



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:23 am GMT

PDB ID : 4QOY
Title : Novel binding motif and new flexibility revealed by structural analysis of a pyruvate dehydrogenase-dihydrolipoyl acetyltransferase sub-complex from the escherichia coli pyruvate dehydrogenase multi-enzyme complex
Authors : Furey, W.; Arjunan, P.
Deposited on : 2014-06-20
Resolution : 2.80 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

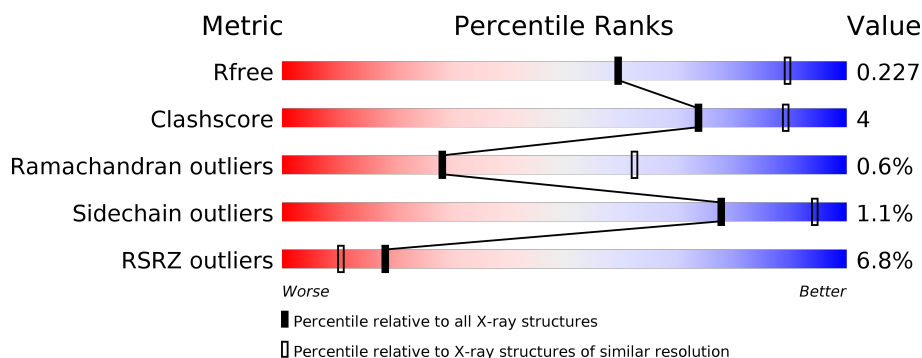
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	886	<div> <div>4%</div> <div>89%</div> <div>8%</div> <div>•</div> </div>
1	B	886	<div> <div>4%</div> <div>88%</div> <div>8%</div> <div>•</div> </div>
1	C	886	<div> <div>9%</div> <div>88%</div> <div>9%</div> <div>•</div> </div>
1	D	886	<div> <div>7%</div> <div>89%</div> <div>7%</div> <div>•</div> </div>
2	E	46	<div> <div>15%</div> <div>85%</div> <div>15%</div> </div>
2	F	46	<div> <div>46%</div> <div>83%</div> <div>17%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 29167 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 Pyruvate dehydrogenase E1 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	862	Total	C	N	O	S	0	0	0
			6824	4318	1181	1298	27			
1	B	854	Total	C	N	O	S	0	0	0
			6772	4287	1170	1288	27			
1	C	864	Total	C	N	O	S	0	0	0
			6826	4317	1183	1299	27			
1	D	849	Total	C	N	O	S	0	0	0
			6722	4254	1163	1278	27			

- Molecule 2 is a protein called Pyruvate dehydrogenase (Dihydrolipoyltransacetylase component).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	46	Total	C	N	O	0	0	0
			365	230	76	59			
2	F	46	Total	C	N	O	0	0	0
			365	230	76	59			

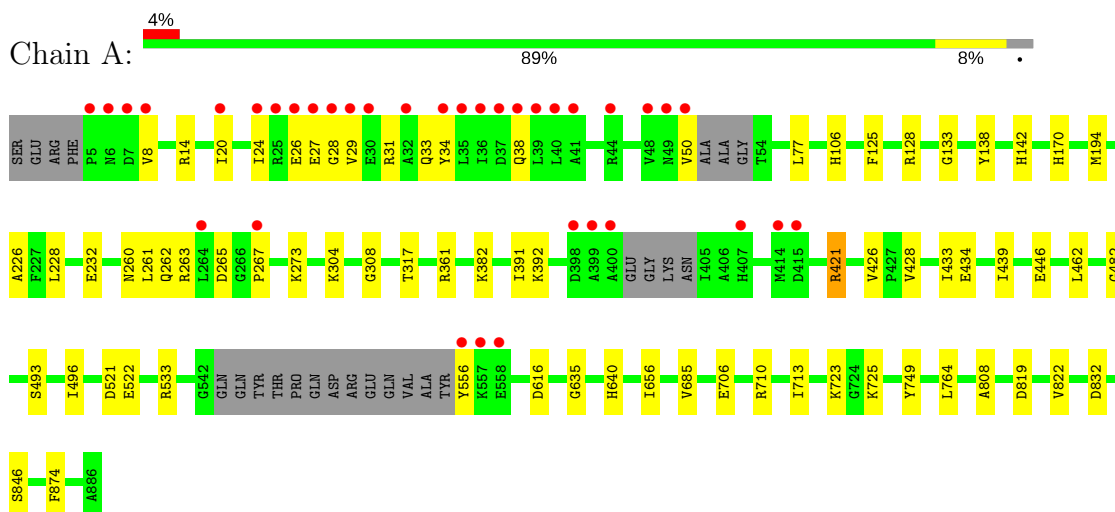
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	401	Total	O	0	0
			401	401		
3	B	436	Total	O	0	0
			436	436		
3	C	224	Total	O	0	0
			224	224		
3	D	224	Total	O	0	0
			224	224		
3	E	5	Total	O	0	0
			5	5		
3	F	3	Total	O	0	0
			3	3		

