



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 11, 2016 – 06:59 PM EDT

PDB ID : 5ERY
Title : Crystal Structure of APO MenD from M. tuberculosis - P212121
Authors : Johnston, J.M.; Jirgis, E.N.M.; Bashiri, G.; Bulloch, E.M.M.; Baker, E.N.
Deposited on : 2015-11-16
Resolution : 2.25 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
<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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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) : rb-20027790

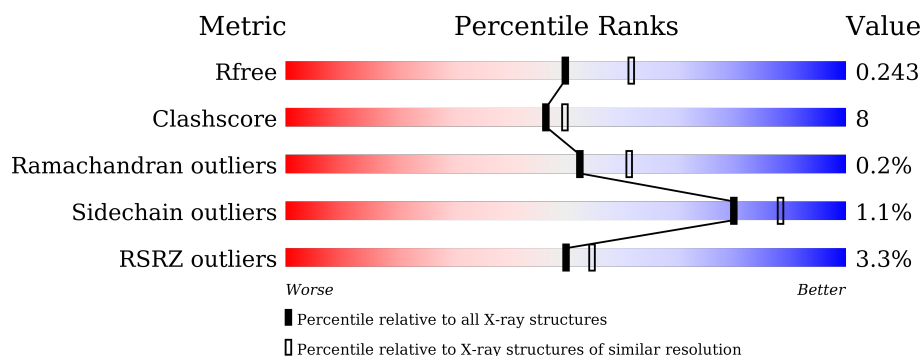
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 ≥ 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	574	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>12%</div> </div> </div>
1	B	574	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>14%</div> </div> </div>
1	C	574	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>13%</div> <div>18%</div> </div> </div>
1	D	574	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div>13%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14779 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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	3	0
			3691	2308	684	690	9			
1	D	498	Total	C	N	O	S	0	3	0
			3658	2284	682	683	9			
1	C	473	Total	C	N	O	S	0	3	0
			3478	2179	645	645	9			
1	B	496	Total	C	N	O	S	0	4	0
			3641	2276	676	680	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P9WK11
A	-18	GLY	-	expression tag	UNP P9WK11
A	-17	SER	-	expression tag	UNP P9WK11
A	-16	SER	-	expression tag	UNP P9WK11
A	-15	HIS	-	expression tag	UNP P9WK11
A	-14	HIS	-	expression tag	UNP P9WK11
A	-13	HIS	-	expression tag	UNP P9WK11
A	-12	HIS	-	expression tag	UNP P9WK11
A	-11	HIS	-	expression tag	UNP P9WK11
A	-10	HIS	-	expression tag	UNP P9WK11
A	-9	SER	-	expression tag	UNP P9WK11
A	-8	SER	-	expression tag	UNP P9WK11
A	-7	GLY	-	expression tag	UNP P9WK11
A	-6	LEU	-	expression tag	UNP P9WK11
A	-5	VAL	-	expression tag	UNP P9WK11
A	-4	PRO	-	expression tag	UNP P9WK11
A	-3	ARG	-	expression tag	UNP P9WK11
A	-2	GLY	-	expression tag	UNP P9WK11
A	-1	SER	-	expression tag	UNP P9WK11
A	0	HIS	-	expression tag	UNP P9WK11

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP P9WK11
D	-18	GLY	-	expression tag	UNP P9WK11
D	-17	SER	-	expression tag	UNP P9WK11
D	-16	SER	-	expression tag	UNP P9WK11
D	-15	HIS	-	expression tag	UNP P9WK11
D	-14	HIS	-	expression tag	UNP P9WK11
D	-13	HIS	-	expression tag	UNP P9WK11
D	-12	HIS	-	expression tag	UNP P9WK11
D	-11	HIS	-	expression tag	UNP P9WK11
D	-10	HIS	-	expression tag	UNP P9WK11
D	-9	SER	-	expression tag	UNP P9WK11
D	-8	SER	-	expression tag	UNP P9WK11
D	-7	GLY	-	expression tag	UNP P9WK11
D	-6	LEU	-	expression tag	UNP P9WK11
D	-5	VAL	-	expression tag	UNP P9WK11
D	-4	PRO	-	expression tag	UNP P9WK11
D	-3	ARG	-	expression tag	UNP P9WK11
D	-2	GLY	-	expression tag	UNP P9WK11
D	-1	SER	-	expression tag	UNP P9WK11
D	0	HIS	-	expression tag	UNP P9WK11
C	-19	MET	-	initiating methionine	UNP P9WK11
C	-18	GLY	-	expression tag	UNP P9WK11
C	-17	SER	-	expression tag	UNP P9WK11
C	-16	SER	-	expression tag	UNP P9WK11
C	-15	HIS	-	expression tag	UNP P9WK11
C	-14	HIS	-	expression tag	UNP P9WK11
C	-13	HIS	-	expression tag	UNP P9WK11
C	-12	HIS	-	expression tag	UNP P9WK11
C	-11	HIS	-	expression tag	UNP P9WK11
C	-10	HIS	-	expression tag	UNP P9WK11
C	-9	SER	-	expression tag	UNP P9WK11
C	-8	SER	-	expression tag	UNP P9WK11
C	-7	GLY	-	expression tag	UNP P9WK11
C	-6	LEU	-	expression tag	UNP P9WK11
C	-5	VAL	-	expression tag	UNP P9WK11
C	-4	PRO	-	expression tag	UNP P9WK11
C	-3	ARG	-	expression tag	UNP P9WK11
C	-2	GLY	-	expression tag	UNP P9WK11
C	-1	SER	-	expression tag	UNP P9WK11
C	0	HIS	-	expression tag	UNP P9WK11
B	-19	MET	-	initiating methionine	UNP P9WK11
B	-18	GLY	-	expression tag	UNP P9WK11

