



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:02 PM 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

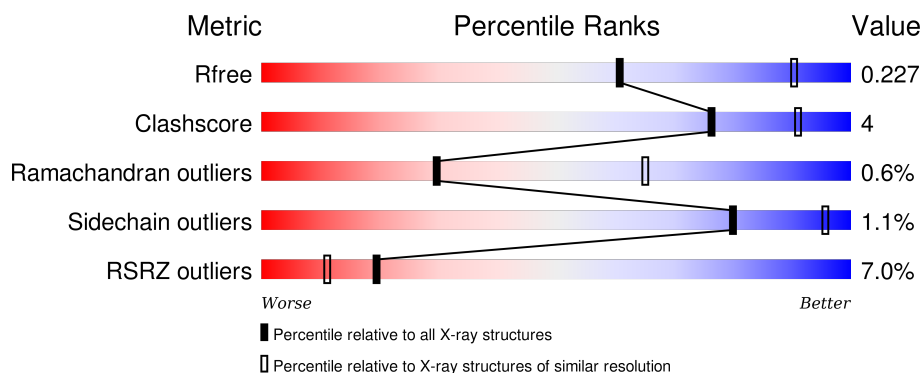
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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>5%</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>17%</div> <div>85%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	46	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: red (46%), green (83%), and yellow (17%). The percentages are labeled above the corresponding segments.

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			

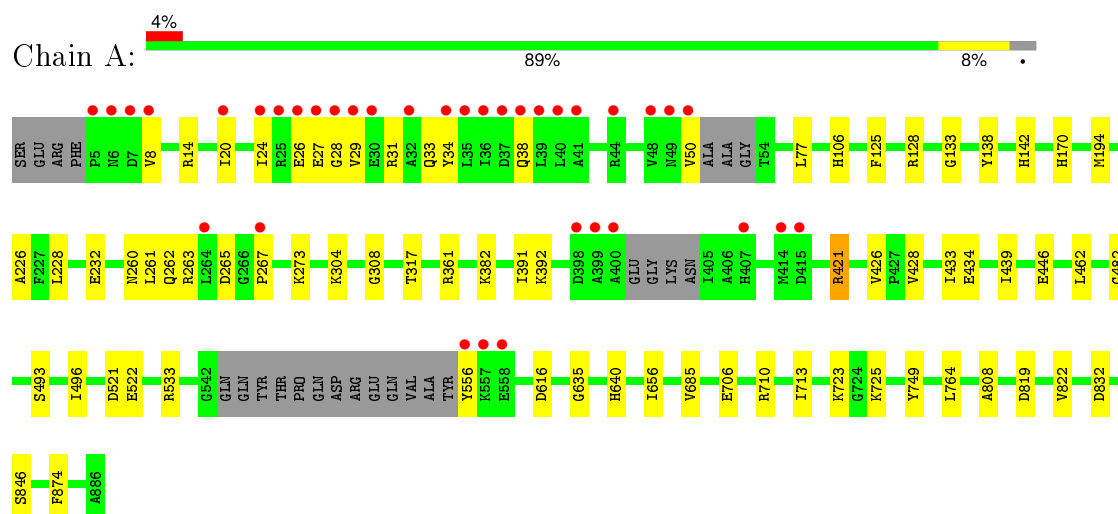
- Molecule 3 is water.

