



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2020 – 10:39 PM EST

PDB ID : 6VB9
Title : Covalent adduct of cis-2,3-epoxysuccinic acid with Isocitrate Lyase-1 from Mycobacterium tuberculosis
Authors : Krieger, I.V.; Pham, T.V.; Meek, T.D.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2019-12-18
Resolution : 1.88 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 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)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
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)	:	2.16

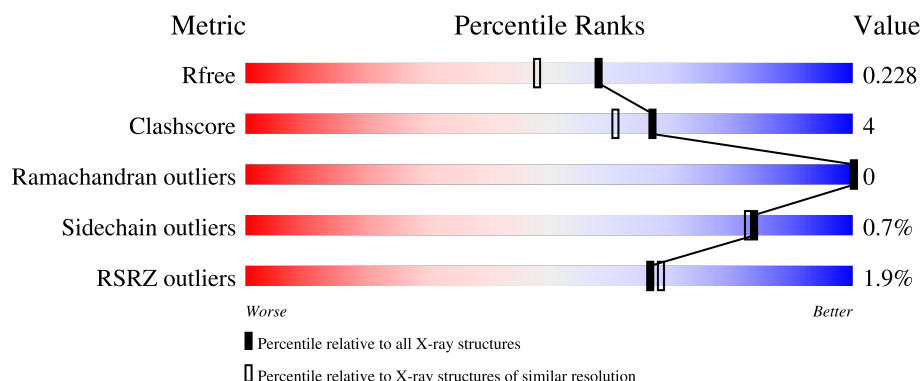
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

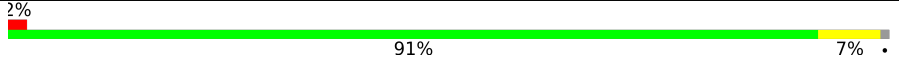
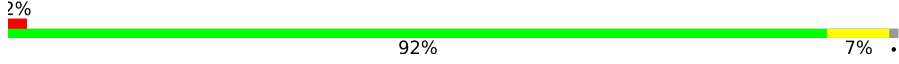
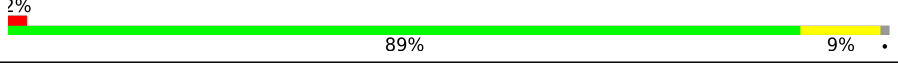
The reported resolution of this entry is 1.88 Å.

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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	431	
1	B	431	
1	C	431	
1	D	431	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACY	B	505	-	-	X	-
5	PEG	B	502[B]	-	-	X	-
5	PEG	C	503	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14419 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 Isocitrate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	4	0
			3340	2098	579	654	9			
1	B	427	Total	C	N	O	S	0	3	0
			3335	2096	579	651	9			
1	C	427	Total	C	N	O	S	0	2	0
			3333	2092	581	651	9			
1	D	427	Total	C	N	O	S	0	3	0
			3337	2096	581	651	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A045H6H0
A	-1	SER	-	expression tag	UNP A0A045H6H0
A	0	HIS	-	expression tag	UNP A0A045H6H0
B	-2	GLY	-	expression tag	UNP A0A045H6H0
B	-1	SER	-	expression tag	UNP A0A045H6H0
B	0	HIS	-	expression tag	UNP A0A045H6H0
C	-2	GLY	-	expression tag	UNP A0A045H6H0
C	-1	SER	-	expression tag	UNP A0A045H6H0
C	0	HIS	-	expression tag	UNP A0A045H6H0
D	-2	GLY	-	expression tag	UNP A0A045H6H0
D	-1	SER	-	expression tag	UNP A0A045H6H0
D	0	HIS	-	expression tag	UNP A0A045H6H0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

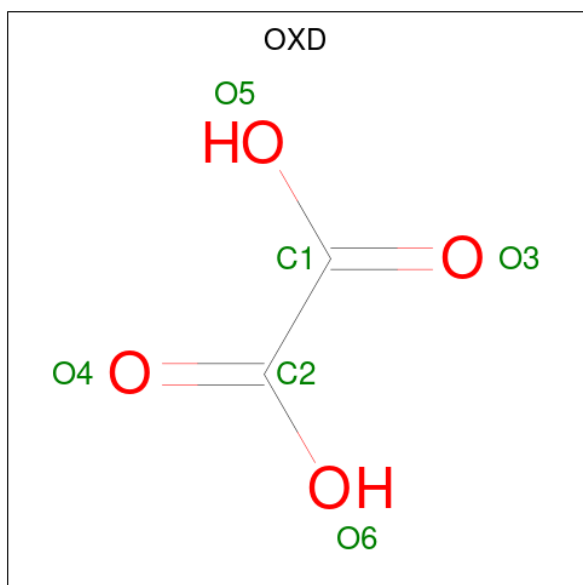
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		