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP P9WK11
B	-16	SER	-	expression tag	UNP P9WK11
B	-15	HIS	-	expression tag	UNP P9WK11
B	-14	HIS	-	expression tag	UNP P9WK11
B	-13	HIS	-	expression tag	UNP P9WK11
B	-12	HIS	-	expression tag	UNP P9WK11
B	-11	HIS	-	expression tag	UNP P9WK11
B	-10	HIS	-	expression tag	UNP P9WK11
B	-9	SER	-	expression tag	UNP P9WK11
B	-8	SER	-	expression tag	UNP P9WK11
B	-7	GLY	-	expression tag	UNP P9WK11
B	-6	LEU	-	expression tag	UNP P9WK11
B	-5	VAL	-	expression tag	UNP P9WK11
B	-4	PRO	-	expression tag	UNP P9WK11
B	-3	ARG	-	expression tag	UNP P9WK11
B	-2	GLY	-	expression tag	UNP P9WK11
B	-1	SER	-	expression tag	UNP P9WK11
B	0	HIS	-	expression tag	UNP P9WK11

- Molecule 2 is water.

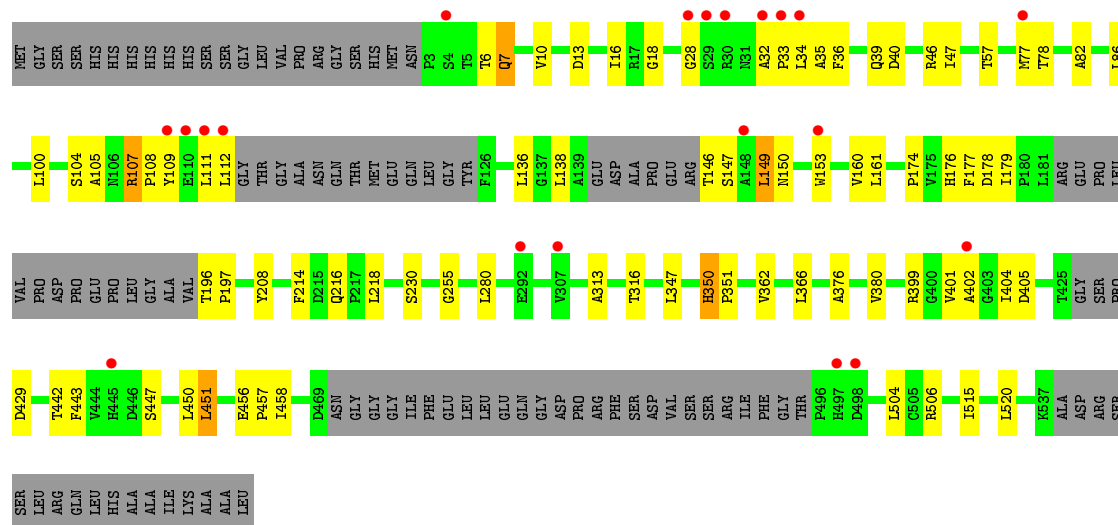
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	85	Total O 85 85	0	0
2	D	86	Total O 86 86	0	0
2	C	58	Total O 58 58	0	0
2	B	82	Total O 82 82	0	0

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.

