Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 02:14 PM EST

PDB ID	:	1L1O
Title	:	Structure of the human Replication Protein A (RPA) trimerization core
Authors	:	Bochkareva, E.V.; Korolev, S.; Lees-Miller, S.P.; Bochkarev, A.
Deposited on	:	2002-02-19
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

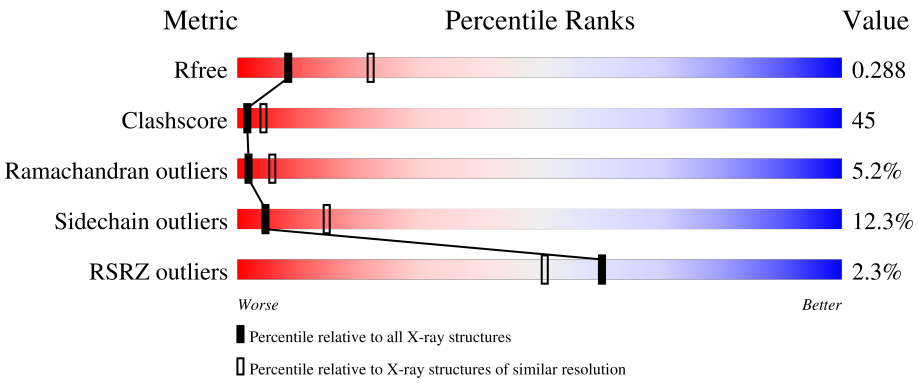
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	121	44% 46% 5% 5%
1	D	121	47% 42% 6% 5%
2	B	128	3% 38% 49% 9% • •
2	E	128	3% 30% 51% 14% • •
3	C	181	5% 33% 50% 13% •

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Mol	Chain	Length	Quality of chain
3	F	181	% 25% 59% 9% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6569 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 Replication protein A 14 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	115	901	580	146	168	7	0	0	0
1	D	115	901	580	146	168	7	0	0	0

- Molecule 2 is a protein called Replication protein A 32 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	123	966	616	163	181	6	0	0	0
2	E	123	966	616	163	181	6	0	0	0

- Molecule 3 is a protein called Replication protein A 70 kDa DNA-binding subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	173	1426	900	245	270	11	0	0	0
3	F	171	1407	887	243	266	11	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

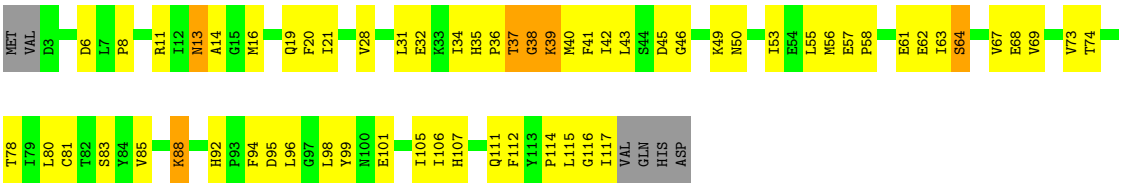
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	C	1	1	1	0	0
4	F	1	1	1	0	0

3 Residue-property plots (i)

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

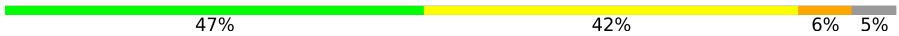
• Molecule 1: Replication protein A 14 kDa subunit

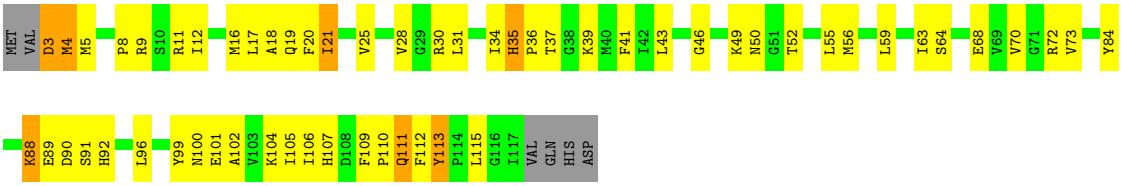
Chain A:



• Molecule 1: Replication protein A 14 kDa subunit

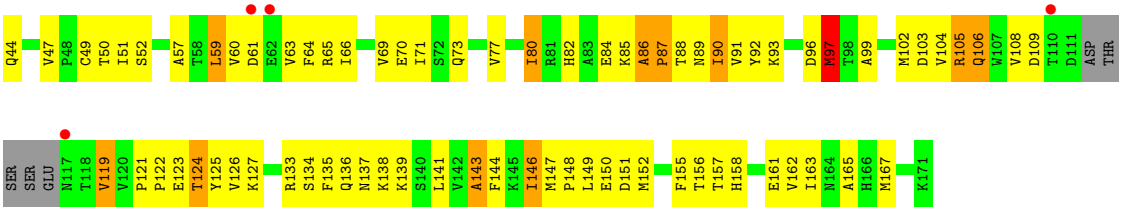
Chain D:





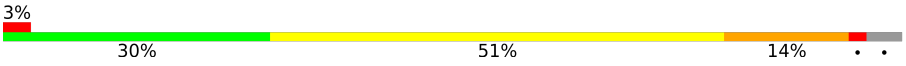
• Molecule 2: Replication protein A 32 kDa subunit

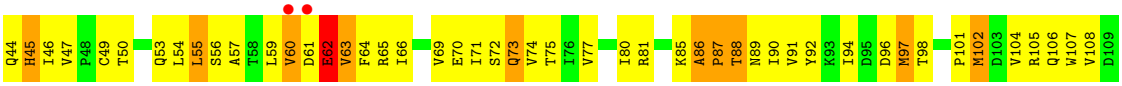
Chain B:

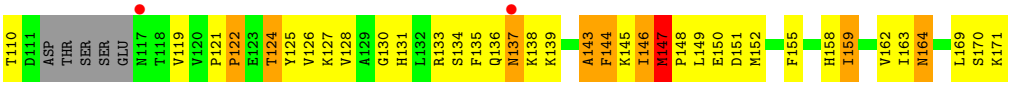


• Molecule 2: Replication protein A 32 kDa subunit

Chain E:

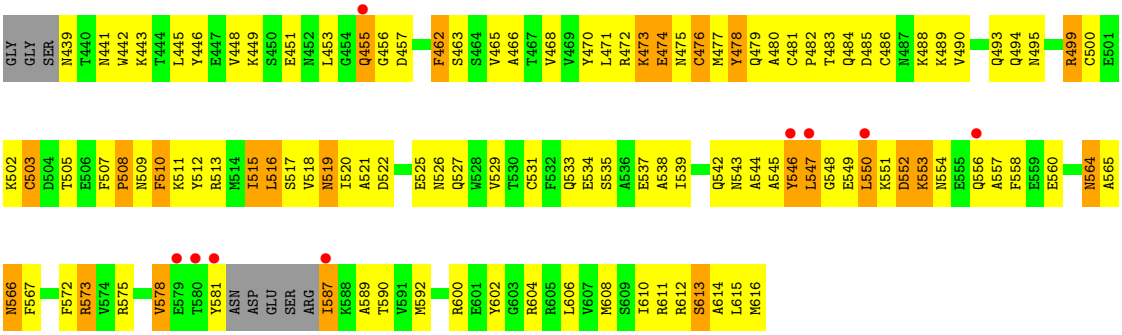






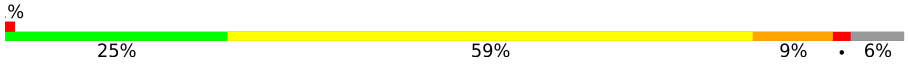
• Molecule 3: Replication protein A 70 kDa DNA-binding subunit

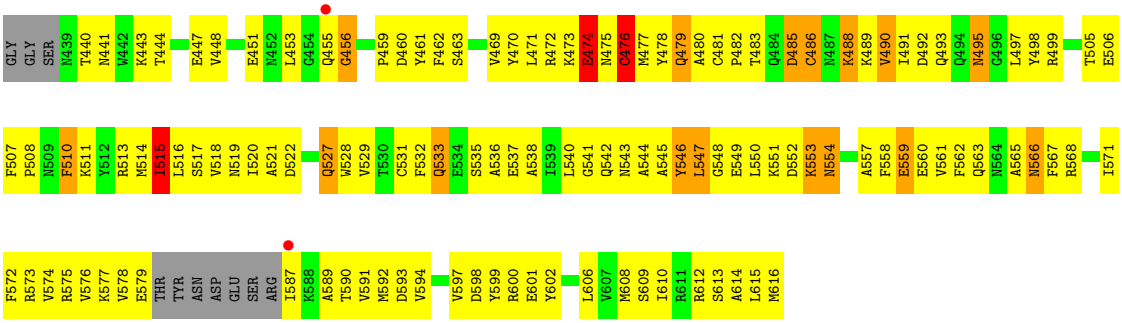
Chain C:



• Molecule 3: Replication protein A 70 kDa DNA-binding subunit

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	88.53Å 88.53Å 341.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.92 – 2.80 28.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.3 (19.92-2.80) 96.4 (28.98-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.68Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.236 , 0.282 0.243 , 0.288	Depositor DCC
R_{free} test set	4373 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å^2)	59.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 76.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6569	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.96	0/920	0.98	0/1242
1	D	0.91	0/920	1.01	0/1242
2	B	0.99	1/983 (0.1%)	1.08	3/1337 (0.2%)
2	E	0.89	0/983	1.06	3/1337 (0.2%)
3	C	0.80	0/1452	0.95	2/1953 (0.1%)
3	F	0.82	0/1432	1.02	3/1925 (0.2%)
All	All	0.89	1/6690 (0.0%)	1.02	11/9036 (0.1%)

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
2	E	0	1
3	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	165	ALA	CA-CB	-5.10	1.41	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	486	CYS	N-CA-C	-7.58	90.53	111.00
2	B	143	ALA	N-CA-C	6.16	127.64	111.00
3	C	573	ARG	N-CA-C	-5.70	95.60	111.00
3	F	483	THR	N-CA-C	-5.67	95.68	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	611	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	E	81	ARG	NE-CZ-NH2	-5.57	117.52	120.30
2	E	147	MET	CB-CG-SD	5.57	129.10	112.40
2	E	143	ALA	N-CA-C	5.56	126.00	111.00
3	F	485	ASP	N-CA-C	5.43	125.66	111.00
2	B	99	ALA	N-CA-C	-5.04	97.38	111.00
2	B	66	ILE	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	92	TYR	Sidechain
3	F	599	TYR	Sidechain

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	901	0	903	67	0
1	D	901	0	903	75	0
2	B	966	0	980	98	0
2	E	966	0	980	105	0
3	C	1426	0	1386	139	0
3	F	1407	0	1370	143	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
All	All	6569	0	6522	588	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 45.