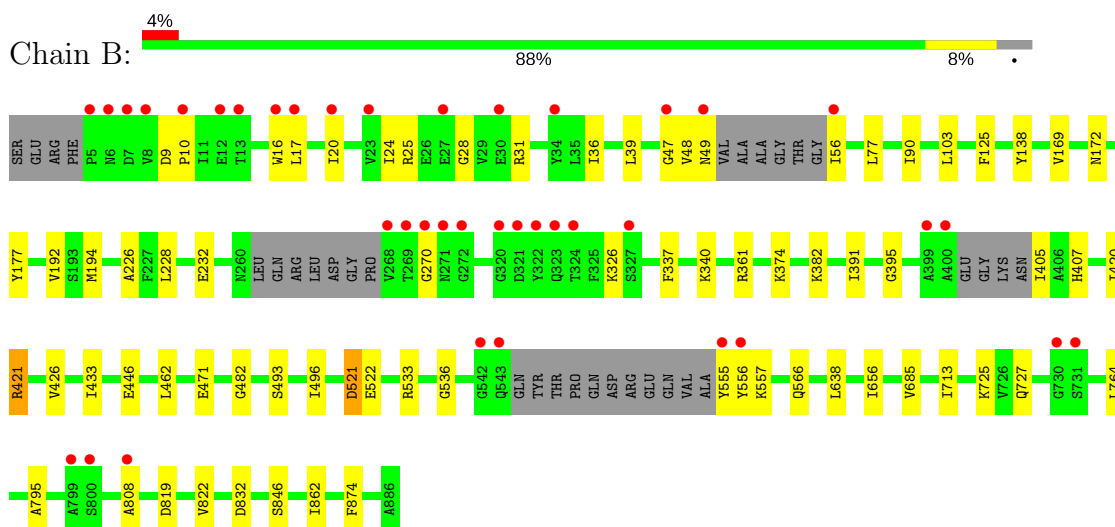
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

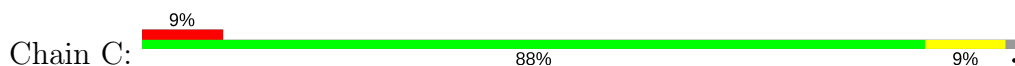
• Molecule 1: Pyruvate dehydrogenase E1 component

