W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:41 PM GMT

PDB ID	:	4J4X
Title	:	Crystal structure of GraVN
Authors	:	Jiao, L.; Ouyang, S.; Liang, M.; Niu, F.; Shaw, N.; Wu, W.; Ding, W.; Jin, C.; Zhu, Y.; Zhang, F.; Wang, T.; Li, C.; Zuo, X.; Luan, C.H.; Li, D.; Liu, Z.J.
Deposited on	:	2013-02-07
Resolution	:	2.51 Å(reported)

The following versions of software and data (see references (i)) 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
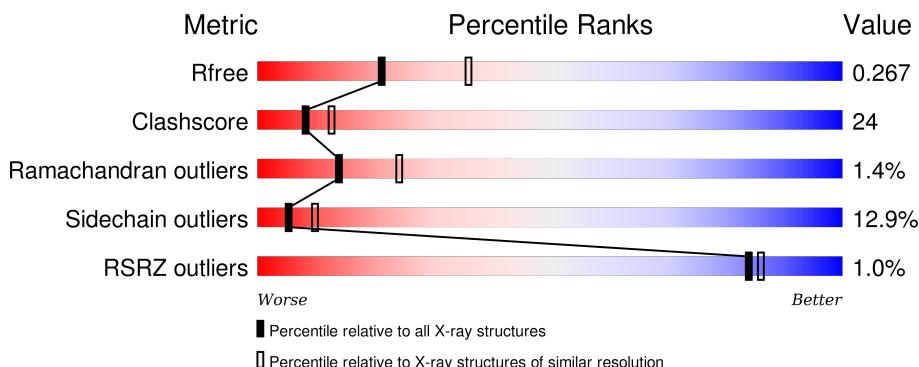
1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.51 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	Percentile Ranks	Value
Rfree		0.267
Clashscore		24
Ramachandran outliers		1.4%
Sidechain outliers		12.9%
RSRZ outliers		1.0%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	257	63% 30% 5% ·
1	B	257	67% 25% 5% ·
1	C	257	2% 53% 33% 8% · ·
1	D	257	% 61% 30% 6% ·
1	E	257	3% 52% 35% 9% · ·

Mol	Chain	Length	Quality of chain
1	F	257	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11737 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 NP protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1938	1230	332	362	14			
1	B	248	Total	C	N	O	S	0	0	0
			1921	1220	329	358	14			
1	C	246	Total	C	N	O	S	0	0	0
			1910	1213	327	356	14			
1	D	249	Total	C	N	O	S	0	0	0
			1930	1226	331	359	14			
1	E	250	Total	C	N	O	S	0	0	0
			1938	1229	331	364	14			
1	F	248	Total	C	N	O	S	0	0	0
			1921	1220	329	358	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP E2DQZ4
A	-1	ASN	-	EXPRESSION TAG	UNP E2DQZ4
A	0	ALA	-	EXPRESSION TAG	UNP E2DQZ4
B	-2	SER	-	EXPRESSION TAG	UNP E2DQZ4
B	-1	ASN	-	EXPRESSION TAG	UNP E2DQZ4
B	0	ALA	-	EXPRESSION TAG	UNP E2DQZ4
C	-2	SER	-	EXPRESSION TAG	UNP E2DQZ4
C	-1	ASN	-	EXPRESSION TAG	UNP E2DQZ4
C	0	ALA	-	EXPRESSION TAG	UNP E2DQZ4
D	-2	SER	-	EXPRESSION TAG	UNP E2DQZ4
D	-1	ASN	-	EXPRESSION TAG	UNP E2DQZ4
D	0	ALA	-	EXPRESSION TAG	UNP E2DQZ4
E	-2	SER	-	EXPRESSION TAG	UNP E2DQZ4
E	-1	ASN	-	EXPRESSION TAG	UNP E2DQZ4
E	0	ALA	-	EXPRESSION TAG	UNP E2DQZ4
F	-2	SER	-	EXPRESSION TAG	UNP E2DQZ4
F	-1	ASN	-	EXPRESSION TAG	UNP E2DQZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	EXPRESSION TAG	UNP E2DQZ4
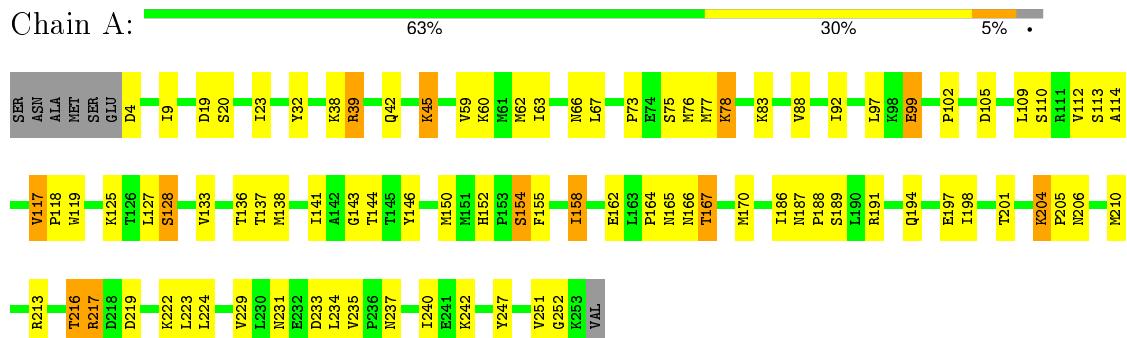
- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	47	Total 47	O 47	0	0
2	B	40	Total 40	O 40	0	0
2	C	19	Total 19	O 19	0	0
2	D	27	Total 27	O 27	0	0
2	E	23	Total 23	O 23	0	0
2	F	23	Total 23	O 23	0	0
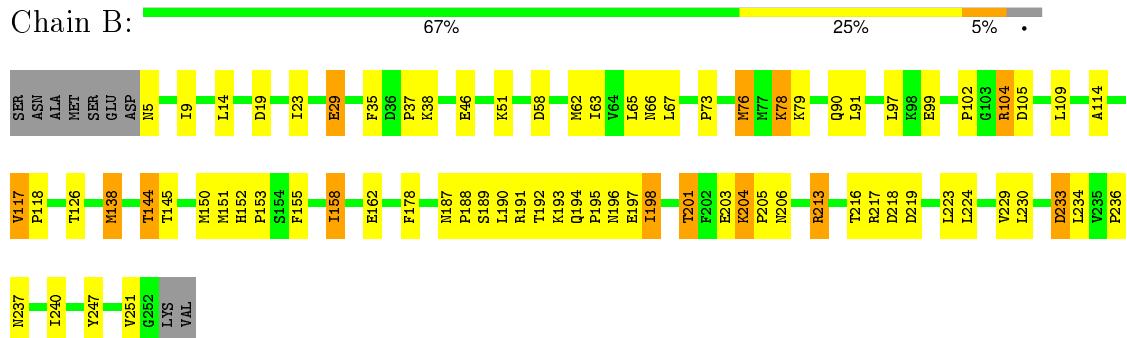
3 Residue-property plots ⓘ