All (588) 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)
2:B:97:MET:SD	2:B:97:MET:CE	2.04	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:LEU:HD22	1:D:63:ILE:HG22	1.18	1.11
3:F:514:MET:HG2	3:F:544:ALA:HB2	1.31	1.07
2:B:91:VAL:HG22	2:B:105:ARG:HB3	1.43	1.00
2:B:87:PRO:HD2	2:B:88:THR:HG22	1.47	0.96
3:F:572:PHE:CD2	3:F:594:VAL:HG12	2.03	0.94
1:D:35:HIS:ND1	1:D:36:PRO:HD2	1.81	0.94
3:F:495:ASN:HD21	3:F:497:LEU:HB2	1.30	0.94
3:F:448:VAL:HG13	3:F:453:LEU:HD12	1.49	0.94
3:C:548:GLY:O	3:C:551:LYS:HB3	1.67	0.94
3:C:612:ARG:HH12	3:F:612:ARG:HH22	1.13	0.92
1:D:21:ILE:HD12	1:D:21:ILE:H	1.34	0.92
3:F:514:MET:HG2	3:F:544:ALA:CB	1.98	0.92
3:C:508:PRO:HG2	3:C:509:ASN:H	1.33	0.92
2:B:63:VAL:HG12	2:B:64:PHE:H	1.33	0.92
3:C:531:CYS:HB3	3:C:535:SER:OG	1.70	0.92
2:B:80:ILE:HG22	2:B:122:PRO:HA	1.51	0.91
3:F:531:CYS:HB3	3:F:535:SER:OG	1.69	0.91
1:D:88:LYS:HZ1	2:E:125:TYR:H	1.20	0.90
1:A:117:ILE:O	1:A:117:ILE:HG22	1.72	0.90
3:F:543:ASN:OD1	3:F:546:TYR:HB3	1.73	0.88
3:F:479:GLN:HB3	3:F:510:PHE:CZ	2.09	0.87
2:B:59:LEU:HD23	2:B:59:LEU:H	1.41	0.86
3:F:479:GLN:HB3	3:F:510:PHE:CE2	2.11	0.85
3:F:514:MET:CG	3:F:544:ALA:HB2	2.05	0.85
3:F:540:LEU:HD22	3:F:561:VAL:HG12	1.57	0.85
1:D:37:THR:OG1	1:D:39:LYS:HG2	1.77	0.84
1:D:88:LYS:H	1:D:88:LYS:HD2	1.41	0.84
2:B:91:VAL:CG2	2:B:105:ARG:HB3	2.08	0.83
3:C:499:ARG:HG2	3:C:499:ARG:HH11	1.42	0.83
1:D:11:ARG:O	1:D:107:HIS:HE1	1.61	0.83
3:C:481:CYS:SG	3:C:483:THR:OG1	2.36	0.82
1:D:106:ILE:HD11	2:E:159:ILE:HG21	1.60	0.82
3:C:480:ALA:O	3:C:511:LYS:HB3	1.80	0.81
3:C:515:ILE:HG23	3:C:515:ILE:O	1.79	0.81
3:C:503:CYS:O	3:C:505:THR:HG23	1.80	0.81
2:E:121:PRO:O	2:E:124:THR:HG23	1.80	0.81
2:B:82:HIS:HE1	2:B:84:GLU:HG3	1.45	0.81
2:E:131:HIS:HD1	2:E:144:PHE:HE2	1.29	0.81
2:E:64:PHE:O	2:E:70:GLU:HA	1.80	0.81
1:D:35:HIS:ND1	1:D:36:PRO:CD	2.43	0.81
1:D:11:ARG:HH11	1:D:11:ARG:HG2	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:475:ASN:O	3:F:477:MET:N	2.14	0.80
1:A:88:LYS:HD3	2:B:152:MET:HE1	1.63	0.80
3:F:479:GLN:CD	3:F:510:PHE:HZ	1.83	0.80
2:B:150:GLU:HG3	2:B:151:ASP:H	1.45	0.80
3:F:572:PHE:HD2	3:F:594:VAL:HG12	1.45	0.79
2:B:138:LYS:HD2	2:B:138:LYS:N	1.99	0.78
3:F:495:ASN:ND2	3:F:497:LEU:HB2	1.98	0.78
2:E:80:ILE:HG22	2:E:122:PRO:HA	1.64	0.78
2:E:73:GLN:NE2	2:E:144:PHE:HE1	1.81	0.78
3:C:543:ASN:O	3:C:547:LEU:HD22	1.83	0.77
2:E:63:VAL:HG13	2:E:70:GLU:HG3	1.66	0.77
1:D:21:ILE:HD12	1:D:21:ILE:N	1.98	0.77
3:C:543:ASN:ND2	3:C:545:ALA:HB3	1.99	0.76
3:F:527:GLN:HE21	3:F:527:GLN:HA	1.51	0.76
3:F:540:LEU:HB3	3:F:561:VAL:HG11	1.66	0.76
1:A:88:LYS:HD3	2:B:152:MET:CE	2.15	0.76
2:B:89:ASN:HA	2:B:108:VAL:HG12	1.67	0.76
3:C:546:TYR:HE2	3:C:550:LEU:HD11	1.50	0.76
3:F:444:THR:OG1	3:F:447:GLU:HG3	1.86	0.75
2:E:91:VAL:HG22	2:E:105:ARG:HG2	1.70	0.74
3:C:479:GLN:CG	3:C:510:PHE:HZ	2.00	0.74
2:E:149:LEU:HD12	2:E:149:LEU:N	2.03	0.74
3:C:546:TYR:O	3:C:550:LEU:HG	1.88	0.74
3:C:508:PRO:HG2	3:C:509:ASN:N	2.03	0.73
2:B:87:PRO:HD2	2:B:88:THR:H	1.53	0.72
1:D:88:LYS:H	1:D:88:LYS:CD	2.02	0.72
2:E:164:ASN:C	2:E:164:ASN:HD22	1.91	0.72
2:B:86:ALA:HB3	2:B:89:ASN:O	1.89	0.72
3:F:472:ARG:HD3	3:F:474:GLU:CD	2.10	0.72
1:D:31:LEU:HD22	1:D:63:ILE:CG2	2.11	0.72
3:F:572:PHE:CE2	3:F:594:VAL:HG12	2.25	0.72
3:C:479:GLN:HG2	3:C:510:PHE:HZ	1.54	0.71
2:B:121:PRO:O	2:B:124:THR:HG23	1.90	0.71
2:E:158:HIS:O	2:E:162:VAL:HG23	1.91	0.71
3:C:546:TYR:CE2	3:C:550:LEU:HD11	2.25	0.71
1:D:89:GLU:O	1:D:91:SER:N	2.23	0.71
1:A:88:LYS:CD	1:A:88:LYS:H	2.04	0.71
3:C:508:PRO:CG	3:C:509:ASN:H	2.02	0.71
3:C:474:GLU:HG3	3:C:475:ASN:H	1.56	0.70
3:C:449:LYS:HE2	3:C:525:GLU:OE2	1.91	0.70
2:B:89:ASN:HB2	2:B:106:GLN:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:469:VAL:HG21	3:F:521:ALA:HB3	1.73	0.70
1:D:106:ILE:HD11	2:E:159:ILE:CG2	2.21	0.70
3:F:479:GLN:CD	3:F:510:PHE:CZ	2.65	0.70
2:B:108:VAL:HG22	2:B:109:ASP:N	2.07	0.69
2:B:87:PRO:CD	2:B:88:THR:H	2.04	0.69
3:F:546:TYR:CE1	3:F:550:LEU:HD11	2.28	0.69
1:A:20:PHE:O	1:A:73:VAL:HB	1.93	0.69
2:E:59:LEU:H	2:E:59:LEU:HD23	1.58	0.69
3:F:441:ASN:HD21	3:F:443:LYS:HE2	1.57	0.69
3:C:552:ASP:CG	3:C:553:LYS:N	2.46	0.69
2:E:54:LEU:O	2:E:56:SER:N	2.26	0.69
1:A:42:ILE:HD12	1:A:50:ASN:HD22	1.56	0.68
2:B:73:GLN:OE1	2:B:144:PHE:HE1	1.76	0.68
2:E:47:VAL:HG12	2:E:49:CYS:SG	2.33	0.68
1:D:11:ARG:NH1	1:D:99:TYR:OH	2.25	0.68
1:D:88:LYS:NZ	2:E:125:TYR:H	1.90	0.68
1:D:35:HIS:CG	1:D:36:PRO:HD2	2.29	0.68
3:F:537:GLU:HG2	3:F:543:ASN:HA	1.74	0.68
1:D:11:ARG:HG2	1:D:11:ARG:NH1	2.08	0.67
3:F:542:GLN:NE2	3:F:546:TYR:HE2	1.93	0.67
1:A:42:ILE:HD12	1:A:50:ASN:ND2	2.10	0.67
2:B:90:ILE:HG21	2:B:119:VAL:HG22	1.77	0.66
2:B:97:MET:HB2	2:B:97:MET:HE2	1.77	0.66
2:E:144:PHE:HD2	2:E:144:PHE:N	1.93	0.66
2:E:144:PHE:N	2:E:144:PHE:CD2	2.61	0.66
2:B:108:VAL:HG22	2:B:109:ASP:H	1.60	0.66
2:B:157:THR:O	2:B:161:GLU:HG3	1.93	0.66
3:C:479:GLN:HG2	3:C:510:PHE:CZ	2.31	0.66
1:A:21:ILE:HA	1:A:73:VAL:CG1	2.25	0.66
2:B:63:VAL:HG12	2:B:64:PHE:N	2.08	0.66
3:F:541:GLY:O	3:F:542:GLN:OE1	2.13	0.66
3:C:557:ALA:HA	3:C:560:GLU:HG3	1.77	0.66
2:E:89:ASN:CB	2:E:107:TRP:HA	2.25	0.66
1:A:31:LEU:HA	1:A:43:LEU:HD23	1.76	0.66
1:A:14:ALA:HB3	1:A:49:LYS:HB2	1.78	0.66
3:F:557:ALA:HA	3:F:560:GLU:HG2	1.77	0.66
3:C:542:GLN:HB2	3:C:547:LEU:CD1	2.26	0.65
3:F:476:CYS:SG	3:F:477:MET:SD	2.94	0.65
3:C:483:THR:OG1	3:C:486:CYS:HB3	1.97	0.65
1:A:63:ILE:CG2	1:A:67:VAL:HG21	2.26	0.65
2:E:96:ASP:OD1	2:E:98:THR:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:554:ASN:HB3	3:F:557:ALA:HB3	1.78	0.65
2:E:89:ASN:HA	2:E:108:VAL:HG12	1.77	0.65
3:C:612:ARG:HG3	3:F:608:MET:HE2	1.79	0.65
2:E:90:ILE:HG22	2:E:91:VAL:N	2.12	0.64
2:E:164:ASN:C	2:E:164:ASN:ND2	2.48	0.64
1:D:106:ILE:CD1	2:E:159:ILE:HG21	2.28	0.64
3:C:477:MET:SD	3:C:548:GLY:HA2	2.38	0.64
3:F:547:LEU:O	3:F:547:LEU:HD12	1.98	0.64
1:A:28:VAL:HB	1:A:99:TYR:CE2	2.33	0.64
2:B:90:ILE:O	2:B:105:ARG:HA	1.98	0.64
3:C:575:ARG:HG3	3:C:590:THR:HB	1.80	0.64
1:A:39:LYS:HD2	1:A:40:MET:HB2	1.80	0.63
2:B:146:ILE:HG22	2:B:146:ILE:O	1.99	0.63
1:D:88:LYS:HD2	1:D:88:LYS:N	2.12	0.63
3:C:478:TYR:CE1	3:C:513:ARG:HB2	2.33	0.63
3:C:518:VAL:HG12	3:C:519:ASN:N	2.12	0.63
3:C:537:GLU:OE2	3:C:543:ASN:HA	1.99	0.63
2:B:59:LEU:HD23	2:B:59:LEU:N	2.12	0.63
2:B:106:GLN:HB3	2:B:143:ALA:HB3	1.79	0.63
2:E:73:GLN:HE21	2:E:144:PHE:HE1	1.47	0.62
2:B:59:LEU:HA	2:B:63:VAL:O	1.98	0.62
2:E:50:THR:HG23	2:E:162:VAL:HG11	1.81	0.62
2:B:50:THR:HG23	2:B:162:VAL:HG11	1.80	0.62
2:B:64:PHE:HZ	2:B:134:SER:HB2	1.63	0.62
3:F:499:ARG:HB2	3:F:506:GLU:HG2	1.81	0.62
3:F:479:GLN:NE2	3:F:510:PHE:CZ	2.67	0.62
2:E:137:ASN:O	2:E:138:LYS:HG2	1.99	0.62
3:C:486:CYS:SG	3:C:502:LYS:HD3	2.39	0.61
3:F:459:PRO:HG3	3:F:575:ARG:HH21	1.64	0.61
3:F:471:LEU:N	3:F:471:LEU:HD12	2.15	0.61
1:A:57:GLU:CD	1:A:58:PRO:HD2	2.21	0.61
3:C:477:MET:SD	3:C:548:GLY:CA	2.89	0.61
3:C:499:ARG:HG2	3:C:499:ARG:NH1	2.12	0.61
3:C:471:LEU:HD23	3:C:518:VAL:HG13	1.82	0.61
3:C:479:GLN:CG	3:C:510:PHE:CZ	2.84	0.61
3:C:615:LEU:O	3:C:616:MET:HB2	2.00	0.61
2:B:89:ASN:CA	2:B:108:VAL:HG12	2.31	0.60
3:C:478:TYR:HE1	3:C:480:ALA:HB2	1.66	0.60
1:D:18:ALA:O	1:D:21:ILE:HG13	2.01	0.60
1:D:30:ARG:O	1:D:43:LEU:HA	2.01	0.60
3:F:470:TYR:C	3:F:471:LEU:HD12	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:TYR:HB2	2:E:163:ILE:HG12	1.82	0.60
2:E:126:VAL:HG12	2:E:148:PRO:HA	1.83	0.60
1:D:100:ASN:O	1:D:104:LYS:HG3	2.00	0.60
1:A:88:LYS:HD3	1:A:88:LYS:H	1.67	0.60
1:A:88:LYS:CD	2:B:152:MET:HE1	2.31	0.60
2:B:136:GLN:HA	2:B:136:GLN:HE21	1.67	0.60
3:C:564:ASN:OD1	3:C:564:ASN:C	2.40	0.60
3:F:448:VAL:HG11	3:F:462:PHE:CE2	2.38	0.59
3:C:543:ASN:HD22	3:C:545:ALA:HB3	1.66	0.59
2:E:145:LYS:HG3	2:E:146:ILE:N	2.17	0.59
2:E:149:LEU:N	2:E:149:LEU:CD1	2.65	0.59
2:B:125:TYR:HB3	2:B:149:LEU:HD12	1.84	0.59
3:C:493:GLN:O	3:C:495:ASN:N	2.34	0.59
2:E:96:ASP:OD1	2:E:96:ASP:C	2.41	0.59
3:C:516:LEU:HD12	3:C:517:SER:N	2.17	0.59
1:A:63:ILE:O	1:A:64:SER:HB3	2.02	0.59
3:C:533:GLN:HE22	3:C:544:ALA:CB	2.16	0.59
1:A:31:LEU:HD23	1:A:64:SER:HA	1.84	0.59
1:A:41:PHE:CZ	1:A:53:ILE:HG21	2.38	0.59
2:B:90:ILE:HD13	2:B:119:VAL:HG23	1.83	0.59
1:A:88:LYS:CD	1:A:88:LYS:N	2.66	0.59
1:A:14:ALA:HB3	1:A:49:LYS:CB	2.33	0.58
2:B:138:LYS:N	2:B:138:LYS:CD	2.65	0.58
2:E:54:LEU:O	2:E:55:LEU:C	2.40	0.58
2:E:89:ASN:HB3	2:E:107:TRP:HA	1.84	0.58
3:F:479:GLN:NE2	3:F:510:PHE:CE1	2.71	0.58
3:C:481:CYS:HA	3:C:490:VAL:CG1	2.32	0.58
2:B:65:ARG:CZ	2:B:70:GLU:HG2	2.33	0.58
3:C:478:TYR:CD1	3:C:478:TYR:C	2.76	0.58
3:F:550:LEU:HD23	3:F:550:LEU:N	2.18	0.58
2:B:92:TYR:HB2	2:B:104:VAL:HG22	1.85	0.58
3:F:535:SER:O	3:F:538:ALA:HB3	2.04	0.58
