



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:09 PM UTC

PDB ID : 6VK4 / pdb_00006vk4
Title : Crystal Structure of Methylosinus trichosporium OB3b Soluble Methane Monooxygenase Hydroxylase and Regulatory Component Complex
Authors : Jones, J.C.; Banerjee, R.; Shi, K.; Aihara, H.; Lipscomb, J.D.
Deposited on : 2020-01-18
Resolution : 2.35 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

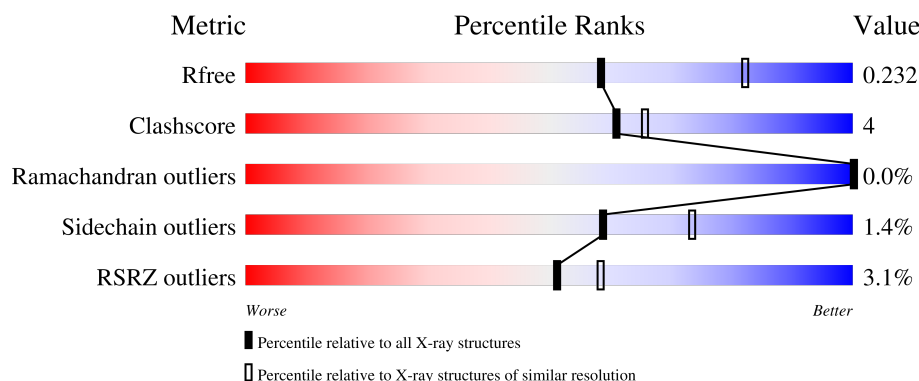
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.



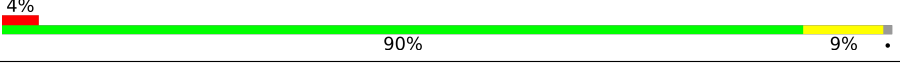
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	526	4% 81% 16% .
1	E	526	3% 85% 12% .
2	B	395	3% 89% 10% .
2	F	395	2% 89% 10% .
3	C	169	0% 89% 9% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	169	 4% 90% 9% 6%
4	D	138	 4% 80% 13% 6%
4	H	138	 6% 83% 12% 6%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 19709 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 Methane monooxygenase component A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			4175	2676	723	764	12			
1	E	515	Total	C	N	O	S	0	0	0
			4175	2676	723	764	12			

- Molecule 2 is a protein called Methane monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	391	Total	C	N	O	S	0	0	0
			3177	2029	554	589	5			
2	F	391	Total	C	N	O	S	0	0	0
			3177	2029	554	589	5			

- Molecule 3 is a protein called Methane monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	167	Total	C	N	O	S	0	0	0
			1357	871	233	252	1			
3	G	167	Total	C	N	O	S	0	0	0
			1357	871	233	252	1			

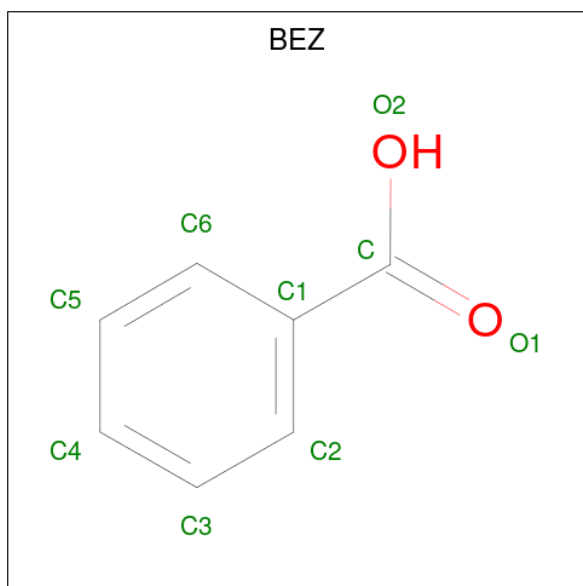
- Molecule 4 is a protein called Methane monooxygenase regulatory protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	130	Total	C	N	O	S	0	0	0
			985	630	157	195	3			
4	H	130	Total	C	N	O	S	0	0	0
			985	630	157	195	3			

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Fe	0	0
			2	2		

- Molecule 6 is BENZOIC ACID (CCD ID: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	7	2		
6	E	1	Total	C	O	0	0
			9	7	2		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	0

