2	1:B:345:ILE:HD12	1.61	0.80
1:B:295:MET:HE3	1:B:345:ILE:HD12	1.66	0.78
1:D:309:THR:HG23	1:D:312:GLY:H	1.49	0.78
1:C:283[A]:THR:HG21	3:C:2243:HOH:O	1.83	0.78
1:C:405:THR:HG21	1:C:428:VAL:HG13	1.68	0.75
1:A:17:GLN:HG3	1:A:63:PHE:CE2	2.23	0.74
1:C:15:HIS:H	1:C:96:ASN:HD21	1.37	0.73
1:B:295:MET:HE3	1:B:345:ILE:CD1	2.18	0.72
1:A:205:LEU:HA	1:A:208[B]:VAL:HG12	1.70	0.72
1:A:405:THR:HG21	1:A:428:VAL:CG1	2.19	0.72
1:C:167:LEU:HD21	1:D:167:LEU:CD2	2.14	0.71
1:B:235:ALA:HB1	1:B:243:LEU:HD12	1.75	0.69
1:D:32:ASN:HD21	1:D:68:ARG:HH21	1.42	0.67
1:B:17:GLN:HG3	1:B:63:PHE:CE2	2.29	0.67
1:D:422:LEU:CD2	1:D:427:VAL:HG21	2.25	0.66
1:D:289:TRP:N	1:D:290:PRO:CD	2.59	0.65
1:D:17:GLN:HG3	1:D:63:PHE:CE2	2.32	0.64
1:A:167:LEU:CD2	1:B:167:LEU:HD21	2.16	0.63
1:C:262:GLN:NE2	1:D:48:GLN:HE22	1.96	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:GLN:HG3	1:C:63:PHE:CE2	2.34	0.62
1:B:210[B]:ILE:HG23	3:B:2191:HOH:O	1.98	0.62
1:C:138:VAL:HG12	1:C:200:MET:HE1	1.81	0.62
1:A:205:LEU:HA	1:A:208[B]:VAL:CG1	2.29	0.61
1:C:83:LEU:HD23	1:C:86:MET:HE3	1.81	0.61
1:A:167:LEU:CD2	1:B:167:LEU:CD2	2.78	0.61
1:C:167:LEU:CD2	1:D:167:LEU:CD2	2.77	0.61
1:A:208[B]:VAL:HG22	1:A:211:LYS:HB2	1.83	0.61
1:D:210:ILE:HD12	3:D:2148:HOH:O	2.00	0.60
1:C:262:GLN:HE22	1:D:48:GLN:HE22	1.47	0.60
1:A:375:ILE:HD13	1:A:400:LEU:HD11	1.84	0.60
1:B:285:ALA:HB3	1:B:288:MET:HG3	1.84	0.58
1:D:296:ILE:HD11	1:D:324:ILE:HG23	1.86	0.57
1:B:205:LEU:HA	1:B:208:VAL:HG22	1.86	0.57
1:A:83:LEU:HD23	1:A:86:MET:HE3	1.87	0.56
1:A:139:TYR:CE2	1:A:142:VAL:HG23	2.40	0.56
1:B:345:ILE:HG23	1:B:346:PRO:HD2	1.88	0.56
1:D:208:VAL:O	1:D:208:VAL:HG12	2.06	0.55
1:A:139:TYR:CE2	1:B:283:THR:OG1	2.55	0.55
1:C:83:LEU:HD23	1:C:86:MET:CE	2.37	0.55
1:A:147:GLY:O	1:A:208[B]:VAL:HG11	2.07	0.55
1:A:32:ASN:HD21	1:A:68:ARG:HH21	1.54	0.55
1:D:210:ILE:H	1:D:210:ILE:HD13	1.72	0.54
1:C:11:LEU:CD1	1:C:36:ILE:HD11	2.33	0.53