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.
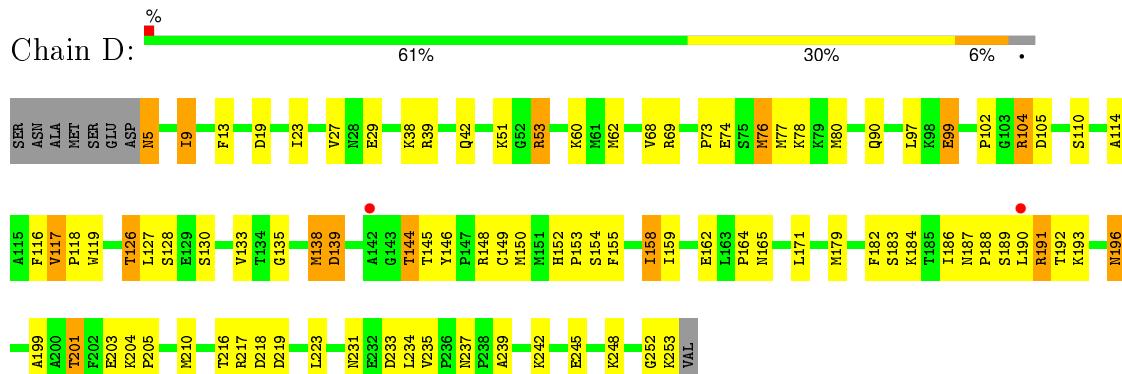
- Molecule 1: NP protein
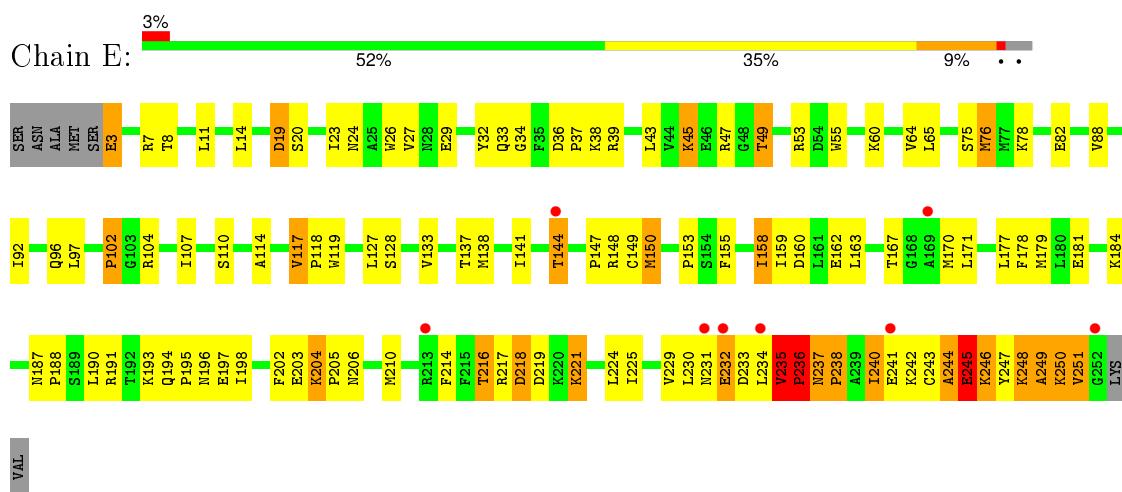
- Molecule 1: NP protein

- Molecule 1: NP protein

• Molecule 1: NP protein

Chain D:

• Molecule 1: NP protein

Chain E:

• Molecule 1: NP protein

Chain F:
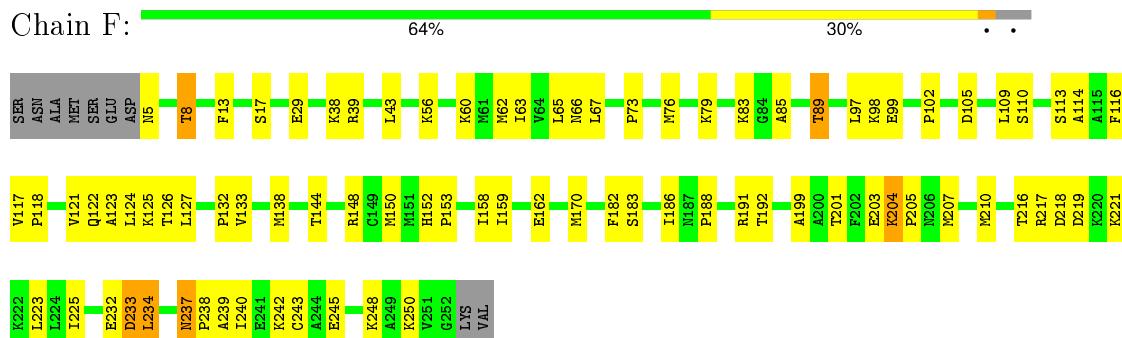
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.29Å 96.34Å 100.80Å 64.57° 81.72° 85.10°	Depositor
Resolution (Å)	49.59 – 2.51 49.59 – 2.51	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.59-2.51) 83.6 (49.59-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.195 , 0.266 0.194 , 0.267	Depositor DCC
R_{free} test set	2981 reflections (5.48%)	DCC
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 57405 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11737	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	1.22	0/1973	0.73	1/2664 (0.0%)
1	B	1.19	0/1956	0.71	0/2642
1	C	1.12	2/1945 (0.1%)	0.76	2/2627 (0.1%)
1	D	1.11	0/1965	0.69	0/2653
1	E	1.03	2/1973 (0.1%)	0.73	2/2665 (0.1%)
1	F	1.11	0/1956	0.72	0/2642
All	All	1.13	4/11768 (0.0%)	0.72	5/15893 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	195	PRO	N-CD	5.49	1.55	1.47
1	C	205	PRO	N-CD	5.37	1.55	1.47
1	E	236	PRO	N-CD	5.36	1.55	1.47
1	E	238	PRO	N-CD	5.24	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	187	ASN	C-N-CD	6.10	141.21	128.40
1	C	204	LYS	C-N-CD	5.64	140.25	128.40
1	E	237	ASN	C-N-CD	5.59	140.13	128.40
1	E	235	VAL	C-N-CD	5.52	139.99	128.40
1	A	252	GLY	N-CA-C	-5.32	99.80	113.10

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	1938	0	1990	63	1
1	B	1921	0	1973	65	0
1	C	1910	0	1959	143	1
1	D	1930	0	1985	85	0
1	E	1938	0	1983	157	0
1	F	1921	0	1970	76	0
2	A	47	0	0	5	0
2	B	40	0	0	2	0
2	C	19	0	0	5	0
2	D	27	0	0	4	0
2	E	23	0	0	12	0
2	F	23	0	0	3	0
All	All	11737	0	11860	572	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 24.