- Molecule 8 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	2	Total Fe 2 2	0	0

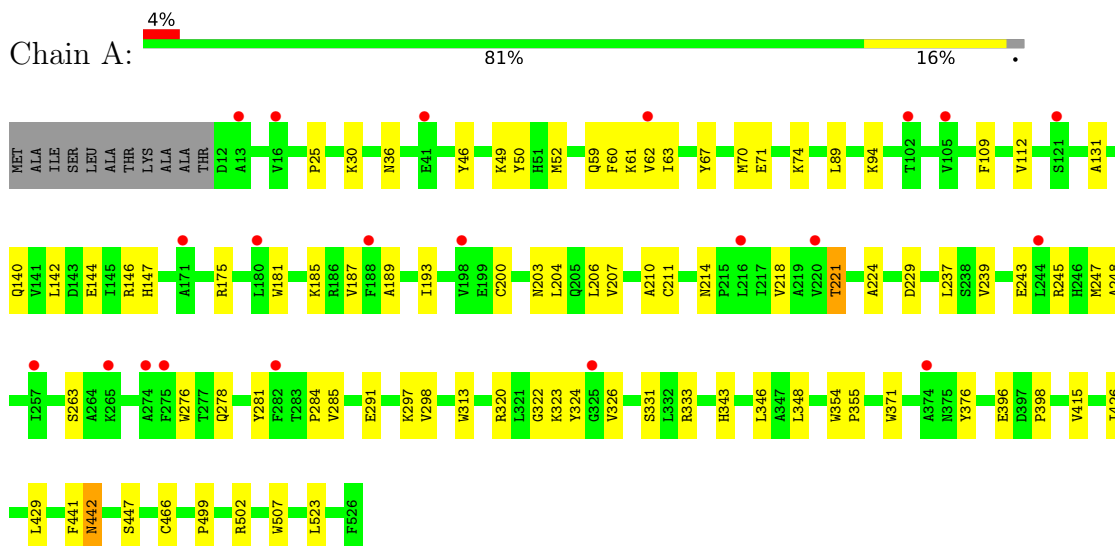
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	71	Total O 71 71	0	0
9	B	55	Total O 55 55	0	0
9	C	17	Total O 17 17	0	0
9	D	4	Total O 4 4	0	0
9	E	61	Total O 61 61	0	0
9	F	62	Total O 62 62	0	0
9	G	17	Total O 17 17	0	0
9	H	8	Total O 8 8	0	0

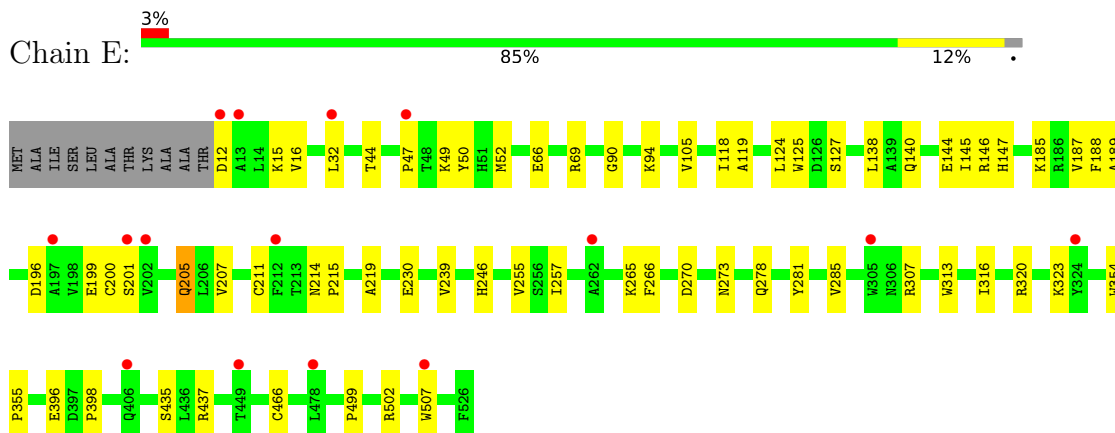
3 Residue-property plots [i](#)

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.

