



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:29 PM GMT

PDB ID : 2V1C
Title : CRYSTAL STRUCTURE AND MUTATIONAL STUDY OF RECOR PROVIDE INSIGHT INTO ITS ROLE IN DNA REPAIR
Authors : Timmins, J.; Leiros, I.; Mcsweeney, S.
Deposited on : 2007-05-23
Resolution : 3.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

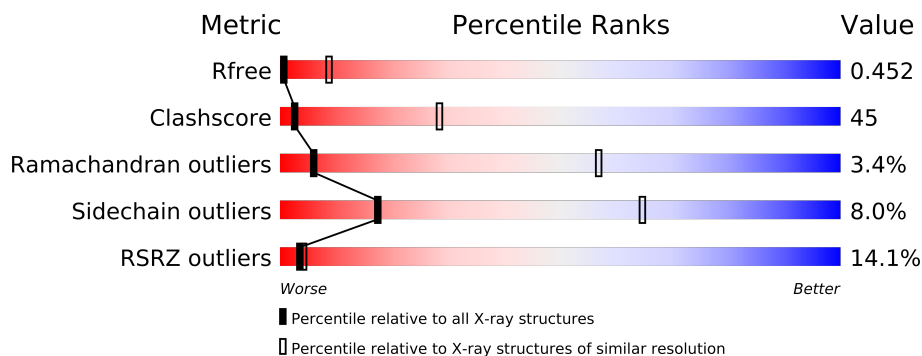
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.80 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}	66092	1162 (4.20-3.40)
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	220	
1	B	220	
2	C	244	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4781 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RECOMBINATION PROTEIN RECR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	1
			1511	952	269	283	7			
1	B	199	Total	C	N	O	S	0	0	1
			1511	952	269	283	7			

- Molecule 2 is a protein called HYPOTHETICAL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	229	Total	C	N	O	S	0	0	0
			1756	1121	320	309	6			

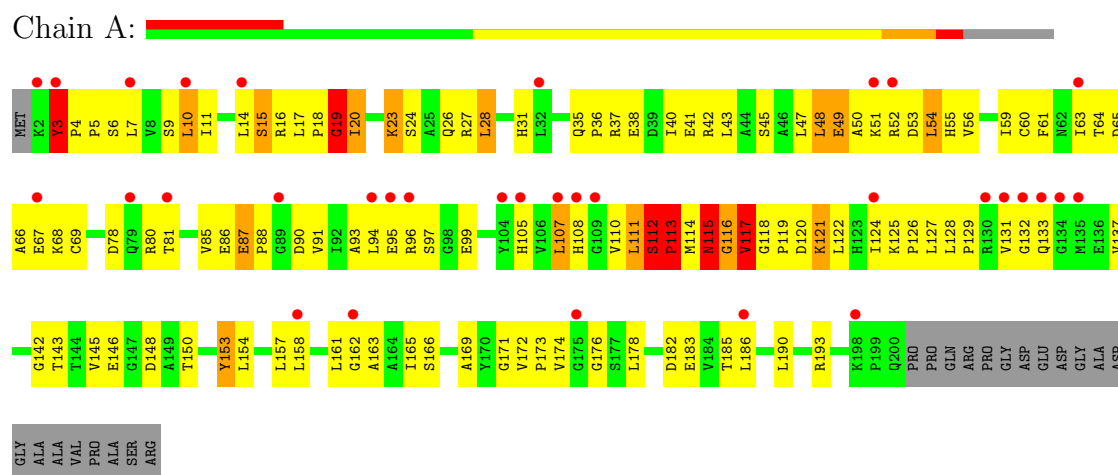
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

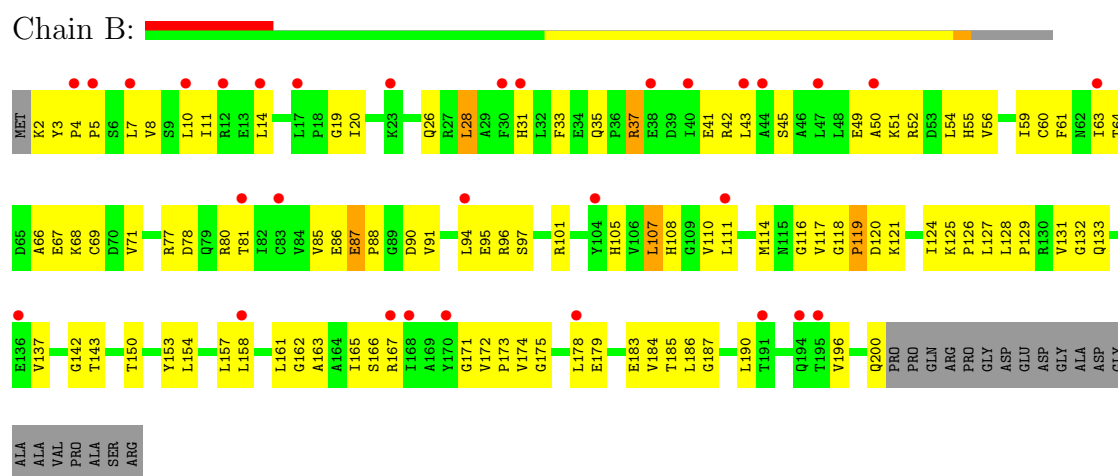
3 Residue-property plots

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.

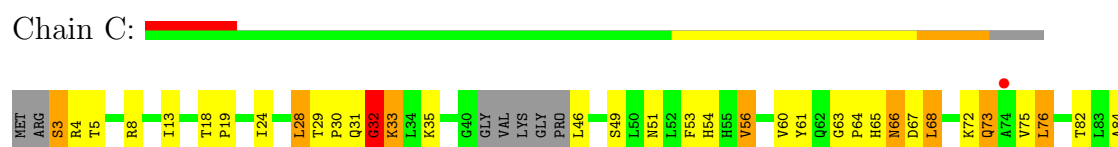
• Molecule 1: RECOMBINATION PROTEIN RECR

