Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 05:56 pm GMT

PDB ID	:	2V8V
Title	:	Crystal structure of mutant R322A of beta-alanine synthase from Saccharomyces kluyveri
Authors	:	Lundgren, S.; Andersen, B.; Piskur, J.; Dobritzsch, D.
Deposited on	:	2007-08-15
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 2.90 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.
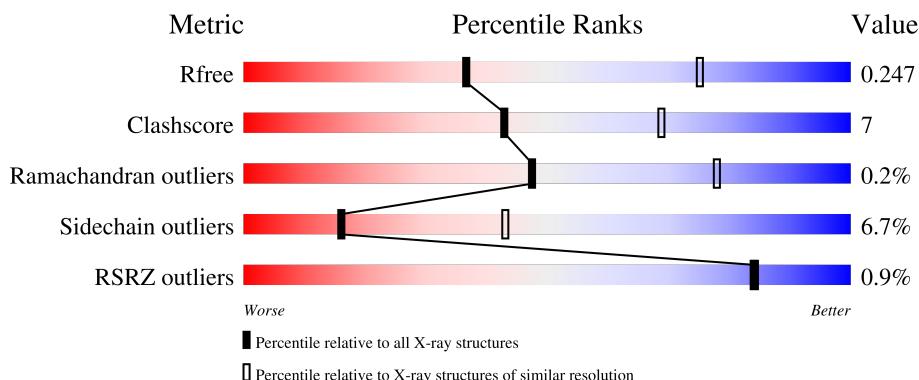
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	474	74% 16% • 8%
1	B	474	.% 74% 15% • 9%
1	C	474	2% 76% 14% • 9%
1	D	474	77% 13% • 8%
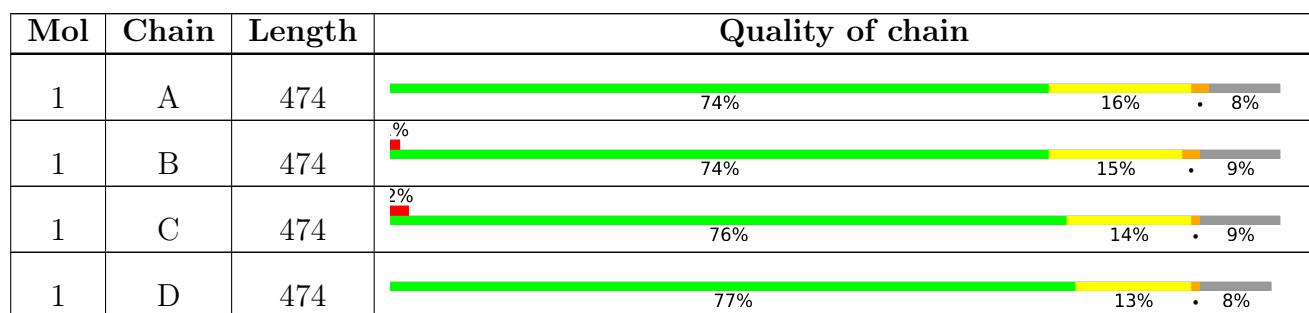
2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 13410 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 BETA-ALANINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total 3360	C 2120	N 575	O 649	S 16	0	1	0
1	B	431	Total 3324	C 2097	N 567	O 644	S 16	0	0	0
1	C	431	Total 3324	C 2097	N 567	O 644	S 16	0	0	0
1	D	435	Total 3355	C 2117	N 572	O 650	S 16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	322	ALA	ARG	engineered mutation	UNP Q96W94
B	322	ALA	ARG	engineered mutation	UNP Q96W94
C	322	ALA	ARG	engineered mutation	UNP Q96W94
D	322	ALA	ARG	engineered mutation	UNP Q96W94

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is N-(AMINOCARBONYL)-BETA-ALANINE (three-letter code: URP) (formula: $C_4H_8N_2O_3$).

