Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:49 AM GMT

PDB ID	:	2UVD
Title	:	THE CRYSTAL STRUCTURE OF A 3-OXOACYL-(ACYL CARRIER PROTEIN) REDUCTASE FROM BACILLUS ANTHRACIS (BA3989)
Authors	:	Zaccai, N.R.; Carter, L.G.; Berrow, N.S.; Sainsbury, S.; Nettleship, J.E.; Walter, T.S.; Harlos, K.; Owens, R.J.; Wilson, K.S.; Stuart, D.I.; Esnouf, R.M.; Oxford Protein Production Facility (Oppf); Structural Proteomics in Europe (Spine)
Deposited on	:	2007-03-09
Resolution	:	2.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

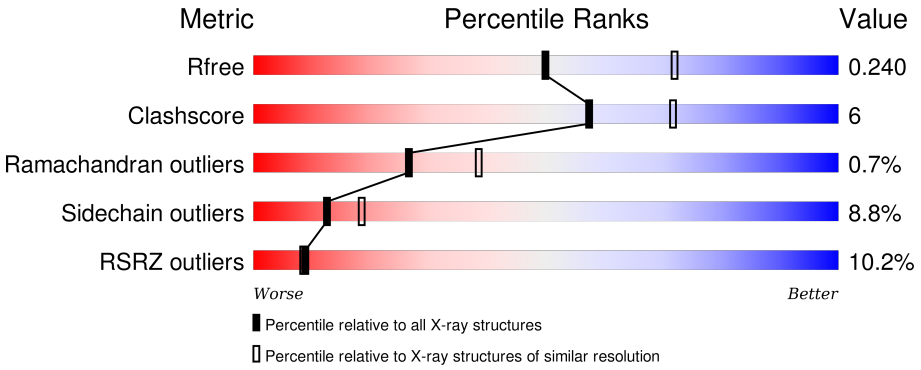
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 <=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	246	13% 83% 13%
1	B	246	11% 87% 11%
1	C	246	11% 83% 16%
1	D	246	10% 85% 13%
1	E	246	9% 78% 17%

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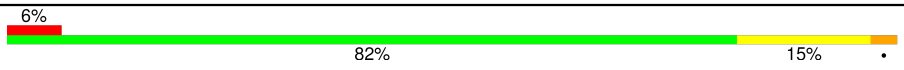
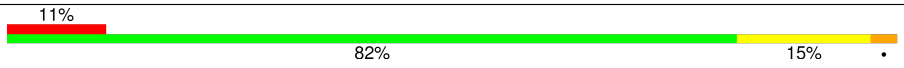
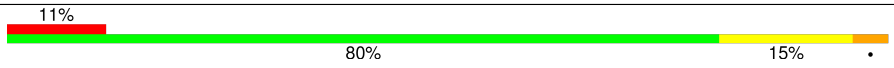
Mol	Chain	Length	Quality of chain
1	F	246	
1	G	246	
1	H	246	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15199 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 3-OXOACYL-(ACYL-CARRIER-PROTEIN) REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1828	1140	322	355	11			
1	B	246	Total	C	N	O	S	0	0	0
			1828	1140	322	355	11			
1	C	246	Total	C	N	O	S	0	0	0
			1828	1140	322	355	11			
1	D	246	Total	C	N	O	S	0	0	0
			1828	1140	322	355	11			
1	E	246	Total	C	N	O	S	0	0	0
			1828	1140	322	355	11			
1	F	246	Total	C	N	O	S	0	0	0
			1828	1140	322	355	11			
1	G	246	Total	C	N	O	S	0	0	0
			1828	1140	322	355	11			
1	H	246	Total	C	N	O	S	0	0	0
			1828	1140	322	355	11			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	84	Total	O	0	0
			84	84		
2	B	93	Total	O	0	0
			93	93		
2	C	60	Total	O	0	0
			60	60		
2	D	75	Total	O	0	0
			75	75		
2	E	96	Total	O	0	0
			96	96		
2	F	65	Total	O	0	0
			65	65		

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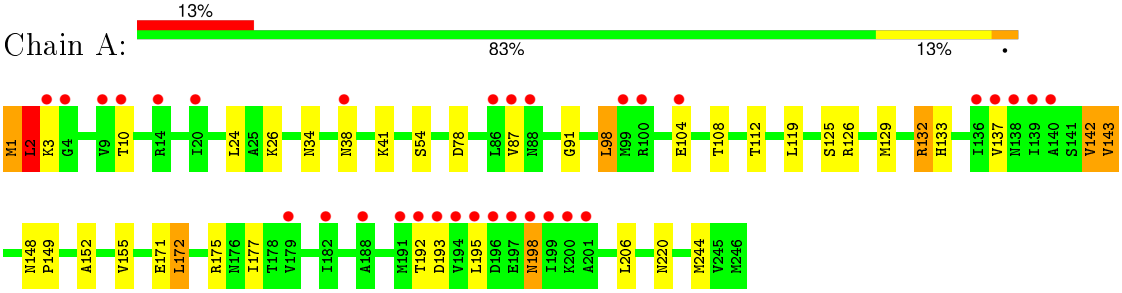
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	47	Total O 47 47	0	0
2	H	55	Total O 55 55	0	0

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.