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		

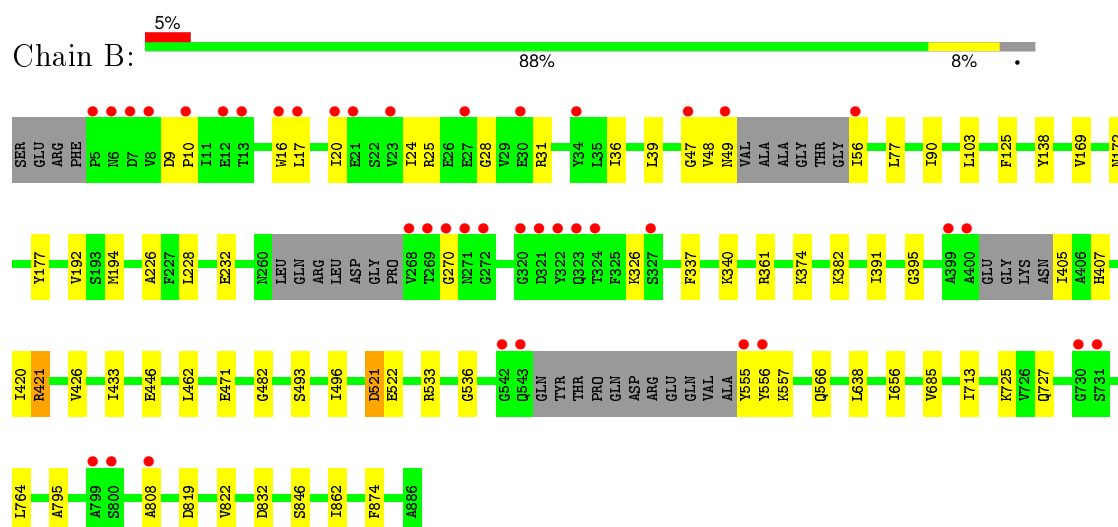
3 Residue-property plots [i](#)

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

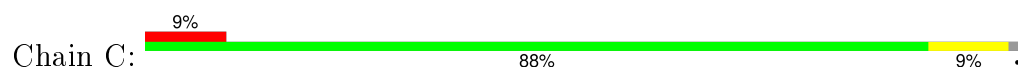
• Molecule 1: Pyruvate dehydrogenase E1 component

