



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:05 AM GMT

PDB ID : 3KRT  
Title : CRYSTAL STRUCTURE OF putative crotonyl CoA reductase from Streptomyces coelicolor A3(2)  
Authors : Malashkevich, V.N.; Patskovsky, Y.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYS-GXRC)  
Deposited on : 2009-11-19  
Resolution : 2.19 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](mailto: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

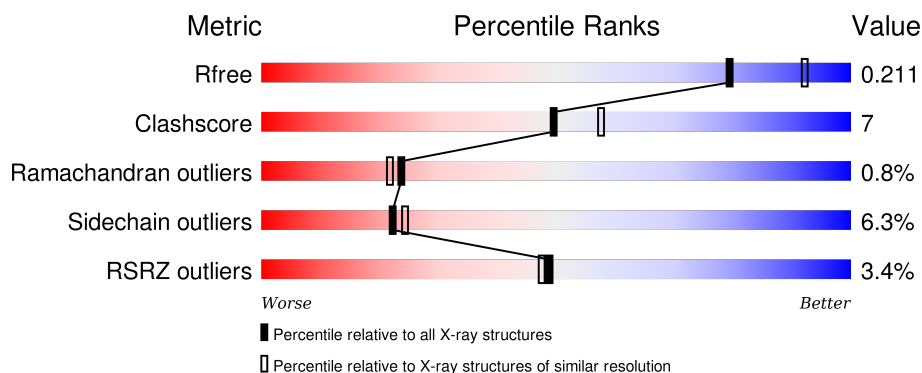
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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  $\geq 3$ , 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	456	<div> <div>4%</div> <div>81%14%..</div> </div>
1	B	456	<div> <div>2%</div> <div>83%12%..</div> </div>
1	C	456	<div> <div>5%</div> <div>82%13%..</div> </div>
1	D	456	<div> <div>2%</div> <div>81%15%..</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14270 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 Crotonyl CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3457	2165	619	660	13			
1	B	446	Total	C	N	O	S	0	0	0
			3457	2165	619	660	13			
1	C	444	Total	C	N	O	S	0	0	0
			3443	2156	617	657	13			
1	D	445	Total	C	N	O	S	0	0	0
			3451	2162	618	658	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9ZBK1
A	2	SER	-	expression tag	UNP Q9ZBK1
A	3	LEU	-	expression tag	UNP Q9ZBK1
A	88	HIS	TRP	engineered	UNP Q9ZBK1
A	449	GLU	-	expression tag	UNP Q9ZBK1
A	450	GLY	-	expression tag	UNP Q9ZBK1
A	451	HIS	-	expression tag	UNP Q9ZBK1
A	452	HIS	-	expression tag	UNP Q9ZBK1
A	453	HIS	-	expression tag	UNP Q9ZBK1
A	454	HIS	-	expression tag	UNP Q9ZBK1
A	455	HIS	-	expression tag	UNP Q9ZBK1
A	456	HIS	-	expression tag	UNP Q9ZBK1
B	1	MET	-	expression tag	UNP Q9ZBK1
B	2	SER	-	expression tag	UNP Q9ZBK1
B	3	LEU	-	expression tag	UNP Q9ZBK1
B	88	HIS	TRP	engineered	UNP Q9ZBK1
B	449	GLU	-	expression tag	UNP Q9ZBK1
B	450	GLY	-	expression tag	UNP Q9ZBK1
B	451	HIS	-	expression tag	UNP Q9ZBK1
B	452	HIS	-	expression tag	UNP Q9ZBK1
B	453	HIS	-	expression tag	UNP Q9ZBK1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	454	HIS	-	expression tag	UNP Q9ZBK1
B	455	HIS	-	expression tag	UNP Q9ZBK1
B	456	HIS	-	expression tag	UNP Q9ZBK1
C	1	MET	-	expression tag	UNP Q9ZBK1
C	2	SER	-	expression tag	UNP Q9ZBK1
C	3	LEU	-	expression tag	UNP Q9ZBK1
C	88	HIS	TRP	engineered	UNP Q9ZBK1
C	449	GLU	-	expression tag	UNP Q9ZBK1
C	450	GLY	-	expression tag	UNP Q9ZBK1
C	451	HIS	-	expression tag	UNP Q9ZBK1
C	452	HIS	-	expression tag	UNP Q9ZBK1
C	453	HIS	-	expression tag	UNP Q9ZBK1
C	454	HIS	-	expression tag	UNP Q9ZBK1
C	455	HIS	-	expression tag	UNP Q9ZBK1
C	456	HIS	-	expression tag	UNP Q9ZBK1
D	1	MET	-	expression tag	UNP Q9ZBK1
D	2	SER	-	expression tag	UNP Q9ZBK1
D	3	LEU	-	expression tag	UNP Q9ZBK1
D	88	HIS	TRP	engineered	UNP Q9ZBK1
D	449	GLU	-	expression tag	UNP Q9ZBK1
D	450	GLY	-	expression tag	UNP Q9ZBK1
D	451	HIS	-	expression tag	UNP Q9ZBK1
D	452	HIS	-	expression tag	UNP Q9ZBK1
D	453	HIS	-	expression tag	UNP Q9ZBK1
D	454	HIS	-	expression tag	UNP Q9ZBK1
D	455	HIS	-	expression tag	UNP Q9ZBK1
D	456	HIS	-	expression tag	UNP Q9ZBK1

