



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:43 PM UTC

PDB ID : 2VJQ / pdb_00002vjq
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

<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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

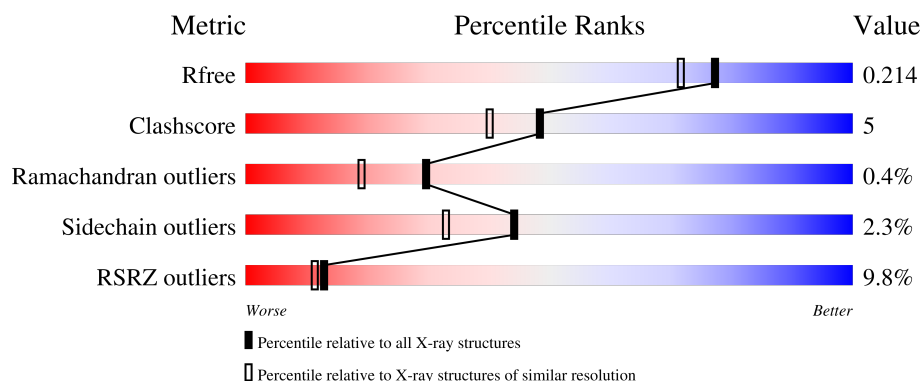
1 Overall quality at a glance

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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	428	4% 90% 9%
1	B	428	16% 88% 11%
1	C	428	4% 87% 12%
1	D	428	16% 89% 9%

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 (CCD ID: 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		

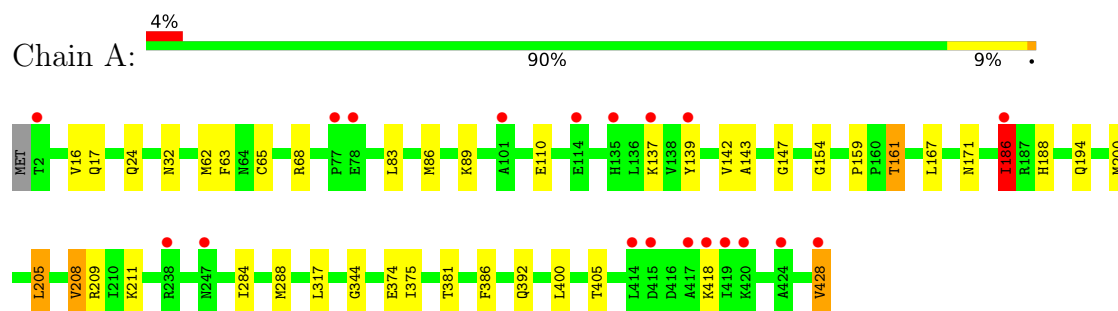
- Molecule 3 is water.

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		

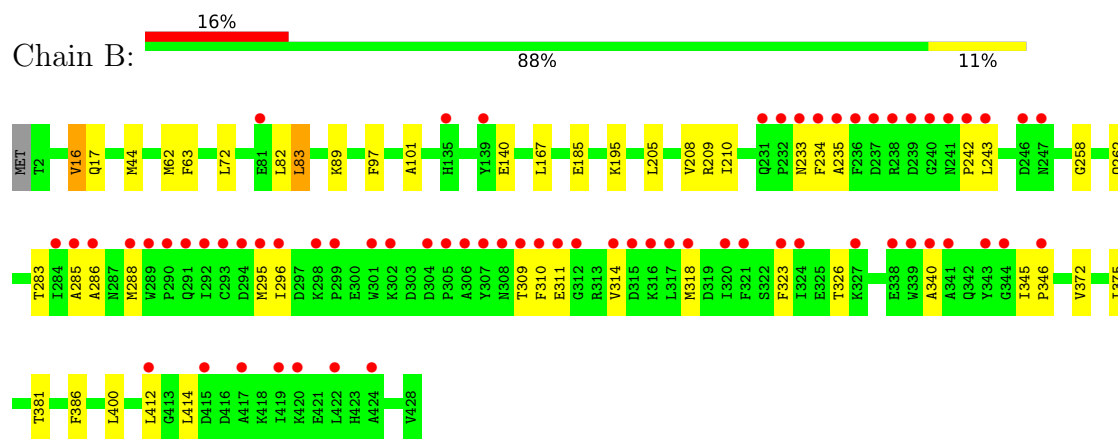
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