All (572) 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:E:194:GLN:CB	1:E:197:GLU:OE2	1.71	1.39
1:C:139:ASP:OD2	1:C:148:ARG:NH1	1.60	1.34
1:E:194:GLN:HB2	1:E:197:GLU:OE2	1.15	1.32
1:C:250:LYS:O	2:C:315:HOH:O	1.52	1.26
1:E:20:SER:O	1:E:24:ASN:ND2	1.65	1.25
1:B:104:ARG:NH1	1:C:80:MET:O	1.71	1.22
1:C:194:GLN:O	1:C:197:GLU:OE2	1.62	1.15
1:B:194:GLN:O	1:B:197:GLU:HB2	1.49	1.13
1:A:62:MET:CE	1:A:97:LEU:HD11	1.79	1.12
1:E:38:LYS:HG2	1:E:214:PHE:CE1	1.84	1.12
1:F:123:ALA:O	1:F:126:THR:OG1	1.65	1.10
1:E:217:ARG:O	1:E:221:LYS:HG3	1.50	1.09
1:C:213:ARG:HB3	1:C:213:ARG:HH11	1.18	1.08
1:A:152:HIS:HD2	1:A:154:SER:HB2	1.18	1.07
1:C:197:GLU:N	1:C:197:GLU:OE2	1.87	1.06
1:C:188:PRO:HG3	1:C:191:ARG:HD2	1.40	1.04
1:E:194:GLN:N	1:E:197:GLU:OE2	1.90	1.04
1:E:229:VAL:O	1:E:230:LEU:HD23	1.58	1.04
1:B:198:ILE:O	1:B:201:THR:HB	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ARG:NH1	1:D:80:MET:O	1.92	1.02
1:F:182:PHE:O	1:F:186:ILE:HG12	1.60	1.01
1:F:133:VAL:HG11	1:F:138:MET:HE1	1.39	1.01
1:E:231:ASN:OD1	1:E:232:GLU:N	1.93	1.01
1:F:132:PRO:HD3	2:F:307:HOH:O	1.59	1.00
1:E:247:TYR:O	1:E:251:VAL:HG23	1.62	0.99
1:C:237:ASN:OD1	1:C:239:ALA:N	1.95	0.99
1:D:152:HIS:HD2	1:D:154:SER:HB2	1.26	0.99
1:C:231:ASN:HD21	1:C:235:VAL:CB	1.76	0.99
1:E:170:MET:HE3	1:E:240:ILE:HG22	1.46	0.97
1:A:62:MET:HE2	1:A:97:LEU:HD11	1.44	0.97
1:E:216:THR:HG22	1:E:219:ASP:H	1.30	0.96
1:C:231:ASN:HD21	1:C:235:VAL:CG2	1.79	0.96
1:C:231:ASN:ND2	1:C:235:VAL:HB	1.81	0.96
1:C:194:GLN:HB2	1:C:197:GLU:OE1	1.63	0.95
1:D:182:PHE:O	1:D:186:ILE:HG12	1.63	0.95
1:B:62:MET:HE2	1:B:97:LEU:HD11	1.48	0.95
1:B:62:MET:CE	1:B:97:LEU:HD11	1.97	0.95
1:C:179:MET:O	1:C:183:SER:OG	1.86	0.94
1:E:194:GLN:CA	1:E:197:GLU:OE2	2.16	0.93
1:E:155:PHE:HE2	1:E:159:ILE:HD11	1.32	0.93
1:E:147:PRO:HB2	1:E:150:MET:HG3	1.48	0.93
1:F:216:THR:HB	1:F:219:ASP:OD2	1.68	0.92
1:E:38:LYS:HG2	1:E:214:PHE:HE1	1.33	0.92
1:A:152:HIS:CD2	1:A:154:SER:HB2	2.04	0.92
1:C:213:ARG:HB3	1:C:213:ARG:NH1	1.83	0.91
1:E:65:LEU:HD21	1:E:76:MET:HE1	1.50	0.91
1:B:188:PRO:HA	1:B:191:ARG:HE	1.36	0.91
1:E:170:MET:CE	1:E:240:ILE:HG22	2.02	0.90
1:C:164:PRO:O	1:C:165:ASN:HB2	1.70	0.90
1:D:237:ASN:OD1	1:D:239:ALA:N	2.03	0.90
1:B:29:GLU:OE1	1:C:81:SER:OG	1.90	0.89
1:E:231:ASN:HB3	1:E:235:VAL:HG11	1.54	0.89
1:C:188:PRO:CG	1:C:191:ARG:HD2	2.01	0.89
1:C:194:GLN:O	1:C:197:GLU:CD	2.11	0.89
1:F:133:VAL:HG11	1:F:138:MET:CE	2.03	0.89
1:F:237:ASN:ND2	1:F:239:ALA:H	1.70	0.88
1:E:244:ALA:O	1:E:246:LYS:N	2.08	0.87
1:C:242:LYS:O	1:C:246:LYS:CG	2.23	0.87
1:C:140:SER:OG	2:C:312:HOH:O	1.90	0.87
1:C:188:PRO:HG3	1:C:191:ARG:CD	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:PRO:HB3	1:C:191:ARG:HB2	1.55	0.87
1:C:138:MET:CE	1:C:178:PHE:HA	2.04	0.87
1:D:231:ASN:ND2	1:D:235:VAL:HB	1.91	0.86
1:F:237:ASN:HB3	1:F:240:ILE:HD12	1.58	0.86
1:F:98:LYS:HA	1:F:98:LYS:HE3	1.56	0.86
1:E:231:ASN:HB3	1:E:235:VAL:CG1	2.05	0.86
1:F:62:MET:HE2	1:F:97:LEU:HD11	1.57	0.85
1:B:216:THR:HG22	1:B:218:ASP:H	1.41	0.85
1:E:43:LEU:O	1:E:47:ARG:HB2	1.75	0.85
1:F:114:ALA:O	1:F:117:VAL:CG2	2.25	0.84
1:F:133:VAL:CG1	1:F:138:MET:CE	2.55	0.84
1:E:194:GLN:HB2	1:E:197:GLU:CD	1.97	0.84
1:C:231:ASN:HD21	1:C:235:VAL:HG23	1.41	0.84
1:D:62:MET:CE	1:D:97:LEU:HD11	2.08	0.84
1:C:62:MET:HE3	1:C:97:LEU:HD11	1.59	0.83
1:E:170:MET:HE1	1:E:241:GLU:HB2	1.60	0.83
1:E:149:CYS:SG	2:E:321:HOH:O	2.38	0.82
1:C:187:ASN:O	1:C:190:LEU:HD12	1.79	0.82
1:E:137:THR:O	1:E:141:ILE:HG12	1.80	0.82
1:A:128:SER:OG	2:A:331:HOH:O	1.97	0.82
1:C:188:PRO:HA	1:C:190:LEU:N	1.95	0.81
1:D:135:GLY:O	1:D:139:ASP:OD1	1.99	0.81
1:C:72:LYS:O	1:C:76:MET:HG3	1.80	0.81
1:F:237:ASN:HD22	1:F:238:PRO:N	1.79	0.81
1:F:188:PRO:O	1:F:191:ARG:HG3	1.81	0.81
1:E:155:PHE:CE2	1:E:159:ILE:HD11	2.15	0.80
1:E:187:ASN:HB3	1:E:190:LEU:HD12	1.64	0.80
1:F:237:ASN:HD22	1:F:239:ALA:H	1.29	0.79
1:F:207:MET:HA	1:F:210:MET:HE2	1.61	0.79
1:C:138:MET:HE1	1:C:178:PHE:HA	1.62	0.79
1:E:45:LYS:O	1:E:49:THR:OG1	2.00	0.79
1:D:149:CYS:SG	2:D:307:HOH:O	2.39	0.79
1:A:45:LYS:HD3	2:A:347:HOH:O	1.81	0.79
1:E:33:GLN:OE1	2:E:304:HOH:O	2.01	0.79
1:C:231:ASN:ND2	1:C:235:VAL:CB	2.42	0.78
1:C:62:MET:CE	1:C:97:LEU:HD11	2.14	0.78
1:D:216:THR:HG23	2:D:315:HOH:O	1.83	0.78
1:B:19:ASP:O	1:B:23:ILE:HG12	1.84	0.77
1:C:62:MET:HE1	1:C:97:LEU:HD21	1.67	0.77
1:D:152:HIS:CD2	1:D:154:SER:HB2	2.16	0.77
1:C:148:ARG:HD2	1:C:151:MET:CE	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ASN:HD21	1:D:235:VAL:HB	1.48	0.76
1:E:114:ALA:O	1:E:117:VAL:HG22	1.85	0.76
1:E:133:VAL:HG11	1:E:138:MET:HE1	1.67	0.76
1:A:204:LYS:HB3	1:A:205:PRO:HD3	1.68	0.76
1:A:63:ILE:HD11	1:A:112:VAL:HG12	1.67	0.76
1:E:144:THR:HG21	1:E:242:LYS:HE3	1.68	0.75
1:E:217:ARG:O	1:E:221:LYS:CG	2.32	0.75
1:D:248:LYS:O	1:D:252:GLY:N	2.19	0.75
1:C:181:GLU:O	1:C:184:LYS:HB2	1.87	0.75
1:F:85:ALA:O	1:F:89:THR:OG1	2.04	0.75
1:C:148:ARG:HA	1:C:151:MET:CE	2.17	0.75
1:E:181:GLU:OE2	1:E:184:LYS:NZ	2.20	0.75
1:C:229:VAL:O	1:C:230:LEU:HD23	1.87	0.75
1:F:133:VAL:CG1	1:F:138:MET:HE1	2.15	0.74
1:E:216:THR:HG21	1:E:218:ASP:OD2	1.86	0.74
1:E:194:GLN:CG	1:E:197:GLU:OE2	2.34	0.74
1:D:133:VAL:HG11	1:D:138:MET:CE	2.17	0.74
1:B:114:ALA:O	1:B:117:VAL:HG22	1.87	0.74
1:C:231:ASN:OD1	1:C:233:ASP:N	2.21	0.73
1:E:194:GLN:H	1:E:197:GLU:CD	1.91	0.73
1:E:234:LEU:O	1:E:234:LEU:HD23	1.89	0.73
1:D:62:MET:HE2	1:D:97:LEU:HD11	1.70	0.72
1:E:38:LYS:CG	1:E:214:PHE:CE1	2.69	0.72
1:A:125:LYS:O	2:A:331:HOH:O	2.06	0.72
1:E:233:ASP:H	1:E:235:VAL:HG12	1.53	0.72
1:B:194:GLN:O	1:B:197:GLU:CB	2.35	0.72
1:D:233:ASP:O	1:D:234:LEU:HB2	1.87	0.72
1:F:117:VAL:N	1:F:118:PRO:CD	2.52	0.71
1:E:229:VAL:C	1:E:230:LEU:HD23	2.09	0.71
1:E:3:GLU:CG	2:E:318:HOH:O	2.38	0.71
1:C:188:PRO:CB	1:C:191:ARG:HB2	2.21	0.71
1:B:65:LEU:HD11	1:B:76:MET:CE	2.20	0.71
1:C:188:PRO:HA	1:C:190:LEU:H	1.53	0.71
1:C:152:HIS:ND1	1:C:154:SER:HB2	2.06	0.70
1:C:142:ALA:O	1:C:144:THR:N	2.23	0.70
1:E:216:THR:CG2	1:E:218:ASP:CG	2.60	0.70
1:B:158:ILE:HD11	1:B:223:LEU:HD13	1.73	0.70
1:E:60:LYS:HG2	1:E:119:TRP:CE2	2.26	0.70
1:C:62:MET:CE	1:C:97:LEU:HD21	2.21	0.70
1:C:165:ASN:O	1:C:166:ASN:HB2	1.92	0.69