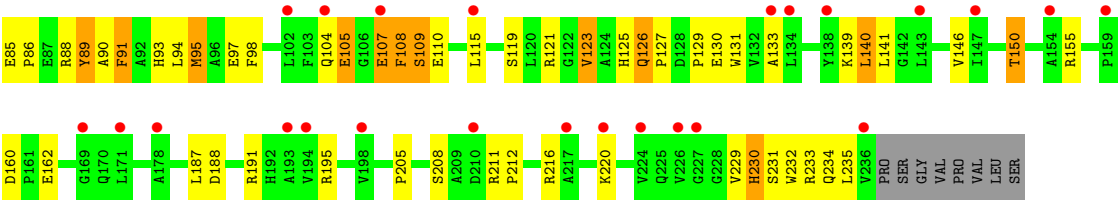


• Molecule 1: RECOMBINATION PROTEIN RECR



• Molecule 2: HYPOTHETICAL PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.00Å 83.20Å 66.60Å 90.00° 106.90° 90.00°	Depositor
Resolution (Å)	71.25 – 3.80 44.30 – 3.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (71.25-3.80) 95.4 (44.30-3.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.459 , 0.443 0.435 , 0.452	Depositor DCC
R_{free} test set	329 reflections (4.80%)	DCC
Wilson B-factor (Å ²)	128.2	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Outliers	1 of 7180 reflections (0.014%)	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	4781	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	1.12	4/1539 (0.3%)	1.20	14/2091 (0.7%)
1	B	0.40	0/1539	0.70	2/2091 (0.1%)
2	C	0.60	0/1801	0.86	6/2454 (0.2%)
All	All	0.76	4/4879 (0.1%)	0.94	22/6636 (0.3%)

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
2	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	LEU	C-N	-24.32	0.78	1.34
1	A	19	GLY	C-N	-20.59	0.86	1.34
1	A	15	SER	C-N	19.61	1.79	1.34
1	A	54	LEU	C-N	-10.98	1.08	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	LEU	O-C-N	-25.73	81.53	122.70
1	A	54	LEU	CA-C-N	18.05	156.90	117.20
1	A	54	LEU	C-N-CA	17.13	164.52	121.70
1	A	48	LEU	O-C-N	11.38	140.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	LEU	CA-C-N	-9.55	96.19	117.20
1	A	48	LEU	C-N-CA	-9.09	98.97	121.70
1	A	117	VAL	N-CA-C	-6.32	93.95	111.00
1	A	19	GLY	O-C-N	-5.94	113.19	122.70
1	A	60	CYS	N-CA-C	-5.87	95.15	111.00
1	B	60	CYS	N-CA-C	-5.86	95.17	111.00
1	A	107	LEU	N-CA-C	-5.85	95.21	111.00
1	B	107	LEU	N-CA-C	-5.83	95.25	111.00
2	C	188	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	113	PRO	N-CA-CB	5.66	110.09	103.30
2	C	160	ASP	CB-CG-OD2	5.54	123.28	118.30
2	C	91	PHE	C-N-CA	-5.48	108.00	121.70
2	C	32	GLY	CA-C-N	-5.46	105.18	117.20
1	A	115	ASN	N-CA-C	-5.40	96.42	111.00
2	C	32	GLY	C-N-CA	5.26	134.86	121.70
1	A	113	PRO	CA-N-CD	-5.15	104.29	111.50
1	A	112	SER	CA-C-N	5.06	131.27	117.10
2	C	32	GLY	N-CA-C	5.04	125.69	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	GLY	Mainchain
2	C	3	SER	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1511	0	1537	257	3
1	B	1511	0	1541	137	10
2	C	1756	0	1763	170	6
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
All	All	4781	0	4841	429	16

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 45.

All (429) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:LEU:CD2	1:B:178:LEU:CD1	1.87	1.50
1:A:48:LEU:C	1:A:49:GLU:CA	1.76	1.49
1:A:115:ASN:HB2	2:C:234:GLN:CB	1.39	1.49
1:A:174:VAL:HG23	1:B:185:THR:CB	1.44	1.48
1:A:94:LEU:HD21	1:B:178:LEU:CD1	0.98	1.45
1:A:48:LEU:CA	1:A:49:GLU:N	1.79	1.44
1:A:174:VAL:CG2	1:B:185:THR:CA	1.97	1.41
1:A:115:ASN:HB2	2:C:234:GLN:CG	1.49	1.40
1:A:15:SER:C	1:A:16:ARG:N	1.79	1.36
2:C:86:PRO:O	2:C:89:TYR:CD2	1.82	1.32
1:A:174:VAL:CG2	1:B:185:THR:HA	1.55	1.31
1:A:174:VAL:HG21	1:B:185:THR:N	1.43	1.30
2:C:107:GLU:O	2:C:108:PHE:CB	1.80	1.28
1:A:94:LEU:CD2	1:B:178:LEU:HD13	1.47	1.27
1:A:115:ASN:CB	2:C:234:GLN:CB	2.11	1.25
1:A:174:VAL:HG23	1:B:185:THR:CA	1.55	1.25
1:A:174:VAL:CG2	1:B:185:THR:OG1	1.85	1.24
1:A:174:VAL:HG23	1:B:185:THR:OG1	1.13	1.23
1:A:19:GLY:C	1:A:20:ILE:CA	2.10	1.20
1:A:115:ASN:CB	2:C:234:GLN:HG3	1.72	1.20
2:C:94:LEU:CA	2:C:235:LEU:HD13	1.69	1.19
1:A:45:SER:O	1:A:49:GLU:HG3	1.41	1.19
1:A:99:GLU:OE2	1:B:187:GLY:HA2	1.43	1.19
1:A:174:VAL:N	1:B:185:THR:OG1	1.75	1.18
2:C:88:ARG:NH2	2:C:126:GLN:O	1.76	1.18
1:A:19:GLY:O	1:A:20:ILE:N	1.76	1.17
2:C:94:LEU:HA	2:C:235:LEU:CD1	1.74	1.17
2:C:3:SER:N	2:C:4:ARG:HA	1.58	1.17
2:C:232:TRP:O	2:C:235:LEU:HB2	1.44	1.16
1:A:94:LEU:CD2	1:B:178:LEU:HD12	1.72	1.14
1:A:124:ILE:HD13	1:A:153:TYR:CE2	1.83	1.14
1:A:19:GLY:CA	1:A:20:ILE:N	2.12	1.12
2:C:94:LEU:HD13	2:C:235:LEU:CB	1.80	1.11
1:A:94:LEU:CG	1:B:178:LEU:HD12	1.79	1.11