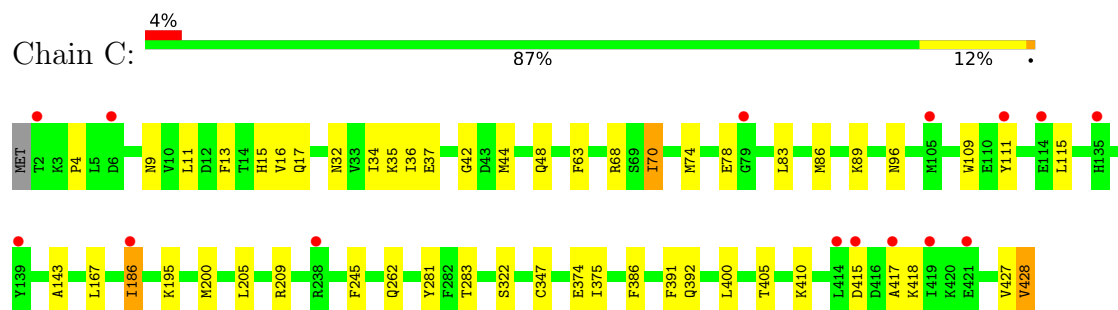
• Molecule 1: FORMYL-COENZYME A TRANSFERASE



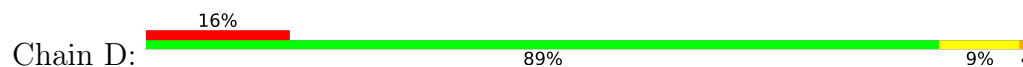
• Molecule 1: FORMYL-COENZYME A TRANSFERASE