URP
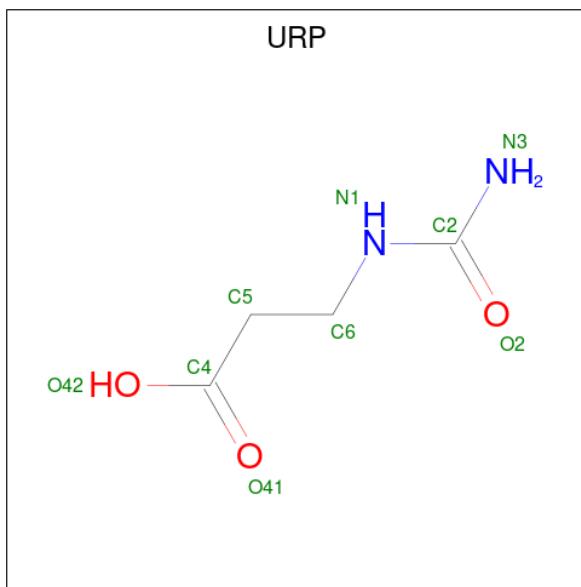
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 9	C 4	N 2	O 3	0	0
3	C	1	Total 9	C 4	N 2	O 3	0	0
3	D	1	Total 9	C 4	N 2	O 3	0	0

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).

DTT
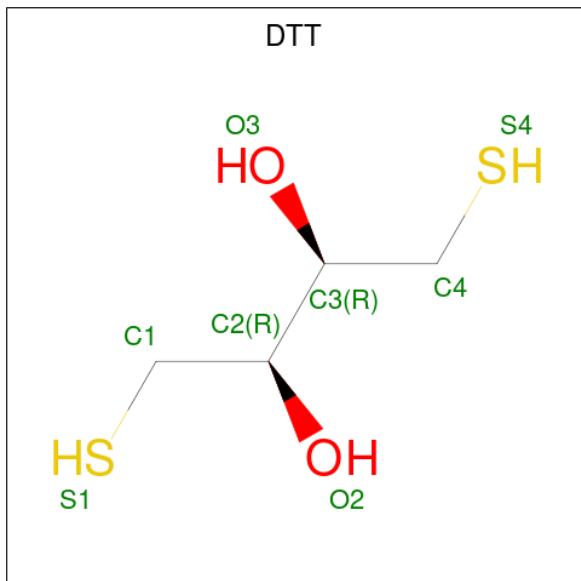
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total 8	C 4	O 2	S 2	0	0

- Molecule 5 is water.

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

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: BETA-ALANINE SYNTHASE

Chain A:

• Molecule 1: BETA-ALANINE SYNTHASE

Chain B:

• Molecule 1: BETA-ALANINE SYNTHASE

Chain C:

E181 G190 E191 D192 K193 S196 T210 H222 F223 E224 P231 N250 V259 R271 K272 M277 N293 A303 Y306 I311 V315 S316 F317 T318 L319 D320 F321 A322 H323 P324 S325 M332 L333 K334 L352 E357 V361 S362 F367 H368 E369

V370 C371 I372 E373 S376 R377 D386 R389 Q390 A395 G396 T402 A403 V406 P407 T408 S409 M410 D417 G418 L419 N422 Y423 E430 E433 I452 R453 GLY HIS GLN PHE PRO GLY ASP ASP ASP LYS HIS HIS HIS HIS HIS HIS HIS HIS SER GLY ASP

• Molecule 1: BETA-ALANINE SYNTHASE

Chain D:

77%　　　　　　　　　13%　•　8%

SER LYS ASP VAL SER SER THR ILE THR THR VAL SER ALA SER PRO ASP GLY T19 L20 N21 L22 P23 L28 E55 E58 F59 S83 K89 T111 H114 L115 D116 K123 Y124 D125 V130 L134 E135 R138 N143 N144 N158 F164 A165 R166

S172 S179 D192 T210 E216 A221 H222 F223 H226 I227 V243 V246 T266 R269 L270 R271 M277 E287 R291 H292 N293 D302 A303 K304 I311 F317 T318 L319 D327 T331 K334 E335 D348 C371 I372 S376 R377