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:148:ASP:OD1	2:C:84:ALA:HB1	1.50	1.11
1:A:124:ILE:HD13	1:A:153:TYR:HE2	0.99	1.10
1:A:148:ASP:OD1	2:C:84:ALA:CB	1.98	1.09
1:A:115:ASN:CB	2:C:234:GLN:HB2	1.76	1.09
1:A:172:VAL:O	1:B:171:GLY:O	1.68	1.09
1:A:115:ASN:CB	2:C:234:GLN:CG	2.26	1.08
1:A:115:ASN:HB2	2:C:234:GLN:HB2	1.13	1.08
2:C:86:PRO:HA	2:C:89:TYR:CD2	1.87	1.08
1:A:166:SER:HA	1:B:196:VAL:HG22	1.33	1.08
1:A:115:ASN:HB2	2:C:234:GLN:HG3	1.28	1.08
1:B:175:GLY:HA3	2:C:51:ASN:HD21	1.17	1.08
1:A:183:GLU:OE1	2:C:76:LEU:HB3	1.51	1.07
2:C:232:TRP:HB2	2:C:235:LEU:HD12	1.36	1.06
2:C:94:LEU:HD13	2:C:235:LEU:HB2	1.32	1.06
1:A:18:PRO:HB2	2:C:19:PRO:CG	1.85	1.05
2:C:97:GLU:HB2	2:C:235:LEU:HD11	1.37	1.05
1:A:48:LEU:O	1:A:49:GLU:N	1.89	1.04
1:A:64:THR:HG21	1:A:69:CYS:HA	1.37	1.04
1:B:64:THR:HG21	1:B:69:CYS:HA	1.37	1.03
2:C:30:PRO:O	2:C:109:SER:O	1.77	1.03
1:A:153:TYR:CZ	1:A:157:LEU:HD12	1.94	1.02
1:A:112:SER:O	2:C:93:HIS:NE2	1.92	1.02
1:A:148:ASP:CG	2:C:84:ALA:HB1	1.80	1.02
1:A:94:LEU:HD21	1:B:178:LEU:HD11	1.38	1.02
1:B:175:GLY:HA3	2:C:51:ASN:ND2	1.74	1.02
1:A:94:LEU:HD21	1:B:178:LEU:HD12	1.29	1.01
1:A:174:VAL:HG21	1:B:185:THR:CA	1.75	1.01
1:B:85:VAL:HG11	1:B:90:ASP:HB2	1.39	1.01
2:C:107:GLU:O	2:C:108:PHE:HB2	1.11	1.00
1:A:85:VAL:HG11	1:A:90:ASP:HB2	1.38	1.00
1:A:115:ASN:HD22	1:A:116:GLY:N	1.59	0.99
2:C:86:PRO:O	2:C:89:TYR:CE2	2.16	0.99
1:A:165:ILE:O	1:B:196:VAL:HG23	1.61	0.98
1:A:165:ILE:O	1:B:196:VAL:CG2	2.13	0.97
1:A:48:LEU:O	1:A:49:GLU:CA	2.10	0.97
1:A:115:ASN:C	1:A:115:ASN:HD22	1.68	0.96
1:A:112:SER:OG	2:C:89:TYR:HE1	1.46	0.96
2:C:86:PRO:O	2:C:89:TYR:HD2	1.49	0.96
1:A:173:PRO:HD3	1:B:173:PRO:HB3	1.48	0.95
1:A:115:ASN:HA	2:C:234:GLN:HB2	1.48	0.94
1:A:174:VAL:CB	1:B:185:THR:OG1	2.15	0.94
2:C:86:PRO:HA	2:C:89:TYR:HD2	1.34	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:182:ASP:OD2	2:C:76:LEU:HG	1.66	0.93
1:A:133:GLN:HG2	1:A:162:GLY:HA3	1.51	0.92
1:B:133:GLN:HG2	1:B:162:GLY:HA3	1.51	0.92
1:A:48:LEU:O	1:A:49:GLU:C	2.08	0.92
2:C:86:PRO:C	2:C:89:TYR:HD2	1.73	0.92
1:A:153:TYR:OH	1:A:157:LEU:HD12	1.70	0.92
1:A:19:GLY:C	1:A:20:ILE:N	0.86	0.91
1:A:115:ASN:CA	2:C:234:GLN:HB2	1.99	0.91
1:A:113:PRO:HA	2:C:93:HIS:CE1	2.05	0.90
1:A:124:ILE:CD1	1:A:153:TYR:CE2	2.54	0.90
1:A:174:VAL:CG2	1:B:185:THR:N	2.21	0.90
1:A:124:ILE:CD1	1:A:153:TYR:HE2	1.85	0.89
2:C:94:LEU:CD1	2:C:235:LEU:HB2	2.01	0.89
2:C:56:VAL:CG2	2:C:75:VAL:O	2.21	0.89
1:A:174:VAL:H	1:B:185:THR:HG1	0.99	0.89
2:C:86:PRO:C	2:C:89:TYR:CD2	2.46	0.88
1:A:153:TYR:OH	1:A:157:LEU:CD1	2.22	0.88
1:A:94:LEU:HG	1:B:178:LEU:HD12	1.55	0.88
1:A:49:GLU:O	1:A:52:ARG:N	2.07	0.87
2:C:56:VAL:HG23	2:C:75:VAL:O	1.75	0.87
1:A:99:GLU:OE2	1:B:187:GLY:CA	2.22	0.86
2:C:86:PRO:CA	2:C:89:TYR:HD2	1.87	0.86
1:A:173:PRO:HB3	1:B:173:PRO:HD3	1.55	0.86
2:C:232:TRP:CB	2:C:235:LEU:HD12	2.06	0.85
1:A:145:VAL:HG21	2:C:53:PHE:CE2	2.12	0.84
1:A:111:LEU:HD23	1:A:122:LEU:CD1	2.07	0.84
1:A:174:VAL:HG21	1:B:184:VAL:C	1.96	0.84
2:C:94:LEU:CD1	2:C:235:LEU:CB	2.56	0.84
1:A:53:ASP:O	1:A:65:ASP:HA	1.78	0.84
1:A:48:LEU:C	1:A:49:GLU:N	0.78	0.83
1:A:111:LEU:HD23	1:A:122:LEU:HD12	1.59	0.83
2:C:232:TRP:O	2:C:235:LEU:CB	2.25	0.83
1:A:115:ASN:CG	2:C:234:GLN:HG3	1.98	0.82
2:C:86:PRO:CA	2:C:89:TYR:CD2	2.60	0.82
1:A:86:GLU:OE1	1:A:110:VAL:HG22	1.80	0.82
1:A:18:PRO:CB	2:C:19:PRO:HG2	2.10	0.82
1:B:117:VAL:HA	1:B:121:LYS:HD3	1.62	0.81
2:C:33:LYS:HD3	2:C:105:GLU:O	1.80	0.81
2:C:94:LEU:HB2	2:C:235:LEU:HB3	1.63	0.80
1:A:19:GLY:O	1:A:20:ILE:HG13	1.82	0.80
1:A:18:PRO:HB2	2:C:19:PRO:CD	2.11	0.80
1:A:115:ASN:ND2	1:A:116:GLY:N	2.30	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:18:PRO:CB	2:C:19:PRO:CG	2.59	0.80
1:A:43:LEU:O	1:A:47:LEU:HG	1.82	0.80
2:C:29:THR:OG1	2:C:32:GLY:N	2.14	0.80
1:A:48:LEU:C	1:A:49:GLU:C	2.39	0.80
2:C:94:LEU:HA	2:C:235:LEU:HD13	0.84	0.79
1:A:18:PRO:HB2	2:C:19:PRO:HG2	1.62	0.79
2:C:94:LEU:HD13	2:C:235:LEU:HB3	1.63	0.79
1:A:115:ASN:OD1	2:C:234:GLN:NE2	2.16	0.79
1:A:112:SER:HG	2:C:89:TYR:HE1	0.78	0.78
1:A:85:VAL:CG1	1:A:90:ASP:HB2	2.13	0.78
2:C:229:VAL:O	2:C:229:VAL:HG13	1.84	0.78
1:A:115:ASN:CG	2:C:234:GLN:CG	2.51	0.78
2:C:32:GLY:O	2:C:33:LYS:HG2	1.83	0.78
1:A:174:VAL:HG22	1:B:185:THR:HA	1.65	0.77
2:C:97:GLU:HB2	2:C:235:LEU:CD1	2.13	0.77
1:A:174:VAL:CA	1:B:185:THR:OG1	2.33	0.77
1:B:85:VAL:CG1	1:B:90:ASP:HB2	2.13	0.76
1:A:115:ASN:CB	2:C:234:GLN:HB3	2.13	0.76
1:A:186:LEU:HD13	1:B:94:LEU:HD23	1.68	0.76
1:A:48:LEU:N	1:A:49:GLU:N	2.34	0.76
2:C:33:LYS:CD	2:C:105:GLU:O	2.34	0.76
2:C:93:HIS:HB3	2:C:235:LEU:HD22	1.66	0.75
1:A:114:MET:O	1:A:115:ASN:HB3	1.84	0.75
1:A:171:GLY:O	1:B:172:VAL:O	2.04	0.75
1:A:111:LEU:HG	1:A:150:THR:HG23	1.69	0.75
1:A:115:ASN:OD1	2:C:234:GLN:HG3	1.85	0.75
1:A:166:SER:CA	1:B:196:VAL:HG22	2.16	0.75
1:A:115:ASN:C	1:A:115:ASN:ND2	2.41	0.75
1:B:7:LEU:O	1:B:11:ILE:HG12	1.87	0.74
1:A:19:GLY:O	1:A:20:ILE:CA	2.28	0.74
1:B:2:LYS:HE2	1:B:8:VAL:HG22	1.70	0.74
1:A:7:LEU:O	1:A:11:ILE:HG12	1.87	0.73
1:A:171:GLY:N	1:B:172:VAL:O	2.19	0.73
1:A:112:SER:HB2	2:C:93:HIS:CD2	2.24	0.73
1:A:145:VAL:HG21	2:C:53:PHE:HE2	1.54	0.73
1:B:105:HIS:CG	1:B:127:LEU:HD23	2.25	0.72
1:B:183:GLU:CD	1:B:183:GLU:H	1.93	0.72
1:A:18:PRO:C	2:C:19:PRO:HG2	2.10	0.72
1:A:183:GLU:CD	1:A:183:GLU:H	1.93	0.71
1:A:105:HIS:CG	1:A:127:LEU:HD23	2.25	0.71
2:C:75:VAL:HG12	2:C:76:LEU:N	2.06	0.71
1:A:124:ILE:HG21	1:A:153:TYR:OH	1.90	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:SER:O	1:A:49:GLU:CG	2.32	0.71
1:A:112:SER:O	2:C:93:HIS:CE1	2.44	0.71
2:C:93:HIS:HB3	2:C:235:LEU:CD2	2.20	0.71
1:B:51:LYS:HD3	1:B:51:LYS:O	1.90	0.71
2:C:212:PRO:O	2:C:216:ARG:HG2	1.91	0.71