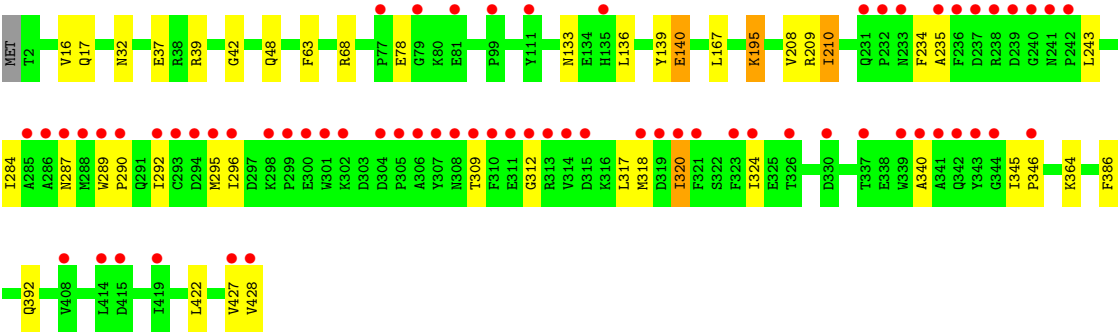


• Molecule 1: FORMYL-COENZYME A TRANSFERASE



• 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	214.16Å 98.92Å 152.53Å 90.00° 135.27° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 30.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.8 (30.00-1.80) 91.8 (30.00-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.212 0.185 , 0.214	Depositor DCC
R_{free} test set	9536 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
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
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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.55	0/3428	0.73	1/4634 (0.0%)
1	B	0.53	0/3432	0.73	1/4640 (0.0%)
1	C	0.54	0/3478	0.73	1/4701 (0.0%)
1	D	0.52	0/3423	0.72	0/4626
All	All	0.54	0/13761	0.73	3/18601 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	ILE	CB-CA-C	-5.65	104.52	112.14
1	A	186	ILE	CB-CA-C	-5.38	104.80	112.22
1	B	258	GLY	N-CA-C	5.35	120.25	113.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3337	0	3290	44	0
1	B	3341	0	3295	42	0
1	C	3369	0	3335	40	0
1	D	3335	0	3285	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	D	271	0	0	5	0
All	All	14791	0	13239	146	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 (146) 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:B:295:MET:HE3	1:B:345:ILE:HD12	1.25	1.16
1:A:167:LEU:HD21	1:B:167:LEU:HD21	1.24	1.11
1:D:295:MET:HE3	1:D:345:ILE:HD12	1.23	1.10
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:HE3	1:B:345:ILE:CD1	1.97	0.95
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: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: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:B:295:MET:HE2	1:B:340:ALA:HA	1.67	0.76
1:C:405:THR:HG21	1:C:428:VAL:HG13	1.68	0.75
1:C:143:ALA:HB2	1:C:200:MET:HE2	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:A:137:LYS:NZ	1:B:288:MET:HE1	2.04	0.72
1:D:295:MET:HE2	1:D:340:ALA:HA	1.71	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:D:295:MET:HE3	1:D:345:ILE:CD1	2.12	0.71
1:C:167:LEU:HD21	1:D:167:LEU:CD2	2.14	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ALA:HB1	1:B:243:LEU:HD12	1.75	0.69
1:B:16:VAL:HG22	1:B:44[B]:MET:HE2	1.75	0.67
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:C:74:MET:HE3	1:C:83:LEU:HD11	1.77	0.66
1:D:289:TRP:N	1:D:290:PRO:CD	2.59	0.65
1:C:83:LEU:HD23	1:C:86:MET:HE3	1.78	0.64
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
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:A:205:LEU:HA	1:A:208[B]:VAL:CG1	2.29	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:137:LYS:HZ3	1:B:288:MET:HE1	1.70	0.57
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:234:PHE:CZ	1:D:318:MET:HE2	2.41	0.56
1:D:208:VAL:HG12	1:D:208:VAL:O	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:32:ASN:HD21	1:A:68:ARG:HH21	1.54	0.55