3:C:521:ALA:HA	3:C:526:ASN:HA	1.86	0.58
2:E:145:LYS:HG3	2:E:146:ILE:H	1.67	0.58
3:F:516:LEU:HD12	3:F:517:SER:N	2.18	0.58
3:F:492:ASP:OD2	3:F:498:TYR:HE2	1.87	0.58
1:D:31:LEU:HD23	1:D:64:SER:HA	1.85	0.57
1:A:117:ILE:O	1:A:117:ILE:CG2	2.43	0.57
2:B:61:ASP:O	2:B:63:VAL:HG23	2.05	0.57
2:E:90:ILE:HD13	2:E:119:VAL:HG22	1.87	0.57
3:F:543:ASN:O	3:F:547:LEU:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:VAL:HG13	1:A:81:CYS:SG	2.44	0.57
2:E:89:ASN:HB2	2:E:106:GLN:O	2.04	0.57
3:F:592:MET:HE3	3:F:592:MET:HA	1.87	0.57
2:B:138:LYS:HD2	2:B:138:LYS:H	1.68	0.56
2:B:138:LYS:CD	2:B:138:LYS:H	2.18	0.56
3:C:515:ILE:O	3:C:515:ILE:CG2	2.53	0.56
2:E:47:VAL:HG12	2:E:47:VAL:O	2.05	0.56
3:C:552:ASP:CG	3:C:553:LYS:H	2.07	0.56
2:E:89:ASN:HA	2:E:108:VAL:H	1.71	0.56
2:E:97:MET:N	2:E:97:MET:HE2	2.20	0.56
1:A:112:PHE:HE1	2:B:167:MET:HG3	1.70	0.56
3:C:542:GLN:HB2	3:C:547:LEU:HD13	1.88	0.56
3:C:468:VAL:HG13	3:C:518:VAL:CG1	2.35	0.56
3:C:516:LEU:HD12	3:C:516:LEU:C	2.25	0.56
3:F:472:ARG:HB3	3:F:474:GLU:HG3	1.88	0.56
3:F:527:GLN:HE21	3:F:527:GLN:CA	2.18	0.56
2:B:60:VAL:HG12	2:B:61:ASP:OD1	2.06	0.56
3:C:472:ARG:HH11	3:C:472:ARG:HG2	1.70	0.56
3:C:557:ALA:HA	3:C:560:GLU:CG	2.35	0.55
3:F:472:ARG:HG2	3:F:472:ARG:HH11	1.71	0.55
2:E:94:ILE:HD12	2:E:104:VAL:HG21	1.88	0.55
3:C:549:GLU:O	3:C:551:LYS:N	2.40	0.55
1:A:101:GLU:O	1:A:105:ILE:HG13	2.05	0.55
3:C:549:GLU:C	3:C:551:LYS:H	2.09	0.55
3:C:478:TYR:C	3:C:478:TYR:HD1	2.09	0.55
3:C:479:GLN:HB3	3:C:510:PHE:CE2	2.42	0.55
2:E:59:LEU:HA	2:E:63:VAL:O	2.07	0.55
2:E:147:MET:SD	3:F:568:ARG:NH1	2.80	0.55
3:F:559:GLU:O	3:F:563:GLN:HG2	2.06	0.55
2:E:88:THR:O	2:E:107:TRP:HD1	1.89	0.55
3:C:448:VAL:HA	3:C:453:LEU:HD22	1.89	0.55
3:C:612:ARG:HH12	3:F:612:ARG:NH2	1.93	0.55
3:F:557:ALA:O	3:F:560:GLU:HB2	2.06	0.55
2:B:64:PHE:CZ	2:B:134:SER:HB2	2.41	0.55
2:B:87:PRO:CD	2:B:88:THR:N	2.70	0.55
3:C:448:VAL:HG21	3:C:462:PHE:CE2	2.42	0.54
3:F:531:CYS:HB3	3:F:535:SER:HG	1.71	0.54
1:D:46:GLY:HA2	1:D:96:LEU:HG	1.88	0.54
3:F:473:LYS:HE3	3:F:559:GLU:OE2	2.08	0.54
3:F:535:SER:O	3:F:538:ALA:N	2.38	0.54
3:C:493:GLN:C	3:C:495:ASN:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:614:ALA:O	3:C:616:MET:HG3	2.08	0.54
1:D:35:HIS:CE1	1:D:36:PRO:HD2	2.43	0.54
2:E:126:VAL:HA	2:E:149:LEU:CD1	2.36	0.54
3:F:460:ASP:C	3:F:461:TYR:CD1	2.81	0.54
3:C:462:PHE:CD1	3:C:462:PHE:C	2.81	0.54
1:D:31:LEU:CD2	1:D:63:ILE:HG22	2.13	0.54
2:E:66:ILE:HD11	2:E:71:ILE:HD13	1.90	0.54
2:E:65:ARG:HA	2:E:69:VAL:O	2.08	0.54
1:A:13:ASN:H	1:A:13:ASN:ND2	2.05	0.54
3:C:442:TRP:O	3:C:443:LYS:HD2	2.08	0.54
1:D:112:PHE:HB2	2:E:163:ILE:HG23	1.90	0.53
1:D:112:PHE:O	2:E:163:ILE:HG12	2.07	0.53
1:A:8:PRO:HG2	1:A:116:GLY:O	2.09	0.53
3:C:566:ASN:O	3:C:567:PHE:HB2	2.09	0.53
1:D:88:LYS:HZ1	2:E:125:TYR:N	1.98	0.53
2:E:152:MET:O	2:E:155:PHE:HB3	2.08	0.53
2:B:97:MET:CE	2:B:97:MET:HB2	2.38	0.53
2:B:135:PHE:CZ	2:B:136:GLN:HG2	2.43	0.53
3:F:533:GLN:HE22	3:F:544:ALA:HB3	1.73	0.53
2:B:69:VAL:HG12	2:B:71:ILE:HG23	1.89	0.53
3:C:507:PHE:HB3	3:C:508:PRO:HD2	1.90	0.53
3:C:479:GLN:HB3	3:C:510:PHE:HE2	1.74	0.53
1:D:99:TYR:O	1:D:102:ALA:HB3	2.09	0.53
1:D:105:ILE:HG23	1:D:109:PHE:CD1	2.43	0.53
3:F:491:ILE:O	3:F:498:TYR:HA	2.08	0.53
3:F:606:LEU:O	3:F:610:ILE:HG13	2.09	0.53
1:A:13:ASN:H	1:A:13:ASN:HD22	1.57	0.52
3:C:479:GLN:CD	3:C:510:PHE:HZ	2.12	0.52
1:D:18:ALA:HB3	1:D:19:GLN:NE2	2.24	0.52
1:A:21:ILE:HA	1:A:73:VAL:HG12	1.91	0.52
2:B:90:ILE:HG21	2:B:119:VAL:CG2	2.39	0.52
2:E:62:GLU:O	2:E:63:VAL:HG23	2.09	0.52
2:E:144:PHE:HD2	2:E:144:PHE:H	1.52	0.52
3:F:463:SER:HA	3:F:572:PHE:O	2.08	0.52
1:D:21:ILE:H	1:D:21:ILE:CD1	1.97	0.52
1:D:16:MET:O	1:D:17:LEU:C	2.48	0.52
3:F:532:PHE:HE1	3:F:590:THR:CG2	2.23	0.52
2:B:64:PHE:HZ	2:B:134:SER:CB	2.22	0.52
3:C:575:ARG:HG2	3:C:592:MET:SD	2.49	0.52
1:D:105:ILE:HG23	1:D:109:PHE:CE1	2.45	0.52
2:B:126:VAL:HG12	2:B:148:PRO:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:LEU:C	2:E:56:SER:N	2.63	0.52
2:B:65:ARG:HA	2:B:69:VAL:O	2.08	0.52
3:C:533:GLN:HE22	3:C:544:ALA:HB3	1.73	0.52
3:C:542:GLN:HB2	3:C:547:LEU:HD11	1.91	0.52
3:F:546:TYR:CZ	3:F:550:LEU:HD11	2.44	0.52
1:A:55:LEU:N	1:A:55:LEU:HD12	2.25	0.52
2:E:53:GLN:O	2:E:66:ILE:HG23	2.09	0.52
1:A:63:ILE:HG22	1:A:64:SER:N	2.25	0.52
2:B:63:VAL:CG1	2:B:64:PHE:H	2.16	0.52
2:B:82:HIS:O	2:B:92:TYR:HA	2.10	0.51
2:B:92:TYR:HB2	2:B:104:VAL:CG2	2.40	0.51
3:F:476:CYS:SG	3:F:477:MET:HG2	2.50	0.51
3:F:471:LEU:HD23	3:F:516:LEU:HD21	1.91	0.51
3:F:516:LEU:HD12	3:F:517:SER:H	1.73	0.51
3:C:471:LEU:HD23	3:C:518:VAL:HG22	1.92	0.51
3:F:593:ASP:OD1	3:F:594:VAL:N	2.44	0.51
3:C:566:ASN:ND2	3:C:567:PHE:H	2.09	0.51
3:F:561:VAL:C	3:F:563:GLN:H	2.13	0.51
1:A:98:LEU:O	1:A:99:TYR:C	2.49	0.51
3:C:518:VAL:CG1	3:C:519:ASN:N	2.74	0.51
2:B:47:VAL:HG12	2:B:49:CYS:SG	2.51	0.51
3:F:461:TYR:CD1	3:F:461:TYR:N	2.79	0.51
1:D:88:LYS:CD	1:D:88:LYS:N	2.74	0.51
2:B:108:VAL:CG2	2:B:109:ASP:N	2.74	0.50
3:C:604:ARG:NH1	3:F:615:LEU:O	2.44	0.50
1:A:13:ASN:HD22	1:A:13:ASN:C	2.12	0.50
1:A:46:GLY:HA2	1:A:96:LEU:HG	1.93	0.50
2:E:44:GLN:HG3	2:E:45:HIS:N	2.26	0.50
2:E:73:GLN:NE2	2:E:144:PHE:CE1	2.68	0.50
3:F:480:ALA:O	3:F:481:CYS:C	2.49	0.50
3:F:598:ASP:OD1	3:F:601:GLU:HG3	2.11	0.50
3:F:515:ILE:HG12	3:F:515:ILE:O	2.12	0.50
3:F:549:GLU:HG2	3:F:553:LYS:HE2	1.93	0.50
3:C:478:TYR:CE1	3:C:480:ALA:HB2	2.47	0.50
3:C:556:GLN:O	3:C:560:GLU:HG2	2.12	0.50
2:E:69:VAL:CG1	2:E:169:LEU:HD13	2.41	0.50
2:E:69:VAL:HG11	2:E:169:LEU:HD13	1.92	0.50
3:F:492:ASP:HA	3:F:498:TYR:HD2	1.76	0.50
1:A:53:ILE:N	1:A:53:ILE:HD12	2.27	0.50
2:B:59:LEU:H	2:B:59:LEU:CD2	2.19	0.50
3:C:472:ARG:HG2	3:C:472:ARG:NH1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:549:GLU:C	3:C:551:LYS:N	2.63	0.50
2:E:170:SER:O	2:E:171:LYS:CB	2.58	0.50
3:F:548:GLY:O	3:F:551:LYS:HB3	2.12	0.50
3:C:564:ASN:OD1	3:C:565:ALA:N	2.44	0.50
3:C:578:VAL:HA	3:C:587:ILE:HA	1.93	0.50
2:B:82:HIS:CE1	2:B:84:GLU:HG3	2.36	0.50
2:B:90:ILE:HD13	2:B:119:VAL:CG2	2.42	0.50
3:C:543:ASN:C	3:C:547:LEU:HD22	2.31	0.50
1:D:55:LEU:HD21	1:D:59:LEU:CD2	2.42	0.49
2:E:135:PHE:O	2:E:136:GLN:HB2	2.12	0.49
2:E:125:TYR:O	2:E:149:LEU:HD13	2.12	0.49
3:C:508:PRO:CG	3:C:509:ASN:N	2.65	0.49
3:F:575:ARG:O	3:F:576:VAL:HG13	2.12	0.49
3:C:475:ASN:O	3:C:477:MET:N	2.45	0.49
2:E:46:ILE:HD11	2:E:75:THR:HG23	1.94	0.49
2:B:157:THR:O	2:B:157:THR:HG22	2.12	0.49
3:C:445:LEU:O	3:C:446:TYR:C	2.50	0.49
3:C:488:LYS:HD2	3:C:489:LYS:H	1.76	0.49
1:D:101:GLU:O	1:D:105:ILE:HG13	2.13	0.49
3:F:540:LEU:HD22	3:F:561:VAL:CG1	2.36	0.49
3:F:577:LYS:NZ	3:F:577:LYS:HB3	2.28	0.49
3:C:480:ALA:HB3	3:C:511:LYS:O	2.12	0.49
1:D:110:PRO:HG2	1:D:111:GLN:H	1.77	0.49
2:E:90:ILE:HG22	2:E:91:VAL:H	1.76	0.49
3:F:488:LYS:CD	3:F:489:LYS:H	2.26	0.49
1:A:45:ASP:C	1:A:45:ASP:OD2	2.51	0.49
2:B:135:PHE:O	2:B:136:GLN:HB2	2.12	0.49
1:D:91:SER:HG	1:D:92:HIS:CE1	2.31	0.49
2:E:63:VAL:HG13	2:E:70:GLU:CG	2.40	0.49
1:A:11:ARG:NH2	1:A:68:GLU:OE2	2.46	0.48
1:D:84:TYR:CD1	1:D:84:TYR:C	2.86	0.48
1:D:113:TYR:O	1:D:113:TYR:CD2	2.66	0.48
2:B:108:VAL:CG2	2:B:109:ASP:H	2.26	0.48
3:C:543:ASN:ND2	3:C:546:TYR:H	2.10	0.48
3:C:441:ASN:H	3:C:573:ARG:HH12	1.60	0.48
1:D:35:HIS:CE1	1:D:36:PRO:HG2	2.48	0.48
3:F:572:PHE:CE2	3:F:594:VAL:CG1	2.96	0.48
3:F:594:VAL:HG23	3:F:594:VAL:O	2.13	0.48
3:C:575:ARG:CG	3:C:590:THR:HB	2.42	0.48
3:F:493:GLN:HG3	3:F:506:GLU:OE2	2.14	0.48
2:B:64:PHE:O	2:B:70:GLU:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:492:ASP:HA	3:F:498:TYR:CD2	2.49	0.48
1:A:36:PRO:C	1:A:38:GLY:H	2.17	0.48
2:E:63:VAL:HG22	2:E:70:GLU:OE2	2.13	0.48
1:D:9:ARG:CZ	2:E:97:MET:HG3	2.44	0.47
2:E:53:GLN:HB3	2:E:66:ILE:HG21	1.96	0.47
2:E:60:VAL:HG12	2:E:61:ASP:H	1.78	0.47
3:F:505:THR:HB	3:F:507:PHE:CE1	2.49	0.47
3:F:550:LEU:O	3:F:551:LYS:C	2.52	0.47
1:A:92:HIS:CD2	2:B:151:ASP:HB2	2.49	0.47
2:B:57:ALA:O	2:B:139:LYS:HE2	2.13	0.47
3:C:608:MET:SD	3:F:615:LEU:CD1	3.03	0.47
3:F:614:ALA:C	3:F:616:MET:H	2.16	0.47
1:A:105:ILE:HG22	2:B:163:ILE:HD13	1.97	0.47
3:F:578:VAL:HG22	3:F:579:GLU:N	2.29	0.47
3:F:551:LYS:HA	3:F:558:PHE:CD1	2.49	0.47
3:F:571:ILE:HG13	3:F:597:VAL:HA	1.97	0.47
3:C:493:GLN:C	3:C:495:ASN:N	2.67	0.47
1:D:34:ILE:O	1:D:34:ILE:HG23	2.15	0.47
2:E:59:LEU:HD23	2:E:59:LEU:N	2.29	0.47
3:F:443:LYS:HA	3:F:447:GLU:OE1	2.14	0.47
1:A:88:LYS:HE3	2:B:152:MET:HE1	1.96	0.47
1:D:109:PHE:O	1:D:110:PRO:C	2.51	0.47
1:A:112:PHE:CE1	2:B:167:MET:HG3	2.50	0.47
3:C:472:ARG:HD3	3:C:474:GLU:OE2	2.14	0.47
3:C:557:ALA:O	3:C:560:GLU:HB2	2.15	0.46
3:C:612:ARG:HH22	3:F:612:ARG:HH12	1.62	0.46
1:D:21:ILE:N	1:D:21:ILE:CD1	2.65	0.46