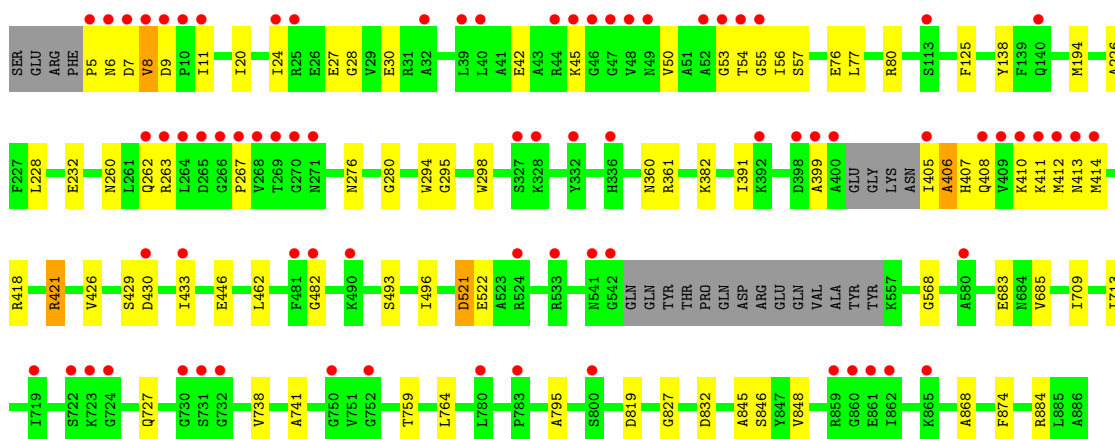


• Molecule 1: Pyruvate dehydrogenase E1 component

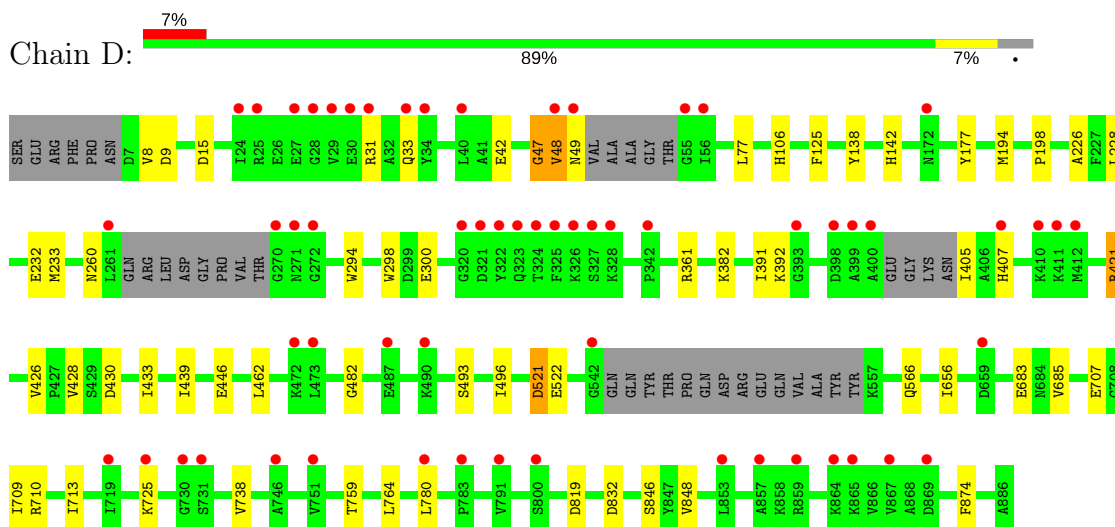


• Molecule 1: Pyruvate dehydrogenase E1 component

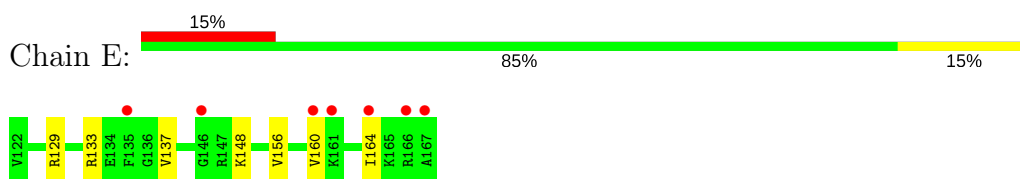




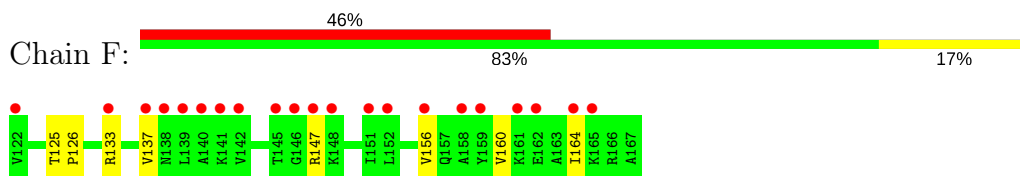
• Molecule 1: Pyruvate dehydrogenase E1 component



• Molecule 2: Pyruvate dehydrogenase (Dihydrolipoyltransacetylase component)



• Molecule 2: Pyruvate dehydrogenase (Dihydrolipoyltransacetylase component)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	210.94Å 326.84Å 77.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.29 – 2.80 32.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (32.29-2.80) 94.4 (32.29-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.198 , 0.233 0.197 , 0.227	Depositor DCC
R_{free} test set	6292 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29167	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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](#)

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	0.45	0/6973	0.62	0/9425
1	B	0.47	0/6920	0.62	0/9351
1	C	0.43	0/6975	0.60	0/9429
1	D	0.44	0/6867	0.61	0/9277
2	E	0.48	0/368	0.56	0/490
2	F	0.46	0/368	0.59	0/490
All	All	0.45	0/28471	0.61	0/38462

