



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2024 – 05:11 PM EST

PDB ID : 3FSX
Title : Structure of tetrahydrodipicolinate N-succinyltransferase (Rv1201c; DapD) from *Mycobacterium tuberculosis*
Authors : Schuldt, L.; Weyand, S.; Kefala, G.; Weiss, M.S.
Deposited on : 2009-01-12
Resolution : 2.15 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), 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

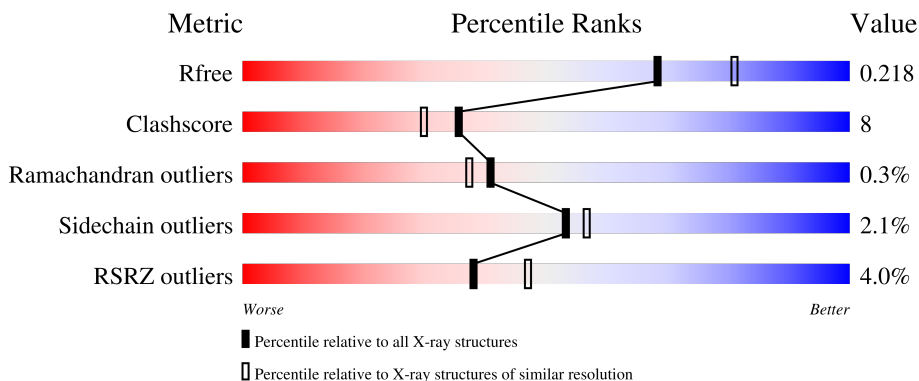
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	332	 2% 77% 13% • 10%
1	B	332	 2% 83% 9% • 8%
1	C	332	 2% 77% 13% • 10%
1	D	332	 3% 84% 8% • 8%
1	E	332	 9% 70% 16% • 13%

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
2	ACY	C	331	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11497 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 Tetrahydrodipicolinate N-succinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	300	Total 2179	C 1353	N 399	O 419	S 8	0	1	0
1	B	306	Total 2206	C 1367	N 404	O 427	S 8	0	0	0
1	C	300	Total 2168	C 1345	N 397	O 418	S 8	0	0	0
1	D	307	Total 2214	C 1373	N 405	O 428	S 8	0	0	0
1	E	290	Total 2107	C 1309	N 385	O 405	S 8	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP O05302
A	0	ALA	-	expression tag	UNP O05302
A	1	VAL	-	expression tag	UNP O05302
A	318	GLY	-	expression tag	UNP O05302
A	319	VAL	-	expression tag	UNP O05302
A	320	PRO	-	expression tag	UNP O05302
A	321	ARG	-	expression tag	UNP O05302
A	322	GLY	-	expression tag	UNP O05302
A	323	LEU	-	expression tag	UNP O05302
A	324	GLU	-	expression tag	UNP O05302
A	325	HIS	-	expression tag	UNP O05302
A	326	HIS	-	expression tag	UNP O05302
A	327	HIS	-	expression tag	UNP O05302
A	328	HIS	-	expression tag	UNP O05302
A	329	HIS	-	expression tag	UNP O05302
A	330	HIS	-	expression tag	UNP O05302
B	-1	MET	-	expression tag	UNP O05302
B	0	ALA	-	expression tag	UNP O05302
B	1	VAL	-	expression tag	UNP O05302

Continued on next page...

Continued from previous page...