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

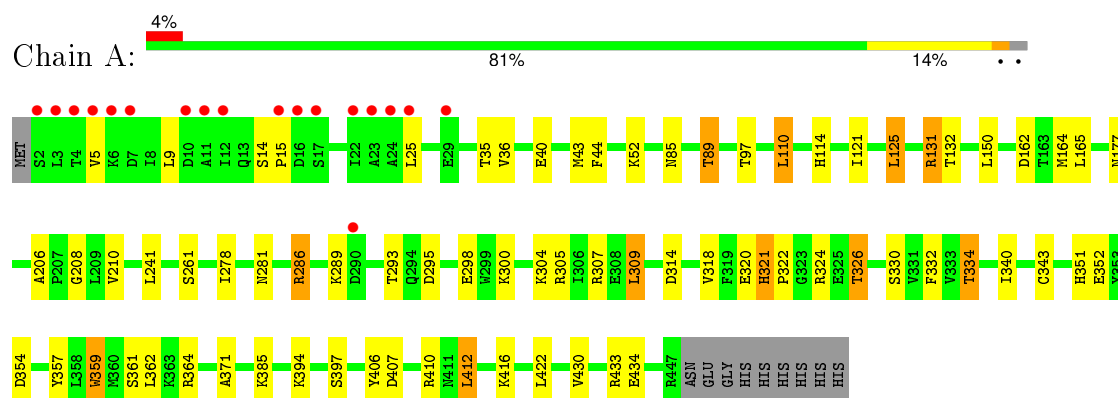
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total 124	O 124	0	0
3	B	128	Total 128	O 128	0	0
3	C	88	Total 88	O 88	0	0
3	D	118	Total 118	O 118	0	0

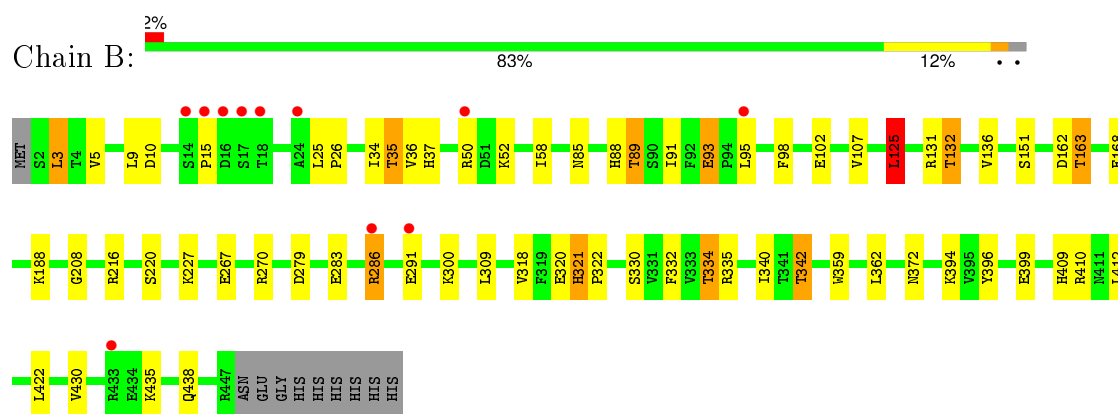
### 3 Residue-property plots

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.