1:B:309:THR:HG22	1:B:311:GLU:H	1.74	0.52
1:D:295:MET:HE2	1:D:340:ALA:HA	1.90	0.52
1:B:295:MET:HE1	1:B:340:ALA:HA	1.92	0.52
1:A:139:TYR:CZ	1:A:142:VAL:CG2	2.92	0.52
1:D:195:LYS:NZ	3:D:2142:HOH:O	2.42	0.51
1:A:139:TYR:CE1	1:B:346:PRO:HB2	2.45	0.51
1:C:35:LYS:O	1:C:70[A]:ILE:HD13	2.10	0.51
1:B:235:ALA:HB3	1:B:243:LEU:HB2	1.94	0.50
1:C:9[A]:ASN:HD22	1:C:32:ASN:HB3	1.77	0.50
1:C:34:ILE:CG2	1:C:70[A]:ILE:HD12	2.42	0.49
1:A:186:ILE:HD12	1:A:194:GLN:NE2	2.26	0.49
1:B:89:LYS:HE2	1:B:412:LEU:HD23	1.95	0.49
1:B:72:LEU:CD2	1:B:83:LEU:HD13	2.42	0.48
1:A:139:TYR:CZ	1:A:142:VAL:HG23	2.49	0.48
1:C:32:ASN:HD21	1:C:68:ARG:HH21	1.62	0.47
1:A:205:LEU:HD23	1:A:208[B]:VAL:HG13	1.96	0.47
1:B:323:PHE:O	1:B:326:THR:OG1	2.25	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ASN:HA	1:B:242:PRO:HB3	1.95	0.47
1:A:139:TYR:CZ	1:A:142:VAL:HG21	2.49	0.47
1:B:295:MET:HE1	1:B:340:ALA:CB	2.45	0.47
1:D:309:THR:HG23	1:D:312:GLY:N	2.24	0.47
1:C:83:LEU:HA	1:C:86:MET:HE3	1.97	0.47
1:B:262:GLN:HE22	1:B:286:ALA:H	1.62	0.47
1:D:289:TRP:N	1:D:290:PRO:HD2	2.29	0.47
1:A:83:LEU:HD23	1:A:86:MET:CE	2.43	0.47
1:D:427:VAL:HG23	1:D:428:VAL:HG13	1.97	0.46
1:D:345:ILE:HG23	1:D:346:PRO:HD2	1.97	0.46
1:D:37:GLU:HB3	1:D:42:GLY:HA2	1.97	0.46
1:B:372:VAL:HG22	1:C:322[A]:SER:OG	2.15	0.46
1:B:295:MET:HE3	1:B:345:ILE:HD13	1.95	0.46
1:C:78:GLU:HB2	1:C:427:VAL:HG21	1.96	0.46
1:A:205:LEU:HA	1:A:208[A]:VAL:HG22	1.98	0.46
1:B:296:ILE:O	1:B:296:ILE:HG22	2.15	0.45
1:A:63:PHE:CZ	1:B:209:ARG:HD2	2.50	0.45
1:A:24:GLN:HE21	1:A:65:CYS:H	1.64	0.45
1:A:159:PRO:O	1:A:161:THR:HG22	2.17	0.45
1:B:235:ALA:CB	1:B:243:LEU:HD12	2.44	0.45
1:A:208[B]:VAL:CG2	1:A:211:LYS:HB2	2.46	0.45
1:D:235:ALA:HB1	1:D:243:LEU:HD12	2.00	0.44
1:A:169:ASP:OD1	1:A:200:MET:HE3	2.17	0.44
1:C:245:PHE:O	3:C:2200:HOH:O	2.21	0.44
1:A:205:LEU:CA	1:A:208[B]:VAL:HG12	2.46	0.44
1:D:422:LEU:HD22	1:D:427:VAL:CG2	2.42	0.43
1:D:210:ILE:N	1:D:210:ILE:HD13	2.33	0.43