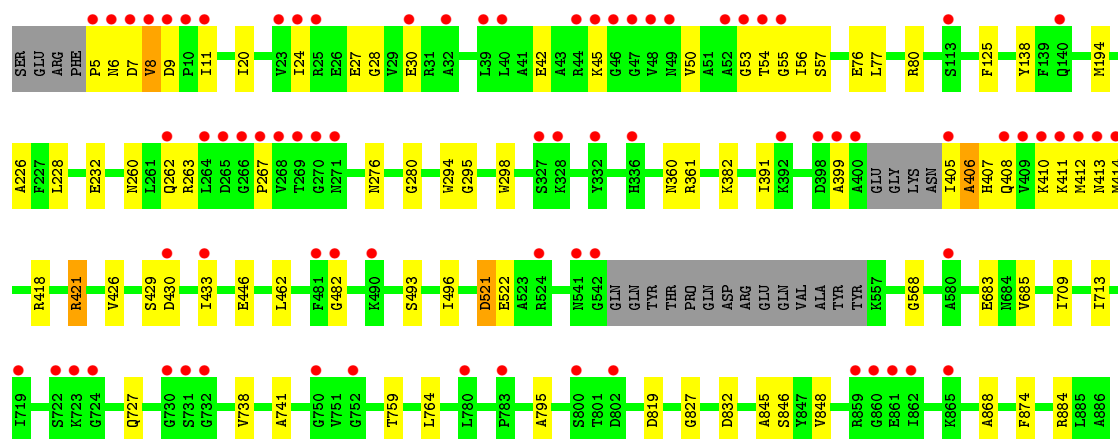


• Molecule 1: Pyruvate dehydrogenase E1 component

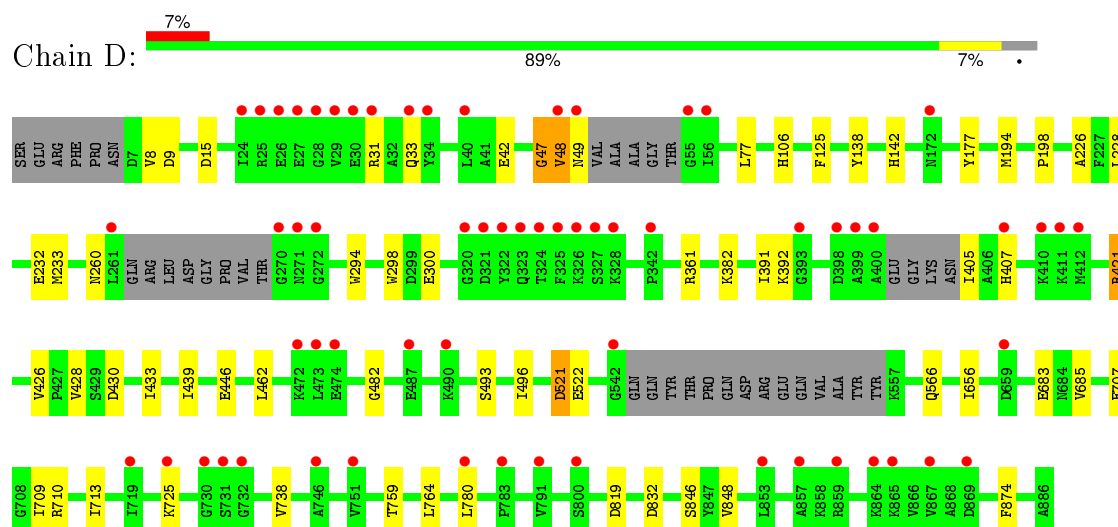


• Molecule 1: Pyruvate dehydrogenase E1 component

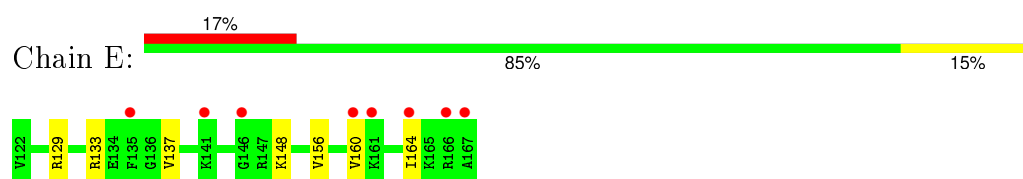




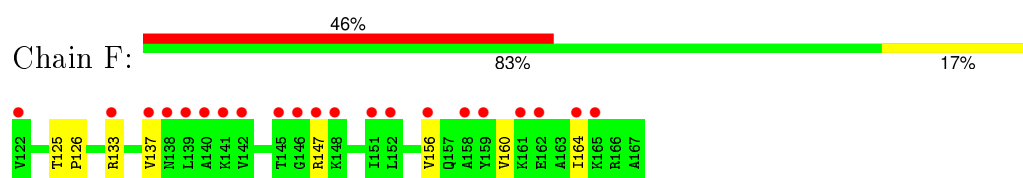
• Molecule 1: Pyruvate dehydrogenase E1 component



• 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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 124909 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.45	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

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

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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:D:15:ASP:HB3	2:F:125:THR:HG21	1.31	1.10
1:C:408:GLN:HB2	1:C:413:ASN:HB3	1.26	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

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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:C:408:GLN:HB2	1:C:413:ASN:CB	2.18	0.62
1:A:846:SER:HB2	1:A:874:PHE:HB3	1.80	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: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:B:395:GLY:O	1:B:420:ILE:HG22	2.03	0.58
1:D:228:LEU:HD22	1:D:232:GLU:CD	2.24	0.57
2:F:125:THR:HG23	2:F:126:PRO:HD2	1.86	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
1:D:683:GLU:HB3	1:D:685:VAL:HG12	1.87	0.56

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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
2:F:125:THR:CG2	2:F:126:PRO:HD2	2.35	0.55
1:A:656:ILE:CG1	1:A:685:VAL:CG1	2.84	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:D:194:MET:HB3	1:D:232:GLU:HG3	1.94	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:C:54:THR:O	1:C:54:THR:HG23	2.10	0.50