- Molecule 3 is OXALIC ACID (three-letter code: OXD) (formula: $C_2H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			11	4	7		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	1
			11	4	7		
3	D	1	Total	C	O	0	1
			11	4	7		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	1
			14	8	6		
5	C	1	Total	C	O	0	0
			7	4	3		

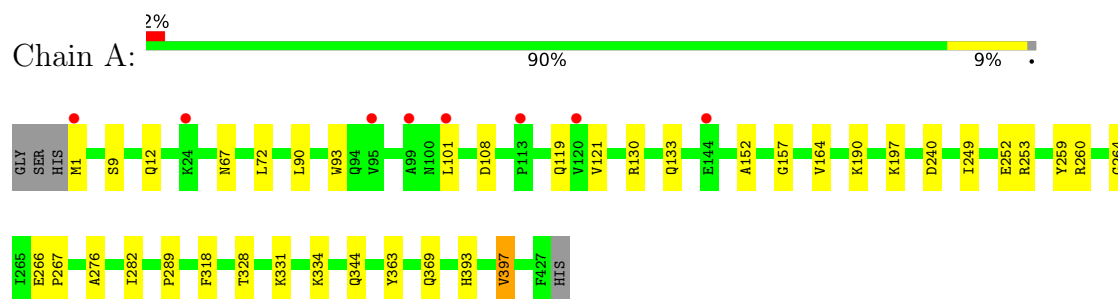
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	257	Total	O	0	0
			257	257		
6	B	249	Total	O	0	0
			249	249		
6	C	244	Total	O	0	0
			244	244		
6	D	221	Total	O	0	0
			221	221		

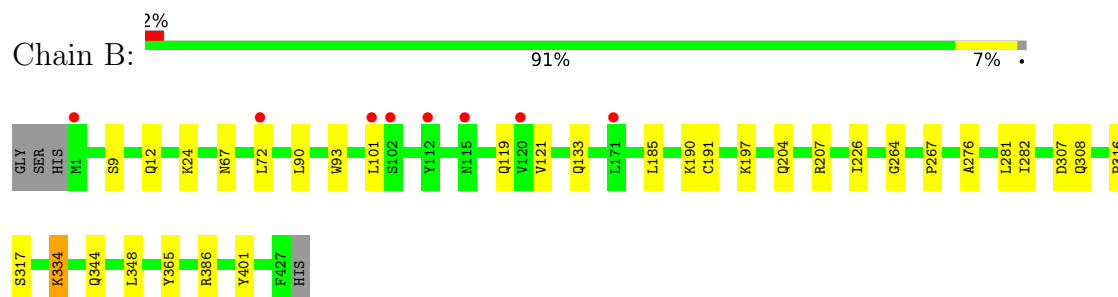
3 Residue-property plots [i](#)

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.