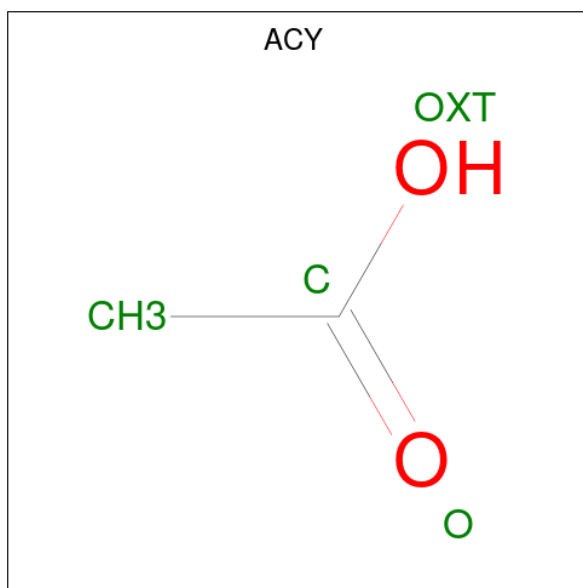
Chain	Residue	Modelled	Actual	Comment	Reference
B	318	GLY	-	expression tag	UNP O05302
B	319	VAL	-	expression tag	UNP O05302
B	320	PRO	-	expression tag	UNP O05302
B	321	ARG	-	expression tag	UNP O05302
B	322	GLY	-	expression tag	UNP O05302
B	323	LEU	-	expression tag	UNP O05302
B	324	GLU	-	expression tag	UNP O05302
B	325	HIS	-	expression tag	UNP O05302
B	326	HIS	-	expression tag	UNP O05302
B	327	HIS	-	expression tag	UNP O05302
B	328	HIS	-	expression tag	UNP O05302
B	329	HIS	-	expression tag	UNP O05302
B	330	HIS	-	expression tag	UNP O05302
C	-1	MET	-	expression tag	UNP O05302
C	0	ALA	-	expression tag	UNP O05302
C	1	VAL	-	expression tag	UNP O05302
C	318	GLY	-	expression tag	UNP O05302
C	319	VAL	-	expression tag	UNP O05302
C	320	PRO	-	expression tag	UNP O05302
C	321	ARG	-	expression tag	UNP O05302
C	322	GLY	-	expression tag	UNP O05302
C	323	LEU	-	expression tag	UNP O05302
C	324	GLU	-	expression tag	UNP O05302
C	325	HIS	-	expression tag	UNP O05302
C	326	HIS	-	expression tag	UNP O05302
C	327	HIS	-	expression tag	UNP O05302
C	328	HIS	-	expression tag	UNP O05302
C	329	HIS	-	expression tag	UNP O05302
C	330	HIS	-	expression tag	UNP O05302
D	-1	MET	-	expression tag	UNP O05302
D	0	ALA	-	expression tag	UNP O05302
D	1	VAL	-	expression tag	UNP O05302
D	318	GLY	-	expression tag	UNP O05302
D	319	VAL	-	expression tag	UNP O05302
D	320	PRO	-	expression tag	UNP O05302
D	321	ARG	-	expression tag	UNP O05302
D	322	GLY	-	expression tag	UNP O05302
D	323	LEU	-	expression tag	UNP O05302
D	324	GLU	-	expression tag	UNP O05302
D	325	HIS	-	expression tag	UNP O05302
D	326	HIS	-	expression tag	UNP O05302
D	327	HIS	-	expression tag	UNP O05302

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	328	HIS	-	expression tag	UNP O05302
D	329	HIS	-	expression tag	UNP O05302
D	330	HIS	-	expression tag	UNP O05302
E	-1	MET	-	expression tag	UNP O05302
E	0	ALA	-	expression tag	UNP O05302
E	1	VAL	-	expression tag	UNP O05302
E	318	GLY	-	expression tag	UNP O05302
E	319	VAL	-	expression tag	UNP O05302
E	320	PRO	-	expression tag	UNP O05302
E	321	ARG	-	expression tag	UNP O05302
E	322	GLY	-	expression tag	UNP O05302
E	323	LEU	-	expression tag	UNP O05302
E	324	GLU	-	expression tag	UNP O05302
E	325	HIS	-	expression tag	UNP O05302
E	326	HIS	-	expression tag	UNP O05302
E	327	HIS	-	expression tag	UNP O05302
E	328	HIS	-	expression tag	UNP O05302
E	329	HIS	-	expression tag	UNP O05302
E	330	HIS	-	expression tag	UNP O05302

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



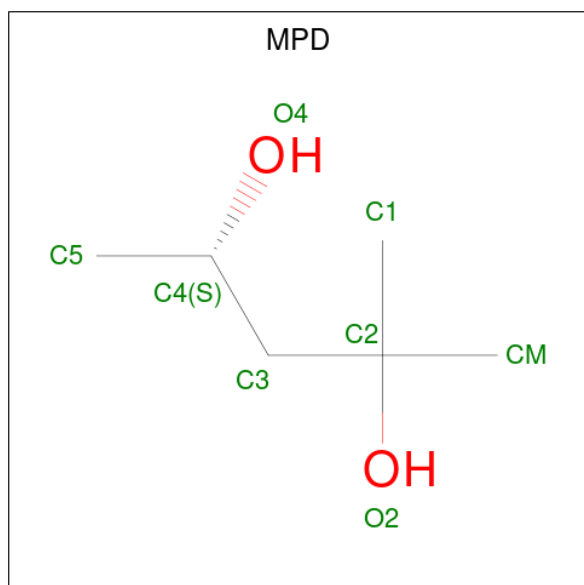
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	3	Total 3	Mg 3	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Na 1	0	0
5	B	1	Total 1	Na 1	0	0
5	D	1	Total 1	Na 1	0	0
5	E	1	Total 1	Na 1	0	0

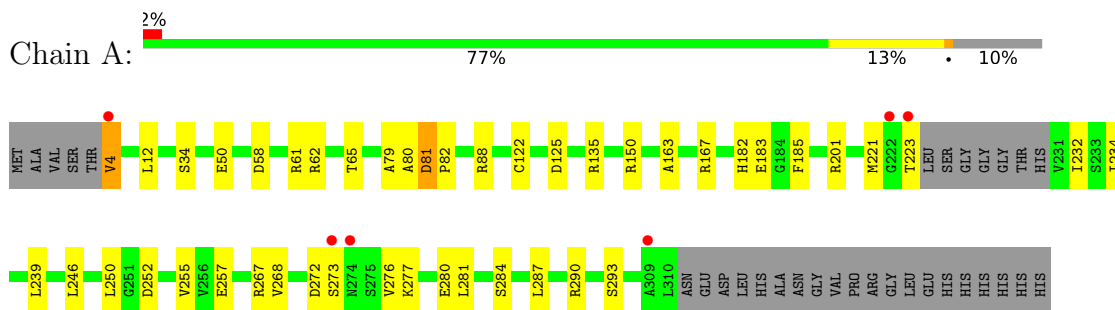
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	125	Total 125	O 125	0	0
6	B	145	Total 145	O 145	0	0
6	C	121	Total 121	O 121	0	0
6	D	157	Total 157	O 157	0	0
6	E	22	Total 22	O 22	0	0