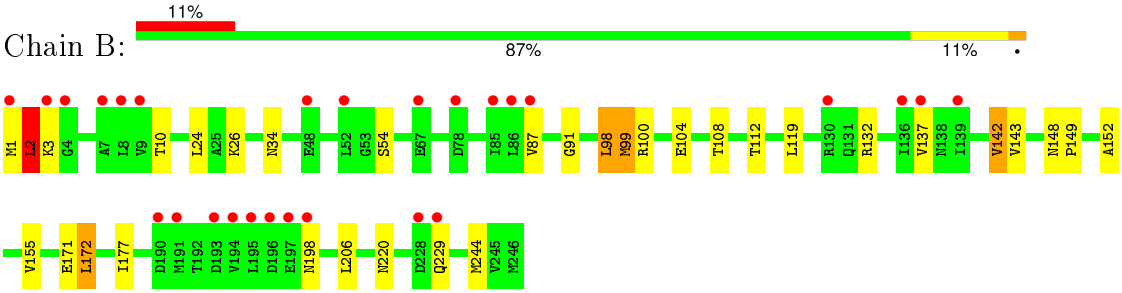
- Molecule 1: 3-OXOACYL-(ACYL-CARRIER-PROTEIN) REDUCTASE

Chain A:



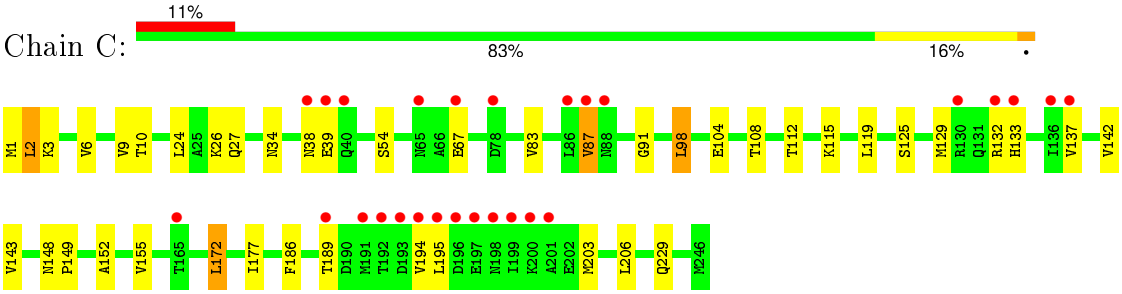
- Molecule 1: 3-OXOACYL-(ACYL-CARRIER-PROTEIN) REDUCTASE

Chain B:



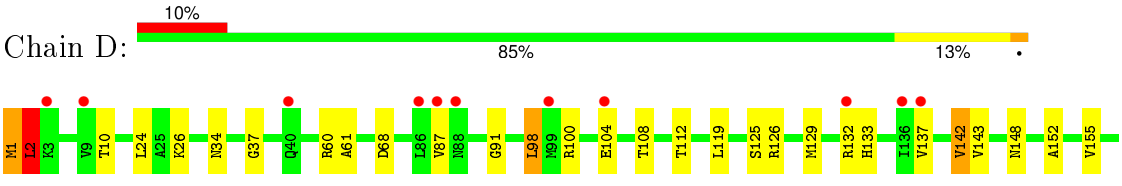
- Molecule 1: 3-OXOACYL-(ACYL-CARRIER-PROTEIN) REDUCTASE

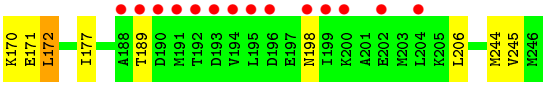
Chain C:



- Molecule 1: 3-OXOACYL-(ACYL-CARRIER-PROTEIN) REDUCTASE

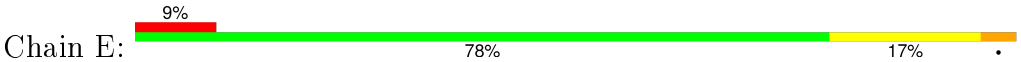
Chain D:

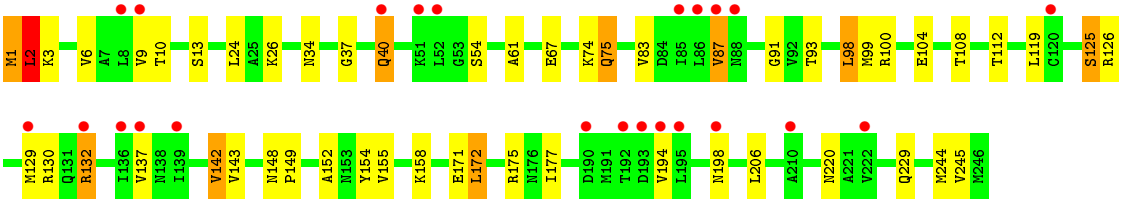




• Molecule 1: 3-OXOACYL-(ACYL-CARRIER-PROTEIN) REDUCTASE

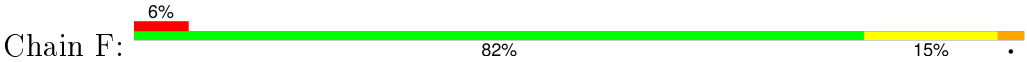
Chain E:

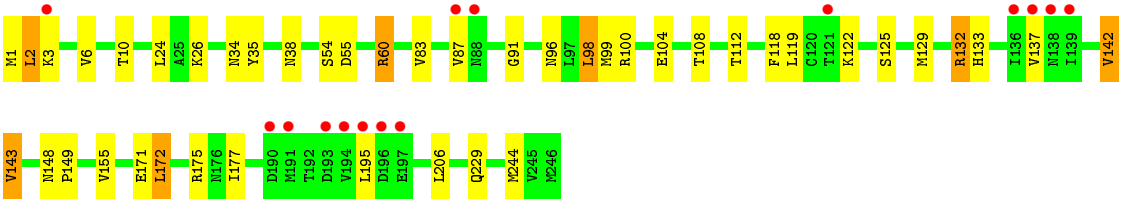




• Molecule 1: 3-OXOACYL-(ACYL-CARRIER-PROTEIN) REDUCTASE

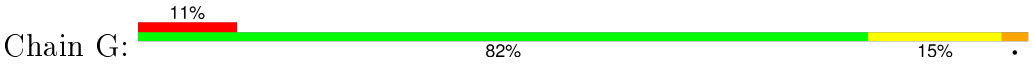
Chain F:

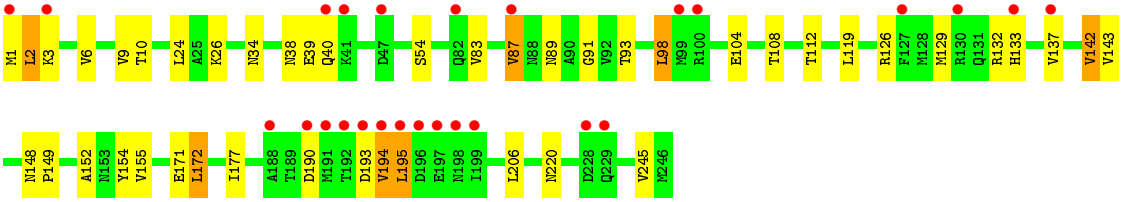




• Molecule 1: 3-OXOACYL-(ACYL-CARRIER-PROTEIN) REDUCTASE

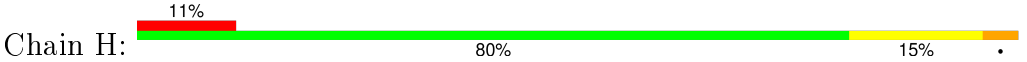
Chain G:

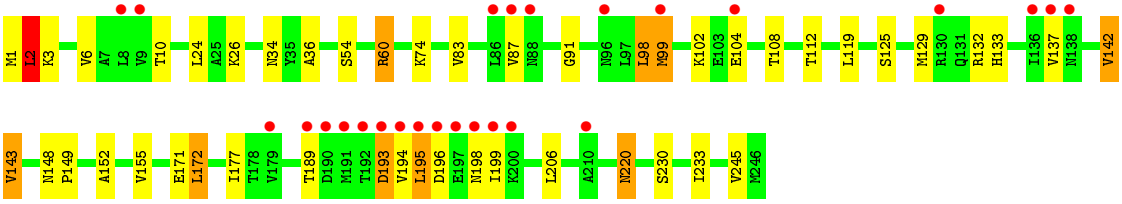




• Molecule 1: 3-OXOACYL-(ACYL-CARRIER-PROTEIN) REDUCTASE

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.62Å 120.65Å 136.38Å 90.00° 104.42° 90.00°	Depositor
Resolution (Å)	27.77 – 2.40 27.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.0 (27.77-2.40) 94.0 (27.76-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.180 , 0.225 0.204 , 0.240	Depositor DCC
R_{free} test set	4131 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.6	EDS
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 81329 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15199	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.62	0/1843	0.71	0/2489
1	B	0.64	0/1843	0.74	1/2489 (0.0%)
1	C	0.59	0/1843	0.70	0/2489
1	D	0.58	0/1843	0.70	0/2489
1	E	0.67	1/1843 (0.1%)	0.72	0/2489
1	F	0.62	0/1843	0.73	1/2489 (0.0%)
1	G	0.59	0/1843	0.69	0/2489
1	H	0.60	0/1843	0.70	0/2489
All	All	0.61	1/14744 (0.0%)	0.71	2/19912 (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	A	0	1
1	D	0	1
1	E	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	75	GLN	CD-NE2	-5.36	1.19	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	98	LEU	CB-CG-CD2	6.42	121.91	111.00
1	B	99	MET	CA-CB-CG	5.04	121.87	113.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide
1	D	1	MET	Peptide
1	E	1	MET	Peptide

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	1828	0	1880	22	0
1	B	1828	0	1880	19	0
1	C	1828	0	1880	21	0
1	D	1828	0	1880	19	0
1	E	1828	0	1880	40	0
1	F	1828	0	1880	24	1
1	G	1828	0	1880	25	0
1	H	1828	0	1880	28	1
2	A	84	0	0	3	0
2	B	93	0	0	3	0
2	C	60	0	0	1	0
2	D	75	0	0	1	0
2	E	96	0	0	5	0
2	F	65	0	0	1	0
2	G	47	0	0	0	0
2	H	55	0	0	3	0
All	All	15199	0	15040	179	1

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 6.