1:A:147:GLY:O	1:A:208[B]:VAL:HG11	2.07	0.55
1:D:210:ILE:HD13	1:D:210:ILE:H	1.72	0.54
1:A:83:LEU:HD23	1:A:86:MET:HE3	1.90	0.54
1:A:137:LYS:HZ1	1:B:288:MET:HE1	1.71	0.54
1:B:323:PHE:O	1:B:326:THR:OG1	2.25	0.53
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: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:B:234:PHE:CZ	1:B:318:MET:HE2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:TYR:CE1	1:B:346:PRO:HB2	2.45	0.51
1:A:143:ALA:HB2	1:A:200:MET:HE2	1.93	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:16:VAL:CG2	1:B:44[B]:MET:HE2	2.44	0.47
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:262:GLN:HE22	1:B:286:ALA:H	1.62	0.47
1:D:309:THR:HG23	1:D:312:GLY:N	2.24	0.47
1:A:83:LEU:HD23	1:A:86:MET:CE	2.43	0.47
1:D:289:TRP:N	1:D:290:PRO:HD2	2.29	0.47
1:D:427:VAL:HG23	1:D:428:VAL:HG13	1.97	0.46
1:B:372:VAL:HG22	1:C:322[A]:SER:OG	2.15	0.46
1:D:37:GLU:HB3	1:D:42:GLY:HA2	1.97	0.46
1:D:345:ILE:HG23	1:D:346:PRO:HD2	1.97	0.46
1:C:143:ALA:CB	1:C:200:MET:HE2	2.42	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:A:288:MET:HE1	1:A:344:GLY:C	2.41	0.45
1:B:296:ILE:O	1:B:296:ILE:HG22	2.15	0.45
1:A:24:GLN:HE21	1:A:65:CYS:H	1.64	0.45
1:A:63:PHE:CZ	1:B:209:ARG:HD2	2.50	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: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:A:188:HIS:HE1	1:B:185:GLU:OE1	2.00	0.43
1:D:210:ILE:HD13	1:D:210:ILE:N	2.33	0.43
1:A:154:GLY:HA3	1:A:161:THR:HG23	2.00	0.43
1:C:44[A]:MET:HE2	1:C:48:GLN:OE1	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ASN:HB3	1:D:136:LEU:HD12	2.00	0.43
1:C:83:LEU:HA	1:C:86:MET:HE3	2.01	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:D:139:TYR:O	1:D:140:GLU:C	2.63	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:B:62:MET:HE3	1:B:381:THR:HA	1.99	0.42
1:A:167:LEU:O	1:A:171:ASN:HB3	2.20	0.42
1:C:111:TYR:CE2	1:C:115:LEU:HD11	2.55	0.41
1:D:210:ILE:CD1	3:D:2148:HOH:O	2.64	0.41
1:C:74:MET:HE3	1:C:83:LEU:CD1	2.48	0.41
1:A:209:ARG:HD2	1:B:63:PHE:CZ	2.55	0.41
1:A:62:MET:HE3	1:A:381:THR:HA	2.03	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:C:281:TYR:O	1:C:347:CYS:HA	2.21	0.41
1:D:78:GLU:HB2	1:D:427:VAL:HG11	2.02	0.41
1:C:375:ILE:HD13	1:C:400:LEU:HD11	2.02	0.41
1:D:292:ILE:HG12	1:D:345:ILE:HD13	2.01	0.41
1:A:284:ILE:HD12	1:A:317:LEU:HD11	2.03	0.41
1:A:288:MET:HE2	1:A:288:MET:HB3	1.92	0.41
1:B:309:THR:HG22	1:B:311:GLU:N	2.36	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:D:48:GLN:CD	3:D:2034:HOH:O	2.63	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%)	43	31
1	B	431/428 (101%)	420 (97%)	9 (2%)	2 (0%)	24	14
1	C	437/428 (102%)	428 (98%)	8 (2%)	1 (0%)	43	31
1	D	430/428 (100%)	418 (97%)	10 (2%)	2 (0%)	24	14
All	All	1729/1712 (101%)	1687 (98%)	36 (2%)	6 (0%)	30	25