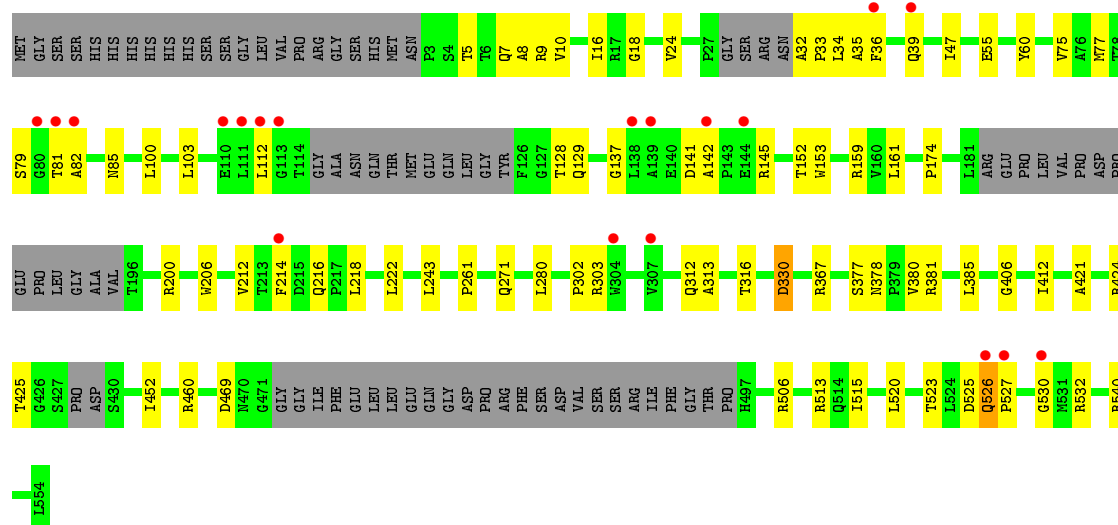
- Chain A:
-
- | Residue Type | Count |
|--------------|-------|
| Green (77%) | 10 |
| Yellow (11%) | 11 |
| Grey (12%) | 12 |
- Legend:
- | Residue | Count |
|---------|-------|
| GLU | 1 |
| LEU | 1 |
| LEU | 1 |
| GLU | 1 |
| GLN | 1 |
| GLY | 1 |
| ASP | 1 |
| PRO | 1 |
| ARG | 1 |
| PHE | 1 |
| SER | 1 |
| D487 | 1 |
| V488 | 1 |
| R491 | 1 |
| ILE | 1 |
| PHE | 1 |
| GLY | 1 |
| THR | 1 |
| P496 | 1 |
| H497 | 1 |
| D498 | 1 |
| V499 | 1 |
| G530 | 1 |
| R544 | 1 |
| H547 | 1 |
| L554 | 1 |
| L218 | 1 |
| L222 | 1 |
| L243 | 1 |
| D256 | 1 |
| P265 | 1 |
| Q270 | 1 |
| L280 | 1 |
| P283 | 1 |
| L288 | 1 |
| R303 | 1 |
| V307 | 1 |
| S308 | 1 |
| G309 | 1 |
| A313 | 1 |
| T316 | 1 |
| R325 | 1 |
| S363 | 1 |
| L366 | 1 |
| V373 | 1 |
| R391 | 1 |
| I404 | 1 |
| D405 | 1 |
| G406 | 1 |
| A421 | 1 |
| T425 | 1 |
| P428 | 1 |
| A436 | 1 |
| L441 | 1 |
| R460 | 1 |
| M470 | 1 |
| G471 | 1 |
| GLY | 1 |
| ILE | 1 |
| PRO | 1 |
| L100 | 1 |
| L103 | 1 |
| M106 | 1 |
| Y109 | 1 |
| E110 | 1 |
| L111 | 1 |
| G115 | 1 |
| ALA | 1 |
| ASN | 1 |
| GLN | 1 |
| VAL | 1 |
| PRO | 1 |
| THR | 1 |
| MET | 1 |
| GLU | 1 |
| GLN | 1 |
| SER | 1 |
| LEU | 1 |
| Y125 | 1 |
| G137 | 1 |
| L138 | 1 |
| A139 | 1 |
| GLU | 1 |
| ASP | 1 |
| ALA | 1 |
| PRO | 1 |
| GLU | 1 |
| ARG | 1 |
| T146 | 1 |
| R159 | 1 |
| P174 | 1 |
| P180 | 1 |
| L181 | 1 |
| R182 | 1 |
| GLU | 1 |
| PRO | 1 |
| LEU | 1 |
| VAL | 1 |
| PRO | 1 |
| ASP | 1 |
| PRO | 1 |
| GLU | 1 |
| PRO | 1 |
| LEU | 1 |
| GLY | 1 |
| ALA | 1 |
| VAL | 1 |
| T196 | 1 |
| V212 | 1 |
| Q216 | 1 |
| T217 | 1 |
| L218 | 1 |
| L222 | 1 |
| L243 | 1 |
| D256 | 1 |
| P265 | 1 |
| Q270 | 1 |
| L280 | 1 |
| P283 | 1 |
| L288 | 1 |
| R303 | 1 |
| V307 | 1 |
| S308 | 1 |
| G309 | 1 |
| A313 | 1 |
| T316 | 1 |
| R325 | 1 |
| S363 | 1 |
| L366 | 1 |
| V373 | 1 |
| R391 | 1 |
| I404 | 1 |
| D405 | 1 |
| G406 | 1 |
| A421 | 1 |
| T425 | 1 |
| P428 | 1 |
| A436 | 1 |
| L441 | 1 |
| R460 | 1 |
| M470 | 1 |
| G471 | 1 |
| GLY | 1 |
| ILE | 1 |
| PRO | 1 |
| L100 | 1 |
| L103 | 1 |
| M106 | 1 |
| Y109 | 1 |
| E110 | 1 |
| L111 | 1 |
| G115 | 1 |
| ALA | 1 |
| ASN | 1 |
| GLN | 1 |
| VAL | 1 |
| PRO | 1 |
| THR | 1 |
| MET | 1 |
| GLU | 1 |
| GLN | 1 |
| SER | 1 |
| LEU | 1 |
| Y125 | 1 |
| G137 | 1 |
| L138 | 1 |
| A139 | 1 |
| GLU | 1 |
| ASP | 1 |
| ALA | 1 |
| PRO | 1 |
| GLU | 1 |
| ARG | 1 |
| T146 | 1 |
| R159 | 1 |
| P174 | 1 |
| P180 | 1 |
| L181 | 1 |
| R182 | 1 |
| GLU | 1 |
| PRO | 1 |
| LEU | 1 |
| VAL | 1 |
| PRO | 1 |
| ASP | 1 |
| PRO | 1 |
| GLU | 1 |
| PRO | 1 |
| LEU | 1 |
| GLY | 1 |
| ALA | 1 |
| VAL | 1 |
| T196 | 1 |
| V212 | 1 |
| Q216 | 1 |
| T217 | 1 |