All (179) 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:104:GLU:OE1	1:E:75:GLN:OE1	1.68	1.08
1:E:129:MET:SD	1:F:99:MET:SD	2.52	1.07
1:C:143:VAL:HG13	1:C:155:VAL:HG22	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:GLU:O	1:H:108:THR:HG22	1.69	0.93
1:B:143:VAL:HG13	1:B:155:VAL:HG22	1.50	0.93
1:E:229:GLN:HB3	1:H:220:ASN:OD1	1.70	0.91
1:E:143:VAL:HG13	1:E:155:VAL:HG22	1.53	0.91
1:G:143:VAL:HG13	1:G:155:VAL:HG22	1.51	0.91
1:A:143:VAL:HG13	1:A:155:VAL:HG22	1.54	0.90
1:D:143:VAL:HG13	1:D:155:VAL:HG22	1.54	0.89
1:H:143:VAL:HG13	1:H:155:VAL:HG22	1.53	0.89
1:F:143:VAL:HG13	1:F:155:VAL:HG22	1.54	0.88
1:A:104:GLU:O	1:A:108:THR:HG22	1.73	0.86
1:C:104:GLU:O	1:C:108:THR:HG22	1.75	0.86
1:D:104:GLU:O	1:D:108:THR:HG22	1.77	0.85
1:E:132:ARG:HG3	1:E:175:ARG:CZ	2.09	0.82
1:H:104:GLU:OE2	2:H:2024:HOH:O	1.98	0.81
1:B:104:GLU:O	1:B:108:THR:HG22	1.80	0.81
1:F:104:GLU:O	1:F:108:THR:HG22	1.80	0.81
1:E:104:GLU:O	1:E:108:THR:HG22	1.81	0.79
1:C:149:PRO:O	1:D:171:GLU:OE2	2.00	0.79
1:F:1:MET:O	1:F:3:LYS:N	2.18	0.77
1:C:143:VAL:HG22	1:C:148:ASN:HB2	1.67	0.77
1:G:104:GLU:O	1:G:108:THR:HG22	1.85	0.76
1:H:143:VAL:HG22	1:H:148:ASN:HB2	1.67	0.76
1:A:143:VAL:HG22	1:A:148:ASN:HB2	1.67	0.76
1:F:143:VAL:HG22	1:F:148:ASN:HB2	1.68	0.76
1:G:143:VAL:HG22	1:G:148:ASN:HB2	1.68	0.75
1:B:143:VAL:HG22	1:B:148:ASN:HB2	1.70	0.74
1:A:78:ASP:OD1	2:A:2027:HOH:O	2.05	0.73
1:A:149:PRO:O	1:B:171:GLU:OE2	2.05	0.73
1:C:1:MET:O	1:C:27:GLN:O	2.07	0.72
1:D:143:VAL:HG22	1:D:148:ASN:HB2	1.73	0.71
1:E:143:VAL:HG22	1:E:148:ASN:HB2	1.73	0.71
1:G:129:MET:SD	1:H:99:MET:HE3	2.33	0.69
1:E:149:PRO:O	1:F:171:GLU:OE2	2.10	0.69
1:E:132:ARG:CG	1:E:175:ARG:CZ	2.71	0.68
1:E:132:ARG:HG3	1:E:175:ARG:NH2	2.11	0.64
1:E:132:ARG:HD2	1:E:175:ARG:NH1	2.12	0.64
1:G:149:PRO:O	1:H:171:GLU:OE2	2.15	0.64
1:A:193:ASP:O	1:A:195:LEU:HD22	1.98	0.62
1:H:74:LYS:NZ	2:H:2019:HOH:O	2.22	0.62
1:G:171:GLU:OE2	1:H:149:PRO:O	2.20	0.59
1:E:171:GLU:OE2	1:F:149:PRO:O	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:MET:HA	1:F:122:LYS:HG3	1.84	0.59
1:E:132:ARG:CD	1:E:175:ARG:NH1	2.67	0.58
1:B:229:GLN:HB2	2:B:2079:HOH:O	2.04	0.58
1:G:193:ASP:O	1:G:195:LEU:HD23	2.05	0.57
1:H:1:MET:O	1:H:3:LYS:N	2.29	0.56
1:G:193:ASP:O	1:G:195:LEU:N	2.39	0.56
1:H:125:SER:O	1:H:129:MET:HG3	2.05	0.56
1:F:132:ARG:HG3	1:F:175:ARG:NH2	2.21	0.56
1:D:125:SER:O	1:D:129:MET:HG3	2.04	0.56
1:B:1:MET:O	1:B:3:LYS:N	2.38	0.55
1:B:91:GLY:HA2	1:B:112:THR:HG22	1.88	0.55
1:E:132:ARG:CD	1:E:175:ARG:CZ	2.84	0.55
1:E:130:ARG:NH1	2:E:2054:HOH:O	2.40	0.55
1:G:129:MET:SD	1:H:99:MET:CE	2.96	0.54
1:H:91:GLY:HA2	1:H:112:THR:HG22	1.90	0.54
1:H:193:ASP:O	1:H:195:LEU:N	2.41	0.54
1:C:125:SER:O	1:C:129:MET:HG3	2.07	0.54
1:E:98:LEU:HD22	1:E:152:ALA:CB	2.37	0.53
1:H:98:LEU:HD22	1:H:152:ALA:HB2	1.91	0.53
1:A:91:GLY:HA2	1:A:112:THR:HG22	1.91	0.53
1:C:91:GLY:HA2	1:C:112:THR:HG22	1.90	0.53
1:D:37:GLY:O	1:D:60:ARG:NH1	2.41	0.52
1:F:91:GLY:HA2	1:F:112:THR:HG22	1.90	0.52
1:G:143:VAL:HG13	1:G:155:VAL:CG2	2.33	0.52
1:F:132:ARG:NH2	2:F:2037:HOH:O	2.42	0.52
1:G:98:LEU:HD22	1:G:152:ALA:HB2	1.92	0.52
1:H:98:LEU:HD22	1:H:152:ALA:CB	2.40	0.52
1:H:196:ASP:HB3	1:H:199:ILE:HD12	1.90	0.52
1:B:98:LEU:HD22	1:B:152:ALA:CB	2.40	0.51
1:A:132:ARG:NH2	2:A:2050:HOH:O	2.43	0.51
1:E:132:ARG:HD2	1:E:175:ARG:CZ	2.39	0.51
1:G:172:LEU:HB3	1:G:177:ILE:HB	1.93	0.51
1:F:172:LEU:HB3	1:F:177:ILE:HB	1.93	0.51
1:F:35:TYR:CZ	1:F:60:ARG:HB3	2.45	0.51
1:C:143:VAL:HG13	1:C:155:VAL:CG2	2.34	0.51
1:D:91:GLY:HA2	1:D:112:THR:HG22	1.92	0.50
1:B:143:VAL:HG13	1:B:155:VAL:CG2	2.31	0.50
1:F:1:MET:HG3	1:F:1:MET:O	2.12	0.50
1:C:98:LEU:HD22	1:C:152:ALA:HB2	1.93	0.50
1:G:1:MET:O	1:G:3:LYS:N	2.45	0.50
1:C:1:MET:O	1:C:3:LYS:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:THR:HA	1:C:34:ASN:HB3	1.94	0.50
1:A:172:LEU:HB3	1:A:177:ILE:HB	1.93	0.49
1:F:35:TYR:O	1:F:60:ARG:HA	2.11	0.49
1:A:98:LEU:HD22	1:A:152:ALA:CB	2.42	0.49
