



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 01:20 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 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

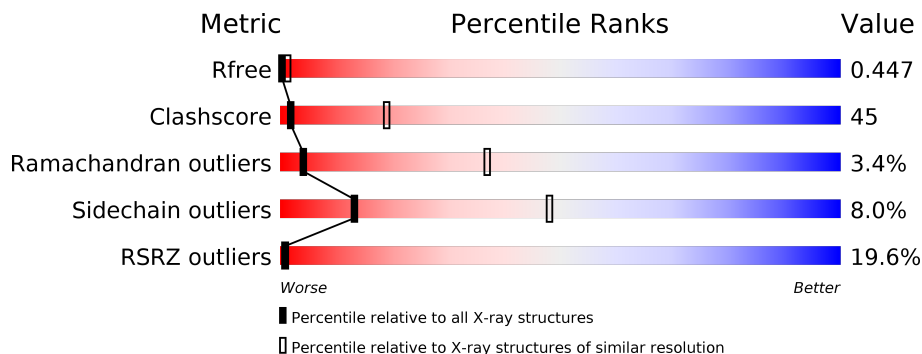
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	111664	1028 (4.02-3.58)
Clashscore	122126	1061 (4.00-3.60)
Ramachandran outliers	120053	1025 (4.00-3.60)
Sidechain outliers	120020	1019 (4.00-3.60)
RSRZ outliers	108989	1021 (4.06-3.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	220	<div> <div>20%</div> <div>36% 45% 6% • 10%</div> </div>
1	B	220	<div> <div>19%</div> <div>44% 45% • 10%</div> </div>
2	C	244	<div> <div>16%</div> <div>58% 27% 8% 6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4781 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 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			

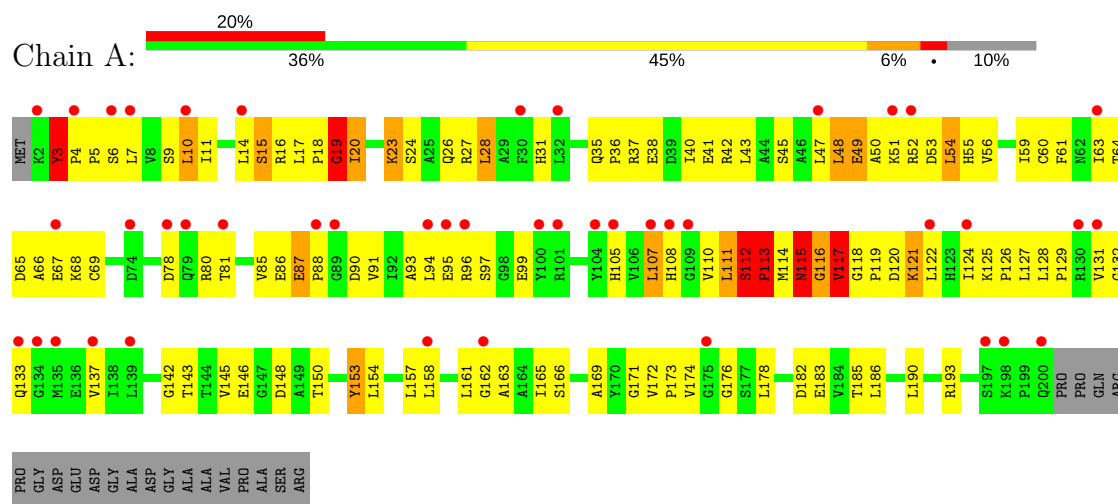
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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		