- [illegible]

- Chain C:  3% 69% 13% 18%



• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.41Å 137.28Å 164.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.25 72.35 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.70-2.25) 100.0 (72.35-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.212 , 0.246 0.208 , 0.243	Depositor DCC
R_{free} test set	5382 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14779	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.34	0/3771	0.58	0/5161
1	B	0.37	0/3722	0.59	0/5096
1	C	0.38	0/3556	0.61	2/4873 (0.0%)
1	D	0.35	0/3743	0.59	0/5126
All	All	0.36	0/14792	0.59	2/20256 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	LEU	CB-CG-CD2	-7.26	98.66	111.00
1	C	34	LEU	CA-CB-CG	5.26	127.41	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	255	GLY	Peptide

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	3691	0	3722	52	0
1	B	3641	0	3682	66	0
1	C	3478	0	3514	62	0
1	D	3658	0	3698	69	0
2	A	85	0	0	4	0
2	B	82	0	0	5	0
2	C	58	0	0	1	0
2	D	86	0	0	1	0
All	All	14779	0	14616	222	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 8.

All (222) 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:367:ARG:NH1	1:B:525:ASP:OD1	1.90	1.05
1:A:39[B]:GLN:OE1	1:A:43:ARG:NH2	2.05	0.89
1:C:36:PHE:O	1:C:39:GLN:HG2	1.74	0.87
1:B:280:LEU:O	1:B:381:ARG:NH2	2.10	0.85
1:B:142:ALA:HB1	1:B:145:ARG:HB2	1.62	0.81
1:C:108:PRO:HG2	1:C:138:LEU:HD22	1.63	0.81
1:C:32:ALA:HB3	1:C:35:ALA:HB2	1.65	0.78
1:A:7:GLN:NE2	1:A:137:GLY:O	2.17	0.77
1:B:77:MET:HE2	1:B:82:ALA:HB1	1.66	0.77
1:A:40:ASP:OD1	1:A:43:ARG:NH1	2.18	0.77
1:D:9:ARG:NH2	1:D:40:ASP:OD2	2.13	0.77
1:A:488:VAL:HG21	1:D:39:GLN:HB2	1.67	0.76
1:C:13:ASP:OD1	1:C:46:ARG:NH2	2.16	0.76
1:C:456:GLU:O	1:C:458:ILE:CD1	2.37	0.73
1:A:498:ASP:OD1	1:D:509:HIS:HD2	1.71	0.72
1:B:330:ASP:OD1	2:B:601:HOH:O	2.08	0.72
1:C:33:PRO:HB3	1:C:105:ALA:HB2	1.73	0.70
1:A:498:ASP:OD1	1:D:509:HIS:CD2	2.45	0.69
1:C:405:ASP:OD1	1:B:85:ASN:ND2	2.26	0.69
1:A:218:LEU:HD22	1:A:313:ALA:HB1	1.75	0.69
1:C:149:LEU:HD21	1:C:153:TRP:CZ2	2.28	0.69
1:B:39:GLN:OE1	1:B:39:GLN:N	2.26	0.67
1:D:214[B]:PHE:HE1	1:B:212:VAL:HG21	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:SER:HB3	1:C:112:LEU:HB2	1.77	0.66
1:D:178:ASP:O	1:D:179:ILE:HD13	1.96	0.66
1:D:469:ASP:HB2	1:D:540:ARG:HG2	1.77	0.66
1:C:32:ALA:HA	1:C:78:THR:HG22	1.76	0.66
1:D:32:ALA:H	1:D:33:PRO:HD2	1.60	0.66
1:B:424:ARG:NH1	2:B:603:HOH:O	2.29	0.65
1:C:515:ILE:HD11	1:C:520:LEU:HD12	1.77	0.65
1:D:149:LEU:HD21	1:D:153:TRP:CZ2	2.32	0.65
1:B:35:ALA:O	1:B:39:GLN:NE2	2.29	0.65
1:D:468:ASN:HB3	1:D:537:LYS:HD3	1.79	0.65
1:B:32:ALA:HB3	1:B:33:PRO:HD3	1.79	0.64
1:D:212:VAL:HG21	1:B:214[A]:PHE:CE1	2.33	0.64
1:C:146:THR:O	1:C:150:ASN:N	2.31	0.63
1:C:456:GLU:O	1:C:458:ILE:HD12	1.98	0.63