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6824	0	6661	55	0
1	B	6772	0	6601	56	0
1	C	6826	0	6666	68	0
1	D	6722	0	6559	48	0
2	E	365	0	401	5	0
2	F	365	0	401	12	0
3	A	401	0	0	2	0
3	B	436	0	0	3	0
3	C	224	0	0	0	0
3	D	224	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	5	0	0	0	0
3	F	3	0	0	0	0
All	All	29167	0	27289	208	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (208) 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:640:HIS:HE1	1:B:192:VAL:HG11	1.14	1.12
1:C:408:GLN:HB2	1:C:413:ASN:HB3	1.26	1.10
1:D:15:ASP:HB3	2:F:125:THR:HG21	1.31	1.10
1:C:295:GLY:HA3	1:C:360:ASN:OD1	1.52	1.07
1:A:640:HIS:HE1	1:B:192:VAL:CG1	1.71	1.03
1:A:640:HIS:CE1	1:B:192:VAL:HG11	1.95	0.99
1:D:430:ASP:O	1:D:433:ILE:HG22	1.64	0.95
1:B:48:VAL:HG12	1:B:49:ASN:H	1.29	0.93
1:D:260:ASN:ND2	1:D:392:LYS:HD2	1.86	0.91
1:C:30:GLU:HA	1:D:49:ASN:ND2	1.87	0.88
1:A:640:HIS:CE1	1:B:192:VAL:CG1	2.55	0.86
1:A:38:GLN:HG3	1:B:17:LEU:HD11	1.56	0.85
1:D:15:ASP:CB	2:F:125:THR:HG21	2.07	0.85
1:C:407:HIS:CE1	1:C:410:LYS:HD3	2.16	0.81
1:B:405:ILE:O	1:B:405:ILE:HG22	1.81	0.80
1:C:11:ILE:HG22	2:F:133:ARG:NH1	1.96	0.80
1:C:429:SER:O	1:C:433:ILE:HG23	1.81	0.79
1:D:198:PRO:HD3	1:D:228:LEU:HD21	1.65	0.78
1:C:407:HIS:NE2	1:C:410:LYS:HD3	1.99	0.78
1:A:24:ILE:HA	1:A:28:GLY:HA3	1.67	0.76
1:D:725:LYS:HE2	3:D:944:HOH:O	1.85	0.76
1:A:106:HIS:NE2	1:A:142:HIS:HD2	1.83	0.75
1:A:106:HIS:NE2	1:A:142:HIS:CD2	2.54	0.74
1:A:656:ILE:HG12	1:A:685:VAL:CG1	2.17	0.74
1:A:20:ILE:HD13	1:B:39:LEU:HG	1.70	0.74
1:B:48:VAL:HG12	1:B:49:ASN:N	2.03	0.73
1:B:24:ILE:HA	1:B:28:GLY:HA3	1.69	0.73
1:B:177:TYR:CB	1:B:192:VAL:CG2	2.67	0.71
1:A:106:HIS:CD2	1:A:142:HIS:HD2	2.08	0.71
1:B:177:TYR:HB3	1:B:192:VAL:CG2	2.22	0.70
1:D:15:ASP:HB3	2:F:125:THR:CG2	2.17	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:PRO:HB3	1:D:228:LEU:HD11	1.73	0.70
1:C:30:GLU:HA	1:D:49:ASN:HD22	1.56	0.69
1:C:399:ALA:HA	1:C:405:ILE:HG21	1.76	0.68
1:D:260:ASN:HD21	1:D:392:LYS:HD2	1.56	0.68
1:A:106:HIS:CD2	1:A:142:HIS:CD2	2.82	0.67
1:C:56:ILE:HD12	1:C:276:ASN:O	1.95	0.67
1:C:24:ILE:HA	1:C:28:GLY:HA3	1.77	0.67
1:B:177:TYR:CB	1:B:192:VAL:HG21	2.25	0.66
1:A:26:GLU:HG2	2:E:148:LYS:HB2	1.78	0.66
1:C:411:LYS:O	1:C:412:MET:HB2	1.97	0.64
1:D:656:ILE:HG12	1:D:685:VAL:CG2	2.29	0.63
1:C:11:ILE:HG21	2:F:133:ARG:CZ	2.30	0.62
1:C:263:ARG:HH12	1:D:566:GLN:NE2	1.97	0.62
1:A:846:SER:HB2	1:A:874:PHE:HB3	1.80	0.62
1:C:408:GLN:HB2	1:C:413:ASN:CB	2.18	0.62
1:C:57:SER:HB3	1:D:49:ASN:O	1.99	0.62
1:A:29:VAL:HG13	1:B:47:GLY:O	1.99	0.61
1:D:656:ILE:HG12	1:D:685:VAL:HG22	1.82	0.61
1:B:405:ILE:CG2	1:B:405:ILE:O	2.48	0.61
1:B:533:ARG:HG2	1:B:556:TYR:HB3	1.81	0.61
1:A:50:VAL:HG22	1:B:56:ILE:HA	1.81	0.61
1:C:399:ALA:O	1:C:405:ILE:HG13	2.01	0.61
1:A:106:HIS:CE1	1:A:142:HIS:HD2	2.18	0.60
1:B:656:ILE:HG12	1:B:685:VAL:HG22	1.83	0.60
1:D:106:HIS:CE1	1:D:142:HIS:CD2	2.90	0.60
1:B:713:ILE:HB	1:B:764:LEU:HD11	1.84	0.60
1:C:414:MET:HB2	1:C:418:ARG:HH21	1.67	0.59
1:C:11:ILE:CG2	2:F:133:ARG:NH1	2.64	0.59
1:C:7:ASP:O	1:C:8:VAL:HB	2.03	0.59
1:B:656:ILE:HG12	1:B:685:VAL:CG2	2.32	0.59
1:C:56:ILE:HD11	1:C:280:GLY:CA	2.33	0.58
1:A:26:GLU:OE1	1:A:26:GLU:O	2.22	0.58
1:B:846:SER:HB2	1:B:874:PHE:HB3	1.84	0.58
1:B:395:GLY:O	1:B:420:ILE:HG22	2.03	0.58
1:C:30:GLU:HA	1:D:49:ASN:HD21	1.69	0.58