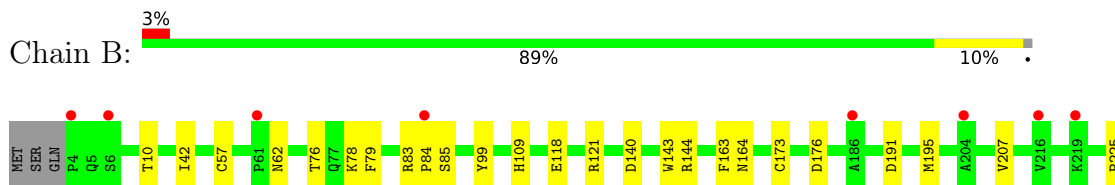
- Molecule 1: Methane monooxygenase component A alpha chain

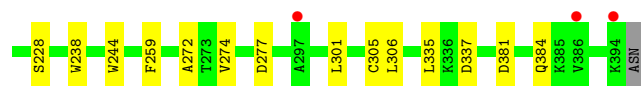


- Molecule 1: Methane monooxygenase component A alpha chain

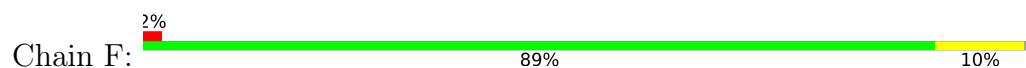


- Molecule 2: Methane monooxygenase

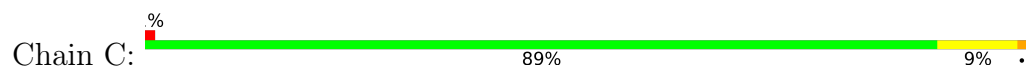




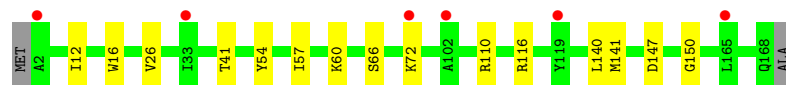
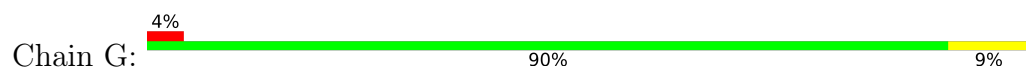
• Molecule 2: Methane monooxygenase



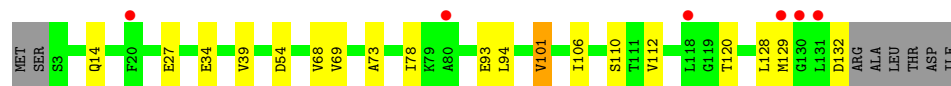
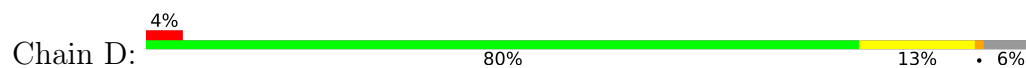
• Molecule 3: Methane monooxygenase



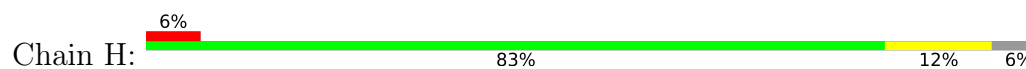
• Molecule 3: Methane monooxygenase



• Molecule 4: Methane monooxygenase regulatory protein B



• Molecule 4: Methane monooxygenase regulatory protein B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.86Å 105.21Å 300.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.59 – 2.35 52.59 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.3 (52.59-2.35) 96.4 (52.59-2.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.20rc2_4400	Depositor
R, R_{free}	0.190 , 0.228 0.199 , 0.232	Depositor DCC
R_{free} test set	6694 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.088 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19709	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: FE2, EDO, FE, BEZ

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	0.23	0/4305	0.42	0/5850
1	E	0.23	0/4305	0.42	0/5850
2	B	0.22	0/3270	0.41	0/4446
2	F	0.22	0/3270	0.41	0/4446
3	C	0.23	0/1383	0.37	0/1870
3	G	0.22	0/1383	0.39	0/1870
4	D	0.19	0/1001	0.35	0/1354
4	H	0.19	0/1001	0.38	0/1354
All	All	0.22	0/19918	0.41	0/27040