S393 Q401 T402 A403 V406 P407 T408 S409 M410 L419 S420 E430 L440 I443 R453 GLY HIS GLN PHE PRO GLY ASP ASP ASP LYS HIS HIS HIS HIS HIS HIS HIS HIS SER GLY ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	77.48Å 84.90Å 104.85Å 67.45° 67.81° 62.75°	Depositor
Resolution (Å)	45.00 – 2.90 43.80 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (45.00-2.90) 84.6 (43.80-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.246 0.198 , 0.247	Depositor DCC
R_{free} test set	2012 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 27.9	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.430 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13410	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, URP, DTT

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	#$\vert Z \vert$ >5	RMSZ	#$\vert Z \vert$ >5
1	A	0.59	0/3440	0.69	1/4666 (0.0%)
1	B	0.53	0/3401	0.64	0/4613
1	C	0.54	0/3401	0.66	0/4613
1	D	0.59	0/3432	0.67	1/4657 (0.0%)
All	All	0.56	0/13674	0.67	2/18549 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	125	ASP	CB-CG-OD1	6.58	124.22	118.30
1	D	125	ASP	CB-CG-OD1	5.87	123.58	118.30

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	3360	0	3252	57	0
1	B	3324	0	3209	50	0
1	C	3324	0	3208	38	0
1	D	3355	0	3243	45	0
2	A	2	0	0	0	0

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W O R L D W I D E
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PROTEIN DATA BANK