1:C:713:ILE:HB	1:C:764:LEU:HD11	1.86	0.58
1:D:228:LEU:HD22	1:D:232:GLU:CD	2.24	0.57
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.86	0.57
1:D:846:SER:HB2	1:D:874:PHE:HB3	1.86	0.57
2:F:125:THR:HG23	2:F:126:PRO:HD2	1.86	0.57
1:D:683:GLU:HB3	1:D:685:VAL:HG12	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:TRP:HB3	1:D:298:TRP:CD1	2.41	0.56
1:A:27:GLU:HG2	2:E:148:LYS:HE2	1.86	0.56
1:D:106:HIS:HE1	1:D:177:TYR:HE1	1.52	0.56
1:C:295:GLY:CA	1:C:360:ASN:OD1	2.41	0.56
1:D:713:ILE:HB	1:D:764:LEU:HD11	1.87	0.55
1:A:656:ILE:CG1	1:A:685:VAL:CG1	2.84	0.55
2:F:125:THR:CG2	2:F:126:PRO:HD2	2.35	0.55
1:C:407:HIS:CE1	1:C:410:LYS:NZ	2.75	0.55
1:C:430:ASP:O	1:C:433:ILE:HG13	2.08	0.54
1:C:430:ASP:O	1:C:433:ILE:CG1	2.55	0.54
1:C:407:HIS:CE1	1:C:410:LYS:CD	2.89	0.54
1:C:53:GLY:O	1:C:54:THR:HG22	2.06	0.54
1:B:48:VAL:CG1	1:B:49:ASN:H	2.10	0.54
1:C:55:GLY:C	1:C:56:ILE:HG12	2.28	0.54
1:C:683:GLU:HB3	1:C:685:VAL:HG22	1.88	0.54
1:B:177:TYR:CG	1:B:192:VAL:HG21	2.42	0.54
1:C:421:ARG:HG2	1:C:426:VAL:HB	1.90	0.54
1:D:421:ARG:HG2	1:D:426:VAL:HB	1.90	0.54
1:D:430:ASP:O	1:D:433:ILE:CG2	2.49	0.54
1:B:90:ILE:HD13	1:B:420:ILE:HD12	1.89	0.53
1:D:738:VAL:HG12	1:D:848:VAL:HG21	1.91	0.53
1:C:846:SER:HB2	1:C:874:PHE:HB3	1.90	0.53
1:C:11:ILE:CG2	2:F:133:ARG:CZ	2.87	0.53
1:B:177:TYR:CG	1:B:192:VAL:CG2	2.91	0.53
1:A:421:ARG:HG2	1:A:426:VAL:HB	1.90	0.53
1:A:616:ASP:OD1	1:B:638:LEU:HD13	2.09	0.53
1:B:421:ARG:HG2	1:B:426:VAL:HB	1.90	0.52
1:C:868:ALA:HB2	1:D:780:LEU:HD23	1.90	0.52
2:E:137:VAL:HG11	2:E:156:VAL:HG13	1.91	0.52
1:B:194:MET:HB3	1:B:232:GLU:HG3	1.91	0.52
1:D:77:LEU:HD21	1:D:446:GLU:HB3	1.92	0.52
1:C:56:ILE:HD11	1:C:280:GLY:HA3	1.91	0.52
1:C:55:GLY:O	1:C:56:ILE:HD13	2.11	0.51
1:C:521:ASP:HB2	1:C:568:GLY:HA2	1.93	0.51
1:A:31:ARG:NH1	1:A:34:TYR:CE2	2.79	0.51
1:B:77:LEU:HD21	1:B:446:GLU:HB3	1.93	0.51
1:B:177:TYR:HB2	1:B:192:VAL:HG21	1.92	0.50
1:C:77:LEU:HD21	1:C:446:GLU:HB3	1.93	0.50
1:C:727:GLN:HG3	1:C:795:ALA:HB3	1.93	0.50
1:D:194:MET:HB3	1:D:232:GLU:HG3	1.94	0.50
1:C:54:THR:O	1:C:54:THR:HG23	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:137:VAL:HG11	2:F:156:VAL:HG13	1.92	0.50
1:C:194:MET:HB3	1:C:232:GLU:HG3	1.92	0.50
1:C:405:ILE:C	1:C:407:HIS:H	2.13	0.50
1:C:56:ILE:CD1	1:C:276:ASN:O	2.60	0.49
1:D:106:HIS:HE1	1:D:177:TYR:CE1	2.30	0.49
1:A:8:VAL:HB	1:B:31:ARG:HH11	1.78	0.49
1:C:8:VAL:HG12	1:C:9:ASP:N	2.28	0.48
1:C:406:ALA:C	1:C:408:GLN:H	2.17	0.48
1:B:192:VAL:HG23	3:B:903:HOH:O	2.14	0.48
1:B:125:PHE:HB3	1:B:462:LEU:HD13	1.95	0.48
1:C:407:HIS:CE1	1:C:410:LYS:CE	2.96	0.48
1:A:635:GLY:HA3	1:B:103:LEU:O	2.14	0.47
1:C:20:ILE:HD11	1:D:42:GLU:HB3	1.96	0.47
1:A:125:PHE:HB3	1:A:462:LEU:HD13	1.96	0.47
1:D:493:SER:H	1:D:496:ILE:HD12	1.79	0.47
1:A:194:MET:HB3	1:A:232:GLU:HG3	1.96	0.47
1:C:125:PHE:HB3	1:C:462:LEU:HD13	1.96	0.47
1:C:407:HIS:CE1	1:C:410:LYS:HZ2	2.31	0.47
1:A:77:LEU:HD21	1:A:446:GLU:HB3	1.95	0.47
1:D:707:GLU:HA	1:D:710:ARG:HH21	1.80	0.47
1:A:656:ILE:CG1	1:A:685:VAL:HG11	2.44	0.47
1:D:125:PHE:HB3	1:D:462:LEU:HD13	1.96	0.47
1:D:47:GLY:O	1:D:48:VAL:HB	2.15	0.47
1:A:493:SER:H	1:A:496:ILE:HD12	1.80	0.47
2:E:129:ARG:O	2:E:133:ARG:HG2	2.15	0.47
1:B:177:TYR:CD2	1:B:192:VAL:HG21	2.51	0.46
1:C:493:SER:H	1:C:496:ILE:HD12	1.80	0.46
1:A:50:VAL:HA	1:B:56:ILE:N	2.30	0.46
1:D:709:ILE:HG23	1:D:759:THR:HG21	1.96	0.46