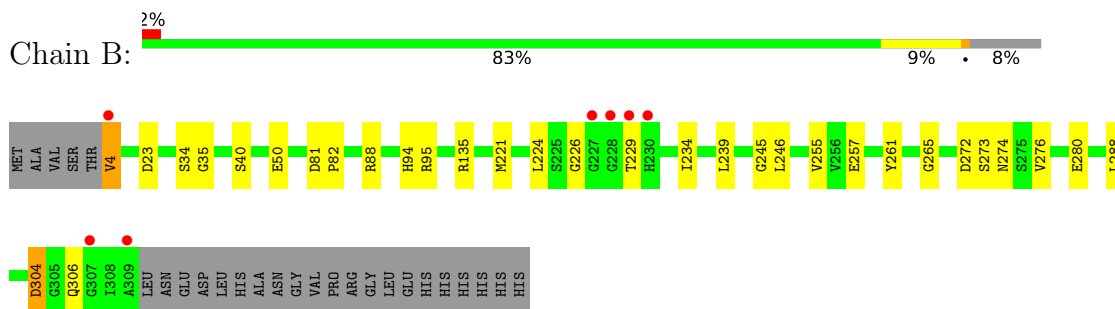
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

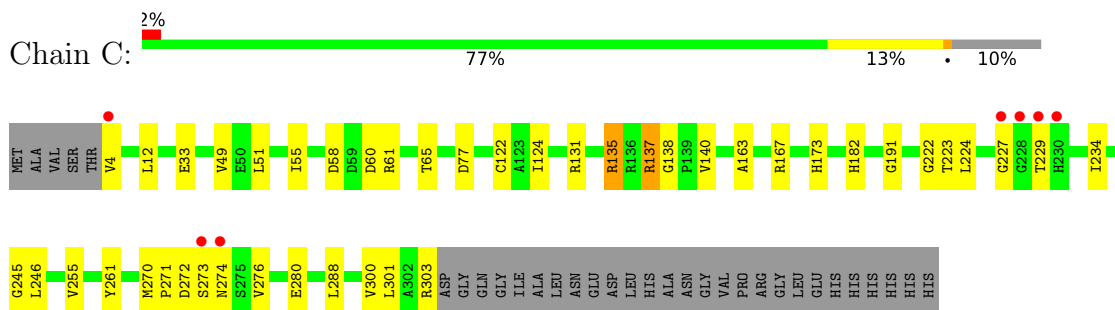
- Molecule 1: Tetrahydrodipicolinate N-succinyltransferase



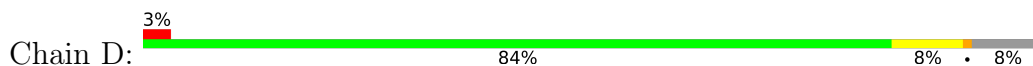
- Molecule 1: Tetrahydrodipicolinate N-succinyltransferase