1:A:488:VAL:CG2	1:D:39:GLN:HB2	2.29	0.63
1:A:363:SER:HA	1:A:366:LEU:HD12	1.82	0.62
1:A:109:TYR:CE1	1:B:152:THR:HG21	2.35	0.62
1:A:109:TYR:OH	1:B:137:GLY:HA3	2.00	0.62
1:C:376:ALA:O	1:C:399:ARG:NH1	2.33	0.62
1:C:7:GLN:HB3	1:C:153:TRP:CH2	2.35	0.61
1:D:214[B]:PHE:CE1	1:B:212:VAL:HG21	2.36	0.61
1:B:10:VAL:HG11	1:B:153:TRP:HE3	1.65	0.61
1:C:39:GLN:HG3	1:C:40:ASP:N	2.14	0.61
1:B:7:GLN:NE2	1:B:137:GLY:O	2.34	0.61
1:A:138:LEU:HD13	1:A:180:PRO:HB2	1.83	0.60
1:D:14:GLU:HB3	1:D:157:THR:HG21	1.84	0.59
1:B:24:VAL:HB	1:B:75:VAL:HG22	1.85	0.59
1:D:77:MET:SD	1:D:86:LEU:HD12	2.43	0.58
1:A:212:VAL:HG21	1:C:214[A]:PHE:CE1	2.39	0.58
1:C:429:ASP:N	1:C:429:ASP:OD1	2.37	0.58
1:A:212:VAL:HG21	1:C:214[A]:PHE:HE1	1.69	0.57
1:A:40:ASP:O	1:A:44:SER:OG	2.21	0.57
1:A:544:ARG:NH2	1:A:547:HIS:HB2	2.19	0.57
1:A:77:MET:HB3	1:A:82:ALA:HB1	1.86	0.57
1:C:7:GLN:HB3	1:C:153:TRP:CZ2	2.40	0.57
1:C:196:THR:HB	1:C:197:PRO:HD3	1.86	0.57
1:B:367:ARG:HH12	1:B:525:ASP:CG	2.06	0.57
1:C:376:ALA:HB1	1:C:402:ALA:HA	1.87	0.57
1:B:34:LEU:HD21	1:B:103:LEU:HD13	1.86	0.57
1:B:421:ALA:O	1:B:425:THR:HG23	2.05	0.57
1:D:136:LEU:HD23	1:D:179:ILE:HD12	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLU:HG2	1:B:77:MET:CE	2.34	0.56
1:A:303:ARG:NH1	2:A:605:HOH:O	2.37	0.56
1:B:377:SER:OG	1:B:378:ASN:N	2.36	0.56
1:D:33:PRO:HA	1:D:36:PHE:CD2	2.41	0.56
1:B:302:PRO:HG2	2:B:641:HOH:O	2.05	0.56
1:C:457:PRO:C	1:C:458:ILE:HD12	2.26	0.56
1:D:200:ARG:HH12	1:B:312:GLN:HA	1.70	0.55
1:A:216:GLN:HB3	1:A:316:THR:HG23	1.87	0.55
1:D:18:GLY:HA3	1:D:161:LEU:HD13	1.88	0.55
1:B:303:ARG:NH2	2:B:602:HOH:O	2.20	0.54
1:C:36:PHE:O	1:C:39:GLN:CG	2.53	0.54
1:B:128:THR:HG23	1:B:129:GLN:HE21	1.73	0.54
1:C:6:THR:O	1:C:10:VAL:HG23	2.08	0.54
1:C:401:VAL:HG11	1:B:81:THR:HG23	1.90	0.54
1:D:494:GLY:O	1:D:495:THR:OG1	2.24	0.54
1:B:10:VAL:HG11	1:B:153:TRP:CE3	2.44	0.53
1:A:441:LEU:HD12	1:A:497[B]:HIS:CE1	2.44	0.53
1:C:107:ARG:HD3	1:C:107:ARG:N	2.24	0.53
1:A:265:PRO:HG3	1:A:283:PRO:HB3	1.91	0.53
1:C:104:SER:HG	1:C:178:ASP:CG	2.12	0.53
1:B:460:ARG:O	1:B:530:GLY:HA2	2.09	0.52
1:A:40:ASP:HA	1:A:43:ARG:NH1	2.25	0.52
1:B:222:LEU:HD22	1:B:243:LEU:HD11	1.92	0.52
1:D:32:ALA:H	1:D:33:PRO:CD	2.23	0.52
1:C:136:LEU:HD22	1:C:153:TRP:HD1	1.74	0.51
1:D:200:ARG:NH2	1:D:206:TRP:CE2	2.78	0.51
1:D:27:PRO:HD2	1:D:52:ARG:O	2.10	0.51
1:B:525:ASP:O	1:B:527:PRO:HD3	2.09	0.51
1:D:30:ARG:O	1:D:31:ASN:HB3	2.10	0.51
1:C:401:VAL:CG1	1:B:81:THR:HG23	2.40	0.51
1:C:447:SER:HB3	1:C:504:LEU:HD21	1.91	0.51
1:B:526:GLN:O	1:B:532:ARG:NH1	2.44	0.51
1:A:441:LEU:HD12	1:A:497[B]:HIS:NE2	2.26	0.51
1:B:218:LEU:HD11	1:B:313:ALA:HB1	1.92	0.51
1:D:196:THR:N	1:D:197:PRO:HD3	2.26	0.51
1:C:146:THR:OG1	1:C:147:SER:N	2.43	0.50
1:A:470:ASN:O	1:A:497[A]:HIS:HD2	1.94	0.50
1:D:54:ASP:HB3	1:D:57:THR:HB	1.94	0.50