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	4175	0	3972	53	0
1	E	4175	0	3972	41	0
2	B	3177	0	3019	23	0
2	F	3177	0	3019	27	0
3	C	1357	0	1395	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1357	0	1395	11	0
4	D	985	0	977	13	0
4	H	985	0	977	10	0
5	A	2	0	0	0	0
6	A	9	0	5	0	0
6	E	9	0	5	0	0
7	C	4	0	6	1	0
8	E	2	0	0	0	0
9	A	71	0	0	1	0
9	B	55	0	0	1	0
9	C	17	0	0	0	0
9	D	4	0	0	0	0
9	E	61	0	0	0	0
9	F	62	0	0	0	0
9	G	17	0	0	1	0
9	H	8	0	0	0	0
All	All	19709	0	18742	161	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 4.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ASN:OD1	4:D:110:SER:OG	2.07	0.70
4:H:54:ASP:HB2	4:H:94:LEU:HD21	1.76	0.66
2:B:259:PHE:HA	2:B:335:LEU:HD21	1.79	0.64
1:E:201:SER:HA	1:E:205:GLN:HG3	1.79	0.64
2:B:42:ILE:HD13	2:B:57:CYS:HB2	1.80	0.63
1:E:44:THR:HB	1:E:127:SER:HA	1.81	0.63
1:E:50:TYR:HB3	1:E:52:MET:HE1	1.81	0.61
1:E:52:MET:HE2	1:E:257:ILE:HA	1.83	0.61
1:A:442:ASN:O	1:A:442:ASN:ND2	2.34	0.59
1:A:396:GLU:OE1	1:A:502:ARG:NH2	2.35	0.58
4:D:93:GLU:HB3	2:F:48:ARG:HG3	1.85	0.58
3:C:168:GLN:HG3	7:C:201:EDO:H22	1.86	0.58
1:E:320:ARG:HH12	1:E:323:LYS:HE2	1.69	0.58
2:B:225:PRO:HA	2:B:228:SER:HB2	1.86	0.57
3:G:26:VAL:HG23	3:G:72:LYS:HD3	1.86	0.56
1:E:214:ASN:OD1	4:H:110:SER:OG	2.16	0.56
1:A:70:MET:HE1	1:A:245:ARG:HE	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:69:VAL:HG22	4:D:78:ILE:HG12	1.87	0.55
1:E:187:VAL:HG23	1:E:278:GLN:HA	1.88	0.55
2:F:42:ILE:HD13	2:F:57:CYS:HB2	1.88	0.55
1:E:66:GLU:OE2	1:E:69:ARG:NH1	2.39	0.55
2:B:79:PHE:HB2	2:B:83:ARG:HB3	1.87	0.55
2:B:121:ARG:HD3	2:F:118:GLU:OE2	2.06	0.55
2:B:381:ASP:HB3	2:B:384:GLN:HB3	1.89	0.55
4:D:101:VAL:HG22	4:D:120:THR:HA	1.89	0.54
1:E:316:ILE:HG12	4:H:37:ALA:O	2.07	0.54
1:A:447:SER:HB3	1:A:523:LEU:HD21	1.90	0.54
3:C:57:ILE:O	3:C:61:ILE:HG13	2.09	0.53
1:E:196:ASP:HB3	1:E:199:GLU:HB2	1.89	0.53
2:B:144:ARG:NH1	2:B:207:VAL:HG11	2.24	0.52
1:E:124:LEU:HD21	1:E:200:CYS:HB2	1.91	0.52
3:C:5:GLU:OE2	3:C:11:SER:OG	2.24	0.52
1:E:119:ALA:HB1	2:F:171:ARG:HD2	1.92	0.52