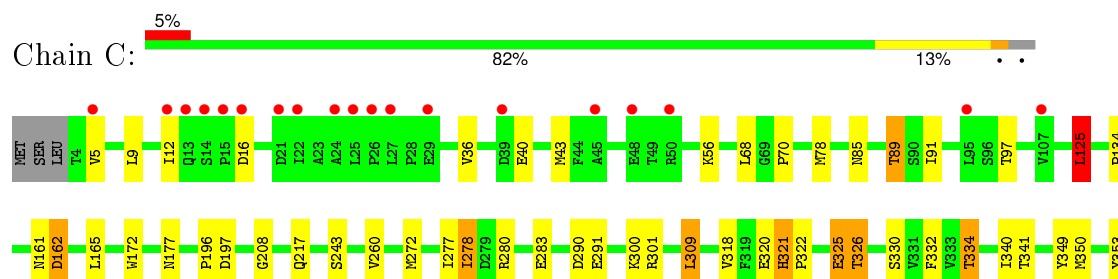
#### • Molecule 1: Crotonyl CoA reductase

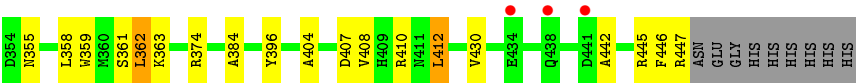


#### • Molecule 1: Crotonyl CoA reductase

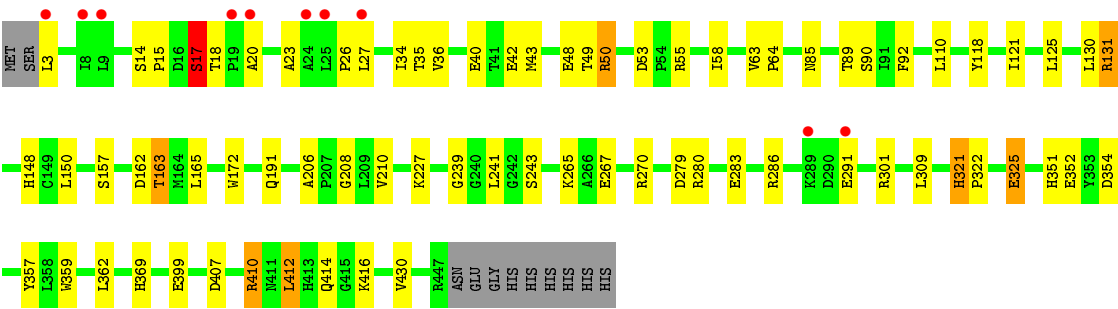
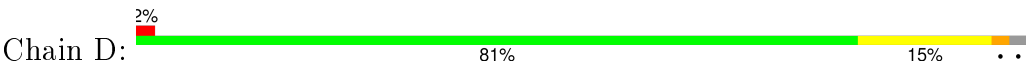


#### • Molecule 1: Crotonyl CoA reductase





● Molecule 1: Crotonyl CoA reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.53Å 117.67Å 187.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.19 39.36 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.19) 99.8 (39.36-2.19)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, $R_{free}$	0.189 , 0.238 0.169 , 0.211	Depositor DCC
$R_{free}$ test set	4742 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.2	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 94719 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14270	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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:  
CL

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	0.56	0/3535	0.69	2/4793 (0.0%)
1	B	0.58	0/3535	0.72	1/4793 (0.0%)
1	C	0.51	0/3521	0.67	2/4774 (0.0%)
1	D	0.56	0/3529	0.67	1/4785 (0.0%)
All	All	0.55	0/14120	0.69	6/19145 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	125	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	324	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	362	LEU	CA-CB-CG	-5.15	103.46	115.30
1	D	362	LEU	CA-CB-CG	-5.14	103.47	115.30
1	C	362	LEU	CA-CB-CG	-5.09	103.59	115.30
1	B	125	LEU	CA-CB-CG	5.05	126.92	115.30

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	3457	0	3364	56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3457	0	3364	41	0
1	C	3443	0	3348	54	0
1	D	3451	0	3359	47	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	124	0	0	2	0
3	B	128	0	0	3	0
3	C	88	0	0	3	0
3	D	118	0	0	1	0
All	All	14270	0	13435	194	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 7.