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 [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	356/351 (101%)	344 (97%)	12 (3%)	32	20
1	B	356/351 (101%)	353 (99%)	3 (1%)	73	70
1	C	362/351 (103%)	351 (97%)	11 (3%)	36	24
1	D	355/351 (101%)	347 (98%)	8 (2%)	44	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1429/1404 (102%)	1395 (98%)	34 (2%)	44 31

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LYS
1	A	110	GLU
1	A	161	THR
1	A	186	ILE
1	A	205	LEU
1	A	208[A]	VAL
1	A	208[B]	VAL
1	A	374	GLU
1	A	386	PHE
1	A	392	GLN
1	A	418	LYS
1	A	428	VAL
1	B	83	LEU
1	B	195	LYS
1	B	386	PHE
1	C	70[A]	ILE
1	C	70[B]	ILE
1	C	89	LYS
1	C	186	ILE
1	C	205	LEU
1	C	374	GLU
1	C	386	PHE
1	C	392	GLN
1	C	410	LYS
1	C	418	LYS
1	C	428	VAL
1	D	39	ARG
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	188	HIS
1	A	247	ASN
1	A	392	GLN
1	B	113	GLN
1	B	233	ASN
1	B	262	GLN
1	B	342	GLN
1	C	15	HIS
1	C	32	ASN
1	C	54	ASN
1	C	85	GLN
1	C	96	ASN
1	C	342	GLN
1	C	392	GLN
1	D	17	GLN
1	D	32	ASN
1	D	48	GLN
1	D	85	GLN
1	D	241	ASN
1	D	342	GLN
1	D	378	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 oligosaccharides 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	D	1429	-	15,15,15	0.86	1 (6%)	19,20,20	0.96	0
2	EPE	B	1429	-	15,15,15	0.86	1 (6%)	19,20,20	1.24	2 (10%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1429	EPE	C10-S	2.96	1.81	1.77
2	B	1429	EPE	C10-S	2.80	1.81	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1429	EPE	C6-N1-C2	3.04	115.39	108.84
2	B	1429	EPE	O1S-S-C10	2.21	110.07	106.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1429	EPE	C8-C7-N4-C5
2	D	1429	EPE	N4-C7-C8-O8
2	B	1429	EPE	N4-C7-C8-O8

There are no ring outliers.

No monomer is involved in short contacts.

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	427/428 (99%)	-0.05	19 (4%) 39 38	8, 19, 41, 48	6 (1%)
1	B	427/428 (99%)	0.44	67 (15%) 5 4	9, 22, 59, 72	6 (1%)
1	C	427/428 (99%)	-0.00	15 (3%) 47 47	7, 20, 41, 48	12 (2%)
1	D	427/428 (99%)	0.57	67 (15%) 5 4	11, 23, 59, 73	5 (1%)
All	All	1708/1712 (99%)	0.24	168 (9%) 13 11	7, 21, 52, 73	29 (1%)