3:F:578:VAL:O	3:F:579:GLU:OE2	2.34	0.46
2:B:161:GLU:HG2	3:C:606:LEU:HD11	1.98	0.46
2:E:53:GLN:HB3	2:E:66:ILE:HD13	1.98	0.46
3:C:519:ASN:HD22	3:C:519:ASN:HA	1.49	0.46
1:D:92:HIS:CG	2:E:151:ASP:HB2	2.50	0.46
1:D:31:LEU:HA	1:D:43:LEU:HD23	1.98	0.46
1:A:39:LYS:HD2	1:A:39:LYS:C	2.36	0.46
1:A:94:PHE:HE1	2:B:156:THR:HG1	1.64	0.46
1:D:96:LEU:HD12	1:D:96:LEU:O	2.16	0.46
3:F:493:GLN:HB2	3:F:495:ASN:ND2	2.31	0.46
1:A:63:ILE:HG22	1:A:64:SER:H	1.79	0.46
2:B:96:ASP:OD1	2:B:96:ASP:C	2.53	0.46
3:F:493:GLN:C	3:F:495:ASN:H	2.19	0.46
1:A:95:ASP:OD1	1:A:95:ASP:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:529:VAL:HG12	3:C:589:ALA:HB1	1.98	0.46
1:D:9:ARG:NH1	2:E:97:MET:HG3	2.31	0.46
1:D:41:PHE:HE1	1:D:43:LEU:HG	1.81	0.46
2:E:73:GLN:C	2:E:74:VAL:HG13	2.36	0.46
1:A:21:ILE:HA	1:A:73:VAL:HG11	1.97	0.45
3:F:460:ASP:HB2	3:F:576:VAL:HG23	1.98	0.45
3:F:591:VAL:O	3:F:591:VAL:HG12	2.14	0.45
3:F:598:ASP:OD1	3:F:601:GLU:CG	2.65	0.45
2:E:50:THR:HB	2:E:98:THR:HG21	1.98	0.45
3:F:476:CYS:O	3:F:514:MET:HA	2.16	0.45
1:A:111:GLN:HG2	1:A:112:PHE:CD2	2.51	0.45
3:C:480:ALA:O	3:C:481:CYS:C	2.53	0.45
3:C:482:PRO:HA	3:C:511:LYS:HB2	1.99	0.45
3:C:612:ARG:HH22	3:F:612:ARG:NH1	2.14	0.45
1:D:113:TYR:O	1:D:113:TYR:HD2	2.00	0.45
3:F:443:LYS:HZ2	3:F:451:GLU:CD	2.20	0.45
2:E:85:LYS:HG2	2:E:119:VAL:HG21	1.98	0.45
3:C:520:ILE:HG21	3:C:572:PHE:CE2	2.52	0.45
2:E:77:VAL:HG23	2:E:158:HIS:CG	2.51	0.45
2:E:72:SER:OG	2:E:73:GLN:N	2.46	0.45
1:D:18:ALA:HB3	1:D:19:GLN:HE22	1.81	0.45
2:E:63:VAL:HG13	2:E:64:PHE:N	2.32	0.45
3:F:495:ASN:C	3:F:495:ASN:HD22	2.20	0.45
1:A:20:PHE:O	1:A:73:VAL:CB	2.63	0.45
2:B:77:VAL:HG23	2:B:158:HIS:CG	2.51	0.45
2:E:55:LEU:CD2	2:E:102:MET:HE3	2.47	0.45
3:C:451:GLU:HB2	3:C:453:LEU:HD13	1.98	0.45
3:C:468:VAL:HG11	3:C:471:LEU:HD21	1.99	0.45
3:F:455:GLN:O	3:F:456:GLY:C	2.56	0.45
1:D:12:ILE:HG21	1:D:20:PHE:CD1	2.52	0.45
1:D:113:TYR:CE1	2:E:159:ILE:HG23	2.52	0.45
3:F:472:ARG:HD3	3:F:474:GLU:OE1	2.16	0.45
3:C:500:CYS:SG	3:C:502:LYS:HB3	2.57	0.44
1:D:3:ASP:O	1:D:4:MET:C	2.56	0.44
2:E:63:VAL:CG1	2:E:64:PHE:N	2.81	0.44
3:F:535:SER:OG	3:F:536:ALA:N	2.49	0.44
1:A:16:MET:HA	1:A:19:GLN:OE1	2.18	0.44
1:A:57:GLU:OE1	1:A:58:PRO:HD2	2.17	0.44
2:B:104:VAL:HG12	2:B:141:LEU:HB3	1.99	0.44
3:C:471:LEU:CD2	3:C:518:VAL:HG22	2.47	0.44
2:E:75:THR:HA	2:E:128:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:86:ALA:HB3	2:E:89:ASN:O	2.18	0.44
3:C:520:ILE:O	3:C:527:GLN:N	2.49	0.44
2:E:147:MET:HB3	3:F:568:ARG:HH12	1.82	0.44
3:C:600:ARG:CZ	3:C:604:ARG:HH21	2.29	0.44
2:E:86:ALA:HB1	2:E:87:PRO:HD2	1.99	0.44
3:F:444:THR:O	3:F:448:VAL:HG23	2.17	0.44
2:B:149:LEU:HD23	2:B:149:LEU:HA	1.81	0.44
3:C:533:GLN:HE22	3:C:544:ALA:HB2	1.83	0.44
3:C:610:ILE:HA	3:C:613:SER:OG	2.17	0.44
1:D:20:PHE:O	1:D:73:VAL:HB	2.18	0.44
3:F:459:PRO:HB3	3:F:577:LYS:HG2	1.99	0.44
2:B:59:LEU:N	2:B:59:LEU:CD2	2.78	0.44
3:C:519:ASN:ND2	3:C:526:ASN:HD22	2.16	0.44
2:E:54:LEU:HA	2:E:54:LEU:HD23	1.73	0.44
3:F:455:GLN:O	3:F:456:GLY:O	2.35	0.44
1:D:41:PHE:CE1	1:D:43:LEU:HG	2.53	0.43
3:F:488:LYS:HD3	3:F:489:LYS:H	1.83	0.43
2:B:161:GLU:HG2	3:C:606:LEU:CD1	2.48	0.43
2:B:161:GLU:OE2	3:C:602:TYR:HE2	2.01	0.43
3:C:558:PHE:C	3:C:560:GLU:N	2.72	0.43
3:F:473:LYS:HE3	3:F:559:GLU:CD	2.39	0.43
3:F:529:VAL:HG12	3:F:589:ALA:CB	2.48	0.43
2:E:130:GLY:HA2	2:E:144:PHE:CD2	2.53	0.43
3:F:529:VAL:HG12	3:F:589:ALA:HB1	2.00	0.43
3:F:554:ASN:HB3	3:F:557:ALA:CB	2.46	0.43
2:B:136:GLN:HB2	2:B:138:LYS:HD3	2.00	0.43
1:A:42:ILE:O	1:A:42:ILE:HG13	2.18	0.43
2:E:64:PHE:CZ	2:E:134:SER:HB2	2.53	0.43
3:F:513:ARG:NH2	3:F:533:GLN:HG2	2.33	0.43
3:F:520:ILE:HD12	3:F:572:PHE:CD1	2.53	0.43
3:C:473:LYS:O	3:C:476:CYS:SG	2.76	0.43
2:E:60:VAL:HG12	2:E:61:ASP:N	2.33	0.43
1:A:88:LYS:N	1:A:88:LYS:HD2	2.32	0.43
3:C:552:ASP:O	3:C:553:LYS:O	2.37	0.43
3:C:556:GLN:C	3:C:558:PHE:N	2.71	0.43
3:F:440:THR:HG22	3:F:441:ASN:N	2.32	0.43
2:B:143:ALA:O	2:B:144:PHE:C	2.55	0.43
1:D:35:HIS:ND1	1:D:36:PRO:N	2.66	0.43
3:F:469:VAL:C	3:F:566:ASN:HD21	2.22	0.43
1:A:111:GLN:OE1	1:A:111:GLN:N	2.40	0.43
2:B:65:ARG:NH2	2:B:70:GLU:HG2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:519:ASN:HD21	3:C:526:ASN:HD22	1.66	0.42
3:C:539:ILE:O	3:C:539:ILE:HG22	2.19	0.42
1:A:16:MET:O	1:A:19:GLN:N	2.44	0.42
1:D:39:LYS:O	1:D:55:LEU:HB2	2.19	0.42
2:E:89:ASN:HB2	2:E:107:TRP:HA	2.00	0.42
3:F:461:TYR:HA	3:F:574:VAL:O	2.19	0.42
3:C:445:LEU:HD23	3:C:445:LEU:HA	1.79	0.42
1:D:11:ARG:NH2	1:D:68:GLU:OE2	2.48	0.42
1:D:68:GLU:O	1:D:84:TYR:HA	2.19	0.42
2:E:47:VAL:CG1	2:E:49:CYS:SG	3.05	0.42
3:F:514:MET:CE	3:F:516:LEU:HB2	2.49	0.42
2:B:127:LYS:HE3	2:B:127:LYS:HB2	1.67	0.42
3:C:449:LYS:CE	3:C:525:GLU:OE2	2.65	0.42
3:C:548:GLY:O	3:C:551:LYS:CB	2.53	0.42
2:B:97:MET:CE	2:B:97:MET:CB	2.97	0.42
1:A:74:THR:N	1:A:78:THR:O	2.43	0.42
3:C:481:CYS:N	3:C:490:VAL:HG13	2.34	0.42
2:E:144:PHE:HD1	3:F:567:PHE:CZ	2.37	0.42
3:C:614:ALA:O	3:C:615:LEU:C	2.57	0.42
2:E:89:ASN:CA	2:E:108:VAL:HG12	2.49	0.42
3:F:558:PHE:C	3:F:560:GLU:H	2.22	0.42
2:B:93:LYS:HD3	2:B:103:ASP:OD1	2.20	0.42
3:F:518:VAL:HG12	3:F:519:ASN:N	2.35	0.42
1:A:114:PRO:C	1:A:115:LEU:HG	2.41	0.42
2:B:85:LYS:O	2:B:86:ALA:HB3	2.19	0.42
2:B:135:PHE:CE1	2:B:136:GLN:HG2	2.55	0.42
2:E:46:ILE:CD1	2:E:75:THR:HG23	2.50	0.42
3:F:441:ASN:O	3:F:443:LYS:HG3	2.19	0.42
3:F:482:PRO:HB3	3:F:510:PHE:O	2.20	0.42
1:A:63:ILE:HG23	1:A:67:VAL:HG21	2.01	0.42
1:A:88:LYS:CE	2:B:152:MET:HE1	2.50	0.42
2:B:65:ARG:HH11	2:B:65:ARG:HG2	1.84	0.42
2:B:136:GLN:HA	2:B:136:GLN:NE2	2.32	0.42
3:C:462:PHE:HD1	3:C:463:SER:N	2.18	0.42
1:D:8:PRO:HB3	2:E:98:THR:O	2.20	0.42
1:D:55:LEU:HD21	1:D:59:LEU:HD23	2.02	0.42
3:F:561:VAL:O	3:F:563:GLN:N	2.53	0.42
1:A:13:ASN:ND2	1:A:13:ASN:N	2.64	0.41
1:A:56:MET:CE	1:A:80:LEU:HD11	2.50	0.41
1:A:106:ILE:HG22	1:A:107:HIS:N	2.33	0.41
2:B:167:MET:CE	3:C:610:ILE:HG23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:522:ASP:OD1	3:C:522:ASP:C	2.58	0.41
3:C:473:LYS:C	3:C:473:LYS:HD2	2.41	0.41
3:F:490:VAL:HB	3:F:498:TYR:HB3	2.03	0.41
2:B:106:GLN:HE21	2:B:106:GLN:HB2	1.61	0.41
3:C:470:TYR:CD2	3:C:471:LEU:N	2.89	0.41
3:F:573:ARG:HD2	3:F:573:ARG:HA	1.82	0.41
3:C:474:GLU:CG	3:C:475:ASN:H	2.29	0.41
3:C:552:ASP:OD2	3:C:553:LYS:N	2.43	0.41
2:E:143:ALA:O	2:E:144:PHE:C	2.57	0.41
3:F:522:ASP:OD1	3:F:522:ASP:C	2.59	0.41
1:A:13:ASN:HD22	1:A:13:ASN:N	2.16	0.41
3:C:455:GLN:NE2	3:C:456:GLY:N	2.68	0.41
3:F:540:LEU:HD23	3:F:565:ALA:CB	2.50	0.41
1:A:88:LYS:HD3	2:B:152:MET:HE2	2.01	0.41
2:B:51:ILE:O	2:B:52:SER:C	2.59	0.41
2:B:73:GLN:OE1	2:B:144:PHE:CE1	2.66	0.41
2:B:121:PRO:O	2:B:124:THR:CG2	2.65	0.41
3:F:558:PHE:O	3:F:560:GLU:N	2.54	0.41
3:F:577:LYS:O	3:F:587:ILE:HA	2.20	0.41
1:A:37:THR:O	1:A:38:GLY:C	2.58	0.41
3:C:448:VAL:HG13	3:C:453:LEU:HD22	2.02	0.41
2:E:59:LEU:O	2:E:60:VAL:O	2.39	0.41
3:F:578:VAL:HG22	3:F:579:GLU:H	1.85	0.41
3:C:482:PRO:HG3	3:C:509:ASN:OD1	2.21	0.41
3:F:519:ASN:HB2	3:F:528:TRP:CZ3	2.56	0.41
1:A:35:HIS:ND1	1:A:37:THR:OG1	2.47	0.41
1:A:40:MET:O	1:A:40:MET:SD	2.79	0.41
3:C:439:ASN:C	3:C:439:ASN:OD1	2.60	0.41
3:C:483:THR:HG23	3:C:507:PHE:CZ	2.56	0.41
3:C:535:SER:O	3:C:538:ALA:N	2.53	0.41
1:D:9:ARG:HD2	1:D:70:VAL:HG11	2.03	0.41
1:D:11:ARG:HH11	1:D:11:ARG:CG	2.17	0.41
1:D:12:ILE:HD13	1:D:25:VAL:HG11	2.03	0.41
1:D:28:VAL:HG21	1:D:99:TYR:CZ	2.56	0.41
1:D:49:LYS:C	1:D:50:ASN:HD22	2.24	0.41
2:E:59:LEU:C	2:E:60:VAL:O	2.58	0.41
3:F:440:THR:CG2	3:F:441:ASN:N	2.82	0.41
3:F:488:LYS:HD2	3:F:489:LYS:N	2.35	0.41
2:E:127:LYS:N	2:E:149:LEU:HD11	2.36	0.41
3:F:478:TYR:CE1	3:F:480:ALA:HB2	2.56	0.41
3:F:495:ASN:ND2	3:F:495:ASN:C	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:602:TYR:CZ	3:F:606:LEU:HD11	2.56	0.41
1:D:9:ARG:HD2	1:D:70:VAL:CG1	2.51	0.40
2:E:73:GLN:O	2:E:74:VAL:CG1	2.69	0.40
2:B:104:VAL:O	2:B:104:VAL:HG23	2.20	0.40
3:C:465:VAL:HG12	3:C:466:ALA:N	2.36	0.40
3:C:566:ASN:HD22	3:C:566:ASN:HA	1.64	0.40
2:E:45:HIS:ND1	2:E:45:HIS:O	2.54	0.40
2:E:69:VAL:HG11	2:E:169:LEU:CD1	2.52	0.40
3:F:516:LEU:HG	3:F:518:VAL:HG22	2.03	0.40
3:F:566:ASN:HD22	3:F:566:ASN:HA	1.57	0.40
1:D:17:LEU:H	1:D:17:LEU:HG	1.74	0.40
2:E:64:PHE:CE2	2:E:134:SER:HB2	2.57	0.40
3:F:558:PHE:C	3:F:560:GLU:N	2.74	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	113/121 (93%)	101 (89%)	9 (8%)	3 (3%)	5 17
1	D	113/121 (93%)	94 (83%)	13 (12%)	6 (5%)	2 6
2	B	119/128 (93%)	103 (87%)	12 (10%)	4 (3%)	3 13
2	E	119/128 (93%)	97 (82%)	14 (12%)	8 (7%)	1 3
3	C	169/181 (93%)	127 (75%)	33 (20%)	9 (5%)	2 6
3	F	167/181 (92%)	130 (78%)	25 (15%)	12 (7%)	1 2
All	All	800/860 (93%)	652 (82%)	106 (13%)	42 (5%)	2 6