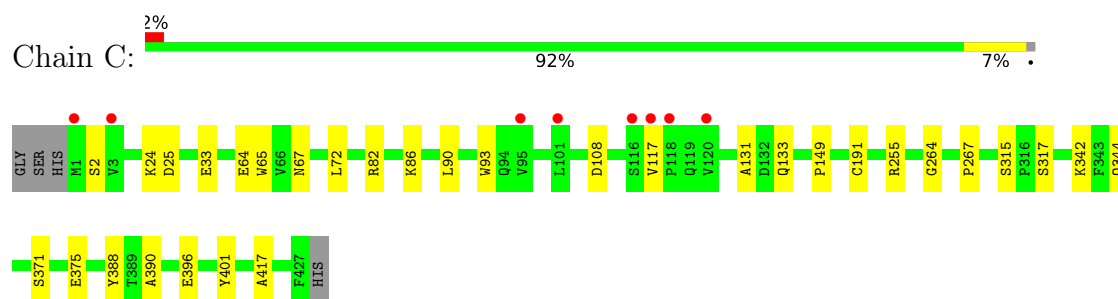
- Molecule 1: Isocitrate lyase



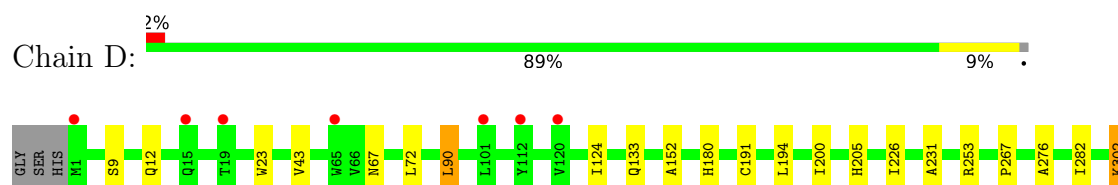
- Molecule 1: Isocitrate lyase

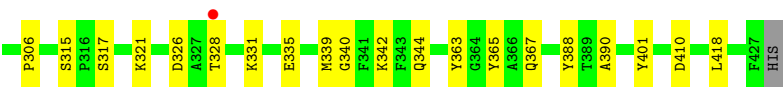


- Molecule 1: Isocitrate lyase



- Molecule 1: Isocitrate lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.06Å 129.06Å 167.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 1.88 48.94 – 1.88	Depositor EDS
% Data completeness (in resolution range)	89.9 (48.94-1.88) 90.7 (48.94-1.88)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.179 , 0.228 0.180 , 0.228	Depositor DCC
R_{free} test set	5970 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14419	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 3.09% 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: OXD, MG, PEG, QVA, ACY

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	0.42	0/3407	0.56	0/4631
1	B	0.40	0/3399	0.55	0/4619
1	C	0.41	0/3394	0.54	0/4612
1	D	0.39	0/3401	0.53	0/4622
All	All	0.40	0/13601	0.55	0/18484