4:D:54:ASP:HB2	4:D:94:LEU:HD21	1.90	0.52
1:A:276:TRP:CE3	1:A:331:SER:HB2	2.46	0.51
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.45	0.51
1:A:147:HIS:CD2	1:A:239:VAL:HG13	2.46	0.51
2:F:272:ALA:HB1	2:F:277:ASP:HB3	1.91	0.51
1:A:207:VAL:O	1:A:211:CYS:HB3	2.10	0.51
2:F:47:LYS:HD3	2:F:47:LYS:H	1.75	0.51
1:A:298:VAL:HG13	2:B:10:THR:HG21	1.93	0.51
2:F:151:TYR:OH	2:F:344:LYS:NZ	2.25	0.50
1:E:49:LYS:NZ	1:E:270:ASP:OD1	2.43	0.50
1:E:118:ILE:HD13	1:E:145:ILE:HG12	1.93	0.50
1:E:185:LYS:O	1:E:189:ALA:HB3	2.12	0.50
1:A:185:LYS:O	1:A:189:ALA:HB3	2.12	0.49
1:A:224:ALA:HB1	1:A:229:ASP:HB3	1.94	0.49
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.48	0.49
2:F:12:ARG:NH2	4:H:73:ALA:O	2.45	0.49
1:A:322:GLY:HA2	1:A:326:VAL:O	2.13	0.49
1:E:140:GLN:HG3	1:E:246:HIS:CE1	2.47	0.49
2:F:11:LYS:O	2:F:19:ARG:NH1	2.46	0.49
1:A:60:PHE:O	1:A:62:VAL:HG13	2.13	0.49
1:A:291:GLU:OE2	1:A:376:TYR:OH	2.30	0.49
2:F:116:LYS:NZ	2:F:191:ASP:OD2	2.43	0.48
1:A:50:TYR:HD1	1:A:263:SER:HB2	1.78	0.48
1:A:218:VAL:O	1:A:221:THR:HB	2.14	0.48
1:A:324:TYR:OH	4:D:132:ASP:OD1	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:44:LYS:NZ	4:H:71:ASP:OD1	2.43	0.48
1:E:211:CYS:HB2	1:E:313:TRP:CD1	2.49	0.48
2:B:78:LYS:HG2	2:B:84:PRO:HA	1.96	0.47
1:E:207:VAL:O	1:E:211:CYS:HB3	2.14	0.47
1:A:193:ILE:HD11	2:B:85:SER:HB3	1.97	0.47
2:B:118:GLU:OE2	2:F:121:ARG:HD3	2.14	0.47
1:A:243:GLU:O	1:A:247:MET:HG3	2.14	0.47
2:F:189:LYS:HD3	2:F:189:LYS:HA	1.74	0.47
2:B:164:ASN:HB3	2:B:238:TRP:CE2	2.50	0.47
1:A:398:PRO:HA	1:A:507:TRP:CE2	2.49	0.47
1:E:211:CYS:HB2	1:E:313:TRP:CE2	2.50	0.47
1:A:203:ASN:OD1	1:A:204:LEU:N	2.47	0.46
1:E:215:PRO:HA	1:E:219:ALA:HB3	1.97	0.46
2:B:191:ASP:O	2:B:195:MET:HG2	2.16	0.46
1:A:59:GLN:HG3	1:A:248:ALA:HB1	1.97	0.46
1:A:320:ARG:HB3	4:D:128:LEU:HD11	1.96	0.46
2:B:173:CYS:HA	2:B:244:TRP:CE2	2.51	0.46
3:C:56:TYR:CZ	3:C:60:LYS:HD2	2.50	0.46
1:E:146:ARG:HB2	2:F:109:HIS:CE1	2.51	0.46
1:E:265:LYS:HE2	1:E:266:PHE:CZ	2.50	0.46
1:A:211:CYS:HB2	1:A:313:TRP:CE2	2.51	0.46
2:F:79:PHE:HB2	2:F:83:ARG:HB3	1.96	0.46