1:A:165:ILE:O	1:B:196:VAL:HG22	1.91	0.70
1:B:78:ASP:OD1	1:B:80:ARG:HG2	1.91	0.70
1:A:169:ALA:O	1:B:172:VAL:HG22	1.90	0.70
1:A:94:LEU:HD21	1:B:178:LEU:HD13	0.70	0.70
2:C:97:GLU:CB	2:C:235:LEU:HD11	2.18	0.70
2:C:230:HIS:O	2:C:233:ARG:HD3	1.92	0.69
1:A:78:ASP:OD1	1:A:80:ARG:HG2	1.91	0.69
2:C:56:VAL:HG22	2:C:75:VAL:O	1.92	0.69
1:A:172:VAL:C	1:B:171:GLY:O	2.31	0.69
1:A:111:LEU:CD2	1:A:122:LEU:HD12	2.23	0.68
2:C:94:LEU:O	2:C:98:PHE:CB	2.41	0.68
1:A:171:GLY:O	1:B:173:PRO:HA	1.93	0.68
1:A:5:PRO:O	1:A:9:SER:HB2	1.92	0.68
2:C:85:GLU:O	2:C:89:TYR:HB3	1.94	0.67
2:C:150:THR:HG21	2:C:191:ARG:HA	1.75	0.67
1:A:171:GLY:O	1:B:172:VAL:C	2.33	0.67
1:A:115:ASN:CG	2:C:234:GLN:CB	2.62	0.67
1:A:51:LYS:HD3	1:A:51:LYS:O	1.94	0.67
1:A:148:ASP:CB	2:C:84:ALA:HB1	2.25	0.67
1:A:48:LEU:C	1:A:49:GLU:HA	2.09	0.66
1:A:23:LYS:O	1:A:27:ARG:HG2	1.95	0.66
2:C:94:LEU:CB	2:C:235:LEU:HB3	2.26	0.66
1:A:5:PRO:O	1:A:9:SER:CB	2.43	0.66
1:A:94:LEU:CG	1:B:178:LEU:CD1	2.53	0.65
1:A:115:ASN:OD1	2:C:234:GLN:CG	2.44	0.65
1:A:115:ASN:CG	2:C:234:GLN:HB3	2.16	0.65
2:C:91:PHE:CZ	2:C:130:GLU:HB2	2.32	0.65
1:A:86:GLU:OE1	1:A:110:VAL:CG2	2.44	0.65
2:C:75:VAL:CG1	2:C:76:LEU:N	2.59	0.64
1:B:111:LEU:HG	1:B:150:THR:HG23	1.79	0.64
1:A:56:VAL:CG2	1:A:61:PHE:HB3	2.28	0.64
1:B:127:LEU:HD12	1:B:158:LEU:HD21	1.80	0.64
1:B:56:VAL:CG2	1:B:61:PHE:HB3	2.28	0.64
1:A:48:LEU:O	1:A:49:GLU:O	2.15	0.63
1:A:127:LEU:HD12	1:A:158:LEU:HD21	1.79	0.63
1:A:35:GLN:HB2	1:A:40:ILE:HD11	1.80	0.63
1:A:53:ASP:O	1:A:65:ASP:CA	2.47	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:11:ILE:HD12	1:A:26:GLN:HA	1.81	0.63
1:B:11:ILE:HD12	1:B:26:GLN:HA	1.81	0.62
2:C:88:ARG:NH2	2:C:126:GLN:C	2.52	0.62
1:A:19:GLY:O	1:A:20:ILE:CG1	2.48	0.62
1:A:185:THR:HA	1:B:174:VAL:HG23	1.81	0.62
2:C:94:LEU:CD1	2:C:235:LEU:HB3	2.26	0.61
1:A:182:ASP:OD2	2:C:76:LEU:CG	2.45	0.61
1:A:107:LEU:HD11	1:A:154:LEU:HD11	1.82	0.61
2:C:107:GLU:O	2:C:108:PHE:HB3	1.95	0.61
1:B:50:ALA:O	1:B:54:LEU:HB2	2.00	0.61
1:A:165:ILE:C	1:B:196:VAL:CG2	2.69	0.61
1:A:114:MET:O	1:A:115:ASN:CB	2.49	0.61
1:B:107:LEU:HD11	1:B:154:LEU:HD11	1.83	0.60
1:A:110:VAL:HG12	1:A:146:GLU:HB3	1.82	0.60
1:A:137:VAL:HG11	1:A:158:LEU:CD1	2.31	0.60
2:C:3:SER:N	2:C:4:ARG:CA	2.48	0.60
1:A:174:VAL:N	1:B:185:THR:HG1	1.74	0.60
1:A:153:TYR:CZ	1:A:157:LEU:CD1	2.79	0.60
1:A:173:PRO:HB3	1:B:173:PRO:CD	2.28	0.60
1:B:137:VAL:HG11	1:B:158:LEU:CD1	2.32	0.60
2:C:63:GLY:O	2:C:65:HIS:N	2.35	0.60
1:A:93:ALA:HB2	1:B:179:GLU:OE1	2.02	0.60
2:C:94:LEU:CD1	2:C:232:TRP:HE3	2.15	0.59
1:B:175:GLY:CA	2:C:51:ASN:HD21	2.04	0.59
1:A:111:LEU:HD23	1:A:122:LEU:HD11	1.83	0.59
1:A:148:ASP:OD1	2:C:84:ALA:HB2	1.94	0.59
2:C:29:THR:OG1	2:C:32:GLY:HA2	2.02	0.59
1:B:64:THR:HG21	1:B:69:CYS:CA	2.23	0.59
1:A:186:LEU:HD13	1:B:94:LEU:CD2	2.32	0.59
2:C:72:LYS:O	2:C:73:GLN:HB2	2.03	0.59
2:C:94:LEU:O	2:C:98:PHE:HB2	2.01	0.59
1:A:183:GLU:OE1	2:C:76:LEU:HD12	2.04	0.58
2:C:94:LEU:HD11	2:C:232:TRP:HE3	1.67	0.58
1:A:116:GLY:H	2:C:234:GLN:HB3	1.68	0.58
1:A:36:PRO:O	1:A:40:ILE:HG12	2.03	0.58
1:A:174:VAL:HG11	1:B:184:VAL:HB	1.86	0.57
2:C:88:ARG:HH21	2:C:126:GLN:C	2.03	0.57
1:A:94:LEU:HD23	1:B:178:LEU:HD13	1.72	0.57
1:A:153:TYR:OH	1:A:157:LEU:HD11	2.04	0.57
1:A:53:ASP:O	1:A:65:ASP:CB	2.52	0.57
1:A:113:PRO:O	2:C:93:HIS:CE1	2.58	0.56
2:C:29:THR:OG1	2:C:32:GLY:CA	2.53	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:229:VAL:O	2:C:229:VAL:CG1	2.53	0.56
2:C:232:TRP:CA	2:C:235:LEU:HD12	2.36	0.56
1:B:117:VAL:HA	1:B:121:LYS:CD	2.35	0.55
1:B:175:GLY:CA	2:C:51:ASN:ND2	2.59	0.55
1:A:18:PRO:CG	2:C:19:PRO:HG2	2.36	0.55
1:B:61:PHE:O	1:B:108:HIS:HE1	1.90	0.55
1:B:77:ARG:NH2	1:B:95:GLU:OE2	2.40	0.55
1:A:94:LEU:CD1	1:B:178:LEU:HD12	2.37	0.55
1:A:115:ASN:HD22	1:A:116:GLY:CA	2.19	0.55
1:A:18:PRO:CG	2:C:19:PRO:CG	2.85	0.55
1:A:61:PHE:O	1:A:108:HIS:HE1	1.90	0.55
1:A:64:THR:HG21	1:A:69:CYS:CA	2.23	0.54
1:B:133:GLN:HG2	1:B:162:GLY:CA	2.32	0.54
1:A:48:LEU:CB	1:A:49:GLU:N	2.68	0.54
1:A:111:LEU:O	1:A:146:GLU:OE1	2.25	0.54
1:A:171:GLY:O	1:B:173:PRO:CA	2.55	0.54
1:B:45:SER:O	1:B:49:GLU:HG3	2.06	0.54
1:B:77:ARG:NH1	1:B:101:ARG:C	2.61	0.54
1:A:18:PRO:HB2	2:C:19:PRO:HG3	1.83	0.54
1:A:18:PRO:HG2	2:C:19:PRO:HG2	1.90	0.54
1:B:87:GLU:HG3	1:B:88:PRO:HD2	1.90	0.54
1:A:67:GLU:HB2	1:A:68:LYS:HD2	1.90	0.54
1:B:67:GLU:HB2	1:B:68:LYS:HD2	1.90	0.53
2:C:29:THR:O	2:C:32:GLY:N	2.40	0.53
2:C:33:LYS:O	2:C:33:LYS:HG3	2.07	0.53
1:B:86:GLU:O	1:B:107:LEU:O	2.27	0.53
1:B:31:HIS:O	1:B:35:GLN:HG2	2.09	0.53
1:A:112:SER:OG	2:C:89:TYR:CE1	2.36	0.53
1:A:86:GLU:O	1:A:107:LEU:O	2.27	0.53
1:B:153:TYR:CE2	1:B:157:LEU:HD12	2.43	0.53
1:A:176:GLY:O	1:B:143:THR:OG1	2.26	0.53
1:A:18:PRO:HB2	2:C:19:PRO:HD3	1.90	0.53
1:A:86:GLU:CD	1:A:110:VAL:HG22	2.29	0.53
1:A:161:LEU:HD12	1:A:161:LEU:H	1.74	0.53
2:C:94:LEU:HD11	2:C:232:TRP:CE3	2.43	0.52
1:A:119:PRO:HB3	1:A:124:ILE:HD12	1.91	0.52
1:B:161:LEU:HD12	1:B:161:LEU:H	1.73	0.52
1:A:133:GLN:HG2	1:A:162:GLY:CA	2.32	0.52
1:B:118:GLY:O	1:B:120:ASP:N	2.38	0.52
1:A:183:GLU:OE1	2:C:76:LEU:CB	2.41	0.52
1:B:119:PRO:HB3	1:B:124:ILE:HD12	1.92	0.52
2:C:91:PHE:CE2	2:C:130:GLU:HA	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:115:ASN:OD1	2:C:234:GLN:CD	2.47	0.52
1:A:148:ASP:HB3	2:C:84:ALA:HB1	1.91	0.52
1:A:87:GLU:HG3	1:A:88:PRO:HD2	1.90	0.52
1:A:173:PRO:CB	1:B:173:PRO:HD3	2.36	0.52
2:C:119:SER:O	2:C:123:VAL:HG13	2.10	0.52
1:A:85:VAL:CG1	1:A:86:GLU:N	2.73	0.51
1:A:174:VAL:CG2	1:B:185:THR:CB	2.34	0.51
1:A:18:PRO:O	2:C:19:PRO:HG2	2.10	0.51
1:B:85:VAL:CG1	1:B:86:GLU:N	2.73	0.51
1:B:56:VAL:HG21	1:B:61:PHE:HB3	1.92	0.51
1:B:131:VAL:HB	1:B:161:LEU:HD22	1.93	0.51