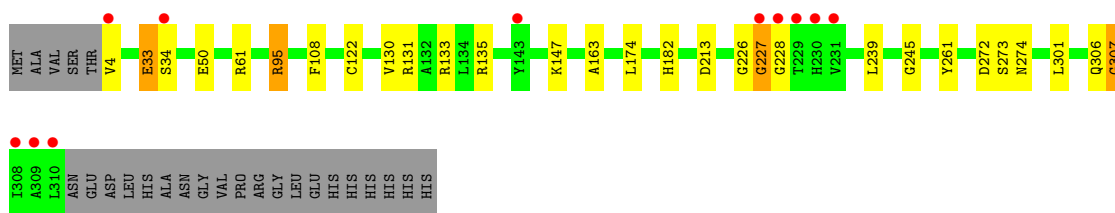


- Molecule 1: Tetrahydrodipicolinate N-succinyltransferase

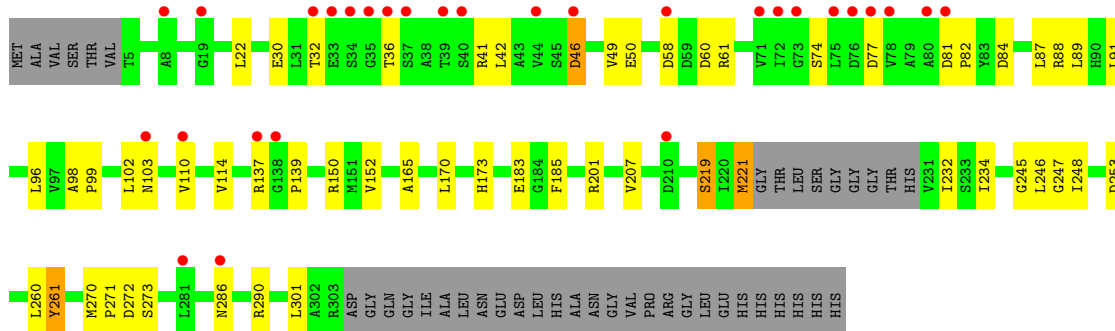


- Molecule 1: Tetrahydrodipicolinate N-succinyltransferase





● Molecule 1: Tetrahydrodipicolinate N-succinyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	216.99Å 216.99Å 216.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15 37.21 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.15) 99.7 (37.21-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.16Å)	Xtrriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.168 , 0.219 0.172 , 0.218	Depositor DCC
R_{free} test set	1127 reflections (1.23%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.015 for -l,-k,-h	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11497	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: MG, ACY, MPD, NA