1:D:7:GLN:HA	1:D:153:TRP:CZ3	2.47	0.50
1:A:404:ILE:HG12	2:A:628:HOH:O	2.11	0.49
1:B:18:GLY:HA3	1:B:161:LEU:HD13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:VAL:HG21	1:B:214[A]:PHE:CD1	2.46	0.49
1:B:5:THR:HG22	1:B:9:ARG:NH1	2.28	0.49
1:D:32:ALA:HB1	1:D:36:PHE:CZ	2.48	0.49
1:C:506:ARG:HH22	1:B:506:ARG:HH11	1.59	0.49
1:D:142:ALA:HB1	1:D:144:GLU:HG2	1.95	0.49
1:B:513:ARG:NH1	1:B:523:THR:HG23	2.28	0.49
1:A:544:ARG:NH1	1:A:544:ARG:O	2.46	0.48
1:C:77:MET:HB3	1:C:82:ALA:HB1	1.94	0.48
1:C:16:ILE:HG12	1:C:47:ILE:HG13	1.96	0.48
1:D:140:GLU:HB2	1:C:109:TYR:CD2	2.48	0.48
1:D:526:GLN:HB3	1:D:527:PRO:HD2	1.94	0.48
1:A:256:ASP:OD2	1:A:391:ARG:CZ	2.62	0.48
1:A:77:MET:SD	1:A:86:LEU:HD11	2.54	0.48
1:B:141:ASP:N	1:B:141:ASP:OD1	2.44	0.48
1:B:79:SER:OG	1:B:82:ALA:HB2	2.13	0.48
1:D:25:LEU:HD23	1:D:26:CYS:N	2.29	0.48
1:A:497[A]:HIS:CE1	1:A:499:VAL:H	2.31	0.47
1:A:288:LEU:HD13	1:A:307:VAL:HG21	1.97	0.47
1:D:290:ASP:O	1:D:310:ASN:ND2	2.47	0.47
1:B:280:LEU:HD11	1:B:380:VAL:HG22	1.97	0.47
1:A:313:ALA:HA	1:C:208:TYR:O	2.15	0.47
1:D:60:TYR:CG	1:D:406:GLY:HA3	2.50	0.47
1:D:513:ARG:HG3	1:D:515:ILE:HG23	1.95	0.47
1:C:451:LEU:HD23	2:C:605:HOH:O	2.15	0.47
1:D:281:HIS:HB3	1:D:283:PRO:HD2	1.96	0.47
1:A:55:GLU:HG2	1:A:77:MET:HE1	1.96	0.46
1:B:142:ALA:HB1	1:B:145:ARG:CB	2.40	0.46
1:C:176:HIS:NE2	1:C:178:ASP:OD2	2.49	0.46
1:A:470:ASN:O	1:A:497[A]:HIS:CD2	2.69	0.46
1:B:36:PHE:HA	1:B:39:GLN:OE1	2.15	0.46
1:C:401:VAL:O	1:C:401:VAL:HG12	2.15	0.46
1:B:412:ILE:HD13	1:B:452:ILE:HD11	1.97	0.46
1:D:10:VAL:HG11	1:D:150:ASN:OD1	2.15	0.46
1:A:159:ARG:HD3	1:B:112:LEU:HD11	1.97	0.46
1:D:100:LEU:O	1:D:174:PRO:HA	2.15	0.46
1:D:280:LEU:HD23	1:D:280:LEU:HA	1.71	0.46
1:D:212:VAL:HG21	1:B:214[A]:PHE:HE1	1.79	0.46
1:A:60:TYR:CG	1:A:406:GLY:HA3	2.51	0.45
1:A:460:ARG:O	1:A:530:GLY:HA2	2.16	0.45
1:B:100:LEU:O	1:B:174:PRO:HA	2.15	0.45
1:B:216:GLN:HB3	1:B:316:THR:HG23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLN:H	1:B:39:GLN:CD	2.13	0.45
1:D:492:ILE:HD11	1:D:493:PHE:CD2	2.51	0.45
1:C:32:ALA:CA	1:C:78:THR:HG22	2.46	0.45
1:B:55:GLU:HB2	1:B:85:ASN:HB3	1.98	0.45
1:D:212:VAL:HG22	1:D:213:THR:N	2.31	0.45
1:A:325:ARG:HB2	1:A:325:ARG:HE	1.59	0.44
1:A:74:CYS:HB3	1:A:103:LEU:HD12	1.99	0.44
1:A:109:TYR:CD1	1:B:152:THR:HG21	2.53	0.44
1:D:373:VAL:O	1:D:436:ALA:HA	2.17	0.44
1:A:270:GLN:HG3	2:A:669:HOH:O	2.16	0.44
1:B:39:GLN:N	1:B:39:GLN:CD	2.70	0.44
1:B:35:ALA:O	1:B:39:GLN:OE1	2.36	0.44
1:C:404:ILE:O	1:C:442:THR:HG23	2.17	0.44
1:C:28:GLY:HA3	1:C:78:THR:HB	1.99	0.44
1:D:302:PRO:HG3	2:D:623:HOH:O	2.17	0.44
1:D:537:LYS:HD3	1:D:537:LYS:HA	1.80	0.44
1:C:149:LEU:HD21	1:C:153:TRP:CH2	2.53	0.44
1:A:404:ILE:HG13	1:A:405:ASP:N	2.32	0.43
1:B:60:TYR:CG	1:B:406:GLY:HA3	2.53	0.43
1:A:222:LEU:HD22	1:A:243:LEU:HD11	2.00	0.43