1:E:38:LYS:CG	1:E:214:PHE:CD1	2.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ASP:OD2	1:C:148:ARG:CZ	2.41	0.69
1:D:117:VAL:N	1:D:118:PRO:CD	2.55	0.69
1:D:133:VAL:HG11	1:D:138:MET:HE2	1.75	0.68
1:E:3:GLU:HG2	2:E:318:HOH:O	1.93	0.68
1:D:216:THR:HB	1:D:219:ASP:OD2	1.93	0.68
1:C:194:GLN:CB	1:C:197:GLU:OE1	2.39	0.68
1:C:137:THR:O	1:C:141:ILE:HG12	1.93	0.68
1:C:216:THR:HG22	1:C:219:ASP:H	1.58	0.68
1:D:146:TYR:O	1:D:148:ARG:NH1	2.27	0.68
1:D:117:VAL:HG23	1:D:118:PRO:HD3	1.75	0.68
1:F:114:ALA:O	1:F:117:VAL:HG22	1.93	0.68
1:A:66:ASN:HB2	1:A:109:LEU:HB3	1.75	0.67
1:B:5:ASN:O	1:B:9:ILE:HG13	1.94	0.67
1:E:160:ASP:HB3	1:E:163:LEU:HG	1.76	0.67
1:C:138:MET:HE2	1:C:178:PHE:HA	1.75	0.67
1:E:38:LYS:HG2	1:E:214:PHE:CD1	2.28	0.67
1:E:216:THR:HB	1:E:219:ASP:OD2	1.95	0.67
1:E:188:PRO:HA	2:E:320:HOH:O	1.95	0.67
1:E:242:LYS:O	1:E:246:LYS:HD2	1.95	0.67
1:C:60:LYS:O	1:C:64:VAL:HG23	1.94	0.67
1:F:62:MET:CE	1:F:97:LEU:HD21	2.24	0.66
1:D:9:ILE:CD1	1:E:55:TRP:HH2	2.08	0.66
1:C:195:PRO:O	1:C:197:GLU:N	2.28	0.66
1:D:158:ILE:HD11	1:D:223:LEU:HD13	1.77	0.66
1:E:104:ARG:HG2	2:E:304:HOH:O	1.95	0.66
1:F:62:MET:HE1	1:F:97:LEU:HD21	1.77	0.66
1:B:65:LEU:HD11	1:B:76:MET:HE1	1.78	0.65
1:D:188:PRO:O	1:D:191:ARG:CG	2.44	0.65
1:C:242:LYS:O	1:C:246:LYS:HG3	1.95	0.65
1:A:198:ILE:O	1:A:201:THR:HB	1.97	0.65
1:A:165:ASN:O	1:A:166:ASN:HB2	1.96	0.65
1:C:188:PRO:HB3	1:C:190:LEU:C	2.16	0.65
1:B:233:ASP:O	1:B:234:LEU:HB2	1.96	0.65
1:C:144:THR:O	1:C:145:THR:OG1	2.11	0.65
1:E:204:LYS:N	1:E:205:PRO:CD	2.58	0.65
1:D:158:ILE:HD11	1:D:223:LEU:CD1	2.26	0.64
1:C:194:GLN:N	1:C:197:GLU:OE1	2.31	0.64
1:C:148:ARG:HD2	1:C:151:MET:HE2	1.78	0.64
1:D:216:THR:HG22	1:D:218:ASP:N	2.11	0.64
1:F:152:HIS:CD2	1:F:153:PRO:HD2	2.33	0.64
1:C:63:ILE:O	1:C:67:LEU:HG	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:PRO:O	1:C:198:ILE:N	2.27	0.64
1:F:133:VAL:HG12	1:F:138:MET:CE	2.26	0.64
1:D:117:VAL:HG13	1:D:154:SER:OG	1.98	0.64
1:C:148:ARG:HA	1:C:151:MET:HE2	1.80	0.63
1:F:237:ASN:C	1:F:237:ASN:HD22	2.01	0.63
1:B:194:GLN:O	1:B:197:GLU:N	2.31	0.63
1:E:216:THR:HG22	1:E:219:ASP:N	2.09	0.63
1:A:133:VAL:HG11	1:A:138:MET:CE	2.28	0.63
1:E:247:TYR:O	1:E:251:VAL:CG2	2.41	0.63
1:B:158:ILE:HG23	1:B:224:LEU:HD21	1.81	0.63
1:A:75:SER:HA	1:A:78:LYS:HE3	1.79	0.63
1:F:233:ASP:O	1:F:234:LEU:HB2	1.98	0.63
1:E:104:ARG:HB2	1:E:104:ARG:NH1	2.13	0.62
1:B:216:THR:HG22	1:B:218:ASP:N	2.13	0.62
1:E:216:THR:CG2	1:E:218:ASP:OD2	2.48	0.62
1:A:63:ILE:HD12	1:A:113:SER:HA	1.81	0.62
1:A:62:MET:HE3	1:A:97:LEU:HD11	1.76	0.62
1:E:177:LEU:HD22	1:E:243:CYS:HB3	1.80	0.62
1:E:191:ARG:NE	2:E:320:HOH:O	2.33	0.62
1:E:170:MET:HE1	1:E:241:GLU:CB	2.30	0.62
1:A:63:ILE:CD1	1:A:112:VAL:HG12	2.30	0.62
1:E:230:LEU:HD22	1:E:236:PRO:HA	1.81	0.62
1:F:98:LYS:CA	1:F:98:LYS:HE3	2.30	0.61
1:C:237:ASN:HB3	1:C:240:ILE:HD13	1.81	0.61
1:C:141:ILE:CD1	2:C:312:HOH:O	2.47	0.61
1:E:97:LEU:HD23	1:E:107:ILE:HG22	1.82	0.61
1:D:74:GLU:HA	1:D:77:MET:HE2	1.81	0.61
1:F:133:VAL:CG1	1:F:138:MET:HE2	2.31	0.61
1:C:237:ASN:HB3	1:C:240:ILE:CD1	2.30	0.61
1:E:19:ASP:N	1:E:19:ASP:OD2	2.15	0.61
1:E:188:PRO:O	1:E:191:ARG:HG3	2.00	0.61
1:C:186:ILE:O	1:C:187:ASN:HB3	1.99	0.60
1:D:188:PRO:HA	1:D:191:ARG:HE	1.66	0.60
1:A:114:ALA:O	1:A:117:VAL:HG22	2.01	0.60
1:E:147:PRO:CB	1:E:150:MET:HG3	2.28	0.60
1:E:236:PRO:O	2:E:316:HOH:O	2.15	0.60
1:C:191:ARG:CG	1:C:191:ARG:HH11	2.14	0.60
1:E:245:GLU:O	1:E:249:ALA:N	2.26	0.60
1:C:19:ASP:OD2	1:C:22:THR:OG1	2.18	0.60
1:F:221:LYS:O	1:F:225:ILE:HG13	2.02	0.60
1:E:19:ASP:OD2	2:E:302:HOH:O	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:ILE:HD12	1:C:240:ILE:N	2.17	0.59
1:C:213:ARG:HH11	1:C:213:ARG:CB	2.05	0.59
1:E:231:ASN:CA	1:E:235:VAL:HG13	2.32	0.59
1:D:188:PRO:O	1:D:191:ARG:HG2	2.01	0.59
1:C:101:ASN:N	1:C:102:PRO:CD	2.66	0.59
1:D:231:ASN:HD21	1:D:235:VAL:CB	2.13	0.59
1:F:114:ALA:O	1:F:117:VAL:HG23	2.02	0.59
1:B:237:ASN:HB3	1:B:240:ILE:HD12	1.84	0.59
1:A:62:MET:HE2	1:A:97:LEU:CD1	2.25	0.59
1:C:242:LYS:O	1:C:246:LYS:HG2	2.01	0.59
1:F:63:ILE:O	1:F:67:LEU:HG	2.03	0.59
1:E:225:ILE:HA	1:E:230:LEU:O	2.03	0.59
1:B:204:LYS:HB3	1:B:205:PRO:HD3	1.85	0.59
1:A:216:THR:HB	1:A:219:ASP:OD2	2.02	0.58
1:E:231:ASN:HB3	1:E:235:VAL:HG13	1.84	0.58
1:E:231:ASN:N	1:E:235:VAL:HG13	2.19	0.58
1:C:170:MET:HG2	1:C:240:ILE:HG22	1.84	0.58
1:C:188:PRO:HB3	1:C:190:LEU:O	2.03	0.58
1:F:98:LYS:CE	1:F:98:LYS:HA	2.24	0.58
1:A:117:VAL:N	1:A:118:PRO:CD	2.66	0.58
1:E:170:MET:CE	1:E:240:ILE:CG2	2.79	0.58
1:B:144:THR:HG22	1:B:145:THR:H	1.68	0.58
1:F:117:VAL:N	1:F:118:PRO:HD3	2.19	0.58
1:B:138:MET:HE1	1:B:178:PHE:HA	1.85	0.58
1:E:202:PHE:C	1:E:205:PRO:HD2	2.24	0.57
1:D:204:LYS:HB2	1:D:205:PRO:HD3	1.86	0.57
1:A:237:ASN:HB3	1:A:240:ILE:HD12	1.87	0.57
1:C:194:GLN:C	1:C:197:GLU:OE2	2.41	0.57
1:E:230:LEU:CD2	1:E:236:PRO:HA	2.35	0.57
1:E:144:THR:CG2	1:E:242:LYS:HE3	2.33	0.57
1:F:152:HIS:CG	1:F:153:PRO:HD2	2.39	0.57
1:B:192:THR:O	1:B:193:LYS:HD2	2.05	0.57
1:F:239:ALA:O	1:F:243:CYS:SG	2.58	0.57
1:E:188:PRO:O	1:E:191:ARG:CG	2.53	0.57
1:D:190:LEU:HD11	1:D:201:THR:HG21	1.87	0.57
1:C:186:ILE:HG22	1:C:187:ASN:HD22	1.69	0.57
1:D:153:PRO:HG3	1:D:179:MET:HE1	1.85	0.57
1:B:230:LEU:HD23	1:B:236:PRO:HA	1.87	0.57
1:D:144:THR:HG22	1:D:145:THR:H	1.69	0.57
1:C:142:ALA:C	1:C:144:THR:H	2.08	0.57
1:E:184:LYS:O	1:E:187:ASN:O	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:LYS:HG3	1:C:214:PHE:CE1	2.40	0.57
1:D:199:ALA:O	1:D:203:GLU:HG3	2.05	0.57
1:C:148:ARG:HA	1:C:151:MET:HE3	1.86	0.56
1:C:223:LEU:O	1:C:227:ILE:HG12	2.04	0.56
1:C:141:ILE:HD13	2:C:312:HOH:O	2.04	0.56
1:B:216:THR:HB	1:B:219:ASP:CG	2.26	0.56
1:E:138:MET:HE2	1:E:138:MET:CA	2.36	0.56
1:F:216:THR:HG22	1:F:218:ASP:N	2.19	0.56
1:E:153:PRO:HD3	1:E:179:MET:HE1	1.88	0.56
1:D:182:PHE:CE2	1:D:186:ILE:HG13	2.40	0.56
1:C:188:PRO:HG3	1:C:191:ARG:HB2	1.88	0.56
1:B:117:VAL:N	1:B:118:PRO:CD	2.68	0.56
1:D:184:LYS:O	1:D:187:ASN:O	2.23	0.56
1:B:73:PRO:HA	1:B:76:MET:HG3	1.88	0.56
1:C:198:ILE:O	1:C:201:THR:HG22	2.06	0.56
1:E:159:ILE:HD12	1:E:171:LEU:HB3	1.87	0.56
1:F:159:ILE:HB	1:F:210:MET:HG2	1.87	0.56
1:E:104:ARG:HH11	1:E:104:ARG:HB2	1.71	0.56
1:E:231:ASN:O	1:E:233:ASP:N	2.38	0.55
1:F:97:LEU:O	1:F:98:LYS:HD2	2.06	0.55