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	3340	0	3219	32	0
1	B	3335	0	3220	26	0
1	C	3333	0	3211	26	0
1	D	3337	0	3220	25	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	0	0	0
3	C	11	0	0	0	0
3	D	11	0	0	0	0
4	A	8	0	6	0	0
4	B	12	0	9	4	0
4	C	4	0	3	0	0
4	D	12	0	9	2	0
5	B	14	0	19	5	0
5	C	7	0	10	7	0
6	A	257	0	0	6	0
6	B	249	0	0	2	0
6	C	244	0	0	2	0
6	D	221	0	0	1	0
All	All	14419	0	12926	103	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 (103) 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:207:ARG:HD3	4:B:505:ACY:O	1.50	1.08
1:B:204:GLN:HE22	5:B:502[B]:PEG:H22	1.39	0.88
1:C:82:ARG:HE	5:C:503:PEG:H41	1.46	0.81
1:C:24:LYS:HE3	1:C:25:ASP:HB2	1.76	0.67
1:A:334:LYS:NZ	6:A:603:HOH:O	2.26	0.65
1:C:64:GLU:HG2	1:C:65:TRP:HE3	1.61	0.65
1:C:64:GLU:HG2	1:C:65:TRP:CE3	2.31	0.65
1:A:1:MET:N	6:A:605:HOH:O	2.30	0.63
1:B:207:ARG:CD	4:B:505:ACY:O	2.38	0.63
1:A:264:GLY:HA3	6:A:607:HOH:O	2.00	0.61
1:C:82:ARG:HH21	5:C:503:PEG:H41	1.66	0.60
1:C:82:ARG:NE	5:C:503:PEG:H41	2.15	0.58
1:D:90:LEU:HD22	1:D:124:ILE:HD12	1.86	0.58
1:B:204:GLN:HE22	5:B:502[B]:PEG:C2	2.14	0.57
1:C:264:GLY:O	1:C:267:PRO:HD2	2.04	0.56
1:B:226:ILE:HG12	1:B:281:LEU:HB2	1.87	0.56
1:C:371:SER:O	1:C:375:GLU:HG3	2.07	0.55
4:B:505:ACY:H3	1:D:410:ASP:OD2	2.06	0.55
1:C:396:GLU:CD	5:C:503:PEG:H32	2.26	0.55
1:B:9:SER:OG	1:B:12:GLN:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:TYR:CZ	1:C:390:ALA:HB3	2.42	0.54
1:A:90:LEU:HD23	1:A:121:VAL:HG22	1.88	0.54
1:C:24:LYS:HE2	6:C:815:HOH:O	2.09	0.53
1:B:185:LEU:CD1	5:B:502[B]:PEG:H21	2.39	0.53
1:B:207:ARG:NH1	4:B:505:ACY:O	2.42	0.53
1:A:252:GLU:HG2	1:A:260:ARG:HB2	1.91	0.52
1:A:369:GLN:OE1	1:B:334:LYS:NZ	2.32	0.52
1:A:101:LEU:HD11	1:A:119:GLN:HG3	1.91	0.52
1:A:253:ARG:HD3	1:A:259:TYR:CE2	2.45	0.52
1:A:266:GLU:CD	1:A:266:GLU:H	2.15	0.50
1:B:67:ASN:HA	1:B:344:GLN:O	2.12	0.50
1:A:157:GLY:HA3	1:A:164:VAL:HG22	1.93	0.50
1:C:82:ARG:HE	5:C:503:PEG:C4	2.22	0.50
1:A:363:TYR:CZ	1:B:386:ARG:HG2	2.47	0.49
1:C:82:ARG:NH2	5:C:503:PEG:H41	2.27	0.49
1:C:93:TRP:CD1	1:C:108:ASP:HB2	2.47	0.49
1:A:252:GLU:OE1	6:A:601:HOH:O	2.20	0.49
1:D:363:TYR:O	1:D:367:GLN:HG2	2.13	0.49
1:C:24:LYS:HE3	1:C:25:ASP:CB	2.42	0.49
1:D:253:ARG:NH2	6:D:602:HOH:O	2.25	0.49
1:A:9:SER:OG	1:A:12:GLN:HG3	2.12	0.48
1:B:24:LYS:NZ	1:B:307:ASP:OD2	2.45	0.48
1:A:289:PRO:HD3	1:A:318:PHE:CG	2.48	0.48
1:C:90:LEU:HD22	1:C:117:VAL:HG13	1.94	0.48
1:C:255:ARG:N	1:C:255:ARG:HD2	2.29	0.48
1:D:133:GLN:HB3	1:D:401:TYR:CE1	2.48	0.48
1:A:253:ARG:HD3	1:A:259:TYR:CD2	2.49	0.48
1:D:23:TRP:HZ2	4:D:504:ACY:H2	1.79	0.47
1:C:67:ASN:HA	1:C:344:GLN:O	2.14	0.47
1:C:67:ASN:HB2	1:D:365:TYR:OH	2.13	0.47
1:D:388:TYR:CZ	1:D:390:ALA:HB3	2.50	0.47