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	0.96	0/2213	0.92	3/3009 (0.1%)
1	B	0.99	1/2239 (0.0%)	0.92	3/3046 (0.1%)
1	C	0.91	0/2201	0.91	5/2995 (0.2%)
1	D	1.01	0/2247	0.93	2/3057 (0.1%)
1	E	0.66	0/2138	0.73	0/2908
All	All	0.91	1/11038 (0.0%)	0.89	13/15015 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	257	GLU	CB-CG	-5.14	1.42	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	C	131	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	C	131	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	B	88	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	81	ASP	CB-CG-OD1	6.46	124.11	118.30
1	C	167	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	D	131	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	D	95	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	77	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	304	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	252	ASP	CB-CG-OD1	5.09	122.88	118.30
1	C	137	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	B	88	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	2179	0	2192	58	0
1	B	2206	0	2208	32	0
1	C	2168	0	2174	29	0
1	D	2214	0	2219	19	0
1	E	2107	0	2115	45	0
2	A	4	0	3	0	0
2	B	4	0	3	1	0
2	C	4	0	3	2	0
2	D	4	0	3	0	0
3	A	8	0	14	0	0
3	B	8	0	14	0	0
3	D	8	0	14	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	125	0	0	1	0
6	B	145	0	0	7	0
6	C	121	0	0	1	0
6	D	157	0	0	0	0
6	E	22	0	0	2	0
All	All	11497	0	10962	177	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 (177) 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:4:VAL:HG22	1:A:34:SER:HB3	1.20	1.15
1:A:4:VAL:HG22	1:A:34:SER:CB	1.93	0.99
1:A:80:ALA:HB3	6:A:514:HOH:O	1.62	0.99
1:A:201[B]:ARG:HG2	1:A:201[B]:ARG:HH11	1.27	0.95
1:C:272:ASP:O	1:C:273:SER:HB2	1.67	0.94
1:B:234:ILE:HD11	1:B:246:LEU:CD2	1.99	0.93
1:A:201[B]:ARG:HH11	1:A:201[B]:ARG:CG	1.81	0.92
1:A:276:VAL:HG23	1:A:280:GLU:CD	1.90	0.92
1:D:272:ASP:O	1:D:273:SER:HB2	1.68	0.91
1:C:234:ILE:HD11	1:C:246:LEU:CD2	2.02	0.88
1:B:276:VAL:HG22	1:B:280:GLU:CD	1.94	0.88
1:A:234:ILE:HD11	1:A:246:LEU:HD21	1.57	0.87
1:A:183:GLU:HG3	1:A:201[B]:ARG:NH2	1.89	0.86
1:B:221:MET:CE	6:B:529:HOH:O	2.22	0.86
1:A:234:ILE:HD11	1:A:246:LEU:CD2	2.09	0.81
1:B:221:MET:HE1	6:B:529:HOH:O	1.79	0.81
1:A:272:ASP:O	1:A:273:SER:HB3	1.80	0.80
1:B:234:ILE:HD11	1:B:246:LEU:HD21	1.64	0.79
1:A:4:VAL:CG2	1:A:34:SER:HB3	2.09	0.79
1:B:135:ARG:HD2	6:B:411:HOH:O	1.83	0.79
1:A:183:GLU:OE2	1:A:201[B]:ARG:NH2	2.16	0.78
1:B:276:VAL:CG2	1:B:280:GLU:CD	2.53	0.78
1:B:276:VAL:CG2	1:B:280:GLU:OE1	2.33	0.77
1:E:232:ILE:HD11	1:E:247:GLY:C	2.06	0.76
1:A:267:ARG:NH2	1:A:277:LYS:HE2	2.01	0.75
1:A:201[B]:ARG:HG2	1:A:201[B]:ARG:NH1	1.99	0.74
1:C:272:ASP:O	1:C:273:SER:CB	2.36	0.74
1:D:33:GLU:HG3	1:D:34:SER:N	2.01	0.74
1:A:276:VAL:CG2	1:A:280:GLU:CD	2.56	0.73
1:E:234:ILE:HD11	1:E:246:LEU:CD2	2.19	0.73
1:C:234:ILE:HD11	1:C:246:LEU:HD21	1.71	0.72
1:D:226:GLY:O	1:D:228:GLY:N	2.22	0.72
1:B:226:GLY:HA2	1:D:306:GLN:HE21	1.54	0.71
1:A:276:VAL:CG2	1:A:280:GLU:HB2	2.20	0.71
1:A:234:ILE:HD12	1:A:250:LEU:HB2	1.73	0.70
1:A:50:GLU:OE2	1:A:50:GLU:N	2.17	0.70
2:B:331:ACY:H1	6:B:466:HOH:O	1.90	0.69
1:D:213:ASP:HB2	1:D:239:LEU:CD1	2.23	0.69
1:E:60:ASP:OD2	1:E:137:ARG:NE	2.27	0.67
1:A:272:ASP:O	1:A:273:SER:CB	2.42	0.67
1:B:265:GLY:H	1:D:306:GLN:HE22	1.42	0.66
1:A:267:ARG:HH21	1:A:277:LYS:HE2	1.59	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:MET:HB2	1:E:271:PRO:CD	2.25	0.66
1:A:183:GLU:CG	1:A:201[B]:ARG:NH2	2.59	0.66
1:B:239:LEU:HD11	1:C:223:THR:HG21	1.78	0.66
1:A:4:VAL:CG2	1:A:34:SER:CB	2.69	0.64
1:E:301:LEU:N	1:E:301:LEU:HD12	2.12	0.64
1:E:77:ASP:O	1:E:103:ASN:HB3	1.98	0.63
1:E:232:ILE:HD11	1:E:248:ILE:N	2.12	0.63
1:B:272:ASP:O	1:B:273:SER:HB3	1.99	0.62
1:B:221:MET:HE2	6:B:529:HOH:O	1.92	0.62
1:E:58:ASP:OD2	1:E:61:ARG:HD3	2.00	0.62
1:A:276:VAL:HG23	1:A:280:GLU:OE1	2.00	0.61
1:E:152:VAL:HG21	1:E:165:ALA:HB1	1.81	0.60
1:B:276:VAL:HG23	1:B:280:GLU:OE1	2.00	0.60
1:C:12:LEU:HD11	1:C:55:ILE:HD13	1.84	0.59
1:D:213:ASP:HB2	1:D:239:LEU:HD13	1.83	0.59
1:E:234:ILE:HD11	1:E:246:LEU:HD23	1.85	0.59
1:A:276:VAL:HG22	1:A:280:GLU:HB2	1.84	0.58
1:B:239:LEU:HD11	1:C:223:THR:CG2	2.34	0.58
1:A:276:VAL:HG21	1:A:280:GLU:HB2	1.85	0.58
1:E:270:MET:HB2	1:E:271:PRO:HD2	1.85	0.57
1:B:234:ILE:HD11	1:B:246:LEU:HD23	1.83	0.57
1:C:222:GLY:CA	2:C:331:ACY:H3	2.35	0.57
1:A:183:GLU:HG3	1:A:201[B]:ARG:HH21	1.66	0.57
1:A:183:GLU:CD	1:A:201[B]:ARG:NH2	2.59	0.56
1:E:89:LEU:HB3	1:E:170:LEU:HG	1.87	0.56
1:D:95:ARG:HD3	1:D:174:LEU:O	2.06	0.56
1:C:270:MET:HB3	1:C:271:PRO:HD2	1.87	0.56
1:D:108:PHE:O	1:D:147:LYS:NZ	2.34	0.56
1:C:222:GLY:HA2	2:C:331:ACY:H3	1.88	0.56
1:E:152:VAL:HG21	1:E:165:ALA:CB	2.36	0.55
1:E:245:GLY:HA3	1:E:261:TYR:CD1	2.42	0.55
1:A:183:GLU:CD	1:A:201[B]:ARG:HH21	2.10	0.55
1:A:12:LEU:HG	1:A:65:THR:CG2	2.38	0.54
1:A:167:ARG:NH2	1:A:201[B]:ARG:HE	2.06	0.53