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	B	9	0	7	0	0
3	C	9	0	7	2	0
3	D	9	0	7	0	0
4	C	8	0	9	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	13410	0	12942	178	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 (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:ALA:HA	1:D:408:THR:CG2	2.04	0.86
1:A:265:THR:HG21	1:B:229:GLN:O	1.77	0.84
1:A:403:ALA:HA	1:A:408:THR:HG23	1.59	0.83
1:C:57:HIS:O	1:C:123:LYS:NZ	2.12	0.82
1:D:22:LEU:HB2	1:D:23:PRO:HD2	1.64	0.77
1:B:57:HIS:O	1:B:123:LYS:NZ	2.17	0.77
1:D:22:LEU:HD23	1:D:22:LEU:H	1.48	0.76
1:C:403:ALA:HA	1:C:408:THR:CG2	2.16	0.75
1:B:403:ALA:HA	1:B:408:THR:HG23	1.69	0.75
1:D:406:VAL:O	1:D:408:THR:HG22	1.87	0.74
1:A:406:VAL:O	1:A:408:THR:HG22	1.87	0.74
1:C:403:ALA:HA	1:C:408:THR:HG23	1.68	0.74
1:A:309:ASN:HD22	1:A:309:ASN:C	1.91	0.74
1:D:291:ARG:NH2	1:D:335:GLU:OE1	2.19	0.74
1:A:266:THR:HG23	1:B:231:PRO:HG3	1.70	0.74
1:A:403:ALA:HA	1:A:408:THR:CG2	2.17	0.73
1:A:59:PHE:O	1:A:123:LYS:HE2	1.89	0.73
1:D:22:LEU:N	1:D:22:LEU:CD2	2.55	0.70
1:D:22:LEU:H	1:D:22:LEU:CD2	2.03	0.70
1:B:403:ALA:HA	1:B:408:THR:CG2	2.22	0.69
1:B:84:LEU:HD21	1:B:138:ARG:HG3	1.73	0.69
1:C:59:PHE:O	1:C:123:LYS:HE2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:ALA:HA	1:D:408:THR:HG21	1.76	0.68
1:A:28:LEU:HD12	1:A:440:LEU:HD11	1.76	0.67
1:B:309:ASN:HD22	1:B:309:ASN:H	1.42	0.67
1:C:317:PHE:HE1	1:C:319:LEU:HD21	1.59	0.67
1:D:55:GLU:HB2	1:D:58:GLU:HG3	1.77	0.66
1:B:262:HIS:HB3	1:B:265:THR:HG22	1.78	0.66
1:A:277:MET:HG3	1:A:352:LEU:HD22	1.77	0.66
1:C:395:ALA:HA	3:C:1457:URP:H51	1.79	0.64
1:C:231:PRO:HG3	1:D:266:THR:HG23	1.79	0.64
1:B:317:PHE:HE1	1:B:319:LEU:HD21	1.63	0.64
1:D:403:ALA:HA	1:D:408:THR:HG23	1.80	0.64
1:A:222:HIS:HB3	1:A:408:THR:HB	1.82	0.61
1:A:302:ASP:OD2	1:B:306:TYR:OH	2.19	0.60
1:A:135:GLU:HA	1:A:135:GLU:OE1	2.00	0.60
1:C:317:PHE:CE1	1:C:319:LEU:HD21	2.37	0.59
1:D:172:SER:HA	1:D:401:GLN:HE21	1.68	0.59
1:A:229:GLN:O	1:B:265:THR:HG21	2.03	0.59
1:A:171:SER:OG	1:A:398:ASP:OD1	2.19	0.58
1:A:371:CYS:HB2	1:A:409:SER:HB2	1.84	0.58
1:A:25:ALA:HB2	1:A:445:ASN:HD21	1.69	0.57
1:C:306:TYR:OH	1:D:302:ASP:OD2	2.21	0.57
1:C:389:ARG:HG2	1:C:390:GLN:O	2.05	0.57
1:D:28:LEU:HD12	1:D:440:LEU:HD11	1.88	0.56
1:C:406:VAL:O	1:C:408:THR:HG22	2.06	0.56
1:A:246:VAL:HG22	1:A:393:SER:HB3	1.88	0.55
1:B:371:CYS:HB3	1:B:409:SER:HB3	1.88	0.55
1:A:271:ARG:HG2	1:A:311:ILE:HD13	1.89	0.55
1:A:371:CYS:CB	1:A:409:SER:HB2	2.37	0.55
1:C:259:VAL:HG23	1:C:272:LYS:HD2	1.89	0.55
1:A:262:HIS:HB3	1:A:265:THR:HG22	1.89	0.54
1:B:252:GLN:HB2	1:B:319:LEU:HB2	1.89	0.53
1:C:373:GLU:O	1:C:377:ARG:HB2	2.08	0.53
1:B:317:PHE:CE1	1:B:319:LEU:HD21	2.43	0.53
1:C:271:ARG:HG2	1:C:311:ILE:HD13	1.91	0.53
1:D:317:PHE:CE1	1:D:319:LEU:HD21	2.44	0.53
1:D:222:HIS:HB3	1:D:408:THR:HB	1.90	0.53
1:B:371:CYS:O	1:B:375:VAL:HG23	2.09	0.52
1:B:90:VAL:O	1:B:210:THR:HG23	2.10	0.52
1:D:403:ALA:CA	1:D:408:THR:HG21	2.39	0.52
1:B:406:VAL:O	1:B:408:THR:HG22	2.10	0.52
1:B:323:HIS:ND1	1:B:324:PRO:HD2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:GLU:O	1:B:377:ARG:HB2	2.10	0.52
1:D:22:LEU:HD23	1:D:22:LEU:N	2.16	0.52
1:B:222:HIS:HB3	1:B:408:THR:HB	1.92	0.52
1:A:309:ASN:C	1:A:309:ASN:ND2	2.61	0.51
1:D:403:ALA:N	1:D:408:THR:HG21	2.25	0.51
1:A:51[B]:ARG:NH1	1:A:53:GLY:O	2.35	0.51
1:D:158:ASN:HD21	1:D:164:PHE:HB2	1.75	0.51
1:D:372:ILE:O	1:D:376:SER:HB2	2.10	0.51
1:C:181:GLU:H	1:C:181:GLU:CD	2.14	0.51
1:B:402:THR:OG1	1:B:408:THR:HG21	2.12	0.50
1:A:207:ILE:HG22	1:A:207:ILE:O	2.12	0.49
1:B:277:MET:HG3	1:B:352:LEU:HD22	1.93	0.49
1:B:181:GLU:CD	1:B:181:GLU:H	2.15	0.49
1:C:111:THR:HA	1:C:223:PHE:O	2.13	0.49
1:D:158:ASN:ND2	1:D:164:PHE:HB2	2.27	0.49
1:A:378:SER:OG	1:A:441:GLN:HB3	2.12	0.49
1:D:22:LEU:HB2	1:D:23:PRO:CD	2.37	0.49
1:A:90:VAL:O	1:A:210:THR:HG23	2.13	0.49
1:C:422:ASN:OD1	1:C:423:TYR:N	2.46	0.49
1:A:157:PHE:CE1	1:A:201:LEU:HD21	2.48	0.48
1:D:59:PHE:O	1:D:123:LYS:HE2	2.14	0.48
1:A:247:GLN:HE22	1:A:295:LEU:HD12	1.79	0.47
1:A:193:LYS:HE2	1:D:327:ASP:OD2	2.14	0.47
1:A:329:LEU:O	1:A:332:MET:HB2	2.14	0.47
1:C:222:HIS:HB3	1:C:408:THR:HB	1.96	0.47
1:D:371:CYS:HB3	1:D:409:SER:HB3	1.96	0.47
1:D:111:THR:HA	1:D:223:PHE:O	2.14	0.47