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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:405:ILE:C	1:C:407:HIS:H	2.13	0.50
1:C:194:MET:HB3	1:C:232:GLU:HG3	1.92	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:C:20:ILE:HD11	1:D:42:GLU:HB3	1.96	0.47
1:A:635:GLY:HA3	1:B:103:LEU:O	2.14	0.47
1:D:493:SER:H	1:D:496:ILE:HD12	1.79	0.47
1:A:125:PHE:HB3	1:A:462:LEU:HD13	1.96	0.47
1:A:194:MET:HB3	1:A:232:GLU:HG3	1.96	0.47
1:C:407:HIS:CE1	1:C:410:LYS:HZ2	2.31	0.47
1:C:125:PHE:HB3	1:C:462:LEU:HD13	1.96	0.47
1:A:77:LEU:HD21	1:A:446:GLU:HB3	1.95	0.47
1:A:656:ILE:CG1	1:A:685:VAL:HG11	2.44	0.47
1:D:707:GLU:HA	1:D:710:ARG:HH21	1.80	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:493:SER:H	1:B:496:ILE:HD12	1.81	0.46
1:B:20:ILE:HD11	1:B:36:ILE:HD11	1.98	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:20:ILE:HG21	1:B:39:LEU:HD21	1.97	0.45
1:A:361:ARG:HD2	1:A:391:ILE:HG13	1.98	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

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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:D:9:ASP:HB2	2:F:147:ARG:HD2	2.00	0.44
1:C:138:TYR:HB2	1:C:226:ALA:HA	2.00	0.44
1:D:228:LEU:HD13	1:D:233:MET:SD	2.58	0.44
1:A:434:GLU:HG3	3:A:1000:HOH:O	2.17	0.44
1:A:261:LEU:HD11	3:A:919:HOH:O	2.18	0.44
1:C:430:ASP:O	1:C:433:ILE:HG12	2.17	0.43
1:A:723:LYS:HD2	1:A:749:TYR:O	2.18	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
2:E:160:VAL:O	2:E:164:ILE:HG12	2.19	0.43
1:C:741:ALA:HB2	1:C:845:ALA:HA	2.00	0.43
1:B:138:TYR:HB2	1:B:226:ALA:HA	2.01	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:C:5:PRO:HA	1:C:6:ASN:HA	1.58	0.42
1:A:706:GLU:O	1:A:710:ARG:HG3	2.19	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:521:ASP:HA	1:B:566:GLN:OE1	2.21	0.41
1:B:361:ARG:HD2	1:B:391:ILE:HG13	2.02	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:C:406:ALA:C	1:C:408:GLN:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:GLY:HA3	1:B:557:LYS:HB2	2.02	0.41
1:A:128:ARG:HG3	1:A:133:GLY:HA2	2.02	0.41
1:A:170:HIS:HD2	3:B:985:HOH:O	2.04	0.41
1:D:656:ILE:CG1	1:D:685:VAL:HG21	2.51	0.41
1:B:471:GLU:HG2	3:B:1224:HOH:O	2.21	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:C:76:GLU:CD	1:C:80:ARG:HH21	2.24	0.40
1:A:808:ALA:HB3	1:A:822:VAL:HG13	2.04	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
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

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%)	39	74
1	B	844/886 (95%)	798 (94%)	40 (5%)	6 (1%)	26	62
1	C	858/886 (97%)	811 (94%)	41 (5%)	6 (1%)	26	62
1	D	839/886 (95%)	798 (95%)	35 (4%)	6 (1%)	26	62
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%)	30	65

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%)	76	94
1	B	710/735 (97%)	697 (98%)	13 (2%)	66	91
1	C	715/735 (97%)	709 (99%)	6 (1%)	86	97
1	D	704/735 (96%)	700 (99%)	4 (1%)	90	98
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%)	80	95

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

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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(Å²)	Q<0.9
1	A	862/886 (97%)	-0.13	36 (4%)	40	28	41, 61, 116, 158	0
1	B	854/886 (96%)	-0.15	40 (4%)	35	24	38, 55, 127, 170	0
1	C	864/886 (97%)	0.29	78 (9%)	12	6	51, 88, 144, 186	0
1	D	849/886 (95%)	0.23	63 (7%)	17	9	48, 89, 143, 185	0
2	E	46/46 (100%)	0.86	8 (17%)	2	1	108, 124, 143, 152	0
2	F	46/46 (100%)	2.11	21 (45%)	0	0	119, 142, 155, 167	0
All	All	3521/3636 (96%)	0.10	246 (6%)	19	11	38, 73, 140, 186	0