1:A:273:LYS:HE3	1:A:317:THR:O	2.15	0.46
1:B:20:ILE:HD11	1:B:36:ILE:HD11	1.98	0.46
1:B:493:SER:H	1:B:496:ILE:HD12	1.81	0.46
1:C:709:ILE:HG23	1:C:759:THR:HG21	1.98	0.46
1:D:656:ILE:CG1	1:D:685:VAL:CG2	2.94	0.46
1:A:262:GLN:HA	1:A:267:PRO:HA	1.98	0.46
1:A:361:ARG:HD2	1:A:391:ILE:HG13	1.98	0.45
1:A:20:ILE:HG21	1:B:39:LEU:HD21	1.97	0.45
1:D:428:VAL:HG23	1:D:439:ILE:HD11	1.97	0.45
1:B:90:ILE:HG21	1:B:420:ILE:HD11	1.97	0.45
1:A:428:VAL:HG23	1:A:439:ILE:HD11	1.98	0.45
1:A:533:ARG:NH2	1:A:556:TYR:CD1	2.84	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:GLN:HA	1:C:267:PRO:HA	1.99	0.45
1:B:337:PHE:O	1:B:340:LYS:HB2	2.17	0.44
1:C:138:TYR:HB2	1:C:226:ALA:HA	2.00	0.44
1:D:9:ASP:HB2	2:F:147:ARG:HD2	2.00	0.44
1:A:434:GLU:HG3	3:A:1000:HOH:O	2.17	0.44
1:D:228:LEU:HD13	1:D:233:MET:SD	2.58	0.44
1:A:261:LEU:HD11	3:A:919:HOH:O	2.18	0.44
1:A:723:LYS:HD2	1:A:749:TYR:O	2.18	0.43
1:C:430:ASP:O	1:C:433:ILE:HG12	2.17	0.43
1:A:31:ARG:HH12	1:A:34:TYR:HE2	1.67	0.43
1:A:138:TYR:HB2	1:A:226:ALA:HA	2.00	0.43
1:A:14:ARG:HD2	1:A:308:GLY:HA3	2.00	0.43
2:F:160:VAL:O	2:F:164:ILE:HG12	2.19	0.43
1:B:656:ILE:CG1	1:B:685:VAL:CG2	2.95	0.43
1:B:90:ILE:HD13	1:B:420:ILE:CD1	2.49	0.43
1:C:42:GLU:HA	1:C:45:LYS:HD2	1.99	0.43
1:B:138:TYR:HB2	1:B:226:ALA:HA	2.01	0.43
1:C:741:ALA:HB2	1:C:845:ALA:HA	2.00	0.43
2:E:160:VAL:O	2:E:164:ILE:HG12	2.19	0.43
1:D:361:ARG:HD2	1:D:391:ILE:HG13	2.02	0.42
1:A:33:GLN:OE1	1:B:49:ASN:N	2.53	0.42
1:D:300:GLU:HB2	3:D:978:HOH:O	2.19	0.42
1:A:706:GLU:O	1:A:710:ARG:HG3	2.19	0.42
1:C:5:PRO:HA	1:C:6:ASN:HA	1.58	0.42
1:A:31:ARG:NH1	1:A:34:TYR:CD2	2.88	0.42
1:B:536:GLY:CA	1:B:557:LYS:HB2	2.49	0.42
1:C:361:ARG:HD2	1:C:391:ILE:HG13	2.01	0.42
1:C:738:VAL:HG13	1:C:848:VAL:HG11	2.01	0.41
1:D:138:TYR:HB2	1:D:226:ALA:HA	2.01	0.41
1:A:26:GLU:CD	1:A:26:GLU:O	2.58	0.41
1:A:20:ILE:HG23	1:B:16:TRP:HH2	1.85	0.41
1:C:8:VAL:HG11	1:D:31:ARG:HD3	2.01	0.41
1:B:361:ARG:HD2	1:B:391:ILE:HG13	2.02	0.41
1:B:521:ASP:HA	1:B:566:GLN:OE1	2.21	0.41
1:D:405:ILE:C	1:D:407:HIS:H	2.22	0.41
1:A:106:HIS:CE1	1:A:142:HIS:CD2	3.01	0.41
1:C:56:ILE:CD1	1:C:280:GLY:CA	2.97	0.41
1:C:294:TRP:HB3	1:C:298:TRP:CD1	2.55	0.41
1:C:827:GLY:CA	1:C:884:ARG:HA	2.51	0.41
1:C:50:VAL:HG21	1:D:33:GLN:OE1	2.21	0.41
1:A:128:ARG:HG3	1:A:133:GLY:HA2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:ALA:C	1:C:408:GLN:N	2.74	0.41
1:A:170:HIS:HD2	3:B:985:HOH:O	2.04	0.41
1:B:536:GLY:HA3	1:B:557:LYS:HB2	2.02	0.41
1:B:471:GLU:HG2	3:B:1224:HOH:O	2.21	0.41
1:D:656:ILE:CG1	1:D:685:VAL:HG21	2.51	0.41
1:C:263:ARG:HD2	1:D:521:ASP:OD1	2.21	0.40
1:B:727:GLN:HG3	1:B:795:ALA:HB3	2.03	0.40
1:A:808:ALA:HB3	1:A:822:VAL:HG13	2.04	0.40
1:C:76:GLU:CD	1:C:80:ARG:HH21	2.24	0.40
1:A:260:ASN:ND2	1:A:392:LYS:HD2	2.36	0.40
1:A:832:ASP:OD2	1:B:169:VAL:HB	2.22	0.40
1:B:405:ILE:C	1:B:407:HIS:H	2.24	0.40
1:B:808:ALA:HB3	1:B:822:VAL:HG13	2.04	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	854/886 (96%)	814 (95%)	37 (4%)	3 (0%)	38	72
1	B	844/886 (95%)	798 (94%)	40 (5%)	6 (1%)	25	59
1	C	858/886 (97%)	811 (94%)	41 (5%)	6 (1%)	25	59
1	D	839/886 (95%)	798 (95%)	35 (4%)	6 (1%)	25	59
2	E	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
2	F	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
All	All	3483/3636 (96%)	3307 (95%)	155 (4%)	21 (1%)	28	62