1:A:111:THR:HA	1:A:223:PHE:O	2.15	0.47
1:B:262:HIS:HB3	1:B:265:THR:CG2	2.43	0.47
1:C:127:ILE:CG2	1:C:131:LEU:HD12	2.44	0.46
1:B:107:LYS:HE3	1:B:220:ASP:OD1	2.14	0.46
1:D:348:ASP:OD2	1:D:348:ASP:N	2.49	0.46
1:A:224:GLU:OE2	1:A:399:SER:OG	2.30	0.46
1:C:323:HIS:ND1	1:C:324:PRO:HD2	2.30	0.46
1:A:263:ALA:O	1:A:271:ARG:NH2	2.48	0.46
1:A:265:THR:HG23	1:B:230:GLY:HA2	1.97	0.46
1:C:55:GLU:HB2	1:C:58:GLU:HG3	1.96	0.46
1:C:419:LEU:HD11	1:C:422:ASN:HD22	1.81	0.46
1:D:226:HIS:HD1	1:D:227:ILE:N	2.13	0.46
1:D:269:ARG:HG2	1:D:270:LEU:HG	1.97	0.46
1:B:60:GLY:HA3	1:B:423:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:GLY:H	3:C:1457:URP:C4	2.29	0.46
1:C:303:ALA:HA	1:C:315:VAL:HG22	1.97	0.46
1:C:371:CYS:HB3	1:C:409:SER:HB3	1.98	0.45
1:D:221:ALA:HB1	1:D:407:PRO:O	2.17	0.45
1:B:60:GLY:HA3	1:B:423:TYR:HD2	1.81	0.45
1:B:111:THR:HA	1:B:223:PHE:O	2.17	0.45
1:A:25:ALA:HB2	1:A:445:ASN:ND2	2.32	0.45
1:B:291:ARG:NH2	1:B:335:GLU:OE1	2.49	0.45
1:A:291:ARG:HG3	1:A:291:ARG:HH11	1.81	0.45
1:D:143:ASN:O	1:D:144:ASN:HB2	2.17	0.45
1:A:91:ASP:OD1	1:A:95:ASN:HB2	2.16	0.45
1:B:100:TYR:HA	1:B:101:PRO:HD3	1.89	0.45
1:C:259:VAL:N	1:C:272:LYS:HB2	2.31	0.44
1:C:367:PHE:HB3	1:C:408:THR:O	2.18	0.44
1:B:401:GLN:NE2	1:B:401:GLN:HA	2.31	0.44
1:D:271:ARG:HG2	1:D:311:ILE:HD13	1.99	0.44
1:D:243:VAL:HB	1:D:410:MET:HB2	2.00	0.44
1:A:90:VAL:HG22	1:A:96:MET:HG2	2.00	0.44
1:B:275:LEU:HB2	1:B:312:PRO:HG2	1.99	0.44
1:A:352:LEU:HD12	1:A:352:LEU:N	2.33	0.44
1:D:114:HIS:HB2	1:D:116:ASP:OD1	2.18	0.44
1:C:127:ILE:HG23	1:C:131:LEU:HD12	2.00	0.44
1:D:277:MET:HE2	1:D:277:MET:HB3	1.67	0.44
1:D:419:LEU:HG	1:D:420:SER:N	2.33	0.44
1:C:361:VAL:HG12	1:C:362:SER:N	2.32	0.43
1:B:55:GLU:HB2	1:B:58:GLU:HG3	2.00	0.43
1:B:301:ILE:HG13	1:B:317:PHE:HB3	2.00	0.43
1:A:339:GLU:OE1	1:A:339:GLU:HA	2.17	0.43
1:B:97:PHE:CD1	1:B:97:PHE:N	2.86	0.43
1:C:323:HIS:CG	1:C:324:PRO:HD2	2.53	0.43
1:B:197:VAL:O	1:B:201:LEU:HG	2.19	0.43
1:D:246:VAL:HG22	1:D:393:SER:HB3	2.01	0.43
1:A:198:TYR:CE2	1:D:293:ASN:HB2	2.53	0.42
1:A:262:HIS:HB3	1:A:265:THR:CG2	2.48	0.42
1:A:277:MET:HE2	1:A:277:MET:HB3	1.66	0.42
1:B:134:LEU:HD22	1:B:138:ARG:HD3	2.01	0.42
1:C:259:VAL:H	1:C:272:LYS:HB2	1.84	0.42
1:D:89:LYS:HB3	1:D:210:THR:HG21	2.00	0.42
1:C:403:ALA:N	1:C:408:THR:HG21	2.35	0.42
1:A:51[B]:ARG:HH11	1:A:51[B]:ARG:HB3	1.84	0.42
1:A:317:PHE:CE1	1:A:319:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LYS:HG2	1:B:193:LYS:O	2.19	0.42
1:A:334:LYS:HB3	1:A:334:LYS:HE2	1.79	0.42
1:A:265:THR:CG2	1:B:229:GLN:O	2.60	0.42
1:A:402:THR:OG1	1:A:408:THR:HG21	2.20	0.42
1:A:127:ILE:O	1:A:131:LEU:HB2	2.20	0.41
1:B:371:CYS:HB3	1:B:409:SER:CB	2.49	0.41
1:A:89:LYS:HB3	1:A:210:THR:HG21	2.02	0.41
1:B:180:LEU:HD11	1:B:184:TYR:CE1	2.56	0.41
1:B:193:LYS:O	1:B:193:LYS:CG	2.68	0.41
1:A:367:PHE:HB3	1:A:408:THR:O	2.20	0.41
1:C:133:GLY:O	1:C:136:VAL:HB	2.21	0.41
1:D:172:SER:HA	1:D:401:GLN:NE2	2.33	0.41
1:C:321:PHE:HD2	1:C:332:MET:HE3	1.86	0.41
1:A:420:SER:HA	1:A:425:GLU:HG3	2.02	0.41
1:B:128:LEU:HD22	1:B:413:ILE:HD11	2.02	0.41
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.88	0.41
1:A:134:LEU:HD22	1:A:138:ARG:HG3	2.03	0.41
1:A:265:THR:HG23	1:B:230:GLY:CA	2.51	0.41
1:B:118:GLN:HB2	1:B:121:ALA:HB2	2.03	0.41
1:B:137:LEU:HD11	1:B:153:VAL:HG23	2.03	0.41
1:D:22:LEU:N	1:D:22:LEU:HD22	2.32	0.41
1:D:135:GLU:HA	1:D:138:ARG:HB2	2.03	0.41
1:A:114:HIS:CE1	1:A:126:GLY:HA3	2.56	0.40
1:B:192:ASP:O	1:B:194:PRO:HD3	2.20	0.40
1:C:224:GLU:HB3	1:C:410:MET:HG2	2.02	0.40
1:A:172:SER:HA	1:A:401:GLN:HE21	1.86	0.40
1:C:372:ILE:O	1:C:376:SER:HB3	2.21	0.40
1:D:111:THR:HB	1:D:443:ILE:HD11	2.03	0.40
1:B:294:GLY:CA	1:B:323:HIS:HD2	2.34	0.40
1:C:402:THR:OG1	1:C:408:THR:HG21	2.21	0.40
1:C:277:MET:HG3	1:C:352:LEU:HD22	2.04	0.40
1:A:157:PHE:CD1	1:A:201:LEU:HD21	2.56	0.40
1:B:306:TYR:HE2	1:D:21:ASN:HD21	1.69	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	434/474 (92%)	423 (98%)	11 (2%)	0	100	100
1	B	429/474 (90%)	412 (96%)	15 (4%)	2 (0%)	29	61
1	C	429/474 (90%)	412 (96%)	16 (4%)	1 (0%)	47	78
1	D	433/474 (91%)	420 (97%)	13 (3%)	0	100	100
All	All	1725/1896 (91%)	1667 (97%)	55 (3%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	ALA
1	C	25	ALA
1	B	158	ASN