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	270	GLY	8.8
1	D	327	SER	8.6
1	D	271	ASN	8.4
1	B	271	ASN	8.0
1	C	48	VAL	7.8
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	D	321	ASP	6.5
1	C	46	GLY	6.4
1	A	7	ASP	6.2
1	D	261	LEU	6.0
1	C	6	ASN	5.9
1	A	29	VAL	5.9
1	D	30	GLU	5.8
1	D	410	LYS	5.7
2	F	152	LEU	5.6
1	C	399	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	5	PRO	5.5
1	B	542	GLY	5.4
1	B	320	GLY	5.3
1	D	399	ALA	5.3
1	D	272	GLY	5.3
1	A	556	TYR	5.1
1	D	400	ALA	5.1
1	B	327	SER	5.0
1	B	269	THR	5.0
1	C	10	PRO	5.0
1	C	413	ASN	4.9
1	C	49	ASN	4.9
1	A	399	ALA	4.9
2	F	139	LEU	4.9
1	B	556	TYR	4.9
2	F	142	VAL	4.9
1	A	5	PRO	4.8
2	F	147	ARG	4.6
1	D	325	PHE	4.6
1	D	28	GLY	4.6
1	B	270	GLY	4.6
1	C	542	GLY	4.4
1	A	37	ASP	4.4
1	C	400	ALA	4.3
1	C	9	ASP	4.3
2	F	164	ILE	4.3
1	B	324	THR	4.2
1	C	410	LYS	4.2
1	C	398	ASP	4.2
1	C	265	ASP	4.2
1	C	269	THR	4.2
1	A	27	GLU	4.2
1	D	398	ASP	4.2
1	C	40	LEU	4.1
1	C	414	MET	4.1
1	C	267	PRO	4.1
1	D	29	VAL	4.1
1	A	30	GLU	4.1
1	D	780	LEU	4.1
1	C	7	ASP	4.1
1	A	400	ALA	4.0
1	A	398	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	7	ASP	4.0
2	F	159	TYR	3.9
1	B	16	TRP	3.9
1	C	5	PRO	3.9
1	C	405	ILE	3.9
1	C	270	GLY	3.9
1	D	27	GLU	3.9
1	D	867	VAL	3.9
1	B	321	ASP	3.9
2	F	138	ASN	3.8
2	F	145	THR	3.8
2	F	151	ILE	3.8
2	E	164	ILE	3.7
1	B	272	GLY	3.7
1	A	28	GLY	3.6
1	A	407	HIS	3.6
1	B	543	GLN	3.6
1	A	50	VAL	3.6
1	B	323	GLN	3.6
1	C	53	GLY	3.6
1	C	411	LYS	3.5
1	D	407	HIS	3.5
1	B	34	TYR	3.5
1	D	25	ARG	3.5
1	A	39	LEU	3.5
2	F	162	GLU	3.5
1	A	44	ARG	3.5
1	C	11	ILE	3.4
1	D	731	SER	3.4
1	D	323	GLN	3.4
1	D	24	ILE	3.4
1	C	723	LYS	3.4
1	C	860	GLY	3.4
1	C	327	SER	3.4
1	B	56	ILE	3.4
1	A	6	ASN	3.4
1	B	399	ALA	3.3
1	D	473	LEU	3.3
2	E	160	VAL	3.3
1	A	267	PRO	3.3
2	E	167	ALA	3.3
1	D	412	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	412	MET	3.3
1	A	26	GLU	3.3
1	C	732	GLY	3.3
1	C	54	THR	3.3
2	F	137	VAL	3.2
1	B	731	SER	3.2
1	A	36	ILE	3.2
1	C	336	HIS	3.2
1	B	27	GLU	3.1
1	D	48	VAL	3.1
1	B	6	ASN	3.1
1	C	752	GLY	3.1
1	D	859	ARG	3.1
1	C	52	ALA	3.1
1	C	332	TYR	3.0
2	F	141	LYS	3.0
1	A	20	ILE	3.0
1	D	487	GLU	3.0
1	D	864	LYS	3.0
1	D	55	GLY	2.9
1	B	555	TYR	2.9