1:C:136:LEU:HD12	1:C:179:ILE:HD12	2.00	0.43
1:D:10:VAL:HG13	1:D:154:ARG:NH2	2.33	0.43
1:D:440:ASP:OD2	1:D:497:HIS:NE2	2.43	0.43
1:A:441:LEU:HD11	1:D:53:ILE:HD13	2.00	0.43
1:D:6:THR:O	1:D:10:VAL:HG23	2.18	0.43
1:B:7:GLN:HG3	1:B:153:TRP:CE2	2.54	0.43
1:C:100:LEU:O	1:C:174:PRO:HA	2.17	0.43
1:C:362:VAL:O	1:C:366:LEU:HG	2.18	0.43
1:D:513:ARG:HG3	1:D:515:ILE:CG2	2.48	0.43
1:D:354:THR:HB	1:D:543:LEU:HD13	2.01	0.43
1:C:347:LEU:HD23	1:C:347:LEU:HA	1.88	0.43
1:C:280:LEU:HD11	1:C:380:VAL:HG22	2.01	0.42
1:D:418:TYR:CE2	1:D:432:PRO:HG2	2.53	0.42
1:A:404:ILE:HG23	2:A:628:HOH:O	2.19	0.42
1:B:8:ALA:HB1	1:B:34:LEU:HA	2.01	0.42
1:A:421:ALA:O	1:A:425:THR:HG23	2.19	0.42
1:B:271:GLN:NE2	2:B:604:HOH:O	2.32	0.42
1:D:3:PRO:HG2	1:D:4:SER:H	1.85	0.42
1:A:8:ALA:HB1	1:A:34:LEU:HA	2.02	0.42
1:D:200:ARG:NH1	1:D:206:TRP:O	2.53	0.42
1:A:544:ARG:NH2	1:A:547:HIS:CB	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ILE:HD11	1:B:520:LEU:HD13	2.01	0.41
1:D:3:PRO:CG	1:D:4:SER:H	2.33	0.41
1:D:5:THR:O	1:D:9:ARG:HG3	2.20	0.41
1:A:106:ASN:O	1:A:180:PRO:HA	2.19	0.41
1:A:373:VAL:O	1:A:436:ALA:HA	2.20	0.41
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.86	0.41
1:D:490:SER:OG	1:D:491:ARG:N	2.54	0.41
1:C:33:PRO:HG3	1:C:104:SER:HA	2.02	0.41
1:C:218:LEU:HD11	1:C:313:ALA:HB1	2.02	0.41
1:B:280:LEU:HD23	1:B:280:LEU:HA	1.78	0.41
1:D:156:ALA:HB2	1:C:111:LEU:HD11	2.02	0.41
1:D:136:LEU:CD2	1:D:179:ILE:HD12	2.49	0.41
1:D:350:HIS:CE1	1:D:546:LEU:HB2	2.56	0.41
1:C:160:VAL:HG21	1:C:177:PHE:CG	2.54	0.41
1:D:3:PRO:HD2	1:D:5:THR:HG23	2.03	0.41
1:C:149:LEU:HD21	1:C:153:TRP:CE2	2.55	0.41
1:D:136:LEU:HD12	1:D:136:LEU:HA	1.90	0.41
1:A:59:GLY:O	1:A:63:ILE:HG12	2.20	0.41
1:B:381:ARG:O	1:B:385:LEU:HG	2.20	0.41
1:B:200:ARG:HE	1:B:206:TRP:HA	1.85	0.41
1:D:140:GLU:HA	1:C:109:TYR:HE2	1.86	0.41
1:C:350:HIS:HA	1:C:351:PRO:HD3	1.98	0.41
1:C:216:GLN:HB3	1:C:316:THR:HG23	2.03	0.40
1:C:515:ILE:HD11	1:C:520:LEU:CD1	2.47	0.40
1:C:77:MET:HG2	1:C:86:LEU:CD1	2.51	0.40
1:D:10:VAL:HG13	1:D:154:ARG:CZ	2.51	0.40
1:D:304:TRP:O	1:B:159:ARG:NH1	2.53	0.40
1:C:108:PRO:CG	1:C:138:LEU:HD22	2.41	0.40
1:B:16:ILE:HG12	1:B:47:ILE:HG23	2.03	0.40
1:C:443:PHE:CZ	1:C:450:LEU:HD11	2.56	0.40
1:D:492:ILE:HD11	1:D:493:PHE:CE2	2.56	0.40
1:A:100:LEU:O	1:A:174:PRO:HA	2.21	0.40
1:B:469:ASP:HB2	1:B:540:ARG:HB2	2.03	0.40
1:C:18:GLY:HA3	1:C:161:LEU:HD13	2.03	0.40
1:D:419:GLU:HG2	1:D:431:PRO:HB2	2.04	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	493/574 (86%)	477 (97%)	16 (3%)	0	100	100
1	B	488/574 (85%)	473 (97%)	14 (3%)	1 (0%)	52	61
1	C	464/574 (81%)	455 (98%)	9 (2%)	0	100	100
1	D	493/574 (86%)	482 (98%)	9 (2%)	2 (0%)	39	43
All	All	1938/2296 (84%)	1887 (97%)	48 (2%)	3 (0%)	52	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	31	ASN
1	D	32	ALA
1	B	526	GLN