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	358/392 (91%)	331 (92%)	27 (8%)	13	37
1	B	354/392 (90%)	330 (93%)	24 (7%)	16	42
1	C	354/392 (90%)	329 (93%)	25 (7%)	14	40
1	D	358/392 (91%)	338 (94%)	20 (6%)	21	52
All	All	1424/1568 (91%)	1328 (93%)	96 (7%)	16	43

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	45	GLN
1	A	51[A]	ARG
1	A	51[B]	ARG
1	A	107	LYS
1	A	113	SER
1	A	130	VAL
1	A	134	LEU
1	A	166	ARG
1	A	188	SER
1	A	192	ASP
1	A	207	ILE
1	A	210	THR
1	A	265	THR
1	A	266	THR
1	A	287	GLU
1	A	304	LYS
1	A	307	SER
1	A	309	ASN
1	A	331	THR
1	A	334	LYS
1	A	348	ASP
1	A	356	SER
1	A	361	VAL
1	A	377	ARG
1	A	408	THR
1	A	430	GLU
1	B	54	GLN
1	B	113	SER
1	B	130	VAL
1	B	134	LEU
1	B	166	ARG
1	B	167	SER
1	B	179	SER
1	B	181	GLU
1	B	193	LYS
1	B	210	THR
1	B	228	GLU
1	B	250	ASN
1	B	265	THR
1	B	286	SER
1	B	309	ASN
1	B	334	LYS