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	87	PRO
3	C	457	ASP
3	C	553	LYS
1	D	90	ASP
3	F	476	CYS
3	F	515	ILE
3	F	545	ALA
1	A	38	GLY
2	B	86	ALA
3	C	474	GLU
3	C	476	CYS
3	C	494	GLN
3	C	508	PRO
1	D	4	MET
1	D	5	MET
1	D	35	HIS
2	E	55	LEU
2	E	57	ALA
2	E	63	VAL
3	F	456	GLY
3	F	511	LYS
3	F	533	GLN
3	F	553	LYS
3	F	562	PHE
1	A	64	SER
3	C	534	GLU
3	C	550	LEU
1	D	111	GLN
2	E	60	VAL
3	F	474	GLU
3	F	508	PRO
3	F	547	LEU
3	C	515	ILE
2	E	62	GLU
3	F	559	GLU
1	A	37	THR
1	D	113	TYR
2	E	86	ALA
2	B	97	MET
2	B	146	ILE
2	E	87	PRO
2	E	146	ILE

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	100/106 (94%)	90 (90%)	10 (10%)	7 22
1	D	100/106 (94%)	93 (93%)	7 (7%)	15 40
2	B	111/117 (95%)	96 (86%)	15 (14%)	4 11
2	E	111/117 (95%)	93 (84%)	18 (16%)	2 7
3	C	156/162 (96%)	134 (86%)	22 (14%)	3 10
3	F	154/162 (95%)	136 (88%)	18 (12%)	5 16
All	All	732/770 (95%)	642 (88%)	90 (12%)	4 15