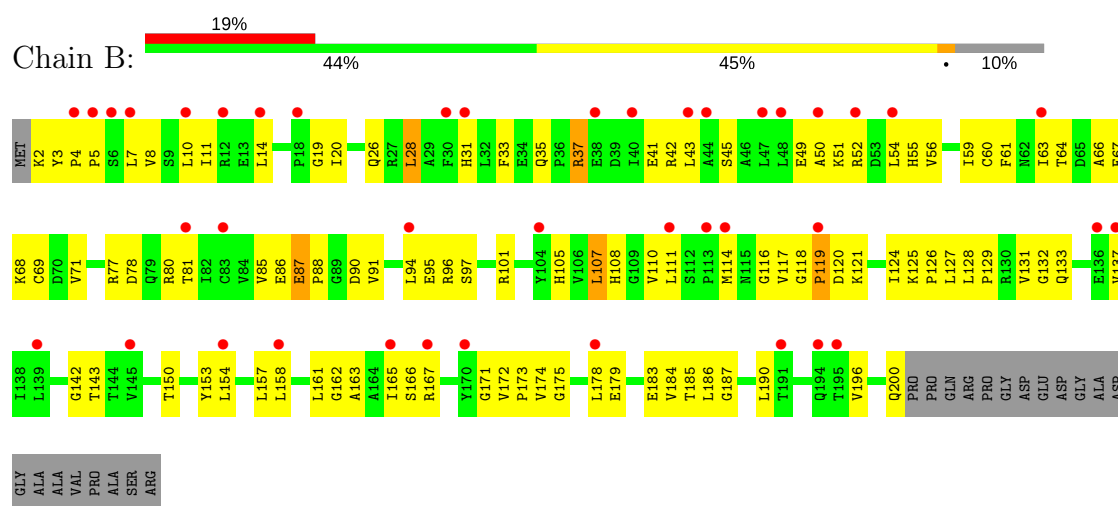
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

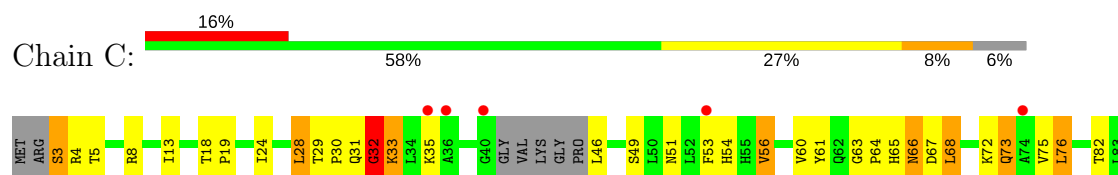
• Molecule 1: RECOMBINATION PROTEIN RECR

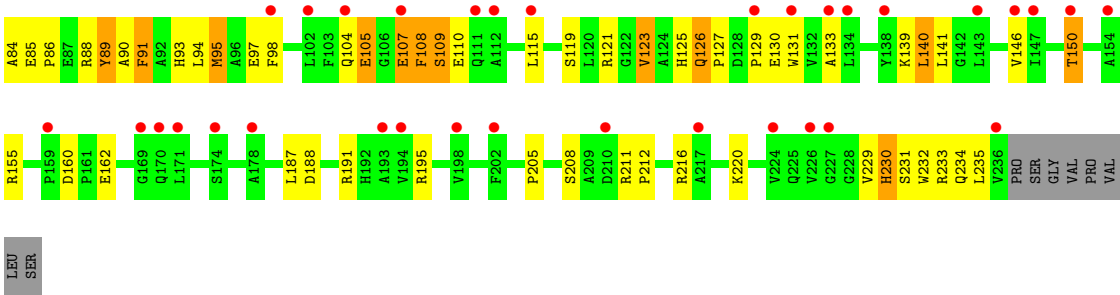


• Molecule 1: RECOMBINATION PROTEIN RECR



• 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 0.426 , 0.447	Depositor DCC
R_{free} test set	329 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	128.2	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Continued on next page...

Continued from previous page...

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 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