2:B:118:GLU:HG2	2:F:118:GLU:HG2	1.98	0.46
1:E:396:GLU:OE1	1:E:502:ARG:NH2	2.45	0.45
1:A:441:PHE:HB2	3:C:162:VAL:HG12	1.97	0.45
2:F:89:GLU:OE2	3:G:116:ARG:NH2	2.46	0.45
1:A:297:LYS:HD2	1:A:371:TRP:CZ3	2.51	0.45
2:B:301:LEU:O	2:B:305:CYS:HB2	2.16	0.45
1:E:255:VAL:HG13	4:H:131:LEU:HG	1.98	0.45
1:A:187:VAL:HG23	1:A:278:GLN:HA	1.97	0.45
1:E:47:PRO:HB2	3:G:141:MET:HE2	1.99	0.45
1:A:221:THR:HG21	1:A:237:LEU:HD11	1.97	0.45
1:A:415:VAL:HG22	1:A:426:ILE:HG12	1.99	0.45
3:C:116:ARG:O	3:C:120:LYS:HB2	2.17	0.45
3:G:147:ASP:OD1	3:G:150:GLY:HA3	2.17	0.45
2:F:47:LYS:H	2:F:47:LYS:CD	2.30	0.45
1:A:140:GLN:O	1:A:144:GLU:HG2	2.17	0.44
1:A:146:ARG:HB2	2:B:109:HIS:CE1	2.52	0.44
1:A:36:ASN:HB2	1:A:131:ALA:HB2	1.98	0.44
1:A:206:LEU:O	1:A:210:ALA:HB3	2.18	0.44
2:F:358:SER:HB2	2:F:390:LEU:HD11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:41:THR:HG22	3:G:54:TYR:CE2	2.51	0.44
1:A:109:PHE:O	1:A:112:VAL:HG12	2.18	0.44
1:E:147:HIS:CD2	1:E:239:VAL:HG13	2.52	0.44
1:E:32:LEU:HD12	1:E:32:LEU:HA	1.82	0.44
2:B:140:ASP:HB3	2:B:143:TRP:HB3	2.00	0.44
2:F:148:LEU:O	2:F:152:PHE:HB3	2.17	0.44
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.53	0.44
1:A:466:CYS:HB2	2:B:76:THR:HA	2.00	0.44
1:A:49:LYS:HG2	3:C:142:GLU:HG2	2.00	0.43
2:B:225:PRO:O	2:B:337:ASP:HB3	2.17	0.43
1:E:435:SER:OG	1:E:437:ARG:NH2	2.50	0.43
4:D:39:VAL:HB	4:D:112:VAL:HB	2.00	0.43
2:F:139:ILE:HG13	2:F:277:ASP:HA	2.00	0.43
1:A:181:TRP:NE1	1:A:185:LYS:HD2	2.34	0.43
2:B:62:ASN:HB2	2:B:99:TYR:OH	2.18	0.43
1:E:398:PRO:HA	1:E:507:TRP:CE2	2.53	0.43
1:A:348:LEU:HD13	1:A:429:LEU:HD13	2.01	0.43
1:E:354:TRP:CG	1:E:355:PRO:HD3	2.53	0.43
1:A:323:LYS:NZ	4:D:34:GLU:OE1	2.38	0.43
3:G:16:TRP:CG	3:G:57:ILE:HD13	2.53	0.43
4:H:129:MET:HE2	4:H:129:MET:HB2	1.93	0.43
1:A:94:LYS:HE2	9:B:453:HOH:O	2.18	0.43
3:C:137:GLY:O	3:C:141:MET:HB2	2.19	0.43
3:C:154:GLU:H	3:C:154:GLU:CD	2.27	0.43
2:F:315:HIS:NE2	3:G:66:SER:OG	2.43	0.43
1:E:281:TYR:CZ	1:E:285:VAL:HG21	2.53	0.43
2:F:195:MET:HE2	2:F:286:GLN:OE1	2.19	0.43