1:B:118:GLY:C	1:B:120:ASP:H	2.13	0.51
2:C:115:LEU:HD23	2:C:140:LEU:HD13	1.92	0.51
2:C:94:LEU:O	2:C:98:PHE:HB3	2.10	0.51
1:A:50:ALA:O	1:A:51:LYS:C	2.48	0.51
2:C:33:LYS:HD2	2:C:105:GLU:HG3	1.92	0.51
2:C:91:PHE:CZ	2:C:130:GLU:CB	2.94	0.51
2:C:89:TYR:CG	2:C:90:ALA:N	2.79	0.51
1:A:18:PRO:HG2	2:C:19:PRO:CG	2.41	0.51
1:A:131:VAL:HB	1:A:161:LEU:HD22	1.93	0.51
1:A:14:LEU:HD22	1:A:28:LEU:HD22	1.93	0.51
1:A:113:PRO:HA	2:C:93:HIS:HE1	1.65	0.51
1:A:113:PRO:CA	2:C:93:HIS:CE1	2.87	0.50
1:A:161:LEU:HD12	1:A:161:LEU:N	2.26	0.50
2:C:86:PRO:HA	2:C:89:TYR:CE2	2.41	0.50
1:A:31:HIS:O	1:A:35:GLN:HG2	2.11	0.50
2:C:29:THR:C	2:C:32:GLY:H	2.15	0.50
1:A:56:VAL:HG21	1:A:61:PHE:HB3	1.92	0.50
1:B:161:LEU:HD12	1:B:161:LEU:N	2.26	0.50
1:A:115:ASN:CA	2:C:234:GLN:CB	2.72	0.50
2:C:121:ARG:O	2:C:125:HIS:HD2	1.92	0.49
1:A:118:GLY:H	1:A:121:LYS:HB2	1.77	0.49
1:A:124:ILE:HG21	1:A:153:TYR:CE2	2.47	0.49
2:C:104:GLN:O	2:C:105:GLU:CB	2.60	0.49
1:A:115:ASN:CG	2:C:234:GLN:HE21	2.17	0.48
1:B:111:LEU:HD12	1:B:150:THR:HA	1.94	0.48
1:B:14:LEU:HD22	1:B:28:LEU:HD22	1.93	0.48
2:C:229:VAL:O	2:C:231:SER:N	2.47	0.48
2:C:75:VAL:CG1	2:C:76:LEU:H	2.27	0.48
1:A:193:ARG:HD2	1:B:166:SER:HB2	1.96	0.47
1:B:42:ARG:NH1	1:B:42:ARG:HB2	2.29	0.47
1:A:85:VAL:HG13	1:A:90:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:117:VAL:HG13	1:B:121:LYS:HD3	1.97	0.47
1:A:166:SER:HA	1:B:196:VAL:CG2	2.24	0.47
1:A:182:ASP:HB2	2:C:49:SER:OG	2.14	0.47
1:A:3:TYR:N	1:A:4:PRO:CD	2.77	0.47
1:B:85:VAL:HG13	1:B:90:ASP:OD2	2.14	0.47
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.79	0.47
1:A:183:GLU:CD	1:A:183:GLU:N	2.65	0.47
1:B:77:ARG:NH1	1:B:101:ARG:HA	2.30	0.47
2:C:95:MET:CE	2:C:133:ALA:HB1	2.45	0.47
1:A:18:PRO:CG	2:C:19:PRO:HG3	2.45	0.46
1:B:37:ARG:O	1:B:41:GLU:HG3	2.15	0.46
1:A:19:GLY:O	1:A:20:ILE:HA	2.14	0.46
2:C:51:ASN:HB2	2:C:54:HIS:CE1	2.51	0.46
1:A:185:THR:HA	1:B:174:VAL:CG2	2.45	0.46
1:A:49:GLU:O	1:A:52:ARG:HB3	2.15	0.46
2:C:30:PRO:HB3	2:C:110:GLU:HG3	1.97	0.46
2:C:13:ILE:HG21	2:C:28:LEU:HD22	1.98	0.46
1:A:117:VAL:HG13	1:A:122:LEU:HG	1.97	0.46
1:B:110:VAL:HG12	1:B:150:THR:OG1	2.16	0.46
2:C:131:TRP:CE2	2:C:205:PRO:HA	2.51	0.46
1:B:78:ASP:OD2	1:B:81:THR:HG23	2.15	0.46
1:A:113:PRO:O	2:C:93:HIS:ND1	2.49	0.46
1:A:23:LYS:HG2	1:A:23:LYS:H	1.46	0.46
1:A:95:GLU:C	1:A:97:SER:H	2.19	0.46
1:A:174:VAL:HG23	1:B:185:THR:HA	1.38	0.45
1:A:78:ASP:OD2	1:A:81:THR:HG23	2.15	0.45
2:C:72:LYS:O	2:C:73:GLN:CB	2.63	0.45
1:B:4:PRO:HA	1:B:5:PRO:HD2	1.84	0.45
1:A:143:THR:OG1	1:B:175:GLY:N	2.46	0.45
2:C:211:ARG:N	2:C:212:PRO:CD	2.79	0.45
2:C:91:PHE:CZ	2:C:130:GLU:HA	2.51	0.45
2:C:18:THR:HB	2:C:19:PRO:HD2	1.99	0.45
1:A:94:LEU:HD11	1:B:178:LEU:CD1	2.46	0.45
1:A:54:LEU:HA	1:A:64:THR:O	2.15	0.45
1:A:4:PRO:O	1:A:5:PRO:C	2.53	0.45
1:A:94:LEU:CD1	1:B:178:LEU:CD1	2.93	0.45
1:B:19:GLY:O	1:B:20:ILE:HG13	2.17	0.45
1:A:173:PRO:HG3	1:B:173:PRO:HG3	1.99	0.45
1:A:5:PRO:O	1:A:9:SER:N	2.50	0.45
1:A:85:VAL:CG1	1:A:90:ASP:OD2	2.66	0.44
1:B:85:VAL:CG1	1:B:90:ASP:OD2	2.66	0.44
1:B:158:LEU:HB2	1:B:165:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:182:ASP:OD2	2:C:49:SER:HB3	2.16	0.44
1:B:95:GLU:C	1:B:97:SER:H	2.20	0.44
2:C:162:GLU:HB3	2:C:187:LEU:HD11	2.00	0.44
1:A:183:GLU:OE1	2:C:76:LEU:CD1	2.66	0.44
1:B:77:ARG:HH12	1:B:101:ARG:HA	1.81	0.44
1:B:85:VAL:HG12	1:B:86:GLU:N	2.33	0.44
1:B:183:GLU:CD	1:B:183:GLU:N	2.65	0.44
1:A:124:ILE:HG21	1:A:153:TYR:CZ	2.52	0.44
1:A:55:HIS:CE1	1:A:66:ALA:O	2.71	0.44
1:A:178:LEU:HD22	1:A:186:LEU:HD21	2.00	0.44
1:A:158:LEU:HB2	1:A:165:ILE:HD11	2.00	0.44
2:C:208:SER:HA	2:C:211:ARG:HD2	2.00	0.44
2:C:29:THR:O	2:C:32:GLY:CA	2.66	0.43
1:A:85:VAL:HG12	1:A:86:GLU:N	2.33	0.43
1:A:68:LYS:N	1:A:68:LYS:HD2	2.33	0.43
1:B:55:HIS:CE1	1:B:66:ALA:O	2.70	0.43
2:C:66:ASN:C	2:C:68:LEU:H	2.22	0.43
1:A:42:ARG:NH1	1:A:42:ARG:HB2	2.33	0.43
1:A:10:LEU:HD22	1:A:14:LEU:CD1	2.49	0.43
1:A:54:LEU:HG	1:A:63:ILE:CG2	2.48	0.43
1:B:85:VAL:CG1	1:B:90:ASP:CB	2.92	0.43
1:B:68:LYS:N	1:B:68:LYS:HD2	2.33	0.43
1:B:178:LEU:HD22	1:B:186:LEU:HD21	2.00	0.43
1:B:96:ARG:HH11	1:B:96:ARG:HG3	1.84	0.43
2:C:162:GLU:HA	2:C:187:LEU:HD21	2.00	0.43
2:C:126:GLN:HG3	2:C:127:PRO:HD2	2.01	0.42
1:A:14:LEU:O	1:A:17:LEU:HB2	2.18	0.42
1:A:165:ILE:C	1:B:196:VAL:HG23	2.30	0.42
2:C:94:LEU:N	2:C:235:LEU:HD13	2.26	0.42
1:A:117:VAL:CG1	1:A:122:LEU:HG	2.50	0.42
1:A:99:GLU:CD	1:B:187:GLY:CA	2.87	0.42
1:A:118:GLY:C	1:A:120:ASP:H	2.22	0.42
1:A:18:PRO:CB	2:C:19:PRO:HG3	2.47	0.42
1:A:37:ARG:O	1:A:41:GLU:HG3	2.20	0.42
1:B:71:VAL:HG13	1:B:77:ARG:CD	2.50	0.42
1:B:71:VAL:HG13	1:B:77:ARG:HD3	2.01	0.42
1:A:193:ARG:HB2	1:B:167:ARG:O	2.19	0.42
1:B:125:LYS:HB3	1:B:126:PRO:CD	2.50	0.42
1:A:4:PRO:HA	1:A:5:PRO:HD2	1.94	0.42
1:A:19:GLY:C	1:A:20:ILE:CB	2.85	0.41
2:C:109:SER:HB2	2:C:110:GLU:H	1.31	0.41
2:C:86:PRO:CA	2:C:89:TYR:CE2	3.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:4:PRO:C	1:A:6:SER:N	2.72	0.41
1:A:125:LYS:HB3	1:A:126:PRO:CD	2.50	0.41
1:A:18:PRO:CA	2:C:19:PRO:HG2	2.50	0.41
1:A:132:GLY:O	1:A:163:ALA:HB2	2.20	0.41
1:A:38:GLU:H	1:A:38:GLU:CD	2.24	0.41
1:B:91:VAL:O	1:B:95:GLU:HB2	2.21	0.41
1:B:132:GLY:O	1:B:163:ALA:HB2	2.20	0.41
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.51	0.41
2:C:29:THR:O	2:C:32:GLY:HA3	2.21	0.41
2:C:32:GLY:HA3	2:C:108:PHE:CE2	2.56	0.41
1:A:19:GLY:C	1:A:20:ILE:HG13	2.41	0.41
1:B:42:ARG:HB2	1:B:42:ARG:HH11	1.85	0.41
2:C:91:PHE:CD1	2:C:129:PRO:HB2	2.56	0.40
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.51	0.40
1:A:117:VAL:HG11	1:A:122:LEU:HD21	2.02	0.40
1:A:91:VAL:O	1:A:95:GLU:HB2	2.21	0.40
2:C:66:ASN:O	2:C:67:ASP:HB2	2.22	0.40