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	13	ASN
1	A	32	GLU
1	A	34	ILE
1	A	39	LYS
1	A	61	GLU
1	A	62	GLU
1	A	83	SER
1	A	85	VAL
1	A	88	LYS
2	B	44	GLN
2	B	59	LEU
2	B	80	ILE
2	B	90	ILE
2	B	97	MET
2	B	102	MET
2	B	105	ARG
2	B	106	GLN
2	B	119	VAL
2	B	123	GLU
2	B	124	THR
2	B	133	ARG

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Mol	Chain	Res	Type
2	B	137	ASN
2	B	147	MET
2	B	155	PHE
3	C	455	GLN
3	C	462	PHE
3	C	473	LYS
3	C	478	TYR
3	C	484	GLN
3	C	485	ASP
3	C	499	ARG
3	C	503	CYS
3	C	510	PHE
3	C	512	TYR
3	C	516	LEU
3	C	519	ASN
3	C	546	TYR
3	C	547	LEU
3	C	552	ASP
3	C	554	ASN
3	C	564	ASN
3	C	566	ASN
3	C	578	VAL
3	C	581	TYR
3	C	587	ILE
3	C	613	SER
1	D	3	ASP
1	D	21	ILE
1	D	52	THR
1	D	56	MET
1	D	72	ARG
1	D	88	LYS
1	D	115	LEU
2	E	45	HIS
2	E	62	GLU
2	E	73	GLN
2	E	88	THR
2	E	97	MET
2	E	101	PRO
2	E	102	MET
2	E	110	THR
2	E	122	PRO
2	E	124	THR