1:A:331:LYS:NZ	6:A:604:HOH:O	2.30	0.47
1:B:90:LEU:HD23	1:B:121:VAL:HG22	1.97	0.47
1:B:191:QVA:O09	1:B:317:SER:OG	2.32	0.47
1:B:204:GLN:NE2	5:B:502[B]:PEG:H22	2.20	0.46
1:C:342:LYS:HE3	6:C:718:HOH:O	2.14	0.46
1:D:321:LYS:NZ	1:D:326:ASP:OD1	2.45	0.46
1:B:101:LEU:HD11	1:B:119:GLN:HG3	1.98	0.46
1:B:276:ALA:HA	1:B:282:ILE:HD11	1.97	0.45
1:C:33:GLU:H	1:C:33:GLU:CD	2.19	0.45
1:D:9:SER:OG	1:D:12:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ALA:HA	1:D:282:ILE:HD11	1.98	0.45
1:D:231:ALA:HB1	1:D:267:PRO:HB2	1.99	0.45
1:D:180:HIS:HB3	1:D:226:ILE:HB	1.99	0.45
1:A:190:LYS:HB2	1:A:197:LYS:HG2	1.98	0.44
1:A:252:GLU:N	6:A:601:HOH:O	2.47	0.44
1:B:133:GLN:HB3	1:B:401:TYR:CE1	2.52	0.44
1:A:264:GLY:O	1:A:267:PRO:HD2	2.17	0.44
1:A:9:SER:H	1:A:12:GLN:HE21	1.65	0.44
1:A:9:SER:H	1:A:12:GLN:NE2	2.15	0.44
1:C:315:SER:OG	1:C:317:SER:HB2	2.18	0.44
1:C:131:ALA:HB1	5:C:503:PEG:H12	2.00	0.43
1:A:328:THR:HA	1:A:331:LYS:HE2	2.00	0.43
1:B:276:ALA:O	6:B:601:HOH:O	2.21	0.43
1:A:67:ASN:HA	1:A:344:GLN:O	2.18	0.43
1:C:417:ALA:HB1	1:D:194:LEU:HD13	2.01	0.43
1:B:316:PRO:HG2	1:B:348:LEU:HB2	2.01	0.43
1:D:90:LEU:HB3	1:D:152:ALA:HA	2.00	0.43
1:D:328:THR:HA	1:D:331:LYS:HE2	2.00	0.43
1:D:43:VAL:HG21	4:D:505:ACY:H2	2.01	0.43
1:D:200:ILE:HD11	1:D:205:HIS:HB2	2.02	0.42
1:D:67:ASN:HA	1:D:344:GLN:O	2.19	0.42
1:A:130:ARG:HD3	1:A:133:GLN:OE1	2.20	0.42
1:D:340:GLY:HA2	1:D:342:LYS:HZ3	1.85	0.42
1:A:240:ASP:HB3	1:A:249:ILE:HD12	2.00	0.42
1:B:185:LEU:HD13	5:B:502[B]:PEG:H21	2.01	0.42
1:D:302:LYS:HE2	1:D:306:PRO:O	2.19	0.42
1:C:133:GLN:HB3	1:C:401:TYR:CE1	2.55	0.41
1:D:315:SER:OG	1:D:317:SER:HB2	2.20	0.41
1:B:308:GLN:NE2	6:B:601:HOH:O	2.20	0.41
1:A:252:GLU:HG3	1:A:260:ARG:HG3	2.02	0.41
1:A:67:ASN:HB2	1:B:365:TYR:OH	2.20	0.41
1:C:86:LYS:O	1:C:149:PRO:HD2	2.20	0.41
1:A:90:LEU:HB3	1:A:152:ALA:HA	2.02	0.40
1:A:93:TRP:CD1	1:A:108:ASP:HB2	2.56	0.40
1:A:393:HIS:HB2	1:B:93:TRP:CH2	2.57	0.40
1:D:335:GLU:O	1:D:339:MET:HG3	2.21	0.40
1:A:276:ALA:HA	1:A:282:ILE:HD11	2.03	0.40
1:B:190:LYS:HB2	1:B:197:LYS:HG2	2.03	0.40
1:B:264:GLY:O	1:B:267:PRO:HD2	2.20	0.40
1:D:418:LEU:HA	1:D:418:LEU:HD23	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/431 (99%)	421 (98%)	7 (2%)	0	100	100
1	B	427/431 (99%)	420 (98%)	7 (2%)	0	100	100
1	C	426/431 (99%)	416 (98%)	10 (2%)	0	100	100
1	D	427/431 (99%)	417 (98%)	10 (2%)	0	100	100
All	All	1708/1724 (99%)	1674 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	340/340 (100%)	337 (99%)	3 (1%)	78	76
1	B	339/340 (100%)	337 (99%)	2 (1%)	86	86
1	C	338/340 (99%)	336 (99%)	2 (1%)	86	86
1	D	339/340 (100%)	336 (99%)	3 (1%)	78	76
All	All	1356/1360 (100%)	1346 (99%)	10 (1%)	84	83