1:E:170:MET:HE3	1:E:241:GLU:CA	2.36	0.55
1:E:206:ASN:O	1:E:210:MET:HG3	2.06	0.55
1:F:162:GLU:OE1	1:F:162:GLU:HA	2.07	0.55
1:E:159:ILE:CD1	1:E:171:LEU:HB3	2.36	0.55
1:B:65:LEU:HD11	1:B:76:MET:HE3	1.87	0.55
1:B:65:LEU:HD21	1:B:76:MET:HE1	1.88	0.55
1:A:247:TYR:O	1:A:251:VAL:HG22	2.07	0.55
1:E:216:THR:HG23	1:E:218:ASP:OD1	2.06	0.55
1:E:3:GLU:HG3	2:E:318:HOH:O	2.05	0.55
1:D:188:PRO:O	1:D:191:ARG:HG3	2.06	0.55
1:E:38:LYS:HG3	1:E:214:PHE:CD1	2.42	0.55
1:D:9:ILE:HD13	1:E:55:TRP:HH2	1.70	0.55
1:E:117:VAL:N	1:E:118:PRO:CD	2.70	0.55
1:F:225:ILE:HD13	1:F:232:GLU:HA	1.89	0.55
1:C:117:VAL:N	1:C:118:PRO:CD	2.70	0.54
1:C:188:PRO:HG2	1:C:191:ARG:HD2	1.89	0.54
1:D:231:ASN:HD21	1:D:235:VAL:CG2	2.20	0.54
1:C:101:ASN:N	1:C:102:PRO:HD3	2.22	0.54
1:C:248:LYS:HD3	1:C:248:LYS:O	2.07	0.54
1:A:158:ILE:HD11	1:A:223:LEU:HD13	1.89	0.54
1:E:233:ASP:N	1:E:235:VAL:HG12	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ASN:HD22	1:C:235:VAL:HB	1.71	0.54
1:D:204:LYS:CB	1:D:205:PRO:HD3	2.38	0.54
1:D:216:THR:HG22	1:D:218:ASP:H	1.73	0.54
1:E:128:SER:HB3	1:E:148:ARG:HG3	1.89	0.54
1:C:148:ARG:HD2	1:C:151:MET:HE1	1.88	0.54
1:A:231:ASN:OD1	1:A:233:ASP:HB2	2.07	0.54
1:E:170:MET:HE2	1:E:240:ILE:CG2	2.38	0.54
1:D:153:PRO:CG	1:D:179:MET:HE1	2.38	0.54
1:A:143:GLY:O	1:A:144:THR:HG23	2.08	0.54
1:D:139:ASP:OD1	1:D:139:ASP:N	2.40	0.53
1:E:138:MET:HA	1:E:138:MET:HE2	1.89	0.53
1:C:188:PRO:CG	1:C:191:ARG:HB2	2.39	0.53
1:A:73:PRO:HA	1:A:76:MET:HG2	1.90	0.53
1:C:170:MET:HG2	1:C:240:ILE:CG2	2.38	0.53
1:D:133:VAL:CG1	1:D:138:MET:HE2	2.37	0.53
1:A:164:PRO:O	1:A:167:THR:OG1	2.24	0.53
1:B:188:PRO:HA	1:B:191:ARG:NE	2.14	0.53
1:E:170:MET:HE3	1:E:241:GLU:HA	1.89	0.53
1:E:231:ASN:CB	1:E:235:VAL:CG1	2.85	0.53
1:F:62:MET:CE	1:F:97:LEU:HD11	2.36	0.53
1:E:104:ARG:CZ	1:E:104:ARG:HB3	2.37	0.53
1:B:158:ILE:HD11	1:B:223:LEU:CD1	2.39	0.53
1:A:144:THR:HG21	1:A:242:LYS:CD	2.40	0.52
1:F:133:VAL:HG12	1:F:138:MET:HE2	1.90	0.52
1:E:231:ASN:C	1:E:233:ASP:H	2.13	0.52
1:C:191:ARG:HG2	1:C:191:ARG:HH11	1.73	0.52
1:C:194:GLN:CA	1:C:197:GLU:OE1	2.58	0.52
1:F:216:THR:HG22	1:F:218:ASP:H	1.74	0.52
1:C:177:LEU:HD13	1:C:243:CYS:O	2.10	0.52
1:C:39:ARG:NH2	1:C:105:ASP:OD2	2.24	0.52
1:A:152:HIS:HD2	1:A:154:SER:CB	2.05	0.52
1:A:231:ASN:OD1	1:A:233:ASP:N	2.33	0.52
1:C:65:LEU:HD21	1:C:76:MET:HE1	1.92	0.52
1:B:63:ILE:O	1:B:67:LEU:HG	2.10	0.52
1:E:195:PRO:HA	1:E:198:ILE:HD12	1.91	0.52
1:D:116:PHE:C	1:D:118:PRO:HD2	2.30	0.51
1:B:204:LYS:CB	1:B:205:PRO:HD3	2.39	0.51
1:D:231:ASN:OD1	1:D:233:ASP:N	2.44	0.51
1:D:216:THR:HG22	1:D:219:ASP:H	1.75	0.51
1:B:14:LEU:HD12	1:C:122:GLN:NE2	2.25	0.51
1:C:242:LYS:O	1:C:246:LYS:CB	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ALA:O	1:C:144:THR:OG1	2.25	0.51
1:E:104:ARG:CZ	1:E:104:ARG:CB	2.88	0.51
1:C:32:TYR:CG	1:C:204:LYS:HE2	2.45	0.51
1:E:245:GLU:O	1:E:248:LYS:N	2.44	0.51
1:E:170:MET:HE2	1:E:240:ILE:HG22	1.90	0.51
1:C:6:TYR:OH	1:D:42:GLN:HG3	2.10	0.51
1:E:104:ARG:NE	2:E:310:HOH:O	1.86	0.51
1:D:114:ALA:O	1:D:117:VAL:HG22	2.10	0.51
1:D:216:THR:CG2	1:D:218:ASP:HB2	2.41	0.51
1:F:199:ALA:O	1:F:203:GLU:HG3	2.11	0.51
1:D:19:ASP:HB2	2:D:311:HOH:O	2.11	0.51
1:F:124:LEU:HD13	1:F:148:ARG:O	2.11	0.51
1:B:62:MET:HE3	1:B:91:LEU:HB3	1.93	0.51
1:E:104:ARG:CB	1:E:104:ARG:NH1	2.73	0.51
1:B:138:MET:CE	1:B:178:PHE:HA	2.41	0.51
1:A:194:GLN:HB2	1:A:197:GLU:OE2	2.11	0.51
1:E:60:LYS:HG2	1:E:119:TRP:CZ2	2.46	0.50
1:A:143:GLY:O	1:A:144:THR:CG2	2.58	0.50
1:E:243:CYS:C	1:E:244:ALA:O	2.45	0.50
1:C:243:CYS:O	1:C:247:TYR:N	2.41	0.50
1:C:231:ASN:ND2	1:C:235:VAL:HG23	2.19	0.50
1:D:216:THR:CG2	1:D:218:ASP:H	2.24	0.50
1:D:164:PRO:O	1:D:165:ASN:HB2	2.11	0.50
1:F:158:ILE:HG22	1:F:158:ILE:O	2.10	0.50
1:C:190:LEU:C	1:C:192:THR:H	2.15	0.50
1:E:231:ASN:CB	1:E:235:VAL:HG13	2.41	0.49
1:A:224:LEU:HD22	1:A:229:VAL:HG11	1.93	0.49
1:E:170:MET:HE3	1:E:241:GLU:N	2.26	0.49
1:E:75:SER:O	1:E:78:LYS:HG3	2.12	0.49
1:C:196:ASN:N	1:C:196:ASN:OD1	2.45	0.49
1:B:216:THR:N	1:B:219:ASP:OD2	2.31	0.49
1:C:60:LYS:HG2	1:C:119:TRP:CE2	2.47	0.49
1:E:170:MET:CE	1:E:241:GLU:CA	2.90	0.49
1:E:144:THR:OG1	1:E:242:LYS:HD2	2.13	0.49
1:C:242:LYS:O	1:C:246:LYS:N	2.34	0.49
1:B:152:HIS:CD2	1:B:153:PRO:HD2	2.47	0.49
1:F:182:PHE:CZ	1:F:186:ILE:HD11	2.48	0.49
1:C:139:ASP:CG	1:C:145:THR:HA	2.32	0.49
1:C:216:THR:HB	1:C:219:ASP:OD2	2.13	0.49
1:D:53:ARG:HH12	1:D:90:GLN:HG2	1.77	0.49
1:A:4:ASP:OD1	1:A:4:ASP:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLU:OE2	1:B:197:GLU:HA	2.13	0.49
1:B:187:ASN:HB3	1:B:190:LEU:HD12	1.94	0.48
1:E:34:GLY:HA2	1:F:79:LYS:HD3	1.94	0.48
1:C:163:LEU:HB3	1:C:164:PRO:HD2	1.94	0.48
1:B:192:THR:C	1:B:193:LYS:HD2	2.33	0.48
1:F:65:LEU:HD21	1:F:76:MET:HE1	1.94	0.48
1:A:144:THR:HG21	1:A:242:LYS:HD3	1.95	0.48
1:F:182:PHE:O	1:F:186:ILE:CG1	2.46	0.48
1:C:231:ASN:OD1	1:C:233:ASP:CA	2.61	0.48
1:F:116:PHE:C	1:F:118:PRO:HD2	2.34	0.48
1:C:142:ALA:C	1:C:144:THR:N	2.66	0.48
1:A:62:MET:CE	1:A:97:LEU:CD1	2.72	0.48
1:E:43:LEU:HB3	1:E:107:ILE:HD11	1.95	0.48
1:A:138:MET:HG3	1:A:146:TYR:CG	2.48	0.48
1:F:186:ILE:O	2:F:321:HOH:O	2.20	0.47
1:C:141:ILE:HD13	1:C:141:ILE:N	2.29	0.47
1:D:69:ARG:HB3	1:D:76:MET:HG2	1.95	0.47
1:D:153:PRO:CA	1:D:179:MET:HE1	2.45	0.47
1:C:114:ALA:O	1:C:117:VAL:HG22	2.14	0.47
1:D:23:ILE:O	1:D:27:VAL:HG23	2.14	0.47
1:D:196:ASN:HD22	1:E:191:ARG:HB3	1.80	0.47
1:D:153:PRO:HA	1:D:179:MET:HE1	1.96	0.47
1:A:231:ASN:HD21	1:A:235:VAL:HB	1.80	0.47
1:E:237:ASN:OD1	1:E:238:PRO:HD2	2.15	0.47
1:A:39:ARG:NH1	1:A:42:GLN:OE1	2.42	0.47
1:C:125:LYS:HG2	1:C:126:THR:N	2.29	0.47
1:B:105:ASP:HB2	2:B:309:HOH:O	2.15	0.47
1:D:159:ILE:HB	1:D:210:MET:HG2	1.97	0.47
1:E:249:ALA:O	1:E:251:VAL:N	2.48	0.47
1:C:38:LYS:HG3	1:C:214:PHE:HE1	1.78	0.47
1:F:158:ILE:HD12	1:F:223:LEU:HD13	1.96	0.47
1:F:150:MET:HE2	1:F:150:MET:HB3	1.66	0.47
1:E:23:ILE:O	1:E:27:VAL:HG23	2.14	0.47
1:D:104:ARG:NH2	1:E:82:GLU:HG3	2.29	0.47
1:D:216:THR:HB	1:D:219:ASP:CG	2.35	0.47
1:A:143:GLY:C	1:A:144:THR:HG23	2.35	0.47
1:E:158:ILE:CG2	1:E:224:LEU:HD21	2.44	0.47
1:B:213:ARG:HG2	1:B:213:ARG:HH11	1.80	0.47
1:F:204:LYS:N	1:F:205:PRO:HD2	2.30	0.47
1:B:66:ASN:HB2	1:B:109:LEU:HB3	1.97	0.47