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

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 (429) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:VAL:O	1:B:171:GLY:O	1.68	1.09
1:A:115:ASN:CB	2:C:234:GLN:HB2	1.76	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:174:VAL:HG21	1:B:185:THR:CA	1.75	1.01
1:A:94:LEU:HD21	1:B:178:LEU:HD12	1.29	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:153:TYR:OH	1:A:157:LEU:HD12	1.70	0.92
2:C:86:PRO:C	2:C:89:TYR:HD2	1.73	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:124:ILE:CD1	1:A:153:TYR:CE2	2.54	0.90
1:A:113:PRO:HA	2:C:93:HIS:CE1	2.05	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
1:A:53:ASP:O	1:A:65:ASP:HA	1.78	0.84
2:C:94:LEU:CD1	2:C:235:LEU:CB	2.56	0.84
1:A:111:LEU:HD23	1:A:122:LEU:HD12	1.59	0.83
1:A:48:LEU:C	1:A:49:GLU:N	0.78	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
1:A:18:PRO:CB	2:C:19:PRO:CG	2.59	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:112:SER:HG	2:C:89:TYR:HE1	0.78	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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
1:B:51:LYS:HD3	1:B:51:LYS:O	1.90	0.71
2:C:93:HIS:HB3	2:C:235:LEU:CD2	2.20	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
1:A:5:PRO:O	1:A:9:SER:CB	2.43	0.66
2:C:94:LEU:CB	2:C:235:LEU:HB3	2.26	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
1:B:111:LEU:HG	1:B:150:THR:HG23	1.79	0.64
2:C:75:VAL:CG1	2:C:76:LEU:N	2.59	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASP:O	1:A:65:ASP:CA	2.47	0.63
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
1:A:182:ASP:OD2	2:C:76:LEU:CG	2.45	0.61
2:C:94:LEU:CD1	2:C:235:LEU:HB3	2.26	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:153:TYR:CZ	1:A:157:LEU:CD1	2.79	0.60
1:A:174:VAL:N	1:B:185:THR:HG1	1.74	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
1:A:111:LEU:HD23	1:A:122:LEU:HD11	1.83	0.59
1:B:175:GLY:CA	2:C:51:ASN:HD21	2.04	0.59
2:C:94:LEU:CD1	2:C:232:TRP:HE3	2.15	0.59
1:A:148:ASP:OD1	2:C:84:ALA:HB2	1.94	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:29:THR:OG1	2:C:32:GLY:HA2	2.02	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:153:TYR:OH	1:A:157:LEU:HD11	2.04	0.57
1:A:94:LEU:HD23	1:B:178:LEU:HD13	1.72	0.57
1:A:53:ASP:O	1:A:65:ASP:CB	2.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PRO:O	2:C:93:HIS:CE1	2.58	0.56
2:C:229:VAL:O	2:C:229:VAL:CG1	2.53	0.56
2:C:29:THR:OG1	2:C:32:GLY:CA	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:61:PHE:O	1:A:108:HIS:HE1	1.90	0.55
1:A:115:ASN:HD22	1:A:116:GLY:CA	2.19	0.55
1:A:94:LEU:CD1	1:B:178:LEU:HD12	2.37	0.55
1:A:18:PRO:CG	2:C:19:PRO:CG	2.85	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:111:LEU:O	1:A:146:GLU:OE1	2.25	0.54
1:A:48:LEU:CB	1:A:49:GLU:N	2.68	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:67:GLU:HB2	1:A:68:LYS:HD2	1.90	0.54
1:B:87:GLU:HG3	1:B:88:PRO:HD2	1.90	0.54
1:A:18:PRO:HG2	2:C:19:PRO:HG2	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:A:176:GLY:O	1:B:143:THR:OG1	2.26	0.53
1:B:153:TYR:CE2	1:B:157:LEU:HD12	2.43	0.53
1:A:161:LEU:HD12	1:A:161:LEU:H	1.74	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:115:ASN:OD1	2:C:234:GLN:CD	2.47	0.52
1:A:87:GLU:HG3	1:A:88:PRO:HD2	1.90	0.52
1:A:148:ASP:HB3	2:C:84:ALA:HB1	1.91	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:B:131:VAL:HB	1:B:161:LEU:HD22	1.93	0.51