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Mol	Chain	Res	Type
1	B	357	GLU
1	B	376	SER
1	B	377	ARG
1	B	390	GLN
1	B	408	THR
1	B	417	ASP
1	B	419	LEU
1	B	430	GLU
1	C	29	SER
1	C	54	GLN
1	C	90	VAL
1	C	113	SER
1	C	130	VAL
1	C	134	LEU
1	C	166	ARG
1	C	193	LYS
1	C	196	SER
1	C	210	THR
1	C	250	ASN
1	C	277	MET
1	C	293	ASN
1	C	325	SER
1	C	334	LYS
1	C	357	GLU
1	C	369	GLU
1	C	376	SER
1	C	377	ARG
1	C	408	THR
1	C	417	ASP
1	C	419	LEU
1	C	430	GLU
1	C	433	GLU
1	C	452	ILE
1	D	22	LEU
1	D	83	SER
1	D	130	VAL
1	D	134	LEU
1	D	166	ARG
1	D	179	SER
1	D	192	ASP
1	D	210	THR
1	D	216	GLU

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Mol	Chain	Res	Type
1	D	266	THR
1	D	269	ARG
1	D	287	GLU
1	D	304	LYS
1	D	331	THR
1	D	334	LYS
1	D	348	ASP
1	D	376	SER
1	D	377	ARG
1	D	408	THR
1	D	430	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	54	GLN
1	A	57	HIS
1	A	143	ASN
1	A	158	ASN
1	A	247	GLN
1	A	309	ASN
1	A	390	GLN
1	A	401	GLN
1	A	445	ASN
1	B	54	GLN
1	B	203	ASN
1	B	250	ASN
1	B	309	ASN
1	B	401	GLN
1	C	54	GLN
1	C	203	ASN
1	C	250	ASN
1	C	366	ASN
1	C	405	HIS
1	C	445	ASN
1	D	57	HIS
1	D	158	ASN
1	D	217	ASN
1	D	250	ASN
1	D	397	HIS
1	D	401	GLN