1:A:183:GLU:CG	1:A:201[B]:ARG:HH21	2.20	0.53
1:B:272:ASP:O	1:B:273:SER:CB	2.56	0.53
1:A:201[B]:ARG:CG	1:A:201[B]:ARG:NH1	2.52	0.53
1:E:272:ASP:O	1:E:273:SER:CB	2.57	0.53
1:B:255:VAL:CG1	1:B:288:LEU:HD12	2.39	0.52
1:A:276:VAL:HG21	1:A:280:GLU:CB	2.39	0.52
1:E:102:LEU:C	1:E:102:LEU:HD12	2.30	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:GLU:HG3	6:E:412:HOH:O	2.09	0.52
1:A:221:MET:HE2	1:A:223:THR:C	2.30	0.52
1:C:49:VAL:HG12	6:C:502:HOH:O	2.09	0.52
1:E:49:VAL:HG23	1:E:50:GLU:OE2	2.09	0.52
1:A:276:VAL:CG2	1:A:280:GLU:CB	2.88	0.52
1:A:284:SER:HB2	1:A:287:LEU:HD11	1.92	0.52
1:E:152:VAL:CG2	1:E:165:ALA:HB1	2.39	0.52
1:A:167:ARG:HH21	1:A:201[B]:ARG:HE	1.57	0.52
1:A:61:ARG:O	1:A:62:ARG:HB2	2.10	0.51
1:C:58:ASP:OD2	1:C:61:ARG:HD3	2.11	0.50
1:E:272:ASP:O	1:E:273:SER:HB2	2.11	0.50
1:B:135:ARG:CD	6:B:411:HOH:O	2.52	0.50
1:E:245:GLY:HA3	1:E:261:TYR:CE1	2.46	0.50
1:A:221:MET:HE2	1:A:223:THR:O	2.11	0.50
1:C:33:GLU:HA	1:C:33:GLU:OE1	2.12	0.50
1:E:150:ARG:HB2	6:E:402:HOH:O	2.11	0.50
1:B:4:VAL:HG12	1:B:34:SER:OG	2.11	0.50
1:A:276:VAL:HG23	1:A:280:GLU:OE2	2.12	0.50
1:E:22:LEU:HD22	1:E:114:VAL:HG22	1.93	0.50
1:B:245:GLY:HA3	1:B:261:TYR:CD1	2.47	0.49
1:C:55:ILE:HG23	1:C:65:THR:O	2.11	0.49
1:E:30:GLU:HG3	1:E:32:THR:CG2	2.43	0.49
1:E:232:ILE:CD1	1:E:248:ILE:N	2.74	0.49
1:A:257:GLU:HG2	1:A:290:ARG:HA	1.93	0.49
1:A:255:VAL:HG13	1:B:224:LEU:HD11	1.95	0.49
1:C:270:MET:HB3	1:C:271:PRO:CD	2.43	0.48
1:C:255:VAL:HB	1:C:288:LEU:HD12	1.95	0.48
1:B:50:GLU:H	1:B:50:GLU:CD	2.17	0.48
1:B:94:HIS:O	1:B:95:ARG:HB2	2.14	0.48
1:A:221:MET:O	1:A:232:ILE:HD12	2.14	0.48
1:B:81:ASP:HB2	1:B:82:PRO:CD	2.44	0.48
1:E:99:PRO:HG2	1:E:207:VAL:HG22	1.96	0.48
1:A:183:GLU:O	1:A:201[B]:ARG:NE	2.47	0.48
1:D:61:ARG:HG2	1:D:122:CYS:SG	2.54	0.48
1:E:81:ASP:HB2	1:E:82:PRO:CD	2.44	0.48
1:C:288:LEU:HD23	1:C:301:LEU:HD13	1.96	0.47
1:C:270:MET:HE2	1:C:274:ASN:O	2.14	0.47
1:B:234:ILE:CD1	1:B:246:LEU:HD21	2.41	0.47
1:E:84:ASP:O	1:E:88:ARG:HG3	2.15	0.47
1:E:185:PHE:HB3	1:E:201:ARG:HG2	1.97	0.47
1:B:304:ASP:OD1	1:B:306:GLN:N	2.42	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:ILE:HD11	1:E:248:ILE:CA	2.45	0.46
1:D:245:GLY:HA3	1:D:261:TYR:CD1	2.50	0.46
1:C:234:ILE:HD11	1:C:246:LEU:HD23	1.92	0.46
1:B:239:LEU:HG	1:C:224:LEU:HD11	1.98	0.46
1:B:265:GLY:H	1:D:306:GLN:NE2	2.10	0.46
1:E:232:ILE:CD1	1:E:247:GLY:C	2.82	0.45
1:B:272:ASP:OD1	1:B:274:ASN:HB2	2.16	0.45
1:C:61:ARG:HG2	1:C:122:CYS:SG	2.55	0.45
1:A:185:PHE:HB3	1:A:201[B]:ARG:CD	2.46	0.45
1:D:50:GLU:CD	1:D:50:GLU:H	2.20	0.45
1:A:4:VAL:CG2	1:A:34:SER:HB2	2.45	0.44
1:D:33:GLU:HG3	1:D:34:SER:O	2.16	0.44
1:E:81:ASP:HB2	1:E:82:PRO:HD2	2.00	0.44
1:A:61:ARG:HG2	1:A:122:CYS:SG	2.57	0.44
1:A:276:VAL:HG22	1:A:277:LYS:O	2.17	0.44
1:C:245:GLY:HA3	1:C:261:TYR:CD1	2.52	0.44
1:E:58:ASP:OD1	1:E:58:ASP:C	2.56	0.44
1:C:276:VAL:CG2	1:C:280:GLU:CD	2.86	0.44
1:A:239:LEU:HD23	1:B:224:LEU:HD21	2.00	0.44
1:E:87:LEU:O	1:E:91:LEU:HG	2.18	0.44
1:A:223:THR:HA	1:A:232:ILE:HG13	2.00	0.43
1:E:81:ASP:C	1:E:110:VAL:CG1	2.86	0.43
1:A:163:ALA:HB1	1:A:182:HIS:CE1	2.54	0.43
1:D:163:ALA:HB1	1:D:182:HIS:CE1	2.54	0.43
1:E:201:ARG:NH2	1:E:219:SER:HB2	2.34	0.43
1:E:221:MET:HE2	1:E:221:MET:HB3	1.83	0.43
1:E:260:LEU:HD22	1:E:290:ARG:HA	2.01	0.43
1:C:163:ALA:HB1	1:C:182:HIS:CE1	2.54	0.42
1:D:301:LEU:HD12	1:D:301:LEU:N	2.34	0.42
1:C:60:ASP:OD2	1:C:137:ARG:NH2	2.47	0.42
1:C:288:LEU:O	1:C:300:VAL:HA	2.20	0.41
1:C:173:HIS:O	1:C:191:GLY:HA3	2.20	0.41
1:A:185:PHE:HB3	1:A:201[B]:ARG:HD3	2.03	0.41
1:C:135:ARG:HA	1:C:138:GLY:O	2.20	0.41
1:C:135:ARG:HG2	1:C:140:VAL:HG23	2.03	0.41
1:A:4:VAL:O	1:A:34:SER:HB3	2.21	0.41
1:B:35:GLY:HA3	6:B:524:HOH:O	2.20	0.41
3:D:340:MPD:H11	3:D:340:MPD:H4	1.92	0.41
1:A:268:VAL:HG21	1:A:281:LEU:CD1	2.51	0.41
1:A:81:ASP:HB2	1:A:82:PRO:CD	2.51	0.41
1:A:223:THR:HA	1:A:232:ILE:CD1	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:ALA:HA	1:E:173:HIS:CD2	2.55	0.41
1:E:301:LEU:N	1:E:301:LEU:CD1	2.83	0.41
1:E:42:LEU:HD22	1:E:46:ASP:HB3	2.02	0.41
1:D:306:GLN:O	1:D:307:GLY:O	2.38	0.40
1:E:270:MET:HE2	1:E:270:MET:HB3	1.91	0.40
1:E:270:MET:CB	1:E:271:PRO:CD	2.92	0.40
1:A:79:ALA:HB2	1:A:88:ARG:HD2	2.03	0.40
1:E:96:LEU:HD23	1:E:96:LEU:HA	1.90	0.40
1:E:253:ASP:HB2	1:E:286:ASN:HD22	1.86	0.40
1:A:58:ASP:OD2	1:A:61:ARG:HD3	2.21	0.40
1:D:226:GLY:O	1:D:227:GLY:C	2.60	0.40
1:D:130:VAL:HG22	1:D:133:ARG:HH21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/332 (90%)	290 (98%)	7 (2%)	0	100	100
1	B	304/332 (92%)	292 (96%)	12 (4%)	0	100	100
1	C	298/332 (90%)	292 (98%)	4 (1%)	2 (1%)	22	15
1	D	305/332 (92%)	297 (97%)	6 (2%)	2 (1%)	22	15
1	E	286/332 (86%)	276 (96%)	9 (3%)	1 (0%)	41	37
All	All	1490/1660 (90%)	1447 (97%)	38 (3%)	5 (0%)	41	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	227	GLY
1	C	229	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	227	GLY
1	E	139	PRO
1	D	307	GLY