1:E:7:ARG:O	1:E:11:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:MET:CA	1:E:138:MET:CE	2.92	0.46
1:E:133:VAL:CG1	1:E:138:MET:HE1	2.41	0.46
1:C:60:LYS:HG2	1:C:119:TRP:CZ2	2.50	0.46
1:B:233:ASP:O	1:B:234:LEU:CB	2.63	0.46
1:A:137:THR:O	1:A:141:ILE:HG12	2.15	0.46
1:C:230:LEU:CD2	1:C:236:PRO:HA	2.46	0.46
1:C:30:PHE:O	1:D:69:ARG:NH1	2.46	0.46
1:C:66:ASN:HB2	1:C:109:LEU:HB3	1.96	0.46
1:C:191:ARG:CG	1:C:191:ARG:NH1	2.73	0.46
1:C:242:LYS:C	1:C:246:LYS:HG3	2.35	0.46
1:E:88:VAL:O	1:E:92:ILE:HG13	2.15	0.46
1:A:170:MET:HG2	1:A:240:ILE:HG22	1.96	0.46
1:C:158:ILE:HD12	1:C:158:ILE:HA	1.72	0.46
1:C:190:LEU:H	1:C:190:LEU:HG	1.60	0.46
1:C:231:ASN:ND2	1:C:235:VAL:H	2.14	0.46
1:B:58:ASP:O	1:B:62:MET:HG3	2.15	0.46
1:A:59:VAL:O	1:A:63:ILE:HG12	2.15	0.46
1:C:158:ILE:HD11	1:C:223:LEU:HD13	1.98	0.46
1:E:195:PRO:O	1:E:198:ILE:N	2.47	0.46
1:D:150:MET:HG2	1:D:155:PHE:CZ	2.50	0.46
1:A:32:TYR:C	1:A:32:TYR:CD1	2.89	0.46
1:C:234:LEU:HD12	1:C:234:LEU:N	2.29	0.46
1:B:158:ILE:CG2	1:B:224:LEU:HD21	2.46	0.46
1:A:119:TRP:HB2	1:F:13:PHE:HB3	1.98	0.46
1:B:35:PHE:O	1:B:37:PRO:HD3	2.16	0.46
1:C:171:LEU:HA	1:C:171:LEU:HD23	1.75	0.45
1:E:97:LEU:CD2	1:E:107:ILE:HG22	2.46	0.45
1:D:62:MET:HE3	1:D:97:LEU:HD11	1.93	0.45
1:C:188:PRO:CA	1:C:190:LEU:N	2.73	0.45
1:C:237:ASN:OD1	1:C:238:PRO:N	2.49	0.45
1:A:233:ASP:O	1:A:234:LEU:HB2	2.17	0.45
1:C:6:TYR:CZ	1:D:42:GLN:HG3	2.52	0.45
1:F:217:ARG:HB2	2:F:308:HOH:O	2.15	0.45
1:E:194:GLN:HB2	1:E:197:GLU:CG	2.47	0.45
1:B:216:THR:HB	1:B:219:ASP:OD2	2.17	0.45
1:C:240:ILE:CD1	1:C:240:ILE:N	2.79	0.45
1:F:62:MET:HE2	1:F:97:LEU:HD21	1.96	0.45
1:E:233:ASP:H	1:E:235:VAL:CG1	2.27	0.45
1:B:138:MET:HG2	1:B:151:MET:CE	2.47	0.45
1:A:9:ILE:HG23	2:A:344:HOH:O	2.17	0.45
1:F:66:ASN:HB2	1:F:109:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLU:HB2	1:A:217:ARG:HH11	1.81	0.45
1:F:242:LYS:HB2	1:F:242:LYS:HE3	1.68	0.45
1:B:229:VAL:HG12	1:B:230:LEU:HG	1.99	0.44
1:C:5:ASN:ND2	2:C:317:HOH:O	2.49	0.44
1:F:237:ASN:HB3	1:F:240:ILE:CD1	2.37	0.44
1:E:240:ILE:CD1	1:E:240:ILE:N	2.81	0.44
1:D:248:LYS:O	1:D:253:LYS:N	2.46	0.44
1:E:202:PHE:O	1:E:205:PRO:HD2	2.18	0.44
1:B:152:HIS:CG	1:B:153:PRO:HD2	2.52	0.44
1:A:234:LEU:CD1	1:A:234:LEU:N	2.80	0.44
1:B:195:PRO:HA	1:B:198:ILE:HG13	1.98	0.44
1:E:233:ASP:HB3	1:E:235:VAL:HB	1.99	0.44
1:C:233:ASP:O	1:C:234:LEU:HB2	2.17	0.44
1:E:170:MET:CE	1:E:241:GLU:N	2.81	0.44
1:F:216:THR:HB	1:F:219:ASP:CG	2.33	0.44
1:D:60:LYS:HG2	1:D:119:TRP:CE2	2.53	0.44
1:B:158:ILE:HD12	1:B:158:ILE:HA	1.77	0.44
1:A:231:ASN:ND2	1:A:235:VAL:HB	2.33	0.44
1:E:231:ASN:C	1:E:235:VAL:CG1	2.86	0.44
1:A:133:VAL:CG1	1:A:138:MET:CE	2.94	0.44
1:C:117:VAL:HG23	1:C:118:PRO:HD3	2.00	0.44
1:E:231:ASN:O	1:E:235:VAL:HG12	2.17	0.43
1:E:7:ARG:NH1	1:F:219:ASP:OD1	2.50	0.43
1:A:204:LYS:CB	1:A:205:PRO:HD3	2.45	0.43
1:C:203:GLU:O	1:C:204:LYS:C	2.54	0.43
1:F:204:LYS:HB2	1:F:204:LYS:HE2	1.80	0.43
1:D:152:HIS:CD2	1:D:154:SER:H	2.35	0.43
1:E:178:PHE:CD2	1:E:179:MET:HE2	2.53	0.43
1:E:32:TYR:CD2	1:E:204:LYS:HD2	2.53	0.43
1:F:62:MET:HE2	1:F:97:LEU:CD1	2.41	0.43
1:D:193:LYS:HA	1:D:193:LYS:HD3	1.91	0.43
1:B:78:LYS:HG2	1:B:79:LYS:HG2	1.99	0.43
1:C:158:ILE:O	1:C:158:ILE:HG23	2.19	0.43
1:D:73:PRO:HD2	1:D:99:GLU:HG2	2.01	0.43
1:C:165:ASN:O	1:C:166:ASN:CB	2.63	0.43
1:B:158:ILE:HG23	1:B:224:LEU:CD2	2.47	0.43
1:D:148:ARG:N	1:D:148:ARG:HD2	2.34	0.43
1:C:234:LEU:CD1	1:C:234:LEU:N	2.82	0.43
1:E:231:ASN:C	1:E:233:ASP:N	2.73	0.43
1:B:216:THR:HG22	1:B:217:ARG:N	2.33	0.43
1:E:163:LEU:HD23	1:E:163:LEU:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:HG11	1:A:138:MET:HE1	2.00	0.42
1:F:43:LEU:HD23	1:F:43:LEU:HA	1.75	0.42
1:D:117:VAL:N	1:D:118:PRO:HD2	2.34	0.42
1:E:171:LEU:HD23	1:E:171:LEU:HA	1.75	0.42
1:C:164:PRO:O	1:C:165:ASN:CB	2.51	0.42
1:D:139:ASP:HA	1:D:144:THR:O	2.20	0.42
1:A:63:ILE:O	1:A:67:LEU:HG	2.19	0.42
1:C:229:VAL:C	1:C:230:LEU:HD23	2.39	0.42
1:D:138:MET:HB3	1:D:146:TYR:CB	2.48	0.42
1:B:5:ASN:HB3	2:B:326:HOH:O	2.19	0.42
1:D:204:LYS:N	1:D:205:PRO:CD	2.82	0.42
1:E:233:ASP:O	1:E:234:LEU:HB3	2.19	0.42
1:D:5:ASN:N	2:D:323:HOH:O	2.51	0.42
1:E:249:ALA:C	1:E:251:VAL:N	2.72	0.42
1:D:9:ILE:HD11	1:E:55:TRP:HH2	1.81	0.42
1:F:73:PRO:HA	1:F:76:MET:HE2	2.01	0.42
1:E:38:LYS:HG3	1:E:214:PHE:HD1	1.85	0.42
1:C:181:GLU:O	1:C:184:LYS:N	2.53	0.42
1:F:5:ASN:ND2	1:F:8:THR:HB	2.34	0.42
1:A:99:GLU:HG2	1:A:99:GLU:H	1.70	0.42
1:D:73:PRO:HA	1:D:76:MET:HE2	2.02	0.42
1:D:245:GLU:HA	1:D:245:GLU:OE2	2.19	0.42
1:F:122:GLN:O	1:F:125:LYS:HG2	2.19	0.42
1:A:206:ASN:O	1:A:210:MET:HG3	2.19	0.42
1:A:62:MET:HE1	1:A:97:LEU:HD21	2.01	0.42
1:F:117:VAL:O	1:F:121:VAL:HG22	2.20	0.42
1:D:13:PHE:HB3	1:E:119:TRP:HB2	2.01	0.42
1:E:23:ILE:O	1:E:26:TRP:HB2	2.20	0.41
1:F:116:PHE:C	1:F:118:PRO:CD	2.88	0.41
1:E:102:PRO:CB	2:E:307:HOH:O	2.68	0.41
1:C:185:THR:HA	1:C:191:ARG:NH2	2.36	0.41
1:E:190:LEU:HA	1:E:193:LYS:HE3	2.02	0.41
1:B:247:TYR:O	1:B:251:VAL:HG22	2.20	0.41
1:A:4:ASP:CB	2:A:336:HOH:O	2.68	0.41
1:A:187:ASN:HA	1:A:188:PRO:HD3	1.76	0.41
1:C:23:ILE:HG21	1:D:126:THR:OG1	2.21	0.41
1:F:182:PHE:CE2	1:F:186:ILE:HG13	2.55	0.41
1:B:62:MET:CE	1:B:97:LEU:HD21	2.51	0.41
1:B:204:LYS:CB	1:B:205:PRO:CD	2.98	0.41
1:F:56:LYS:O	1:F:60:LYS:HG3	2.20	0.41
1:C:138:MET:HE2	1:C:178:PHE:CA	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:PRO:HD2	1:C:188:PRO:O	2.20	0.41
1:E:167:THR:O	1:E:170:MET:HB3	2.21	0.41
1:B:62:MET:HE2	1:B:97:LEU:CD1	2.34	0.41
1:F:170:MET:CE	1:F:240:ILE:HG22	2.51	0.41
1:E:92:ILE:HA	1:E:97:LEU:HD12	2.03	0.41
1:B:117:VAL:N	1:B:118:PRO:HD2	2.36	0.41
1:D:171:LEU:HD23	1:D:171:LEU:HA	1.79	0.41
1:A:88:VAL:O	1:A:92:ILE:HG13	2.21	0.41
1:E:60:LYS:O	1:E:64:VAL:HG23	2.21	0.41
1:F:237:ASN:ND2	1:F:237:ASN:C	2.72	0.40
1:F:65:LEU:HD11	1:F:76:MET:CE	2.51	0.40
1:A:60:LYS:HG2	1:A:119:TRP:CE2	2.56	0.40
1:B:150:MET:HG2	1:B:155:PHE:CZ	2.57	0.40
1:E:229:VAL:HG12	1:E:230:LEU:CD2	2.51	0.40
1:E:141:ILE:H	1:E:141:ILE:HG12	1.59	0.40
1:E:92:ILE:O	1:E:96:GLN:N	2.54	0.40
1:E:36:ASP:HA	1:E:37:PRO:HD2	1.89	0.40
1:A:150:MET:HG2	1:A:155:PHE:CZ	2.56	0.40
1:E:204:LYS:N	1:E:205:PRO:HD2	2.36	0.40
1:D:242:LYS:O	1:D:245:GLU:HB2	2.22	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:A:19:ASP:OD2	1:C:7:ARG:NH2[1_654]	1.95	0.25