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	397[A]	VAL

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Mol	Chain	Res	Type
1	A	397[B]	VAL
1	B	72	LEU
1	B	334	LYS
1	C	2	SER
1	C	72	LEU
1	D	72	LEU
1	D	90	LEU
1	D	302	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	367	GLN
1	B	204	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	QVA	A	191	1	6,14,15	0.90	0	2,18,20	0.76	0
1	QVA	B	191	1	6,14,15	0.73	0	2,18,20	1.16	0
1	QVA	C	191	1	6,14,15	0.67	0	2,18,20	2.24	1 (50%)
1	QVA	D	191	1	6,14,15	0.55	0	2,18,20	1.36	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
1	QVA	A	191	1	-	1/9/19/21	-
1	QVA	B	191	1	-	1/9/19/21	-
1	QVA	C	191	1	-	1/9/19/21	-
1	QVA	D	191	1	-	1/9/19/21	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	QVA	O06-C05-C07	-3.09	103.67	111.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	191	QVA	C02-C04-SG-CB
1	B	191	QVA	C02-C04-SG-CB
1	C	191	QVA	C02-C04-SG-CB
1	D	191	QVA	C02-C04-SG-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	191	QVA	1	0
1	D	191	QVA	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 7 are monoatomic - leaving 19 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	$\# Z > 2$
3	OXD	C	504[A]	2	0,5,5	0.00	-	0,6,6	0.00	-
3	OXD	A	503[A]	2	0,5,5	0.00	-	0,6,6	0.00	-
5	PEG	B	502[A]	-	6,6,6	0.48	0	5,5,5	0.61	0
4	ACY	D	504	-	1,3,3	4.06	1 (100%)	0,3,3	0.00	-
5	PEG	C	503	-	6,6,6	0.48	0	5,5,5	0.41	0
4	ACY	B	504	-	1,3,3	3.91	1 (100%)	0,3,3	0.00	-
4	ACY	A	505	-	1,3,3	3.76	1 (100%)	0,3,3	0.00	-
5	PEG	B	502[B]	-	6,6,6	0.89	0	5,5,5	0.94	0
4	ACY	D	506	-	1,3,3	3.24	1 (100%)	0,3,3	0.00	-
3	OXD	B	503	2	0,5,5	0.00	-	0,6,6	0.00	-
4	ACY	C	505	-	1,3,3	3.38	1 (100%)	0,3,3	0.00	-
4	ACY	D	505	-	1,3,3	4.00	1 (100%)	0,3,3	0.00	-
4	ACY	B	506	-	1,3,3	3.55	1 (100%)	0,3,3	0.00	-
3	OXD	D	503[A]	2	0,5,5	0.00	-	0,6,6	0.00	-
4	ACY	A	504	-	1,3,3	2.94	1 (100%)	0,3,3	0.00	-
3	OXD	A	503[B]	2	0,5,5	0.00	-	0,6,6	0.00	-
4	ACY	B	505	-	1,3,3	3.98	1 (100%)	0,3,3	0.00	-
3	OXD	C	504[B]	2	0,5,5	0.00	-	0,6,6	0.00	-
3	OXD	D	503[B]	2	0,5,5	0.00	-	0,6,6	0.00	-

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
3	OXD	C	504[A]	2	-	0/0/4/4	-
3	OXD	A	503[A]	2	-	0/0/4/4	-
5	PEG	B	502[A]	-	-	3/4/4/4	-
5	PEG	C	503	-	-	4/4/4/4	-
5	PEG	B	502[B]	-	-	3/4/4/4	-
3	OXD	B	503	2	-	0/0/4/4	-
3	OXD	D	503[B]	2	-	0/0/4/4	-
3	OXD	D	503[A]	2	-	0/0/4/4	-
3	OXD	A	503[B]	2	-	0/0/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXD	C	504[B]	2	-	0/0/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	504	ACY	CH3-C	4.06	1.53	1.48
4	D	505	ACY	CH3-C	4.00	1.53	1.48
4	B	505	ACY	CH3-C	3.98	1.53	1.48
4	B	504	ACY	CH3-C	3.91	1.53	1.48
4	A	505	ACY	CH3-C	3.76	1.53	1.48
4	B	506	ACY	CH3-C	3.55	1.53	1.48
4	C	505	ACY	CH3-C	3.38	1.53	1.48
4	D	506	ACY	CH3-C	3.24	1.52	1.48
4	A	504	ACY	CH3-C	2.94	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	503	PEG	O2-C3-C4-O4
5	B	502[A]	PEG	O2-C3-C4-O4
5	B	502[A]	PEG	C4-C3-O2-C2
5	C	503	PEG	O1-C1-C2-O2
5	B	502[B]	PEG	O1-C1-C2-O2
5	B	502[B]	PEG	C1-C2-O2-C3
5	B	502[A]	PEG	C1-C2-O2-C3
5	B	502[B]	PEG	O2-C3-C4-O4
5	C	503	PEG	C4-C3-O2-C2
5	C	503	PEG	C1-C2-O2-C3