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Mol	Chain	Res	Type
1	D	405	HIS
1	D	445	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	URP	C	1457	-	8,8,8	1.23	1 (12%)	9,9,9	1.36	0
4	DTT	C	1456	1	7,7,7	0.38	0	4,8,8	1.28	0
3	URP	B	1456	-	8,8,8	0.94	0	9,9,9	1.14	1 (11%)
3	URP	D	1456	-	8,8,8	1.04	0	9,9,9	1.37	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	URP	C	1457	-	-	5/6/6/6	-
4	DTT	C	1456	1	-	2/8/8/8	-
3	URP	B	1456	-	-	2/6/6/6	-
3	URP	D	1456	-	-	5/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1457	URP	C5-C4	2.68	1.56	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1456	URP	O41-C4-C5	-2.27	115.80	123.08
3	D	1456	URP	N3-C2-N1	2.04	119.01	116.85

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1456	DTT	C2-C3-C4-S4
3	B	1456	URP	O2-C2-N1-C6
3	B	1456	URP	N3-C2-N1-C6
3	C	1457	URP	O2-C2-N1-C6
3	C	1457	URP	N3-C2-N1-C6
3	D	1456	URP	O2-C2-N1-C6
3	D	1456	URP	N3-C2-N1-C6
3	C	1457	URP	C4-C5-C6-N1
3	D	1456	URP	C4-C5-C6-N1
4	C	1456	DTT	O3-C3-C4-S4
3	C	1457	URP	O42-C4-C5-C6
3	C	1457	URP	O41-C4-C5-C6
3	D	1456	URP	O42-C4-C5-C6
3	D	1456	URP	O41-C4-C5-C6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1457	URP	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	435/474 (91%)	-0.36	1 (0%)	95	95	30, 36, 39, 42	0
1	B	431/474 (90%)	-0.12	4 (0%)	84	84	30, 36, 38, 42	0
1	C	431/474 (90%)	-0.11	11 (2%)	56	52	30, 36, 39, 41	0
1	D	435/474 (91%)	-0.35	0	100	100	30, 36, 39, 43	0
All	All	1732/1896 (91%)	-0.24	16 (0%)	84	84	30, 36, 39, 43	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	105	GLY	4.1
1	B	190	GLY	3.9
1	A	105	GLY	2.9
1	C	192	ASP	2.7
1	B	56	SER	2.5
1	C	24	ALA	2.5
1	C	190	GLY	2.5
1	B	50	ALA	2.4
1	C	50	ALA	2.2
1	C	56	SER	2.2
1	C	52	TRP	2.2
1	B	52	TRP	2.1
1	C	54	GLN	2.1
1	C	386	ASP	2.0
1	C	23	PRO	2.0
1	C	193	LYS	2.0

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

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

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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
3	URP	C	1457	9/9	0.90	0.31	52,56,63,64	0
4	DTT	C	1456	8/8	0.92	0.17	54,62,64,67	0
2	ZN	C	1455	1/1	0.93	0.05	36,36,36,36	0
3	URP	D	1456	9/9	0.93	0.28	75,76,77,78	0
3	URP	B	1456	9/9	0.93	0.22	46,49,50,51	0
2	ZN	A	1455	1/1	0.99	0.04	29,29,29,29	0
2	ZN	A	1456	1/1	0.99	0.03	35,35,35,35	0
2	ZN	B	1454	1/1	0.99	0.03	36,36,36,36	0
2	ZN	B	1455	1/1	0.99	0.04	38,38,38,38	0
2	ZN	C	1454	1/1	0.99	0.02	34,34,34,34	0
2	ZN	D	1454	1/1	1.00	0.05	29,29,29,29	0
2	ZN	D	1455	1/1	1.00	0.02	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.