All (16) 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	Distance(Å)	Clash(Å)
1:A:35:GLN:O	1:A:51:LYS:NZ[2_555]	1.68	0.52
1:B:33:PHE:CD1	1:B:63:ILE:CD1[2_555]	1.73	0.47
1:B:2:LYS:CD	1:B:96:ARG:NH2[2_555]	1.85	0.35
1:B:2:LYS:CG	1:B:96:ARG:NH2[2_555]	1.86	0.34
1:B:116:GLY:CA	1:B:119:PRO:CD[2_556]	1.93	0.27
1:B:33:PHE:CE1	1:B:63:ILE:CG1[2_555]	1.95	0.25
1:B:33:PHE:CE1	1:B:63:ILE:CD1[2_555]	1.98	0.22
1:B:114:MET:O	1:B:153:TYR:CD1[2_556]	1.98	0.22
2:C:46:LEU:CD1	2:C:61:TYR:CE2[2_555]	1.99	0.21
2:C:46:LEU:CD1	2:C:61:TYR:OH[2_555]	2.01	0.19
1:A:52:ARG:NH1	1:B:52:ARG:CD[1_545]	2.04	0.16
1:B:200:GLN:N	2:C:155:ARG:O[1_556]	2.09	0.11
2:C:46:LEU:CD1	2:C:61:TYR:CZ[2_555]	2.12	0.08
1:B:37:ARG:CB	1:B:51:LYS:CE[2_555]	2.14	0.06
1:A:24:SER:CA	2:C:19:PRO:O[2_555]	2.15	0.05
2:C:46:LEU:CG	2:C:61:TYR:OH[2_555]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	197/220 (90%)	168 (85%)	21 (11%)	8 (4%)	4	50
1	B	197/220 (90%)	173 (88%)	20 (10%)	4 (2%)	11	68
2	C	225/244 (92%)	204 (91%)	12 (5%)	9 (4%)	5	51
All	All	619/684 (90%)	545 (88%)	53 (9%)	21 (3%)	6	57