All (194) 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:150:LEU:HD22	1:A:164:MET:HE2	1.10	1.07
1:D:50:ARG:H	1:D:50:ARG:HD2	1.26	0.97
3:A:467:HOH:O	1:B:163:THR:HG21	1.64	0.97
3:C:469:HOH:O	1:D:163:THR:HG21	1.64	0.97
1:A:150:LEU:HD22	1:A:164:MET:CE	2.02	0.90
1:B:409:HIS:HD2	1:B:410:ARG:HH11	1.19	0.89
1:B:132:THR:HG23	1:B:136:VAL:HB	1.55	0.88
1:A:278:ILE:HD11	1:A:309:LEU:CD2	2.06	0.85
1:D:50:ARG:N	1:D:50:ARG:HD2	1.92	0.84
1:B:5:VAL:HG12	1:B:422:LEU:HD21	1.58	0.83
1:B:409:HIS:CD2	1:B:410:ARG:HH11	1.96	0.82
1:D:85:ASN:O	1:D:89:THR:HG23	1.80	0.82
1:B:409:HIS:HD2	1:B:410:ARG:NH1	1.79	0.80
1:D:58:ILE:HD11	1:D:90:SER:HB2	1.64	0.79
1:D:40:GLU:HB3	1:D:43:MET:HE2	1.63	0.79
1:C:349:TYR:CD1	1:C:350:MET:HE2	2.18	0.79
1:B:5:VAL:CG1	1:B:422:LEU:HD21	2.12	0.78
1:C:349:TYR:HD1	1:C:350:MET:HE2	1.53	0.71
1:C:320:GLU:OE2	1:C:326:THR:CG2	2.39	0.71
1:B:409:HIS:CD2	1:B:410:ARG:NH1	2.58	0.70
1:D:40:GLU:HB3	1:D:43:MET:CE	2.22	0.69
1:D:35:THR:CG2	1:D:118:TYR:HB2	2.23	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:ARG:NH2	1:D:325:GLU:OE2	2.26	0.69
1:A:40:GLU:HB3	1:A:43:MET:HE2	1.74	0.69
1:D:50:ARG:CD	1:D:50:ARG:H	1.92	0.68
1:D:35:THR:HG21	1:D:118:TYR:HB2	1.73	0.68
1:B:52:LYS:NZ	1:B:93:GLU:OE1	2.27	0.68
1:D:410:ARG:HB3	1:D:412:LEU:HD13	1.77	0.67
1:C:349:TYR:CE1	1:C:350:MET:CE	2.78	0.67
1:C:349:TYR:HE1	1:C:350:MET:HE3	1.60	0.67
1:A:114:HIS:HD2	1:A:177:ASN:H	1.41	0.66
1:C:330:SER:O	1:C:334:THR:HG22	1.95	0.66
1:C:278:ILE:N	1:C:278:ILE:HD13	2.09	0.66
1:C:349:TYR:CE1	1:C:350:MET:HE3	2.31	0.66
1:D:36:VAL:CG1	1:D:92:PHE:HE2	2.09	0.66
1:B:321:HIS:H	1:B:322:PRO:CD	2.09	0.66
1:B:3:LEU:HD13	1:B:26:PRO:HD2	1.78	0.66
1:B:286:ARG:O	1:B:286:ARG:HD2	1.96	0.65
1:C:283:GLU:O	1:C:301:ARG:NH2	2.28	0.65
1:A:114:HIS:CD2	1:A:177:ASN:H	2.14	0.65
1:D:36:VAL:CG1	1:D:92:PHE:CE2	2.80	0.64
1:C:320:GLU:OE2	1:C:326:THR:HG22	1.98	0.64
1:D:279:ASP:O	1:D:283:GLU:HG2	1.98	0.64
1:A:300:LYS:HD3	1:A:332:PHE:CZ	2.33	0.64
1:C:85:ASN:O	1:C:89:THR:HG22	1.98	0.63
1:C:278:ILE:HD11	1:C:309:LEU:HD23	1.81	0.63
1:B:342:THR:CG2	3:B:470:HOH:O	2.46	0.63
1:A:150:LEU:CD2	1:A:164:MET:HE2	2.06	0.62
1:C:361:SER:HB2	1:C:363:LYS:HE3	1.81	0.62