1:A:188:HIS:HE1	1:B:185:GLU:OE1	2.00	0.43
1:A:154:GLY:HA3	1:A:161:THR:HG23	2.00	0.43
1:D:133:ASN:HB3	1:D:136:LEU:HD12	2.00	0.43
1:C:34:ILE:HG22	1:C:70[A]:ILE:HD12	2.01	0.43
1:B:310:PHE:O	1:B:314:VAL:HG23	2.19	0.42
1:C:13:PHE:CE2	1:C:36:ILE:HD12	2.54	0.42
1:B:295:MET:CE	1:B:340:ALA:HA	2.49	0.42
1:C:415:ASP:OD1	1:C:417:ALA:HB3	2.19	0.42
1:B:375:ILE:HG21	1:B:400:LEU:HD21	2.02	0.42
1:A:205:LEU:HD23	1:A:208[B]:VAL:CG1	2.50	0.42
1:B:234:PHE:CE2	1:B:318:MET:HG3	2.54	0.42
1:C:109:TRP:CG	1:C:195:LYS:HE2	2.54	0.42
1:A:167:LEU:O	1:A:171:ASN:HB3	2.20	0.42
1:D:318:MET:HB3	1:D:318:MET:HE3	1.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ILE:CD1	3:D:2148:HOH:O	2.64	0.41
1:C:111:TYR:CE2	1:C:115:LEU:HD11	2.55	0.41
1:A:209:ARG:HD2	1:B:63:PHE:CZ	2.55	0.41
1:D:284:ILE:CD1	1:D:320:ILE:HD13	2.51	0.41
1:C:405:THR:HG21	1:C:428:VAL:CG1	2.46	0.41
1:D:32:ASN:ND2	3:D:2020:HOH:O	2.53	0.41
1:B:306:ALA:HB1	1:B:316:LYS:HZ2	1.86	0.41
1:D:78:GLU:HB2	1:D:427:VAL:HG11	2.02	0.41
1:C:281:TYR:O	1:C:347:CYS:HA	2.21	0.41
1:D:292:ILE:HG12	1:D:345:ILE:HD13	2.01	0.41
1:C:375:ILE:HD13	1:C:400:LEU:HD11	2.02	0.41
1:B:309:THR:HG22	1:B:311:GLU:N	2.36	0.41
1:A:284:ILE:HD12	1:A:317:LEU:HD11	2.03	0.41
1:C:63:PHE:CZ	1:D:209:ARG:HD2	2.56	0.41
1:B:97:PHE:HB3	1:B:101:ALA:HB3	2.03	0.40
1:C:4:PRO:HD3	1:C:391:PHE:CE2	2.56	0.40
1:C:209:ARG:HD2	1:D:63:PHE:CZ	2.56	0.40
1:C:37:GLU:HB3	1:C:42:GLY:HA2	2.03	0.40
1:B:82:LEU:HD21	1:B:414:LEU:HD11	2.03	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	431/428 (101%)	421 (98%)	9 (2%)	1 (0%)	52	35
1	B	431/428 (101%)	420 (97%)	9 (2%)	2 (0%)	34	17
1	C	437/428 (102%)	428 (98%)	8 (2%)	1 (0%)	52	35
1	D	430/428 (100%)	418 (97%)	10 (2%)	2 (0%)	34	17
All	All	1729/1712 (101%)	1687 (98%)	36 (2%)	6 (0%)	39	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	140	GLU
1	D	140	GLU
1	A	16	VAL
1	B	16	VAL
1	C	16	VAL
1	D	16	VAL