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	504	ACY	1	0
5	C	503	PEG	7	0
5	B	502[B]	PEG	5	0
4	D	505	ACY	1	0
4	B	505	ACY	4	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	426/431 (98%)	-0.02	8 (1%) 66 68	15, 24, 38, 62	0
1	B	426/431 (98%)	-0.07	8 (1%) 66 68	14, 25, 39, 64	0
1	C	426/431 (98%)	-0.09	8 (1%) 66 68	14, 25, 38, 63	0
1	D	426/431 (98%)	0.00	8 (1%) 66 68	15, 26, 41, 63	0
All	All	1704/1724 (98%)	-0.04	32 (1%) 66 68	14, 25, 39, 64	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.6
1	D	101	LEU	4.2
1	B	101	LEU	4.0
1	C	1	MET	3.9
1	B	1	MET	3.9
1	A	101	LEU	3.8
1	D	1	MET	3.5
1	C	101	LEU	3.3
1	B	120	VAL	3.0
1	D	328	THR	2.7
1	D	19	THR	2.6
1	A	120	VAL	2.5
1	B	102	SER	2.5
1	D	120	VAL	2.4
1	C	117	VAL	2.4
1	A	113	PRO	2.3
1	C	3	VAL	2.3
1	B	72	LEU	2.3
1	D	112	TYR	2.2
1	D	15	GLN	2.2
1	D	65	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	116	SER	2.2
1	A	99	ALA	2.2
1	C	118	PRO	2.2
1	B	115	ASN	2.1
1	B	112	TYR	2.1
1	A	95	VAL	2.1
1	C	120	VAL	2.1
1	C	95	VAL	2.0
1	A	144	GLU	2.0
1	B	171	LEU	2.0
1	A	24	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	QVA	A	191	15/16	0.96	0.09	13,20,24,25	0
1	QVA	B	191	15/16	0.96	0.09	17,22,26,26	0
1	QVA	D	191	15/16	0.96	0.09	20,25,29,30	0
1	QVA	C	191	15/16	0.97	0.07	19,23,26,28	0

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
5	PEG	B	502[B]	7/7	0.74	0.33	38,40,49,51	7
5	PEG	B	502[A]	7/7	0.74	0.33	38,40,49,51	7
4	ACY	B	505	4/4	0.76	0.30	40,42,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ACY	B	504	4/4	0.78	0.15	36,43,46,48	0
4	ACY	D	505	4/4	0.80	0.19	31,36,40,42	0
4	ACY	A	504	4/4	0.86	0.17	33,45,45,50	0
4	ACY	A	505	4/4	0.87	0.30	46,46,49,58	0
5	PEG	C	503	7/7	0.91	0.34	34,34,39,41	0
4	ACY	B	506	4/4	0.92	0.11	42,48,49,51	0
4	ACY	C	505	4/4	0.92	0.21	37,44,47,48	0
4	ACY	D	504	4/4	0.93	0.09	31,37,40,47	0
4	ACY	D	506	4/4	0.94	0.11	35,43,45,48	0
3	OXD	C	504[B]	6/6	0.96	0.10	21,23,23,24	6
3	OXD	C	504[A]	6/6	0.96	0.10	21,23,23,24	6
3	OXD	A	503[A]	6/6	0.98	0.09	17,18,20,20	6
3	OXD	B	503	6/6	0.98	0.12	21,23,24,26	1
2	MG	C	502	1/1	0.98	0.10	29,29,29,29	0
3	OXD	A	503[B]	6/6	0.98	0.09	17,18,20,20	6
2	MG	A	502	1/1	0.98	0.07	28,28,28,28	0
3	OXD	D	503[B]	6/6	0.98	0.08	23,23,23,25	6
3	OXD	D	503[A]	6/6	0.98	0.08	23,23,23,25	6
2	MG	D	501	1/1	0.98	0.04	30,30,30,30	0
2	MG	A	501	1/1	0.99	0.07	18,18,18,18	0
2	MG	D	502	1/1	0.99	0.10	24,24,24,24	0
2	MG	C	501	1/1	0.99	0.09	21,21,21,21	0
2	MG	B	501	1/1	0.99	0.12	19,19,19,19	0

6.5 Other polymers

There are no such residues in this entry.