1:A:320:GLU:OE1	1:A:326:THR:CG2	2.48	0.61
1:D:321:HIS:H	1:D:322:PRO:CD	2.14	0.61
1:A:89:THR:HG21	3:A:549:HOH:O	2.01	0.60
1:C:321:HIS:H	1:C:322:PRO:CD	2.14	0.60
1:C:330:SER:O	1:C:334:THR:CG2	2.50	0.60
1:A:330:SER:O	1:A:334:THR:CG2	2.49	0.60
1:A:278:ILE:CD1	1:A:309:LEU:HD21	2.32	0.60
1:A:320:GLU:OE1	1:A:326:THR:HG23	2.01	0.60
1:C:349:TYR:HE1	1:C:350:MET:CE	2.15	0.59
1:B:163:THR:HG22	1:B:372:ASN:HB2	1.84	0.58
1:B:89:THR:HG21	3:B:510:HOH:O	2.02	0.58
1:C:40:GLU:HB3	1:C:43:MET:CE	2.35	0.57
1:D:125:LEU:HD23	1:D:172:TRP:CH2	2.39	0.57
1:A:278:ILE:HD11	1:A:309:LEU:HD21	1.82	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TYR:OH	1:A:410:ARG:NH2	2.38	0.57
1:A:278:ILE:HD11	1:A:309:LEU:HD22	1.87	0.57
1:C:442:ALA:HA	1:C:445:ARG:HG3	1.87	0.56
1:C:278:ILE:CD1	1:C:309:LEU:HD23	2.34	0.56
1:A:241:LEU:HD21	1:A:343:CYS:SG	2.45	0.56
1:B:163:THR:HG22	1:B:372:ASN:CB	2.36	0.56
1:B:279:ASP:O	1:B:283:GLU:HG2	2.05	0.56
1:A:40:GLU:O	1:A:43:MET:HB2	2.06	0.56
1:A:150:LEU:HD13	1:A:164:MET:HE1	1.87	0.55
1:C:334:THR:HG21	1:C:340:ILE:HG13	1.88	0.55
1:D:63:VAL:HG13	1:D:64:PRO:HD2	1.88	0.55
1:C:349:TYR:CD1	1:C:350:MET:CE	2.90	0.55
1:A:385:LYS:HD3	3:C:475:HOH:O	2.06	0.55
1:B:394:LYS:HE2	1:B:396:TYR:CZ	2.42	0.54
1:C:396:TYR:OH	1:C:407:ASP:OD2	2.25	0.54
1:A:278:ILE:HD12	1:A:305:ARG:CG	2.38	0.54
1:B:267:GLU:OE2	1:B:270:ARG:NH1	2.41	0.54
1:D:49:THR:HB	1:D:50:ARG:HH21	1.73	0.54
1:D:36:VAL:HG11	1:D:92:PHE:CE2	2.43	0.54
1:A:85:ASN:O	1:A:89:THR:HG22	2.08	0.54
1:A:125:LEU:C	1:A:125:LEU:HD12	2.28	0.54
1:C:40:GLU:HB3	1:C:43:MET:HE2	1.89	0.53
1:A:278:ILE:CD1	1:A:305:ARG:HG3	2.37	0.53
1:A:321:HIS:H	1:A:322:PRO:CD	2.20	0.53
1:A:330:SER:O	1:A:334:THR:HG22	2.07	0.53
1:D:283:GLU:O	1:D:301:ARG:NH2	2.42	0.53
1:C:91:ILE:HG22	1:C:91:ILE:O	2.09	0.53
1:B:334:THR:HG21	1:B:340:ILE:HG13	1.89	0.53
1:B:300:LYS:HG2	1:B:332:PHE:CZ	2.44	0.52
1:C:278:ILE:CD1	1:C:309:LEU:CD2	2.87	0.52
1:A:286:ARG:O	1:A:298:GLU:HG3	2.10	0.52
1:D:265:LYS:HE2	1:D:414:GLN:NE2	2.24	0.52
1:A:40:GLU:HB3	1:A:43:MET:CE	2.39	0.51
1:C:70:PRO:HA	1:C:134:PRO:HD2	1.92	0.51
1:C:358:LEU:HD12	1:C:363:LYS:HB2	1.93	0.51
1:A:85:ASN:O	1:A:89:THR:CG2	2.59	0.51
1:B:318:VAL:HG11	1:B:330:SER:HB3	1.92	0.51