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	356/351 (101%)	348 (98%)	8 (2%)	60	45
1	B	356/351 (101%)	352 (99%)	4 (1%)	80	74
1	C	362/351 (103%)	353 (98%)	9 (2%)	55	39
1	D	355/351 (101%)	345 (97%)	10 (3%)	51	35
All	All	1429/1404 (102%)	1398 (98%)	31 (2%)	61	45

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	A	161	THR
1	A	186	ILE
1	A	205	LEU
1	A	386	PHE
1	A	392	GLN
1	A	418	LYS
1	A	428	VAL
1	B	59	TYR
1	B	83	LEU
1	B	195	LYS
1	B	386	PHE
1	C	59	TYR
1	C	70[A]	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	70[B]	ILE
1	C	186	ILE
1	C	205	LEU
1	C	374	GLU
1	C	386	PHE
1	C	392	GLN
1	C	418	LYS
1	D	39	ARG
1	D	48	GLN
1	D	59	TYR
1	D	195	LYS
1	D	210	ILE
1	D	287	ASN
1	D	320	ILE
1	D	364	LYS
1	D	386	PHE
1	D	392	GLN

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

Mol	Chain	Res	Type
1	A	24	GLN
1	A	188	HIS
1	B	113	GLN
1	B	262	GLN
1	B	342	GLN
1	C	32	ASN
1	C	96	ASN
1	C	262	GLN
1	C	404	HIS
1	D	32	ASN
1	D	342	GLN
1	D	378	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	EPE	B	1429	-	14,15,15	0.46	0	18,20,20	1.43	2 (11%)
2	EPE	D	1429	-	14,15,15	0.37	0	18,20,20	1.18	2 (11%)

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	EPE	B	1429	-	-	0/9/19/19	0/1/1/1
2	EPE	D	1429	-	-	0/9/19/19	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	1429	EPE	O2S-S-C10	2.76	109.26	106.91
2	D	1429	EPE	O1S-S-C10	2.92	109.40	106.91
2	B	1429	EPE	C6-N1-C2	2.99	115.39	108.90
2	B	1429	EPE	O1S-S-C10	3.71	110.07	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	427/428 (99%)	-0.16	2 (0%) 91 90	11, 19, 41, 48	0
1	B	427/428 (99%)	0.18	29 (6%) 20 16	11, 22, 59, 72	0
1	C	427/428 (99%)	-0.16	5 (1%) 81 78	11, 20, 41, 48	0
1	D	427/428 (99%)	0.29	36 (8%) 14 11	11, 23, 59, 73	0
All	All	1708/1712 (99%)	0.04	72 (4%) 40 34	11, 21, 52, 73	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	314	VAL	8.2
1	D	305	PRO	6.3
1	D	238	ARG	5.6
1	D	241	ASN	5.6
1	B	296	ILE	5.5
1	D	306	ALA	5.4
1	D	296	ILE	5.3
1	B	240	GLY	5.2
1	B	238	ARG	5.1
1	B	301	TRP	5.0
1	D	346	PRO	4.8
1	C	139	TYR	4.8
1	D	240	GLY	4.8
1	D	233	ASN	4.6
1	A	139	TYR	4.5
1	D	301	TRP	4.4
1	B	241	ASN	4.3
1	B	305	PRO	4.3
1	B	314	VAL	4.3
1	D	236	PHE	4.2
1	D	307	TYR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	310	PHE	4.1
1	D	293	CYS	4.0
1	C	2	THR	3.9
1	D	343	TYR	3.9
1	D	239	ASP	3.7
1	D	310	PHE	3.6
1	B	298	LYS	3.6
1	B	307	TYR	3.5
1	B	242	PRO	3.5
1	D	298	LYS	3.4
1	B	286	ALA	3.3
1	B	306	ALA	3.3
1	D	323	PHE	3.3
1	B	323	PHE	3.2
1	D	242	PRO	3.2
1	C	238[A]	ARG	3.1
1	D	320	ILE	3.1
1	B	285	ALA	3.1
1	D	299	PRO	3.1
1	B	233	ASN	3.1
1	B	343	TYR	3.0
1	D	342	GLN	2.9
1	D	290	PRO	2.8
1	B	303	ASP	2.8
1	B	239	ASP	2.8
1	A	2	THR	2.7
1	B	290	PRO	2.7
1	B	415	ASP	2.6
1	D	303	ASP	2.6
1	B	294	ASP	2.5
1	B	338	GLU	2.5
1	D	330	ASP	2.4
1	D	341	ALA	2.4
1	B	2	THR	2.4
1	D	237	ASP	2.3
1	D	2	THR	2.3
1	D	315	ASP	2.3
1	B	289	TRP	2.2
1	D	309	THR	2.2
1	B	243	LEU	2.2
1	B	309	THR	2.2
1	D	75	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	189	LYS	2.2
1	B	288	MET	2.1
1	C	186	ILE	2.1
1	D	317	LEU	2.1
1	D	345	ILE	2.1
1	B	346	PRO	2.1
1	D	292	ILE	2.0
1	D	111	TYR	2.0
1	C	418	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	EPE	B	1429	15/15	0.89	0.17	0.45	26,29,30,30	15
2	EPE	D	1429	15/15	0.89	0.17	0.29	34,35,36,36	15

6.5 Other polymers [i](#)

There are no such residues in this entry.