1:A:98:LEU:HD22	1:A:152:ALA:HB2	1.95	0.49
1:E:172:LEU:HB3	1:E:177:ILE:HB	1.95	0.49
1:E:10:THR:HA	1:E:34:ASN:HB3	1.95	0.49
1:H:172:LEU:HB3	1:H:177:ILE:HB	1.95	0.49
1:B:220:ASN:HB2	2:B:2072:HOH:O	2.12	0.48
1:A:171:GLU:OE2	1:B:149:PRO:O	2.30	0.48
1:B:10:THR:HA	1:B:34:ASN:HB3	1.95	0.48
1:F:10:THR:HA	1:F:34:ASN:HB3	1.95	0.48
1:A:10:THR:HA	1:A:34:ASN:HB3	1.95	0.48
1:A:38:ASN:HD22	1:A:41:LYS:HG3	1.77	0.48
1:C:172:LEU:HB3	1:C:177:ILE:HB	1.94	0.48
1:E:40:GLN:OE1	2:E:2013:HOH:O	2.20	0.48
1:C:98:LEU:HD22	1:C:152:ALA:CB	2.44	0.48
1:D:10:THR:HA	1:D:34:ASN:HB3	1.96	0.48
1:G:10:THR:HA	1:G:34:ASN:HB3	1.95	0.48
1:A:132:ARG:HG3	1:A:175:ARG:NH2	2.28	0.47
1:A:220:ASN:HB2	2:A:2067:HOH:O	2.14	0.47
1:B:172:LEU:HB3	1:B:177:ILE:HB	1.96	0.47
1:D:98:LEU:HD22	1:D:152:ALA:HB2	1.96	0.47
1:E:74:LYS:NZ	2:E:2034:HOH:O	2.47	0.47
1:G:98:LEU:HD22	1:G:152:ALA:CB	2.44	0.47
1:D:98:LEU:HD22	1:D:152:ALA:CB	2.45	0.47
1:G:142:VAL:HG13	1:G:245:VAL:HG21	1.97	0.47
1:D:172:LEU:HB3	1:D:177:ILE:HB	1.96	0.47
1:E:98:LEU:HD22	1:E:152:ALA:HB2	1.96	0.46
1:E:2:LEU:H	1:E:2:LEU:HD13	1.79	0.46
1:E:13:SER:OG	2:E:2003:HOH:O	2.20	0.46
1:D:142:VAL:HG13	1:D:245:VAL:HG21	1.97	0.46
1:H:189:THR:HG23	2:H:2043:HOH:O	2.13	0.46
1:H:10:THR:HA	1:H:34:ASN:HB3	1.96	0.46
1:D:1:MET:HG3	1:D:1:MET:O	2.14	0.46
1:A:125:SER:O	1:A:129:MET:HG3	2.15	0.46
1:G:91:GLY:HA2	1:G:112:THR:HG22	1.97	0.46
1:E:125:SER:O	1:E:129:MET:HG3	2.15	0.46
1:B:1:MET:CG	1:B:1:MET:O	2.64	0.46
1:B:104:GLU:CD	1:E:75:GLN:OE1	2.46	0.46
1:A:142:VAL:HG11	1:A:244:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:142:VAL:HG13	1:H:245:VAL:HG21	1.97	0.46
1:B:98:LEU:HD22	1:B:152:ALA:HB2	1.98	0.45
1:B:142:VAL:HG11	1:B:244:MET:HE2	1.98	0.45
1:E:98:LEU:HD13	1:F:118:PHE:CE1	2.52	0.45
1:E:132:ARG:HG3	1:E:175:ARG:NE	2.31	0.45
1:A:1:MET:O	1:A:3:LYS:N	2.45	0.45
1:E:6:VAL:HG22	1:E:83:VAL:HA	1.99	0.45
1:C:9:VAL:HG22	1:C:87:VAL:HG13	1.98	0.45
1:E:1:MET:O	1:E:3:LYS:N	2.43	0.44
1:F:6:VAL:HG22	1:F:83:VAL:HA	2.00	0.44
1:H:2:LEU:H	1:H:2:LEU:HD13	1.82	0.44
1:F:125:SER:O	1:F:129:MET:HG3	2.17	0.44
1:E:158:LYS:NZ	2:E:2063:HOH:O	2.49	0.44
1:C:6:VAL:HG22	1:C:83:VAL:HA	1.99	0.44
1:F:229:GLN:HB3	1:G:220:ASN:ND2	2.33	0.44
1:A:192:THR:O	1:A:195:LEU:HD21	2.18	0.43
1:G:9:VAL:HG22	1:G:87:VAL:HG13	2.00	0.43
1:F:143:VAL:HG13	1:F:155:VAL:CG2	2.36	0.43
1:C:149:PRO:HD3	1:D:170:LYS:HD3	2.00	0.43
1:H:6:VAL:HG22	1:H:83:VAL:HA	1.99	0.43
1:G:126:ARG:HG2	1:H:99:MET:HE2	2.01	0.42
1:H:230:SER:HB2	1:H:233:ILE:HD12	2.01	0.42
1:B:2:LEU:HD13	1:B:2:LEU:H	1.85	0.42
1:F:142:VAL:HG11	1:F:244:MET:HE2	2.01	0.42
1:D:143:VAL:HG13	1:D:155:VAL:CG2	2.37	0.42
1:H:196:ASP:CB	1:H:199:ILE:HD12	2.49	0.42
1:D:2:LEU:HD13	1:D:2:LEU:H	1.85	0.42
1:F:132:ARG:CG	1:F:175:ARG:NH2	2.83	0.42
1:D:61:ALA:HB1	1:D:68:ASP:HB3	2.02	0.42
1:E:91:GLY:HA2	1:E:112:THR:HG22	2.01	0.42
1:H:36:ALA:O	1:H:60:ARG:HD3	2.20	0.42
1:E:132:ARG:NE	1:E:175:ARG:NH1	2.68	0.41
1:G:126:ARG:CG	1:H:99:MET:HE2	2.50	0.41
1:C:186:PHE:CZ	1:C:203:MET:HE3	2.55	0.41
1:F:100:ARG:HA	1:F:100:ARG:HD3	1.91	0.41
1:C:194:VAL:O	1:C:195:LEU:HD22	2.20	0.41
1:E:93:THR:HG22	1:E:154:TYR:CD1	2.55	0.41
1:C:115:LYS:HB2	2:C:2030:HOH:O	2.19	0.41
1:E:9:VAL:HG22	1:E:87:VAL:HG13	2.03	0.41
1:C:186:PHE:CE1	1:C:203:MET:HE3	2.55	0.41
1:G:194:VAL:O	1:G:194:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG13	1:A:155:VAL:CG2	2.36	0.41
1:E:34:ASN:ND2	1:E:61:ALA:HB3	2.36	0.41
1:G:10:THR:O	1:G:89:ASN:HB3	2.21	0.41
1:G:6:VAL:HG22	1:G:83:VAL:HA	2.03	0.41
2:B:2075:HOH:O	1:C:229:GLN:HB2	2.20	0.41
1:E:142:VAL:HG11	1:E:244:MET:HE2	2.02	0.40
1:A:2:LEU:H	1:A:2:LEU:HD13	1.86	0.40
1:D:133:HIS:HB2	2:D:2042:HOH:O	2.20	0.40
1:E:67:GLU:H	1:E:67:GLU:CD	2.24	0.40
1:E:142:VAL:HG13	1:E:245:VAL:HG21	2.03	0.40
1:D:142:VAL:HG11	1:D:244:MET:HE2	2.02	0.40
1:G:93:THR:HG22	1:G:154:TYR:CD1	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:ASP:CB	1:H:102:LYS:NZ[2_746]	2.02	0.18