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	113	PRO
2	C	32	GLY
2	C	33	LYS
2	C	108	PHE
1	A	115	ASN
1	A	142	GLY
1	B	142	GLY
2	C	64	PRO
2	C	73	GLN
2	C	105	GLU
1	A	49	GLU
1	B	3	TYR
2	C	230	HIS
1	A	3	TYR
1	B	119	PRO
2	C	109	SER
1	A	59	ILE
1	B	59	ILE
2	C	107	GLU
1	A	116	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	165/180 (92%)	153 (93%)	12 (7%)	20	69
1	B	165/180 (92%)	159 (96%)	6 (4%)	47	87
2	C	183/195 (94%)	160 (87%)	23 (13%)	7	40
All	All	513/555 (92%)	472 (92%)	41 (8%)	17	64

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	TYR
1	A	10	LEU
1	A	23	LYS
1	A	28	LEU
1	A	87	GLU
1	A	111	LEU
1	A	112	SER
1	A	115	ASN
1	A	117	VAL
1	A	121	LYS
1	A	153	TYR
1	A	190	LEU
1	B	10	LEU
1	B	28	LEU
1	B	37	ARG
1	B	43	LEU
1	B	87	GLU
1	B	190	LEU
2	C	5	THR
2	C	8	ARG
2	C	24	ILE
2	C	28	LEU
2	C	31	GLN
2	C	35	LYS
2	C	56	VAL
2	C	60	VAL
2	C	66	ASN