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	248/257 (96%)	245 (99%)	2 (1%)	1 (0%)	39	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	246/257 (96%)	242 (98%)	3 (1%)	1 (0%)	39	61
1	C	244/257 (95%)	224 (92%)	10 (4%)	10 (4%)	3	4
1	D	247/257 (96%)	242 (98%)	4 (2%)	1 (0%)	39	61
1	E	248/257 (96%)	234 (94%)	8 (3%)	6 (2%)	7	11
1	F	246/257 (96%)	241 (98%)	4 (2%)	1 (0%)	39	61
All	All	1479/1542 (96%)	1428 (97%)	31 (2%)	20 (1%)	14	24

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	145	THR
1	C	190	LEU
1	C	196	ASN
1	C	203	GLU
1	C	143	GLY
1	E	250	LYS
1	C	189	SER
1	C	195	PRO
1	E	232	GLU
1	C	193	LYS
1	E	249	ALA
1	D	102	PRO
1	E	245	GLU
1	A	102	PRO
1	B	102	PRO
1	E	244	ALA
1	C	102	PRO
1	E	102	PRO
1	C	188	PRO
1	F	102	PRO

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	211/217 (97%)	185 (88%)	26 (12%)	6	11
1	B	209/217 (96%)	185 (88%)	24 (12%)	7	13
1	C	208/217 (96%)	181 (87%)	27 (13%)	5	9
1	D	210/217 (97%)	179 (85%)	31 (15%)	4	7
1	E	211/217 (97%)	180 (85%)	31 (15%)	4	7
1	F	209/217 (96%)	186 (89%)	23 (11%)	8	14
All	All	1258/1302 (97%)	1096 (87%)	162 (13%)	5	10