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	314	VAL	8.3
1	B	314	VAL	6.1
1	B	296	ILE	5.9
1	D	299	PRO	5.8
1	A	139	TYR	5.7
1	C	139	TYR	5.2
1	B	301	TRP	5.1
1	D	241	ASN	5.1
1	B	309	THR	5.0
1	B	299	PRO	4.9
1	B	305	PRO	4.9
1	B	240	GLY	4.8
1	D	296	ILE	4.8
1	D	293	CYS	4.8
1	B	285	ALA	4.7
1	B	241	ASN	4.7
1	B	286	ALA	4.7
1	B	310	PHE	4.6
1	D	346	PRO	4.6
1	D	236	PHE	4.6
1	B	292	ILE	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	242	PRO	4.2
1	B	238	ARG	4.2
1	D	289	TRP	4.1
1	B	306	ALA	4.1
1	D	306	ALA	4.1
1	B	289	TRP	4.0
1	B	343	TYR	3.8
1	B	312	GLY	3.8
1	D	240	GLY	3.8
1	B	233	ASN	3.8
1	D	301	TRP	3.8
1	D	308	ASN	3.8
1	B	323	PHE	3.8
1	D	233	ASN	3.8
1	D	305	PRO	3.7
1	B	298	LYS	3.6
1	D	320	ILE	3.6
1	D	309	THR	3.6
1	D	310	PHE	3.6
1	B	293	CYS	3.5
1	B	346	PRO	3.5
1	B	338	GLU	3.5
1	D	343	TYR	3.5
1	D	292	ILE	3.4
1	B	307	TYR	3.4
1	D	111	TYR	3.4
1	D	341	ALA	3.4
1	A	247	ASN	3.3
1	B	304	ASP	3.3
1	B	236	PHE	3.2
1	B	235	ALA	3.2
1	D	295	MET	3.2
1	D	312	GLY	3.2
1	C	415	ASP	3.2
1	D	323	PHE	3.2
1	D	290	PRO	3.1
1	C	2	THR	3.1
1	D	242	PRO	3.1
1	D	238	ARG	3.1
1	B	294	ASP	3.1
1	B	290	PRO	3.1
1	B	344	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	417	ALA	3.1
1	D	304	ASP	3.0
1	D	285	ALA	3.0
1	B	232	PRO	3.0
1	D	307	TYR	2.9
1	B	295	MET	2.9
1	B	341	ALA	2.9
1	D	298	LYS	2.9
1	B	308	ASN	2.9
1	B	234	PHE	2.9
1	D	340	ALA	2.8
1	A	419	ILE	2.8
1	B	243	LEU	2.8
1	B	81	GLU	2.8
1	D	239	ASP	2.8
1	B	321	PHE	2.8
1	D	321	PHE	2.8
1	C	238[A]	ARG	2.8
1	A	414	LEU	2.8
1	B	415	ASP	2.8
1	A	428	VAL	2.7
1	A	101	ALA	2.7
1	B	422	LEU	2.7
1	D	313	ARG	2.7
1	A	77	PRO	2.7
1	A	2	THR	2.6
1	D	81	GLU	2.6
1	D	419	ILE	2.6
1	B	247	ASN	2.6
1	D	330	ASP	2.6
1	B	424	ALA	2.6
1	B	339	TRP	2.6
1	C	414	LEU	2.6
1	D	414	LEU	2.6
1	A	417	ALA	2.6
1	B	135[A]	HIS	2.5
1	C	6	ASP	2.5
1	C	419	ILE	2.5
1	D	235	ALA	2.5
1	D	337	THR	2.5
1	A	424	ALA	2.5
1	D	231	GLN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	418	LYS	2.5
1	A	186	ILE	2.5
1	B	419	ILE	2.5
1	C	186	ILE	2.5
1	A	114	GLU	2.5
1	C	417	ALA	2.5
1	D	286	ALA	2.5
1	C	79	GLY	2.4
1	D	287	ASN	2.4
1	B	231	GLN	2.4
1	B	412	LEU	2.4
1	D	232	PRO	2.4
1	D	311	GLU	2.4
1	D	428	VAL	2.4
1	B	288	MET	2.4
1	C	111	TYR	2.4
1	A	415	ASP	2.4
1	B	284	ILE	2.4
1	B	340	ALA	2.4
1	B	246	ASP	2.3
1	D	294	ASP	2.3
1	D	415	ASP	2.3
1	C	114	GLU	2.3
1	D	300	GLU	2.3
1	B	317	LEU	2.3
1	D	315	ASP	2.3
1	D	339	TRP	2.3
1	C	105	MET	2.3
1	B	302	LYS	2.3
1	C	135[A]	HIS	2.3
1	B	318	MET	2.3
1	D	99	PRO	2.2
1	B	320	ILE	2.2
1	B	324	ILE	2.2
1	A	135[A]	HIS	2.2
1	B	316	LYS	2.2
1	D	135[A]	HIS	2.2
1	D	408	VAL	2.2
1	B	139	TYR	2.2
1	D	288	MET	2.2
1	D	237	ASP	2.2
1	D	77	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	327	LYS	2.2
1	C	421	GLU	2.1
1	D	342	GLN	2.1
1	B	315	ASP	2.1
1	D	344	GLY	2.1
1	A	137	LYS	2.1
1	D	324	ILE	2.1
1	D	79	GLY	2.1
1	D	427	VAL	2.1
1	B	420	LYS	2.1
1	B	237	ASP	2.1
1	A	238	ARG	2.1
1	A	78	GLU	2.1
1	B	239	ASP	2.1
1	D	319	ASP	2.1
1	B	311	GLU	2.0
1	A	420	LYS	2.0
1	D	302	LYS	2.0
1	D	318	MET	2.0
1	B	291	GLN	2.0
1	D	326	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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. 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($\text{\AA}^2$)	Q<0.9
2	EPE	D	1429	15/15	0.82	0.17	34,35,36,36	15
2	EPE	B	1429	15/15	0.87	0.16	26,29,30,30	15

6.5 Other polymers [i](#)

There are no such residues in this entry.