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	386/445 (87%)	383 (99%)	3 (1%)	86	92
1	B	381/445 (86%)	379 (100%)	2 (0%)	92	95
1	C	365/445 (82%)	359 (98%)	6 (2%)	70	81
1	D	384/445 (86%)	377 (98%)	7 (2%)	66	77
All	All	1516/1780 (85%)	1498 (99%)	18 (1%)	80	87

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	48	ARG
1	A	57	THR
1	D	57	THR
1	D	214[A]	PHE
1	D	214[B]	PHE
1	D	230	SER
1	D	282	ARG
1	D	405	ASP
1	D	537	LYS
1	C	7	GLN
1	C	57	THR
1	C	107	ARG
1	C	230	SER
1	C	350	HIS
1	C	451	LEU
1	B	261	PRO
1	B	330	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	445	HIS
1	C	445	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	504/574 (87%)	0.14	13 (2%) 59 63	28, 50, 93, 119	0
1	B	496/574 (86%)	0.18	19 (3%) 44 48	30, 52, 100, 138	0
1	C	473/574 (82%)	0.25	20 (4%) 40 44	29, 52, 100, 126	0
1	D	498/574 (86%)	0.19	13 (2%) 59 63	30, 50, 97, 137	0
All	All	1971/2296 (85%)	0.19	65 (3%) 50 55	28, 51, 98, 138	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	THR	6.7
1	B	82	ALA	6.1
1	B	80	GLY	5.4
1	D	493	PHE	5.1
1	A	111	LEU	4.9
1	C	29	SER	4.4
1	C	111	LEU	4.2
1	D	140	GLU	4.2
1	B	307	VAL	4.1
1	C	109	TYR	3.8
1	A	309	GLY	3.5
1	B	142	ALA	3.4
1	A	554	LEU	3.3
1	C	112	LEU	3.3
1	D	139	ALA	3.3
1	D	77	MET	3.2
1	A	488	VAL	3.2
1	A	498	ASP	3.2
1	A	109	TYR	3.2
1	C	307	VAL	3.2
1	B	36	PHE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	81	THR	3.1
1	C	153	TRP	3.0
1	D	528	GLY	3.0
1	C	77	MET	2.9
1	C	33	PRO	2.9
1	B	527	PRO	2.9
1	B	111	LEU	2.8
1	B	113	GLY	2.8
1	B	139	ALA	2.7
1	B	304	TRP	2.7
1	D	138	LEU	2.7
1	D	428	PRO	2.6
1	B	39	GLN	2.6
1	C	110	GLU	2.6
1	D	29	SER	2.6
1	C	28	GLY	2.6
1	D	495	THR	2.5
1	A	80	GLY	2.4
1	D	426	GLY	2.4
1	C	30	ARG	2.4
1	B	144	GLU	2.4
1	D	147	SER	2.4
1	D	80	GLY	2.4
1	C	34	LEU	2.4
1	A	125	TYR	2.3
1	B	526	GLN	2.3
1	C	148	ALA	2.3
1	B	112	LEU	2.3
1	A	428	PRO	2.3
1	C	4	SER	2.3
1	C	402	ALA	2.3
1	C	32	ALA	2.2
1	C	445	HIS	2.2
1	A	307	VAL	2.2
1	A	32	ALA	2.2
1	A	181	LEU	2.2
1	B	214[A]	PHE	2.2
1	C	292	GLU	2.2
1	D	554	LEU	2.1
1	B	138	LEU	2.1
1	C	497	HIS	2.1
1	C	498	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	110	GLU	2.1
1	B	530	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.