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	244/246 (99%)	231 (95%)	11 (4%)	2 (1%)	24	35
1	B	244/246 (99%)	235 (96%)	8 (3%)	1 (0%)	39	56
1	C	244/246 (99%)	232 (95%)	11 (4%)	1 (0%)	39	56
1	D	244/246 (99%)	234 (96%)	9 (4%)	1 (0%)	39	56
1	E	244/246 (99%)	232 (95%)	9 (4%)	3 (1%)	16	23
1	F	244/246 (99%)	231 (95%)	12 (5%)	1 (0%)	39	56
1	G	244/246 (99%)	232 (95%)	10 (4%)	2 (1%)	24	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	244/246 (99%)	231 (95%)	10 (4%)	3 (1%)	16 23
All	All	1952/1968 (99%)	1858 (95%)	80 (4%)	14 (1%)	26 38

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	B	2	LEU
1	C	2	LEU
1	D	2	LEU
1	E	2	LEU
1	F	2	LEU
1	G	2	LEU
1	G	194	VAL
1	H	2	LEU
1	H	194	VAL
1	H	193	ASP
1	E	194	VAL
1	A	198	ASN
1	E	37	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	193/193 (100%)	177 (92%)	16 (8%)	14 21
1	B	193/193 (100%)	178 (92%)	15 (8%)	16 24
1	C	193/193 (100%)	176 (91%)	17 (9%)	12 18
1	D	193/193 (100%)	178 (92%)	15 (8%)	16 24
1	E	193/193 (100%)	175 (91%)	18 (9%)	11 16
1	F	193/193 (100%)	175 (91%)	18 (9%)	11 16
1	G	193/193 (100%)	175 (91%)	18 (9%)	11 16
1	H	193/193 (100%)	174 (90%)	19 (10%)	10 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1544/1544 (100%)	1408 (91%)	136 (9%)	12 18