1:A:278:ILE:CD1	1:A:309:LEU:CD2	2.83	0.50
1:D:354:ASP:HB3	1:D:357:TYR:HD2	1.75	0.50
1:D:14:SER:O	1:D:17:SER:OG	2.27	0.50
1:A:334:THR:HG21	1:A:340:ILE:HG13	1.92	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:MET:HE3	1:A:371:ALA:O	2.12	0.50
1:B:5:VAL:HG11	1:B:422:LEU:HD21	1.93	0.49
1:C:349:TYR:CE1	1:C:350:MET:HE2	2.45	0.49
1:A:164:MET:HE3	1:A:371:ALA:H	1.78	0.49
1:B:330:SER:O	1:B:334:THR:CG2	2.61	0.49
1:D:48:GLU:HB3	1:D:50:ARG:HG2	1.94	0.48
1:A:89:THR:HB	1:A:97:THR:HG23	1.94	0.48
1:C:85:ASN:O	1:C:89:THR:CG2	2.60	0.48
1:C:334:THR:HG21	1:C:340:ILE:CG1	2.43	0.48
1:A:289:LYS:HG3	1:A:295:ASP:HB2	1.95	0.48
1:C:277:ILE:C	1:C:278:ILE:HD13	2.35	0.48
1:D:210:VAL:HG13	1:D:241:LEU:HA	1.95	0.48
1:A:278:ILE:HD12	1:A:305:ARG:HG3	1.94	0.47
1:B:216:ARG:HA	1:B:220:SER:HB3	1.96	0.47
1:C:280:ARG:NH2	1:C:325:GLU:OE2	2.47	0.47
1:B:5:VAL:HG12	1:B:422:LEU:CD2	2.39	0.47
1:D:34:ILE:HG23	1:D:58:ILE:HG23	1.97	0.47
1:B:125:LEU:C	1:B:125:LEU:HD12	2.34	0.47
1:A:318:VAL:HG21	1:A:334:THR:HG22	1.96	0.47
1:A:351:HIS:O	1:D:352:GLU:HA	2.14	0.47
1:A:261:SER:HB2	1:A:281:ASN:ND2	2.29	0.47
1:A:354:ASP:HB3	1:A:357:TYR:HD2	1.80	0.47
1:A:164:MET:CE	1:A:371:ALA:O	2.63	0.47
1:D:125:LEU:HD12	1:D:125:LEU:C	2.35	0.47
1:B:85:ASN:O	1:B:89:THR:HG23	2.15	0.46
1:A:44:PHE:HB3	1:A:52:LYS:HG2	1.98	0.46
1:A:206:ALA:O	1:A:416:LYS:HE2	2.15	0.46
1:C:125:LEU:C	1:C:125:LEU:HD12	2.35	0.46
1:B:35:THR:CG2	1:B:37:HIS:CD2	2.98	0.46
1:C:318:VAL:HG11	1:C:330:SER:HB3	1.97	0.46
1:C:320:GLU:OE2	1:C:326:THR:HG23	2.16	0.46
1:C:353:TYR:HE1	1:C:355:ASN:HD22	1.63	0.46
1:D:267:GLU:OE2	1:D:270:ARG:NH1	2.45	0.46
1:D:321:HIS:N	1:D:322:PRO:CD	2.79	0.46
1:D:239:GLY:O	1:D:243:SER:HB3	2.15	0.46
1:C:197:ASP:HB2	3:C:515:HOH:O	2.14	0.46
1:D:18:THR:HG22	1:D:20:ALA:N	2.31	0.46
1:C:89:THR:HB	1:C:97:THR:HG21	1.98	0.45
1:D:3:LEU:HD22	1:D:26:PRO:HD2	1.97	0.45
1:B:5:VAL:CG1	1:B:422:LEU:HD11	2.46	0.45
1:B:227:LYS:HE3	1:B:227:LYS:HB3	1.66	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:VAL:HG13	1:D:92:PHE:CE2	2.52	0.45
1:C:196:PRO:HB3	1:C:384:ALA:HA	1.97	0.45
1:D:53:ASP:OD1	1:D:55:ARG:HB2	2.16	0.45
1:B:98:PHE:O	1:B:102:GLU:HG3	2.17	0.45
1:C:290:ASP:OD2	1:C:290:ASP:C	2.55	0.44