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Mol	Chain	Res	Type
2	E	133	ARG
2	E	137	ASN
2	E	139	LYS
2	E	144	PHE
2	E	147	MET
2	E	150	GLU
2	E	159	ILE
2	E	164	ASN
3	F	474	GLU
3	F	476	CYS
3	F	479	GLN
3	F	485	ASP
3	F	486	CYS
3	F	488	LYS
3	F	490	VAL
3	F	495	ASN
3	F	510	PHE
3	F	515	ILE
3	F	527	GLN
3	F	546	TYR
3	F	552	ASP
3	F	554	ASN
3	F	566	ASN
3	F	600	ARG
3	F	609	SER
3	F	613	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	50	ASN
1	A	86	GLN
2	B	44	GLN
2	B	73	GLN
2	B	82	HIS
2	B	106	GLN
2	B	117	ASN
2	B	136	GLN
2	B	137	ASN
2	B	166	HIS
3	C	455	GLN

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Mol	Chain	Res	Type
3	C	519	ASN
3	C	526	ASN
3	C	554	ASN
3	C	566	ASN
1	D	19	GLN
1	D	50	ASN
1	D	107	HIS
2	E	136	GLN
2	E	137	ASN
2	E	166	HIS
3	F	441	ASN
3	F	455	GLN
3	F	479	GLN
3	F	484	GLN
3	F	495	ASN
3	F	527	GLN
3	F	554	ASN
3	F	566	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	115/121 (95%)	-0.32	0	100	100	19, 46, 85, 95	0
1	D	115/121 (95%)	-0.51	0	100	100	23, 42, 74, 88	0
2	B	123/128 (96%)	-0.07	4 (3%)	46	36	18, 45, 83, 106	0
2	E	123/128 (96%)	0.06	4 (3%)	46	36	20, 55, 95, 117	0
3	C	173/181 (95%)	0.17	9 (5%)	27	18	31, 69, 105, 132	0
3	F	171/181 (94%)	0.05	2 (1%)	79	73	35, 69, 99, 111	0
All	All	820/860 (95%)	-0.07	19 (2%)	60	51	18, 56, 98, 132	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	581	TYR	7.1
2	B	110	THR	3.9
2	E	61	ASP	3.7
3	C	580	THR	3.6
3	C	556	GLN	3.3
2	E	137	ASN	3.1
2	E	60	VAL	3.0
3	C	547	LEU	2.8
2	B	62	GLU	2.6
3	C	579	GLU	2.6
3	C	550	LEU	2.6
3	C	455	GLN	2.6
3	F	455	GLN	2.5
3	F	587	ILE	2.4
2	B	61	ASP	2.3
3	C	587	ILE	2.2
2	B	117	ASN	2.2
2	E	117	ASN	2.1
3	C	546	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	F	2	1/1	0.97	0.07	66,66,66,66	0
4	ZN	C	1	1/1	0.99	0.08	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.