1:E:466:CYS:HB2	2:F:76:THR:HA	2.01	0.42
1:A:333:ARG:NH2	4:D:27:GLU:OE2	2.52	0.42
4:H:48:ILE:HD13	4:H:48:ILE:HA	1.92	0.42
1:A:284:PRO:HA	1:A:343:HIS:HB3	2.01	0.42
2:B:272:ALA:HB1	2:B:277:ASP:HB3	1.99	0.42
1:E:187:VAL:HG13	1:E:188:PHE:N	2.35	0.42
3:G:110:ARG:HA	3:G:110:ARG:HD2	1.87	0.42
1:A:175:ARG:HD2	1:A:181:TRP:CZ3	2.54	0.42
2:F:238:TRP:CD1	2:F:238:TRP:C	2.98	0.42
1:E:140:GLN:HG3	1:E:246:HIS:NE2	2.35	0.42
1:A:200:CYS:HA	1:A:203:ASN:OD1	2.20	0.42
4:D:129:MET:HE2	4:D:129:MET:HB2	1.84	0.42
1:E:125:TRP:CZ3	1:E:138:LEU:HD13	2.55	0.41
1:A:67:TYR:CZ	1:A:71:GLU:HG3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:MET:CE	1:E:257:ILE:HG12	2.50	0.41
2:F:47:LYS:HB2	2:F:47:LYS:HE2	1.67	0.41
1:A:89:LEU:HD21	1:E:230:GLU:HG3	2.02	0.41
3:G:60:LYS:HD3	3:G:60:LYS:HA	1.79	0.41
1:E:140:GLN:O	1:E:144:GLU:HG2	2.21	0.41
2:F:80:HIS:HB3	3:G:140:LEU:HD23	2.03	0.41
3:C:110:ARG:HD2	3:C:110:ARG:HA	1.81	0.41
4:D:68:VAL:O	4:D:78:ILE:HA	2.21	0.41
2:F:204:ALA:HB2	2:F:212:ALA:HB2	2.03	0.41
1:A:74:LYS:HE2	4:D:106:ILE:HA	2.02	0.41
1:E:12:ASP:OD2	1:E:15:LYS:N	2.47	0.41
3:G:12:ILE:HD13	9:G:208:HOH:O	2.20	0.41
1:A:25:PRO:HA	1:A:63:ILE:HD13	2.03	0.40
4:H:9:ASN:O	4:H:14:GLN:HG2	2.21	0.40
2:B:301:LEU:O	2:B:306:LEU:HG	2.21	0.40
1:E:354:TRP:CH2	1:E:499:PRO:HD3	2.55	0.40
4:H:3:SER:HB3	4:H:66:SER:HA	2.03	0.40
1:A:46:TYR:HB3	9:A:713:HOH:O	2.21	0.40
1:A:297:LYS:HD2	1:A:371:TRP:CE3	2.57	0.40
1:E:90:GLY:O	1:E:94:LYS:HD3	2.22	0.40
3:C:121:PRO:HD3	3:C:129:PHE:CG	2.57	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	513/526 (98%)	497 (97%)	16 (3%)	0	100	100
1	E	513/526 (98%)	495 (96%)	18 (4%)	0	100	100
2	B	389/395 (98%)	378 (97%)	11 (3%)	0	100	100
2	F	389/395 (98%)	375 (96%)	14 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	165/169 (98%)	160 (97%)	5 (3%)	0	100	100
3	G	165/169 (98%)	160 (97%)	5 (3%)	0	100	100
4	D	128/138 (93%)	121 (94%)	6 (5%)	1 (1%)	16	17
4	H	128/138 (93%)	121 (94%)	7 (6%)	0	100	100
All	All	2390/2456 (97%)	2307 (96%)	82 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	73	ALA