1:B:56:VAL:HG21	1:B:61:PHE:HB3	1.92	0.51
1:B:85:VAL:CG1	1:B:86:GLU:N	2.73	0.51
1:A:18:PRO:O	2:C:19:PRO:HG2	2.10	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:91:PHE:CZ	2:C:130:GLU:CB	2.94	0.51
2:C:33:LYS:HD2	2:C:105:GLU:HG3	1.92	0.51
1:A:131:VAL:HB	1:A:161:LEU:HD22	1.93	0.51
1:A:18:PRO:HG2	2:C:19:PRO:CG	2.41	0.51
1:A:14:LEU:HD22	1:A:28:LEU:HD22	1.93	0.51
2:C:89:TYR:CG	2:C:90:ALA:N	2.79	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
1:A:31:HIS:O	1:A:35:GLN:HG2	2.11	0.50
2:C:86:PRO:HA	2:C:89:TYR:CE2	2.41	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:14:LEU:HD22	1:B:28:LEU:HD22	1.93	0.48
1:B:111:LEU:HD12	1:B:150:THR:HA	1.94	0.48
2:C:229:VAL:O	2:C:231:SER:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:3:TYR:N	1:A:4:PRO:CD	2.77	0.47
1:A:182:ASP:HB2	2:C:49:SER:OG	2.14	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:78:ASP:OD2	1:A:81:THR:HG23	2.15	0.45
1:A:174:VAL:HG23	1:B:185:THR:HA	1.38	0.45
1:B:4:PRO:HA	1:B:5:PRO:HD2	1.84	0.45
2:C:72:LYS:O	2:C:73:GLN:CB	2.63	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: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:HD11	1:B:178:LEU:CD1	2.46	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PRO:O	1:A:9:SER:N	2.50	0.45
1:A:173:PRO:HG3	1:B:173:PRO:HG3	1.99	0.45
1:A:85:VAL:CG1	1:A:90:ASP:OD2	2.66	0.44
1:B:158:LEU:HB2	1:B:165:ILE:HD11	2.00	0.44
1:B:85:VAL:CG1	1:B:90:ASP:OD2	2.66	0.44
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:183:GLU:CD	1:B:183:GLU:N	2.65	0.44
1:B:85:VAL:HG12	1:B:86:GLU:N	2.33	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
1:A:85:VAL:HG12	1:A:86:GLU:N	2.33	0.43
2:C:29:THR:O	2:C:32:GLY:CA	2.66	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
1:A:42:ARG:NH1	1:A:42:ARG:HB2	2.33	0.43
2:C:66:ASN:C	2:C:68:LEU:H	2.22	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:68:LYS:N	1:B:68:LYS:HD2	2.33	0.43
1:B:85:VAL:CG1	1:B:90:ASP:CB	2.92	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
1:A:14:LEU:O	1:A:17:LEU:HB2	2.18	0.42
2:C:126:GLN:HG3	2:C:127:PRO:HD2	2.01	0.42
1:A:165:ILE:C	1:B:196:VAL:HG23	2.30	0.42
1:A:117:VAL:CG1	1:A:122:LEU:HG	2.50	0.42
2:C:94:LEU:N	2:C:235:LEU:HD13	2.26	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:A:193:ARG:HB2	1:B:167:ARG:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LYS:HB3	1:B:126:PRO:CD	2.50	0.42
1:B:71:VAL:HG13	1:B:77:ARG:HD3	2.01	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
1:A:4:PRO:C	1:A:6:SER:N	2.72	0.41
2:C:86:PRO:CA	2:C:89:TYR:CE2	3.01	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:132:GLY:O	1:B:163:ALA:HB2	2.20	0.41
1:B:91:VAL:O	1:B:95:GLU:HB2	2.21	0.41
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.51	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:32:GLY:HA3	2:C:108:PHE:CE2	2.56	0.41
2:C:29:THR:O	2:C:32:GLY:HA3	2.21	0.41
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.51	0.40
2:C:91:PHE:CD1	2:C:129:PRO:HB2	2.56	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	Interatomic distance (Å)	Clash overlap (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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	197/220 (90%)	168 (85%)	21 (11%)	8 (4%)	3	32
1	B	197/220 (90%)	173 (88%)	20 (10%)	4 (2%)	8	47
2	C	225/244 (92%)	204 (91%)	12 (5%)	9 (4%)	3	32
All	All	619/684 (90%)	545 (88%)	53 (9%)	21 (3%)	4	37