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	24	LEU
1	A	26	LYS
1	A	54	SER
1	A	87	VAL
1	A	98	LEU
1	A	119	LEU
1	A	126	ARG
1	A	132	ARG
1	A	133	HIS
1	A	137	VAL
1	A	142	VAL
1	A	143	VAL
1	A	172	LEU
1	A	198	ASN
1	A	206	LEU
1	B	2	LEU
1	B	24	LEU
1	B	26	LYS
1	B	54	SER
1	B	87	VAL
1	B	98	LEU
1	B	99	MET
1	B	100	ARG
1	B	119	LEU
1	B	132	ARG
1	B	137	VAL
1	B	142	VAL
1	B	172	LEU
1	B	198	ASN
1	B	206	LEU
1	C	2	LEU
1	C	24	LEU
1	C	26	LYS
1	C	38	ASN
1	C	39	GLU
1	C	54	SER

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Mol	Chain	Res	Type
1	C	67	GLU
1	C	87	VAL
1	C	98	LEU
1	C	119	LEU
1	C	132	ARG
1	C	133	HIS
1	C	137	VAL
1	C	142	VAL
1	C	172	LEU
1	C	189	THR
1	C	206	LEU
1	D	2	LEU
1	D	24	LEU
1	D	26	LYS
1	D	87	VAL
1	D	98	LEU
1	D	100	ARG
1	D	119	LEU
1	D	126	ARG
1	D	132	ARG
1	D	137	VAL
1	D	142	VAL
1	D	172	LEU
1	D	189	THR
1	D	198	ASN
1	D	206	LEU
1	E	2	LEU
1	E	24	LEU
1	E	26	LYS
1	E	40	GLN
1	E	54	SER
1	E	87	VAL
1	E	98	LEU
1	E	100	ARG
1	E	119	LEU
1	E	125	SER
1	E	126	ARG
1	E	132	ARG
1	E	137	VAL
1	E	142	VAL
1	E	172	LEU
1	E	198	ASN

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Mol	Chain	Res	Type
1	E	206	LEU
1	E	220	ASN
1	F	2	LEU
1	F	24	LEU
1	F	26	LYS
1	F	38	ASN
1	F	54	SER
1	F	60	ARG
1	F	87	VAL
1	F	96	ASN
1	F	98	LEU
1	F	119	LEU
1	F	132	ARG
1	F	133	HIS
1	F	137	VAL
1	F	142	VAL
1	F	143	VAL
1	F	172	LEU
1	F	195	LEU
1	F	206	LEU
1	G	2	LEU
1	G	24	LEU
1	G	26	LYS
1	G	38	ASN
1	G	39	GLU
1	G	40	GLN
1	G	54	SER
1	G	87	VAL
1	G	98	LEU
1	G	119	LEU
1	G	132	ARG
1	G	133	HIS
1	G	137	VAL
1	G	142	VAL
1	G	172	LEU
1	G	190	ASP
1	G	195	LEU
1	G	206	LEU
1	H	2	LEU
1	H	24	LEU
1	H	26	LYS
1	H	54	SER