1:B:321:HIS:N	1:B:322:PRO:CD	2.78	0.44
1:C:300:LYS:HG2	1:C:332:PHE:CZ	2.52	0.44
1:B:151:SER:OG	1:B:188:LYS:HE3	2.17	0.44
1:A:89:THR:HB	1:A:97:THR:CG2	2.47	0.43
1:C:243:SER:HB2	1:C:272:MET:HE1	1.99	0.43
1:C:272:MET:HE3	1:C:446:PHE:HE1	1.82	0.43
1:D:14:SER:HA	1:D:15:PRO:HD3	1.79	0.43
1:C:217:GLN:HG2	1:C:341:THR:HG23	2.01	0.43
1:C:278:ILE:HD12	1:C:309:LEU:CD2	2.48	0.43
1:A:14:SER:HA	1:A:15:PRO:HD3	1.83	0.43
1:C:125:LEU:HD23	1:C:172:TRP:CH2	2.53	0.43
1:B:399:GLU:HG3	3:B:509:HOH:O	2.19	0.43
1:D:23:ALA:O	1:D:131:ARG:NH1	2.52	0.43
1:C:161:ASN:O	1:C:162:ASP:HB2	2.19	0.43
1:D:35:THR:HG22	1:D:36:VAL:N	2.33	0.43
1:A:307:ARG:NH2	1:A:314:ASP:OD1	2.52	0.43
1:D:15:PRO:HD2	3:D:572:HOH:O	2.18	0.42
1:A:25:LEU:O	1:A:131:ARG:NH2	2.53	0.42
1:D:407:ASP:HA	1:D:412:LEU:HD22	2.01	0.42
1:A:278:ILE:HD11	1:A:305:ARG:HG3	2.01	0.42
1:D:148:HIS:CE1	1:D:150:LEU:HB3	2.55	0.42
1:A:210:VAL:HG13	1:A:241:LEU:HA	2.01	0.42
1:C:161:ASN:O	1:C:162:ASP:CB	2.68	0.42
1:B:34:ILE:HG23	1:B:58:ILE:HG23	2.01	0.42
1:B:330:SER:O	1:B:334:THR:HG23	2.20	0.41
1:A:407:ASP:HA	1:A:412:LEU:HD22	2.02	0.41
1:A:304:LYS:HA	1:A:304:LYS:HD2	1.87	0.41
1:A:352:GLU:HA	1:D:351:HIS:O	2.20	0.41
1:B:85:ASN:O	1:B:89:THR:CG2	2.69	0.41
1:A:5:VAL:HG11	1:A:422:LEU:HD21	2.02	0.41
1:C:410:ARG:HB3	1:C:412:LEU:HD13	2.03	0.41
1:C:260:VAL:O	1:C:280:ARG:HG2	2.21	0.41
1:C:12:ILE:HD13	1:C:78:MET:HE2	2.03	0.41
1:B:5:VAL:HG13	1:B:422:LEU:HD11	2.03	0.41
1:A:110:LEU:HD12	1:A:110:LEU:HA	1.96	0.40
1:C:404:ALA:O	1:C:408:VAL:HG23	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:LYS:O	1:B:438:GLN:HB3	2.22	0.40
1:D:148:HIS:CD2	1:D:191:GLN:HA	2.56	0.40
1:A:357:TYR:O	1:A:361:SER:HB2	2.22	0.40
1:B:88:HIS:O	1:B:91:ILE:O	2.39	0.40
1:C:321:HIS:N	1:C:322:PRO:CD	2.83	0.40
1:A:359:TRP:O	1:D:369:HIS:HB2	2.22	0.40
1:D:206:ALA:O	1:D:416:LYS:HE2	2.21	0.40
1:C:374:ARG:HB2	1:D:157:SER:O	2.21	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	444/456 (97%)	430 (97%)	11 (2%)	3 (1%)	26	25
1	B	444/456 (97%)	427 (96%)	13 (3%)	4 (1%)	21	19
1	C	442/456 (97%)	428 (97%)	11 (2%)	3 (1%)	26	25
1	D	443/456 (97%)	423 (96%)	16 (4%)	4 (1%)	21	19
All	All	1773/1824 (97%)	1708 (96%)	51 (3%)	14 (1%)	24	22