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	482	GLY
1	A	522	GLU
1	B	482	GLY
1	C	482	GLY
1	C	522	GLU
1	D	482	GLY
1	B	522	GLU
1	C	8	VAL
1	D	48	VAL
1	D	522	GLU
1	A	521	ASP
1	B	270	GLY
1	B	521	ASP
1	C	521	ASP
1	D	521	ASP
1	B	9	ASP
1	C	27	GLU
1	D	47	GLY
1	B	10	PRO
1	C	406	ALA
1	D	8	VAL

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	716/735 (97%)	707 (99%)	9 (1%)	73	93
1	B	710/735 (97%)	697 (98%)	13 (2%)	64	90
1	C	715/735 (97%)	709 (99%)	6 (1%)	85	96
1	D	704/735 (96%)	700 (99%)	4 (1%)	89	97
2	E	36/36 (100%)	36 (100%)	0	100	100
2	F	36/36 (100%)	36 (100%)	0	100	100
All	All	2917/3012 (97%)	2885 (99%)	32 (1%)	78	94

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	LEU
1	A	263	ARG
1	A	265	ASP
1	A	304	LYS
1	A	382	LYS
1	A	421	ARG
1	A	433	ILE
1	A	725	LYS
1	A	819	ASP
1	B	25	ARG
1	B	172	ASN
1	B	228	LEU
1	B	326	LYS
1	B	374	LYS
1	B	382	LYS
1	B	421	ARG
1	B	433	ILE
1	B	555	TYR
1	B	725	LYS
1	B	819	ASP
1	B	832	ASP
1	B	862	ILE
1	C	228	LEU
1	C	260	ASN
1	C	382	LYS
1	C	421	ARG
1	C	819	ASP
1	C	832	ASP
1	D	382	LYS
1	D	421	ARG
1	D	819	ASP
1	D	832	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	142	HIS
1	A	407	HIS
1	A	408	GLN
1	A	640	HIS
1	B	213	HIS
1	B	737	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	49	ASN
1	D	106	HIS
1	D	142	HIS
1	D	566	GLN