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	426/433 (98%)	419 (98%)	7 (2%)	55	70
1	E	426/433 (98%)	421 (99%)	5 (1%)	63	77
2	B	323/327 (99%)	320 (99%)	3 (1%)	70	82
2	F	323/327 (99%)	316 (98%)	7 (2%)	45	59
3	C	145/146 (99%)	144 (99%)	1 (1%)	76	86
3	G	145/146 (99%)	145 (100%)	0	100	100
4	D	103/110 (94%)	101 (98%)	2 (2%)	50	65
4	H	103/110 (94%)	101 (98%)	2 (2%)	50	65
All	All	1994/2032 (98%)	1967 (99%)	27 (1%)	59	73

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	52	MET
1	A	61	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	142	LEU
1	A	221	THR
1	A	346	LEU
1	A	442	ASN
2	B	163	PHE
2	B	176	ASP
2	B	274	VAL
3	C	141	MET
4	D	14	GLN
4	D	101	VAL
1	E	16	VAL
1	E	105	VAL
1	E	205	GLN
1	E	273	ASN
1	E	307	ARG
2	F	8	GLN
2	F	47	LYS
2	F	95	THR
2	F	156	LEU
2	F	163	PHE
2	F	176	ASP
2	F	274	VAL
4	H	12	ILE
4	H	28	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	388	ASN
2	B	88	ASN
2	B	110	HIS
1	E	156	HIS
1	E	472	GLN
1	E	486	HIS
2	F	362	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	BEZ	A	603	5	9,9,9	0.76	0	11,11,11	0.90	1 (9%)
6	BEZ	E	603	8	9,9,9	0.82	0	11,11,11	1.03	2 (18%)
7	EDO	C	201	-	3,3,3	0.49	0	2,2,2	0.24	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BEZ	A	603	5	-	0/4/4/4	0/1/1/1
6	BEZ	E	603	8	-	0/4/4/4	0/1/1/1
7	EDO	C	201	-	-	0/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	603	BEZ	O2-C-O1	-2.55	117.87	123.35
6	E	603	BEZ	O2-C-C1	2.13	120.31	114.84
6	A	603	BEZ	O2-C-C1	2.09	120.20	114.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	201	EDO	1	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	515/526 (97%)	0.70	21 (4%)	41 47	47, 60, 85, 117	0
1	E	515/526 (97%)	0.58	15 (2%)	53 60	50, 61, 81, 107	0
2	B	391/395 (98%)	0.54	11 (2%)	55 61	49, 60, 77, 105	0
2	F	391/395 (98%)	0.49	6 (1%)	72 77	52, 61, 78, 118	0
3	C	167/169 (98%)	0.45	2 (1%)	76 81	56, 67, 79, 89	0
3	G	167/169 (98%)	0.58	6 (3%)	46 52	59, 69, 83, 99	0
4	D	130/138 (94%)	0.67	6 (4%)	37 43	63, 74, 96, 118	0
4	H	130/138 (94%)	0.81	8 (6%)	26 30	57, 72, 92, 108	0
All	All	2406/2456 (97%)	0.59	75 (3%)	51 58	47, 63, 84, 118	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4	PRO	4.9
1	A	121	SER	4.3
4	H	118	LEU	3.9
2	F	4	PRO	3.8
4	H	129	MET	3.6
1	A	244	LEU	3.3
4	H	4	ALA	3.2
1	A	62	VAL	3.2
1	E	202	VAL	3.2
4	D	118	LEU	3.2
3	G	2	ALA	3.1
2	F	332	VAL	3.0
4	H	101	VAL	2.9
1	A	374	ALA	2.9
4	H	83	ALA	2.9
2	B	216	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	G	33	ILE	2.7
1	A	16	VAL	2.6
1	E	201	SER	2.6
2	B	61	PRO	2.6
1	A	282	PHE	2.5
1	E	47	PRO	2.5
1	A	220	VAL	2.5
2	B	219	LYS	2.5
4	H	57	LEU	2.5
1	A	216	LEU	2.5
2	B	84	PRO	2.5
1	E	478	LEU	2.4
4	D	130	GLY	2.4
2	B	386	VAL	2.4
3	C	162	VAL	2.4
1	A	13	ALA	2.3
1	A	274	ALA	2.3
4	D	20	PHE	2.3
1	A	265	LYS	2.3
1	A	275	PHE	2.3
3	G	165	LEU	2.3
2	B	186	ALA	2.3
3	C	2	ALA	2.3
2	F	373	ALA	2.3
1	A	180	LEU	2.2
2	F	339	VAL	2.3
1	A	102	THR	2.2
2	B	6	SER	2.2
1	E	324	TYR	2.2
1	E	507	TRP	2.2
1	A	198	VAL	2.2
1	E	12	ASP	2.2
2	B	204	ALA	2.2
1	A	41	GLU	2.2
2	B	394	LYS	2.2
2	F	394	LYS	2.2
1	A	325	GLY	2.2
1	E	406	GLN	2.2
3	G	102	ALA	2.2
1	E	32	LEU	2.1
4	H	52	ILE	2.1
1	A	105	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	197	ALA	2.1
1	E	262	ALA	2.1
4	D	131	LEU	2.1
1	A	188	PHE	2.1
4	D	80	ALA	2.1
2	F	149	ASN	2.1
1	E	305	TRP	2.1
1	E	449	THR	2.0
4	H	109	SER	2.0
1	A	171	ALA	2.0
1	E	13	ALA	2.0
2	B	297	ALA	2.0
4	D	129	MET	2.0
3	G	119	TYR	2.0
1	E	212	PHE	2.0
1	A	257	ILE	2.0
3	G	72	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 oligosaccharides 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
7	EDO	C	201	4/4	0.85	0.17	63,63,64,65	0
6	BEZ	E	603	9/9	0.92	0.13	61,63,67,69	0
6	BEZ	A	603	9/9	0.95	0.12	58,61,64,65	0
5	FE	A	602	1/1	0.99	0.03	70,70,70,70	0
8	FE2	E	601	1/1	0.99	0.03	66,66,66,66	0
8	FE2	E	602	1/1	0.99	0.02	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FE	A	601	1/1	1.00	0.01	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.