5.3.2 Protein sidechains [i](#)

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	227/251 (90%)	223 (98%)	4 (2%)	59	63
1	B	229/251 (91%)	225 (98%)	4 (2%)	60	65
1	C	226/251 (90%)	221 (98%)	5 (2%)	52	55
1	D	230/251 (92%)	226 (98%)	4 (2%)	60	65
1	E	220/251 (88%)	213 (97%)	7 (3%)	39	38
All	All	1132/1255 (90%)	1108 (98%)	24 (2%)	53	57

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	125	ASP
1	A	135	ARG
1	A	293	SER
1	B	4	VAL
1	B	23	ASP
1	B	40	SER
1	B	229	THR
1	C	4	VAL
1	C	51	LEU
1	C	124	ILE
1	C	135	ARG
1	C	303	ARG
1	D	4	VAL
1	D	33	GLU
1	D	135	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	274	ASN
1	E	36	THR
1	E	41	ARG
1	E	46	ASP
1	E	74	SER
1	E	219	SER
1	E	221	MET
1	E	261	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	306	GLN
1	D	274	ASN
1	D	306	GLN
1	E	113	ASN
1	E	286	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 13 are monoatomic - leaving 7 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
2	ACY	A	331	-	3,3,3	0.84	0	3,3,3	0.95	0
3	MPD	A	340	-	7,7,7	0.28	0	9,10,10	1.08	0
2	ACY	D	331	-	3,3,3	0.92	0	3,3,3	1.82	1 (33%)
2	ACY	B	331	-	3,3,3	0.88	0	3,3,3	0.51	0
3	MPD	D	340	-	7,7,7	0.48	0	9,10,10	0.45	0
2	ACY	C	331	-	3,3,3	0.73	0	3,3,3	0.41	0
3	MPD	B	340	-	7,7,7	0.47	0	9,10,10	1.12	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
3	MPD	D	340	-	-	3/5/5/5	-
3	MPD	B	340	-	-	3/5/5/5	-
3	MPD	A	340	-	-	4/5/5/5	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	331	ACY	OXT-C-CH3	2.39	125.08	115.18