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Mol	Chain	Res	Type
1	H	60	ARG
1	H	87	VAL
1	H	98	LEU
1	H	99	MET
1	H	119	LEU
1	H	132	ARG
1	H	133	HIS
1	H	137	VAL
1	H	142	VAL
1	H	143	VAL
1	H	172	LEU
1	H	195	LEU
1	H	198	ASN
1	H	206	LEU
1	H	220	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	B	75	GLN
1	E	75	GLN
1	F	75	GLN
1	G	220	ASN
1	H	216	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	246/246 (100%)	0.75	32 (13%) 5 4	46, 57, 86, 116	0
1	B	246/246 (100%)	0.56	27 (10%) 7 7	46, 57, 80, 100	0
1	C	246/246 (100%)	0.65	27 (10%) 7 7	43, 57, 87, 125	0
1	D	246/246 (100%)	0.63	25 (10%) 9 8	41, 57, 83, 121	0
1	E	246/246 (100%)	0.60	23 (9%) 11 10	42, 57, 79, 101	0
1	F	246/246 (100%)	0.54	15 (6%) 25 25	45, 57, 77, 109	0
1	G	246/246 (100%)	0.62	26 (10%) 8 8	42, 57, 81, 117	0
1	H	246/246 (100%)	0.51	26 (10%) 8 8	40, 57, 85, 119	0
All	All	1968/1968 (100%)	0.61	201 (10%) 9 8	40, 57, 84, 125	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	VAL	11.0
1	C	194	VAL	10.5
1	G	193	ASP	9.1
1	A	193	ASP	8.1
1	C	193	ASP	7.5
1	C	192	THR	7.4
1	H	193	ASP	7.3
1	A	195	LEU	7.2
1	G	195	LEU	7.2
1	B	195	LEU	7.0
1	H	195	LEU	6.6
1	G	194	VAL	6.4
1	F	193	ASP	6.2
1	E	194	VAL	5.6
1	C	195	LEU	5.5
1	D	193	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
1	H	191	MET	5.3
1	G	192	THR	5.1
1	B	194	VAL	5.1
1	H	194	VAL	5.1
1	G	99	MET	5.0
1	A	192	THR	5.0
1	A	198	ASN	5.0
1	A	191	MET	4.9
1	E	195	LEU	4.8
1	D	194	VAL	4.8
1	D	192	THR	4.7
1	F	195	LEU	4.7
1	D	189	THR	4.7
1	A	38	ASN	4.6
1	F	194	VAL	4.6
1	C	197	GLU	4.6
1	D	195	LEU	4.5
1	C	199	ILE	4.5
1	D	196	ASP	4.4
1	H	192	THR	4.4
1	B	193	ASP	4.3
1	C	198	ASN	4.2
1	G	198	ASN	4.2
1	A	201	ALA	4.2
1	E	87	VAL	4.1
1	A	137	VAL	4.1
1	G	1	MET	4.1
1	G	191	MET	4.0
1	B	87	VAL	4.0
1	C	191	MET	4.0
1	G	3	LYS	3.9
1	D	40	GLN	3.8
1	G	47	ASP	3.8
1	G	199	ILE	3.8
1	G	40	GLN	3.7
1	G	197	GLU	3.7
1	A	196	ASP	3.7
1	E	198	ASN	3.7
1	C	137	VAL	3.6
1	E	193	ASP	3.5
1	G	196	ASP	3.5
1	E	86	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	87	VAL	3.4
1	B	86	LEU	3.4
1	D	200	LYS	3.4
1	E	9	VAL	3.4
1	H	87	VAL	3.3
1	D	99	MET	3.3
1	H	196	ASP	3.3
1	G	87	VAL	3.3
1	A	87	VAL	3.2
1	E	192	THR	3.2
1	D	191	MET	3.2
1	E	210	ALA	3.2
1	B	9	VAL	3.2
1	F	139	ILE	3.2
1	H	199	ILE	3.2
1	B	198	ASN	3.1
1	A	199	ILE	3.1
1	D	199	ILE	3.1
1	H	136	ILE	3.1
1	B	4	GLY	3.1
1	A	139	ILE	3.1
1	C	65	ASN	3.0
1	D	198	ASN	3.0
1	D	137	VAL	3.0
1	C	201	ALA	3.0
1	B	130	ARG	3.0
1	E	40	GLN	2.9
1	C	133	HIS	2.9
1	G	133	HIS	2.9
1	C	132	ARG	2.9
1	A	197	GLU	2.9
1	B	1	MET	2.9
1	B	85	ILE	2.9
1	H	104	GLU	2.9
1	C	130	ARG	2.8
1	G	82	GLN	2.8
1	C	87	VAL	2.8
1	E	132	ARG	2.8
1	C	78	ASP	2.8
1	D	188	ALA	2.8
1	H	197	GLU	2.8
1	G	41	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	4	GLY	2.8
1	B	197	GLU	2.8
1	B	196	ASP	2.8
1	G	229	GLN	2.8
1	C	38	ASN	2.8
1	F	87	VAL	2.7
1	H	198	ASN	2.7
1	D	104	GLU	2.7
1	E	190	ASP	2.7
1	F	137	VAL	2.7
1	D	132	ARG	2.7
1	E	88	ASN	2.7
1	G	228	ASP	2.7
1	A	100	ARG	2.7
1	D	9	VAL	2.7
1	H	137	VAL	2.7
1	G	100	ARG	2.6
1	E	137	VAL	2.6
1	H	86	LEU	2.6
1	C	196	ASP	2.6
1	B	7	ALA	2.6
1	B	52	LEU	2.6
1	F	136	ILE	2.6
1	H	189	THR	2.6
1	A	104	GLU	2.6
1	A	10	THR	2.6
1	E	120	CYS	2.6
1	A	200	LYS	2.5
1	A	188	ALA	2.5
1	B	3	LYS	2.5
1	B	191	MET	2.5
1	H	190	ASP	2.5
1	A	88	ASN	2.5
1	C	86	LEU	2.5
1	E	222	VAL	2.5
1	E	8	LEU	2.5
1	E	51	LYS	2.5
1	E	136	ILE	2.5
1	F	138	ASN	2.5
1	A	86	LEU	2.5
1	H	210	ALA	2.5
1	B	137	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	88	ASN	2.4
1	A	20	ILE	2.4
1	A	14	ARG	2.4
1	A	3	LYS	2.4
1	D	204	LEU	2.4
1	C	136	ILE	2.4
1	A	140	ALA	2.4
1	B	67	GLU	2.4
1	F	197	GLU	2.4
1	F	3	LYS	2.4
1	B	8	LEU	2.4
1	B	139	ILE	2.4
1	B	78	ASP	2.3
1	D	190	ASP	2.3
1	F	190	ASP	2.3
1	H	130	ARG	2.3
1	A	136	ILE	2.3
1	F	88	ASN	2.3
1	B	190	ASP	2.3
1	D	3	LYS	2.3
1	A	9	VAL	2.3
1	G	137	VAL	2.3
1	A	99	MET	2.2
1	B	136	ILE	2.2
1	H	8	LEU	2.2
1	F	121	THR	2.2
1	A	179	VAL	2.2
1	G	190	ASP	2.2
1	H	9	VAL	2.2
1	E	85	ILE	2.2
1	G	188	ALA	2.2
1	H	138	ASN	2.2
1	C	200	LYS	2.2
1	C	189	THR	2.2
1	E	129	MET	2.1
1	B	229	GLN	2.1
1	H	179	VAL	2.1
1	H	200	LYS	2.1
1	D	88	ASN	2.1
1	C	40	GLN	2.1
1	A	182	ILE	2.1
1	F	196	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	130	ARG	2.1
1	E	139	ILE	2.1
1	C	88	ASN	2.1
1	H	96	ASN	2.1
1	C	39	GLU	2.1
1	D	136	ILE	2.1
1	C	67	GLU	2.1
1	A	138	ASN	2.1
1	B	48	GLU	2.1
1	C	165	THR	2.1
1	B	228	ASP	2.1
1	F	191	MET	2.0
1	E	52	LEU	2.0
1	D	86	LEU	2.0
1	G	127	PHE	2.0
1	D	202	GLU	2.0
1	H	99	MET	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.