1	B	17	LEU	2.9
1	B	49	ASN	2.9
1	D	490	LYS	2.9
1	C	264	LEU	2.8
1	B	20	ILE	2.8
1	C	724	GLY	2.8
1	B	10	PRO	2.8
1	A	557	LYS	2.8
1	D	322	TYR	2.8
1	C	25	ARG	2.8
1	D	320	GLY	2.8
1	D	33	GLN	2.8
2	F	165	LYS	2.8
1	D	31	ARG	2.8
1	A	49	ASN	2.7
1	C	266	GLY	2.7
1	C	780	LEU	2.7
1	B	800	SER	2.7
1	C	408	GLN	2.7
1	D	342	PRO	2.7
1	C	433	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	324	THR	2.7
1	C	140	GLN	2.7
2	F	158	ALA	2.7
1	A	35	LEU	2.6
1	C	262	GLN	2.6
1	C	865	LYS	2.6
1	A	40	LEU	2.6
1	A	41	ALA	2.6
1	A	558	GLU	2.6
1	C	39	LEU	2.6
1	A	264	LEU	2.6
1	D	40	LEU	2.6
2	F	133	ARG	2.6
1	C	731	SER	2.6
1	A	38	GLN	2.5
1	C	44	ARG	2.5
1	C	409	VAL	2.5
1	D	393	GLY	2.5
1	C	800	SER	2.5
1	D	56	ILE	2.5
1	D	865	LYS	2.5
1	A	32	ALA	2.5
1	B	13	THR	2.5
1	D	472	LYS	2.5
1	C	524	ARG	2.5
1	B	730	GLY	2.5
1	C	24	ILE	2.4
2	F	161	LYS	2.4
1	D	751	VAL	2.4
1	D	326	LYS	2.4
1	A	8	VAL	2.4
2	F	148	LYS	2.4
1	C	861	GLU	2.4
2	F	156	VAL	2.4
1	C	392	LYS	2.4
1	C	482	GLY	2.4
2	F	146	GLY	2.4
1	D	328	LYS	2.4
1	C	730	GLY	2.4
1	D	542	GLY	2.4
1	A	34	TYR	2.4
1	C	268	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	23	VAL	2.4
1	D	800	SER	2.4
1	A	415	ASP	2.4
1	A	25	ARG	2.3
1	A	414	MET	2.3
2	F	140	ALA	2.3
1	C	862	ILE	2.3
1	D	411	LYS	2.3
1	D	49	ASN	2.3
1	A	48	VAL	2.3
1	D	791	VAL	2.3
1	D	730	GLY	2.3
1	C	541	ASN	2.3
1	B	47	GLY	2.3
2	E	146	GLY	2.3
1	B	12	GLU	2.3
1	D	783	PRO	2.3
1	C	45	LYS	2.3
1	C	490	LYS	2.3
1	D	869	ASP	2.3
1	D	172	ASN	2.2
1	C	580	ALA	2.2
1	D	853	LEU	2.2
2	E	166	ARG	2.2
1	C	719	ILE	2.2
1	D	719	ILE	2.2
1	C	722	SER	2.2
1	C	750	GLY	2.2
1	C	328	LYS	2.2
1	D	34	TYR	2.2
1	B	799	ALA	2.2
1	D	659	ASP	2.2
1	C	271	ASN	2.2
2	E	135	PHE	2.2
1	A	24	ILE	2.2
1	C	430	ASP	2.2
1	D	725	LYS	2.1
1	B	30	GLU	2.1
1	C	783	PRO	2.1
2	F	122	VAL	2.1
1	C	859	ARG	2.1
1	C	32	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	481	PHE	2.1
2	E	161	LYS	2.1
1	C	55	GLY	2.1
1	C	113	SER	2.1
1	D	474	GLU	2.1
1	B	322	TYR	2.1
1	D	26	GLU	2.1
1	B	8	VAL	2.1
1	B	808	ALA	2.1
1	D	857	ALA	2.0
1	D	732	GLY	2.0
2	E	141	LYS	2.0
1	B	21	GLU	2.0
1	C	30	GLU	2.0
1	C	802	ASP	2.0
1	C	23	VAL	2.0
1	D	746	ALA	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.