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	340	MPD	C1-C2-C3-C4
3	D	340	MPD	O2-C2-C3-C4
3	A	340	MPD	C1-C2-C3-C4
3	D	340	MPD	CM-C2-C3-C4
3	A	340	MPD	O2-C2-C3-C4
3	B	340	MPD	O2-C2-C3-C4
3	A	340	MPD	C2-C3-C4-C5
3	B	340	MPD	C2-C3-C4-C5
3	A	340	MPD	C2-C3-C4-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	340	MPD	C2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	331	ACY	1	0
3	D	340	MPD	1	0
2	C	331	ACY	2	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	300/332 (90%)	-0.25	6 (2%) 65 72	21, 28, 40, 57	0
1	B	306/332 (92%)	-0.17	7 (2%) 60 68	20, 28, 42, 63	0
1	C	300/332 (90%)	-0.21	7 (2%) 60 68	21, 29, 40, 61	0
1	D	307/332 (92%)	-0.21	11 (3%) 42 51	23, 28, 42, 67	0
1	E	290/332 (87%)	0.47	29 (10%) 7 11	21, 30, 40, 47	0
All	All	1503/1660 (90%)	-0.08	60 (3%) 38 47	20, 29, 41, 67	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	229	THR	5.6
1	D	228	GLY	4.8
1	E	36	THR	4.3
1	D	310	LEU	4.2
1	D	34	SER	4.0
1	C	4	VAL	4.0
1	D	4	VAL	3.8
1	E	34	SER	3.8
1	B	309	ALA	3.8
1	E	80	ALA	3.8
1	A	4	VAL	3.7
1	E	78	VAL	3.6
1	C	230	HIS	3.4
1	E	72	ILE	3.4
1	E	40	SER	3.3
1	A	309	ALA	3.2
1	D	227	GLY	3.2
1	B	227	GLY	3.2
1	E	32	THR	3.2
1	D	308	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	71	VAL	3.1
1	C	274	ASN	3.1
1	B	307	GLY	3.0
1	E	73	GLY	3.0
1	E	110	VAL	3.0
1	A	223	THR	2.9
1	E	138	GLY	2.9
1	E	103	ASN	2.9
1	E	33	GLU	2.9
1	D	230	HIS	2.9
1	B	228	GLY	2.8
1	E	76	ASP	2.8
1	E	8	ALA	2.7
1	B	229	THR	2.7
1	C	227	GLY	2.7
1	E	58	ASP	2.6
1	A	222	GLY	2.6
1	E	286	ASN	2.6
1	B	230	HIS	2.6
1	A	274	ASN	2.5
1	E	75	LEU	2.5
1	D	309	ALA	2.4
1	D	229	THR	2.4
1	E	77	ASP	2.4
1	D	143	TYR	2.3
1	E	210	ASP	2.3
1	E	35	GLY	2.2
1	E	39	THR	2.2
1	B	4	VAL	2.2
1	E	46	ASP	2.2
1	E	137	ARG	2.2
1	A	273	SER	2.2
1	C	228	GLY	2.1
1	E	281	LEU	2.1
1	E	37	SER	2.1
1	E	19	GLY	2.1
1	D	231	VAL	2.0
1	C	273	SER	2.0
1	E	44	VAL	2.0
1	E	81	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
4	MG	A	332	1/1	0.82	0.09	43,43,43,43	0
4	MG	B	332	1/1	0.84	0.16	53,53,53,53	0
3	MPD	A	340	8/8	0.90	0.15	32,38,46,48	0
2	ACY	A	331	4/4	0.91	0.45	26,28,28,28	4
4	MG	E	331	1/1	0.92	0.24	54,54,54,54	1
4	MG	E	333	1/1	0.92	0.15	44,44,44,44	1
3	MPD	D	340	8/8	0.93	0.18	30,45,56,61	0
4	MG	A	333	1/1	0.94	0.06	46,46,46,46	0
3	MPD	B	340	8/8	0.95	0.23	27,38,51,52	0
4	MG	C	332	1/1	0.95	0.06	27,27,27,27	0
5	NA	A	334	1/1	0.95	0.26	40,40,40,40	0
5	NA	B	333	1/1	0.95	0.20	32,32,32,32	1
2	ACY	B	331	4/4	0.96	0.11	22,25,26,29	0
4	MG	D	332	1/1	0.96	0.04	21,21,21,21	1
5	NA	E	334	1/1	0.96	0.24	49,49,49,49	1
4	MG	D	333	1/1	0.97	0.09	62,62,62,62	1
2	ACY	D	331	4/4	0.97	0.10	29,32,34,35	0
5	NA	D	334	1/1	0.98	0.56	48,48,48,48	1
2	ACY	C	331	4/4	0.98	0.07	27,29,30,31	0
4	MG	E	332	1/1	1.00	0.16	55,55,55,55	1

6.5 Other polymers [i](#)

There are no such residues in this entry.