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	23	ILE
1	A	38	LYS
1	A	39	ARG
1	A	45	LYS
1	A	77	MET
1	A	78	LYS
1	A	83	LYS
1	A	99	GLU
1	A	105	ASP
1	A	110	SER
1	A	117	VAL
1	A	127	LEU
1	A	128	SER
1	A	136	THR
1	A	154	SER
1	A	158	ILE
1	A	167	THR
1	A	186	ILE
1	A	189	SER
1	A	191	ARG
1	A	204	LYS
1	A	213	ARG
1	A	216	THR
1	A	217	ARG
1	A	222	LYS
1	B	29	GLU
1	B	38	LYS
1	B	46	GLU
1	B	51	LYS

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Mol	Chain	Res	Type
1	B	76	MET
1	B	78	LYS
1	B	90	GLN
1	B	99	GLU
1	B	104	ARG
1	B	117	VAL
1	B	126	THR
1	B	138	MET
1	B	144	THR
1	B	158	ILE
1	B	162	GLU
1	B	189	SER
1	B	196	ASN
1	B	198	ILE
1	B	201	THR
1	B	203	GLU
1	B	204	LYS
1	B	206	ASN
1	B	213	ARG
1	B	233	ASP
1	C	22	THR
1	C	57	LYS
1	C	78	LYS
1	C	79	LYS
1	C	83	LYS
1	C	104	ARG
1	C	105	ASP
1	C	117	VAL
1	C	125	LYS
1	C	127	LEU
1	C	128	SER
1	C	136	THR
1	C	144	THR
1	C	158	ILE
1	C	183	SER
1	C	186	ILE
1	C	189	SER
1	C	190	LEU
1	C	191	ARG
1	C	193	LYS
1	C	195	PRO
1	C	196	ASN

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Mol	Chain	Res	Type
1	C	210	MET
1	C	213	ARG
1	C	216	THR
1	C	217	ARG
1	C	243	CYS
1	D	5	ASN
1	D	9	ILE
1	D	29	GLU
1	D	38	LYS
1	D	39	ARG
1	D	51	LYS
1	D	53	ARG
1	D	68	VAL
1	D	76	MET
1	D	78	LYS
1	D	99	GLU
1	D	104	ARG
1	D	105	ASP
1	D	110	SER
1	D	117	VAL
1	D	126	THR
1	D	127	LEU
1	D	128	SER
1	D	130	SER
1	D	138	MET
1	D	139	ASP
1	D	144	THR
1	D	158	ILE
1	D	162	GLU
1	D	183	SER
1	D	189	SER
1	D	191	ARG
1	D	192	THR
1	D	196	ASN
1	D	201	THR
1	D	217	ARG
1	E	3	GLU
1	E	8	THR
1	E	14	LEU
1	E	19	ASP
1	E	29	GLU
1	E	39	ARG

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Mol	Chain	Res	Type
1	E	45	LYS
1	E	49	THR
1	E	53	ARG
1	E	76	MET
1	E	110	SER
1	E	117	VAL
1	E	127	LEU
1	E	144	THR
1	E	150	MET
1	E	158	ILE
1	E	162	GLU
1	E	196	ASN
1	E	203	GLU
1	E	204	LYS
1	E	216	THR
1	E	218	ASP
1	E	221	LYS
1	E	235	VAL
1	E	236	PRO
1	E	240	ILE
1	E	245	GLU
1	E	246	LYS
1	E	248	LYS
1	E	250	LYS
1	E	251	VAL
1	F	8	THR
1	F	17	SER
1	F	29	GLU
1	F	38	LYS
1	F	39	ARG
1	F	83	LYS
1	F	89	THR
1	F	99	GLU
1	F	105	ASP
1	F	110	SER
1	F	113	SER
1	F	127	LEU
1	F	144	THR
1	F	183	SER
1	F	192	THR
1	F	201	THR
1	F	204	LYS

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Mol	Chain	Res	Type
1	F	233	ASP
1	F	234	LEU
1	F	237	ASN
1	F	245	GLU
1	F	248	LYS
1	F	250	LYS

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	152	HIS
1	C	187	ASN
1	D	66	ASN
1	D	90	GLN
1	D	152	HIS
1	F	237	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 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	250/257 (97%)	-0.16	0	100	100	30, 47, 68, 96	0
1	B	248/257 (96%)	-0.08	0	100	100	30, 48, 74, 87	0
1	C	246/257 (95%)	0.12	5 (2%)	68	72	31, 60, 103, 120	0
1	D	249/257 (96%)	-0.03	2 (0%)	87	89	34, 59, 86, 95	0
1	E	250/257 (97%)	0.14	8 (3%)	51	56	37, 67, 104, 123	0
1	F	248/257 (96%)	-0.10	0	100	100	34, 58, 78, 91	0
All	All	1491/1542 (96%)	-0.02	15 (1%)	84	86	30, 56, 91, 123	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	245	GLU	4.0
1	E	169	ALA	2.8
1	C	192	THR	2.7
1	C	177	LEU	2.7
1	E	144	THR	2.6
1	E	252	GLY	2.5
1	C	142	ALA	2.4
1	D	190	LEU	2.4
1	E	232	GLU	2.4
1	C	244	ALA	2.3
1	D	142	ALA	2.3
1	E	213	ARG	2.3
1	E	234	LEU	2.2
1	E	241	GLU	2.2
1	E	231	ASN	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.