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	15	51
1	B	165/180 (92%)	159 (96%)	6 (4%)	38	70
2	C	183/195 (94%)	160 (87%)	23 (13%)	5	28
All	All	513/555 (92%)	472 (92%)	41 (8%)	13	48

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 [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](#)

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.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	15:SER	C	16:ARG	N	1.79
1	A	54:LEU	C	55:HIS	N	1.08

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	19:GLY	C	20:ILE	N	0.86
1	A	48:LEU	C	49:GLU	N	0.78

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%)	1.11	44 (22%) 0 0	96, 96, 96, 96	0
1	B	199/220 (90%)	0.87	41 (20%) 1 1	96, 96, 96, 96	0
2	C	229/244 (93%)	0.93	38 (16%) 1 2	96, 96, 96, 96	0
All	All	627/684 (91%)	0.97	123 (19%) 1 1	96, 96, 96, 96	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	GLY	8.9
1	B	44	ALA	6.2
1	A	14	LEU	6.1
1	A	7	LEU	5.8
1	A	67	GLU	5.7
1	A	105	HIS	5.6
1	A	134	GLY	5.5
2	C	194	VAL	5.1
1	B	63	ILE	4.9
1	A	162	GLY	4.8
2	C	138	TYR	4.6
1	B	4	PRO	4.5
1	A	63	ILE	4.5
2	C	171	LEU	4.5
1	A	10	LEU	4.4
1	A	2	LYS	4.3
2	C	154	ALA	4.2
1	B	104	TYR	4.2
1	A	200	GLN	4.2
2	C	169	GLY	4.2
2	C	198	VAL	4.1
1	B	7	LEU	4.0
2	C	170	GLN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	104	TYR	3.9
2	C	107	GLU	3.8
2	C	210	ASP	3.7
2	C	202	PHE	3.7
1	A	94	LEU	3.7
1	A	81	THR	3.7
1	B	47	LEU	3.6
2	C	150	THR	3.6
1	B	195	THR	3.5
1	A	198	LYS	3.5
1	B	10	LEU	3.5
1	A	32	LEU	3.5
1	B	111	LEU	3.5
2	C	102	LEU	3.5
2	C	115	LEU	3.4
1	B	136	GLU	3.4
1	A	124	ILE	3.4
1	B	158	LEU	3.4
2	C	74	ALA	3.4
1	A	96	ARG	3.3
1	B	12	ARG	3.2
2	C	178	ALA	3.2
1	A	52	ARG	3.2
1	B	14	LEU	3.1
1	B	113	PRO	3.1
2	C	159	PRO	3.1
1	B	170	TYR	3.1
1	A	51	LYS	3.1
1	A	89	GLY	3.1
1	A	109	GLY	3.0
2	C	236	VAL	2.9
1	B	167	ARG	2.9
2	C	147	ILE	2.9
1	A	135	MET	2.8
1	B	165	ILE	2.8
2	C	226	VAL	2.8
1	A	108	HIS	2.8
1	A	6	SER	2.8
2	C	143	LEU	2.8
1	B	178	LEU	2.8
1	A	131	VAL	2.8
2	C	112	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	193	ALA	2.7
1	A	197	SER	2.7
1	A	107	LEU	2.7
2	C	227	GLY	2.7
1	B	30	PHE	2.7
1	B	50	ALA	2.7
2	C	133	ALA	2.7
1	A	95	GLU	2.7
1	A	74	ASP	2.6
1	B	94	LEU	2.6
1	A	79	GLN	2.6
1	A	158	LEU	2.6
2	C	111	GLN	2.6
1	A	133	GLN	2.6
2	C	53	PHE	2.6
1	B	43	LEU	2.6
1	B	145	VAL	2.6
2	C	104	GLN	2.5
1	B	31	HIS	2.5
2	C	35	LYS	2.5
1	B	81	THR	2.5
1	B	83	CYS	2.5
2	C	174	SER	2.4
2	C	40	GLY	2.4
2	C	134	LEU	2.4
1	B	52	ARG	2.4
1	A	78	ASP	2.4
1	A	130	ARG	2.4
1	B	154	LEU	2.3
1	B	191	THR	2.3
1	B	137	VAL	2.3
1	B	48	LEU	2.3
2	C	217	ALA	2.3
1	B	5	PRO	2.3
2	C	98	PHE	2.3
1	A	100	TYR	2.3
1	B	18	PRO	2.2
1	B	6	SER	2.2
1	B	114	MET	2.2
2	C	224	VAL	2.2
1	B	194	GLN	2.2
1	B	40	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	36	ALA	2.2
1	B	139	LEU	2.2
1	B	119	PRO	2.2
2	C	129	PRO	2.2
1	B	38	GLU	2.2
2	C	131	TRP	2.1
1	A	101	ARG	2.1
1	A	139	LEU	2.1
1	B	54	LEU	2.1
2	C	146	VAL	2.1
1	A	137	VAL	2.1
1	A	122	LEU	2.0
1	A	4	PRO	2.0
1	A	88	PRO	2.0
1	A	30	PHE	2.0
1	A	47	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
3	ZN	C	266	1/1	0.74	0.10	96,96,96,96	0
3	ZN	B	230	1/1	0.75	0.11	96,96,96,96	0
3	ZN	A	230	1/1	0.91	0.07	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.