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Mol	Chain	Res	Type
2	C	68	LEU
2	C	76	LEU
2	C	82	THR
2	C	89	TYR
2	C	95	MET
2	C	123	VAL
2	C	126	GLN
2	C	139	LYS
2	C	140	LEU
2	C	141	LEU
2	C	146	VAL
2	C	150	THR
2	C	195	ARG
2	C	220	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	108	HIS
1	A	115	ASN
1	A	133	GLN
1	A	155	GLN
1	B	55	HIS
1	B	108	HIS
1	B	133	GLN
1	B	155	GLN
2	C	51	ASN
2	C	65	HIS
2	C	125	HIS
2	C	234	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 3 ligands modelled in this entry, 3 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.

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, 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	199/220 (90%)	0.95	33 (16%) 2 3	96, 96, 96, 96	0
1	B	199/220 (90%)	0.86	31 (15%) 3 4	96, 96, 96, 96	0
2	C	229/244 (93%)	0.85	25 (10%) 6 7	96, 96, 96, 96	0
All	All	627/684 (91%)	0.88	89 (14%) 3 4	96, 96, 96, 96	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	44	ALA	5.0
1	A	7	LEU	4.8
1	A	14	LEU	4.8
1	A	175	GLY	4.8
1	A	105	HIS	4.4
1	B	63	ILE	4.2
2	C	138	TYR	4.1
1	B	7	LEU	4.0
1	B	104	TYR	3.9
1	B	14	LEU	3.8
1	A	67	GLU	3.7
1	A	162	GLY	3.7
1	B	10	LEU	3.6
2	C	169	GLY	3.6
1	A	134	GLY	3.6
1	B	4	PRO	3.5
2	C	194	VAL	3.4
1	A	104	TYR	3.4
2	C	178	ALA	3.3
1	A	2	LYS	3.3
1	B	136	GLU	3.3
1	B	12	ARG	3.3
1	A	63	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	47	LEU	3.2
2	C	210	ASP	3.2
2	C	147	ILE	3.1
2	C	171	LEU	3.1
2	C	74	ALA	3.0
1	A	10	LEU	3.0
2	C	115	LEU	2.9
1	A	52	ARG	2.9
1	B	94	LEU	2.9
1	A	130	ARG	2.8
1	A	96	ARG	2.8
1	A	135	MET	2.8
1	A	124	ILE	2.7
2	C	102	LEU	2.7
1	B	30	PHE	2.7
2	C	107	GLU	2.7
1	B	170	TYR	2.7
1	B	111	LEU	2.7
1	B	178	LEU	2.7
1	A	198	LYS	2.6
1	A	131	VAL	2.6
1	B	167	ARG	2.6
1	A	107	LEU	2.6
1	B	31	HIS	2.6
2	C	198	VAL	2.5
2	C	154	ALA	2.5
1	B	158	LEU	2.5
1	B	83	CYS	2.5
1	B	195	THR	2.5
1	A	81	THR	2.5
1	A	95	GLU	2.4
1	A	3	TYR	2.4
1	B	168	ILE	2.4
1	A	32	LEU	2.4
2	C	226	VAL	2.4
2	C	236	VAL	2.4
1	A	108	HIS	2.3
1	A	94	LEU	2.3
1	B	43	LEU	2.3
1	B	38	GLU	2.3
1	B	194	GLN	2.3
1	A	132	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	133	ALA	2.3
1	B	17	LEU	2.2
2	C	193	ALA	2.2
1	B	5	PRO	2.2
2	C	159	PRO	2.2
1	A	186	LEU	2.2
2	C	220	LYS	2.2
1	A	89	GLY	2.2
2	C	143	LEU	2.1
2	C	217	ALA	2.1
1	A	133	GLN	2.1
1	A	79	GLN	2.1
1	B	81	THR	2.1
1	B	191	THR	2.1
1	A	51	LYS	2.1
1	B	40	ILE	2.1
1	A	109	GLY	2.0
2	C	227	GLY	2.0
2	C	224	VAL	2.0
1	B	23	LYS	2.0
1	A	158	LEU	2.0
1	B	50	ALA	2.0
2	C	104	GLN	2.0
2	C	134	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	C	266	1/1	0.10	-	96,96,96,96	0
3	ZN	A	230	1/1	0.06	-	96,96,96,96	0
3	ZN	B	230	1/1	0.09	-	96,96,96,96	0

6.5 Other polymers ⓘ

There are no such residues in this entry.