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ASP
1	A	321	HIS
1	B	321	HIS
1	C	162	ASP
1	C	208	GLY
1	C	321	HIS
1	D	162	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	321	HIS
1	A	208	GLY
1	B	162	ASP
1	B	208	GLY
1	D	208	GLY
1	D	17	SER
1	B	15	PRO

### 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	363/372 (98%)	340 (94%)	23 (6%)	22	24
1	B	363/372 (98%)	336 (93%)	27 (7%)	17	17
1	C	361/372 (97%)	340 (94%)	21 (6%)	25	28
1	D	362/372 (97%)	342 (94%)	20 (6%)	27	30
All	All	1449/1488 (97%)	1358 (94%)	91 (6%)	22	24

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	35	THR
1	A	36	VAL
1	A	89	THR
1	A	110	LEU
1	A	121	ILE
1	A	125	LEU
1	A	131	ARG
1	A	132	THR
1	A	165	LEU
1	A	286	ARG
1	A	293	THR
1	A	309	LEU
1	A	326	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	334	THR
1	A	359	TRP
1	A	364	ARG
1	A	394	LYS
1	A	397	SER
1	A	412	LEU
1	A	430	VAL
1	A	433	ARG
1	A	434	GLU
1	B	3	LEU
1	B	9	LEU
1	B	10	ASP
1	B	25	LEU
1	B	35	THR
1	B	36	VAL
1	B	50	ARG
1	B	89	THR
1	B	93	GLU
1	B	95	LEU
1	B	107	VAL
1	B	125	LEU
1	B	131	ARG
1	B	132	THR
1	B	163	THR
1	B	168	GLU
1	B	286	ARG
1	B	291	GLU
1	B	309	LEU
1	B	320	GLU
1	B	334	THR
1	B	335	ARG
1	B	342	THR
1	B	359	TRP
1	B	362	LEU
1	B	412	LEU
1	B	430	VAL
1	C	5	VAL
1	C	9	LEU
1	C	16	ASP
1	C	36	VAL
1	C	56	LYS
1	C	68	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	89	THR
1	C	125	LEU
1	C	165	LEU
1	C	177	ASN
1	C	278	ILE
1	C	291	GLU
1	C	309	LEU
1	C	325	GLU
1	C	326	THR
1	C	334	THR
1	C	359	TRP
1	C	362	LEU
1	C	412	LEU
1	C	430	VAL
1	C	447	ARG
1	D	17	SER
1	D	27	LEU
1	D	42	GLU
1	D	50	ARG
1	D	110	LEU
1	D	121	ILE
1	D	130	LEU
1	D	131	ARG
1	D	163	THR
1	D	165	LEU
1	D	227	LYS
1	D	286	ARG
1	D	291	GLU
1	D	309	LEU
1	D	325	GLU
1	D	359	TRP
1	D	399	GLU
1	D	410	ARG
1	D	412	LEU
1	D	430	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	140	GLN
1	A	414	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	444	ASN
1	B	228	GLN
1	B	409	HIS
1	B	414	GLN
1	C	198	HIS
1	C	355	ASN
1	C	389	HIS
1	C	414	GLN
1	D	355	ASN
1	D	414	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	446/456 (97%)	0.06	18 (4%) 42 41	19, 29, 50, 69	0
1	B	446/456 (97%)	-0.05	11 (2%) 61 60	18, 27, 48, 70	0
1	C	444/456 (97%)	0.27	22 (4%) 32 32	19, 33, 56, 72	0
1	D	445/456 (97%)	-0.02	10 (2%) 65 64	18, 28, 61, 71	0
All	All	1781/1824 (97%)	0.07	61 (3%) 49 47	18, 29, 53, 72	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	6.4
1	C	15	PRO	5.9
1	D	20	ALA	5.5
1	C	45	ALA	5.3
1	A	3	LEU	4.6
1	D	27	LEU	4.5
1	B	16	ASP	4.3
1	C	27	LEU	4.3
1	C	25	LEU	4.2
1	D	19	PRO	4.0
1	B	15	PRO	3.8
1	C	12	ILE	3.8
1	D	9	LEU	3.7
1	B	95	LEU	3.7
1	C	24	ALA	3.6
1	C	26	PRO	3.5
1	A	16	ASP	3.5
1	A	15	PRO	3.4
1	D	24	ALA	3.4
1	C	16	ASP	3.2
1	C	438	GLN	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	6	LYS	3.0
1	C	50	ARG	3.0
1	B	24	ALA	3.0
1	A	12	ILE	2.9
1	A	17	SER	2.8
1	D	25	LEU	2.8
1	A	10	ASP	2.8
1	B	286	ARG	2.7
1	A	23	ALA	2.7
1	B	291	GLU	2.6
1	B	17	SER	2.6
1	B	433	ARG	2.6
1	C	21	ASP	2.6
1	A	5	VAL	2.5
1	D	291	GLU	2.5
1	C	14	SER	2.5
1	C	107	VAL	2.4
1	C	29	GLU	2.4
1	C	95	LEU	2.4
1	B	18	THR	2.4
1	B	14	SER	2.4
1	A	29	GLU	2.3
1	A	22	ILE	2.3
1	C	434	GLU	2.3
1	C	441	ASP	2.2
1	A	11	ALA	2.2
1	C	48	GLU	2.2
1	D	289	LYS	2.2
1	C	5	VAL	2.2
1	A	290	ASP	2.1
1	A	24	ALA	2.1
1	A	25	LEU	2.1
1	B	50	ARG	2.1
1	A	7	ASP	2.1
1	C	22	ILE	2.1
1	C	39	ASP	2.1
1	A	4	THR	2.1
1	C	13	GLN	2.1
1	D	8	ILE	2.1
1	D	3	LEU	2.1

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	CL	D	501	1/1	0.97	0.09	-1.42	30,30,30,30	0
2	CL	C	501	1/1	0.98	0.07	-1.68	34,34,34,34	0
2	CL	B	501	1/1	0.99	0.06	-2.67	35,35,35,35	0
2	CL	A	501	1/1	0.97	0.06	-3.06	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.