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	862/886 (97%)	-0.14	36 (4%) 37 26	41, 61, 116, 158	0
1	B	854/886 (96%)	-0.16	39 (4%) 33 23	38, 55, 127, 170	0
1	C	864/886 (97%)	0.27	77 (8%) 10 5	51, 88, 144, 186	0
1	D	849/886 (95%)	0.22	60 (7%) 17 9	48, 89, 143, 185	0
2	E	46/46 (100%)	0.85	7 (15%) 2 1	108, 124, 143, 152	0
2	F	46/46 (100%)	2.09	21 (45%) 0 0	119, 142, 155, 167	0
All	All	3521/3636 (96%)	0.08	240 (6%) 18 10	38, 73, 140, 186	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	270	GLY	8.7
1	D	327	SER	8.4
1	D	271	ASN	8.2
1	B	271	ASN	7.8
1	C	48	VAL	7.7
1	B	400	ALA	7.3
1	C	47	GLY	7.2
1	B	268	VAL	6.9
1	C	8	VAL	6.8
1	C	46	GLY	6.4
1	D	321	ASP	6.3
1	A	7	ASP	6.0
1	D	261	LEU	5.9
1	A	29	VAL	5.8
1	C	6	ASN	5.7
1	D	30	GLU	5.7
1	C	399	ALA	5.7
1	D	410	LYS	5.6
2	F	152	LEU	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	399	ALA	5.4
1	B	5	PRO	5.4
1	B	542	GLY	5.3
1	B	320	GLY	5.3
1	D	272	GLY	5.3
1	D	400	ALA	5.1
1	A	556	TYR	5.0
1	B	327	SER	4.9
1	A	399	ALA	4.9
1	B	269	THR	4.9
1	C	10	PRO	4.8
2	F	142	VAL	4.8
2	F	139	LEU	4.8
2	F	147	ARG	4.8
1	C	413	ASN	4.7
1	B	556	TYR	4.7
1	C	49	ASN	4.7
1	A	5	PRO	4.6
1	D	28	GLY	4.5
1	B	270	GLY	4.5
1	D	325	PHE	4.5
1	C	542	GLY	4.4
1	C	400	ALA	4.4
1	A	37	ASP	4.3
2	F	164	ILE	4.2
1	C	9	ASP	4.2
1	C	410	LYS	4.1
1	B	324	THR	4.1
1	C	398	ASP	4.1
1	D	29	VAL	4.1
1	C	40	LEU	4.1
1	A	400	ALA	4.1
1	A	27	GLU	4.1
1	C	269	THR	4.1
1	D	780	LEU	4.1
1	C	265	ASP	4.0
1	C	414	MET	4.0
1	D	398	ASP	4.0
1	A	30	GLU	4.0
1	C	267	PRO	4.0
1	C	7	ASP	3.9
1	A	398	ASP	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	270	GLY	3.8
1	C	405	ILE	3.8
1	D	867	VAL	3.8
1	B	7	ASP	3.8
2	F	159	TYR	3.8
1	B	16	TRP	3.8
1	D	27	GLU	3.8
1	C	5	PRO	3.8
1	B	321	ASP	3.7
2	F	151	ILE	3.7
2	F	138	ASN	3.7
2	E	164	ILE	3.7
1	D	25	ARG	3.7
2	F	145	THR	3.7
1	B	272	GLY	3.6
1	A	44	ARG	3.6
1	A	28	GLY	3.6
1	A	50	VAL	3.6
1	A	407	HIS	3.6
1	C	53	GLY	3.5
1	B	543	GLN	3.5
1	B	323	GLN	3.5
1	D	407	HIS	3.5
1	C	411	LYS	3.4
1	B	34	TYR	3.4
1	A	39	LEU	3.4
1	C	11	ILE	3.4
1	B	399	ALA	3.4
2	F	162	GLU	3.4
2	E	167	ALA	3.4
1	D	731	SER	3.3
1	C	860	GLY	3.3
1	D	24	ILE	3.3
1	B	56	ILE	3.3
2	E	160	VAL	3.3
1	C	723	LYS	3.3
1	D	473	LEU	3.3
1	C	327	SER	3.3
1	D	323	GLN	3.3
1	A	6	ASN	3.2
1	D	859	ARG	3.2
1	D	412	MET	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	732	GLY	3.2
2	F	137	VAL	3.2
1	A	267	PRO	3.2
1	C	412	MET	3.2
1	A	26	GLU	3.2
1	C	54	THR	3.2
1	B	731	SER	3.1
1	D	48	VAL	3.1
1	A	36	ILE	3.1
1	C	52	ALA	3.1
1	C	336	HIS	3.1
1	C	752	GLY	3.1
1	B	27	GLU	3.1
1	B	6	ASN	3.0
1	A	20	ILE	3.0
2	F	141	LYS	3.0
1	C	332	TYR	3.0
1	D	55	GLY	2.9
1	D	864	LYS	2.9
1	D	487	GLU	2.9
1	C	25	ARG	2.9
1	B	17	LEU	2.9
1	D	31	ARG	2.9
1	B	555	TYR	2.9
1	B	49	ASN	2.8
1	D	490	LYS	2.8
1	C	264	LEU	2.8
1	B	20	ILE	2.8
1	C	724	GLY	2.8
1	D	320	GLY	2.7
1	A	557	LYS	2.7
1	D	322	TYR	2.7
1	B	10	PRO	2.7
2	F	165	LYS	2.7
1	C	266	GLY	2.7
2	F	133	ARG	2.7
1	C	780	LEU	2.7
2	F	158	ALA	2.7
1	D	33	GLN	2.7
1	C	433	ILE	2.6
1	C	44	ARG	2.6
1	A	49	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	41	ALA	2.6
1	B	800	SER	2.6
1	A	35	LEU	2.6
1	C	408	GLN	2.6
1	D	342	PRO	2.6
1	D	324	THR	2.6
1	A	40	LEU	2.6
1	C	524	ARG	2.6
1	C	140	GLN	2.6
1	C	39	LEU	2.6
1	C	865	LYS	2.6
1	A	264	LEU	2.5
1	D	40	LEU	2.5
1	C	262	GLN	2.5
1	A	558	GLU	2.5
1	C	409	VAL	2.5
1	A	32	ALA	2.5
1	C	731	SER	2.5
1	D	393	GLY	2.5
1	D	56	ILE	2.5
1	A	38	GLN	2.5
1	C	800	SER	2.4
1	A	25	ARG	2.4
1	D	865	LYS	2.4
1	D	751	VAL	2.4
1	B	730	GLY	2.4
1	C	24	ILE	2.4
1	D	472	LYS	2.4
1	A	8	VAL	2.4
1	B	13	THR	2.4
2	F	156	VAL	2.4
2	F	161	LYS	2.4
1	D	326	LYS	2.4
2	F	148	LYS	2.4
1	C	268	VAL	2.4
1	C	482	GLY	2.4
2	F	146	GLY	2.4
2	F	140	ALA	2.4
1	B	23	VAL	2.3
1	C	730	GLY	2.3
1	D	542	GLY	2.3
1	C	861	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	392	LYS	2.3
1	D	328	LYS	2.3
1	A	34	TYR	2.3
2	E	166	ARG	2.3
1	C	862	ILE	2.3
1	A	48	VAL	2.3
1	D	791	VAL	2.3
1	D	800	SER	2.3
1	D	730	GLY	2.3
1	D	411	LYS	2.3
1	A	414	MET	2.3
1	B	47	GLY	2.3
2	E	146	GLY	2.3
1	A	415	ASP	2.3
1	C	580	ALA	2.3
1	D	49	ASN	2.2
1	B	12	GLU	2.2
1	B	799	ALA	2.2
1	C	45	LYS	2.2
1	C	490	LYS	2.2
1	C	541	ASN	2.2
1	C	859	ARG	2.2
1	D	853	LEU	2.2
1	C	719	ILE	2.2
1	D	719	ILE	2.2
1	D	783	PRO	2.2
1	C	750	GLY	2.2
1	D	869	ASP	2.2
1	D	172	ASN	2.2
1	C	722	SER	2.2
1	C	328	LYS	2.2
1	D	34	TYR	2.2
1	A	24	ILE	2.1
2	E	135	PHE	2.1
1	C	32	ALA	2.1
2	F	122	VAL	2.1
1	D	659	ASP	2.1
1	C	271	ASN	2.1
1	D	725	LYS	2.1
1	C	430	ASP	2.1
1	B	808	ALA	2.1
1	B	30	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	481	PHE	2.1
1	C	783	PRO	2.1
1	D	857	ALA	2.0
1	C	55	GLY	2.0
1	B	8	VAL	2.0
1	C	533	ARG	2.0
2	E	161	LYS	2.0
1	C	263	ARG	2.0
1	D	746	ALA	2.0
1	C	113	SER	2.0
1	B	322	TYR	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 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.