



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:48 PM GMT

PDB ID : 1CN4
Title : ERYTHROPOIETIN COMPLEXED WITH EXTRACELLULAR DOMAINS
OF ERYTHROPOIETIN RECEPTOR
Authors : Stroud, R.M.; Reid, S.W.
Deposited on : 1999-05-25
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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

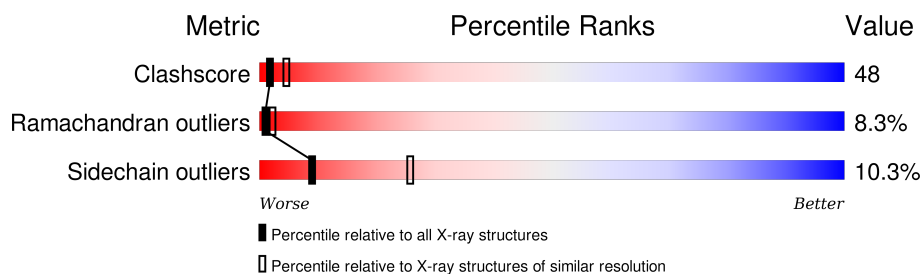
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	228	
1	B	228	
2	C	166	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4604 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 PROTEIN (ERYTHROPOIETIN RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1688	1071	296	314	7			
1	B	218	Total	C	N	O	S	0	0	0
			1695	1075	297	316	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	GLN	ASN	ENGINEERED	UNP P19235
B	52	GLN	ASN	ENGINEERED	UNP P19235
A	164	GLN	ASN	ENGINEERED	UNP P19235
B	164	GLN	ASN	ENGINEERED	UNP P19235
A	211	GLU	ALA	ENGINEERED	UNP P19235
B	211	GLU	ALA	ENGINEERED	UNP P19235

- Molecule 2 is a protein called PROTEIN (ERYTHROPOIETIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	154	Total	C	N	O	S	0	0	0
			1206	767	213	221	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	24	LYS	ASN	ENGINEERED	UNP P01588
C	38	LYS	ASN	ENGINEERED	UNP P01588
C	83	LYS	ASN	ENGINEERED	UNP P01588

- Molecule 3 is water.

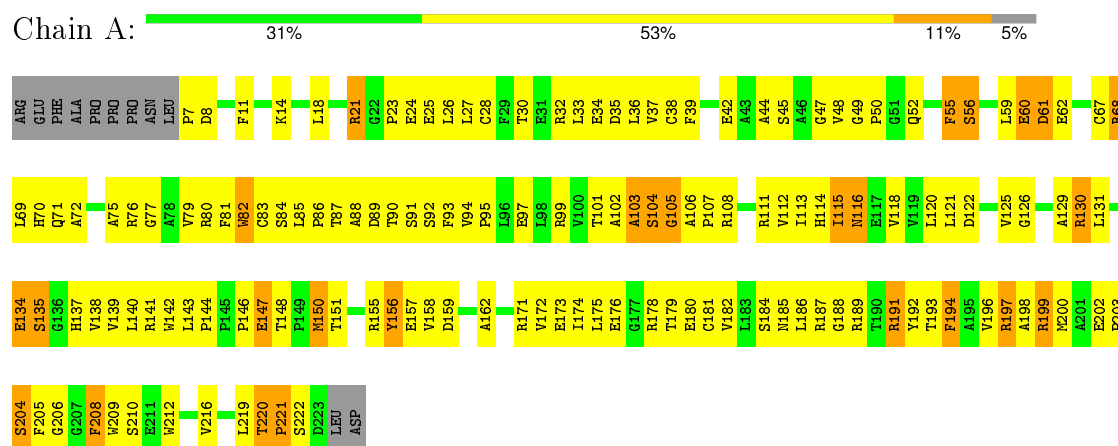
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	O 4	0	0
3	B	5	Total 5	O 5	0	0
3	C	6	Total 6	O 6	0	0

3 Residue-property plots

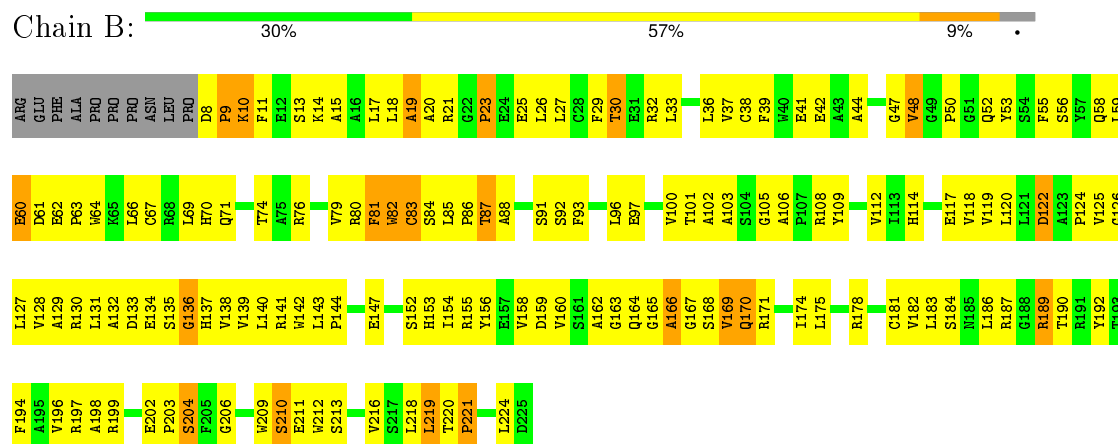
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

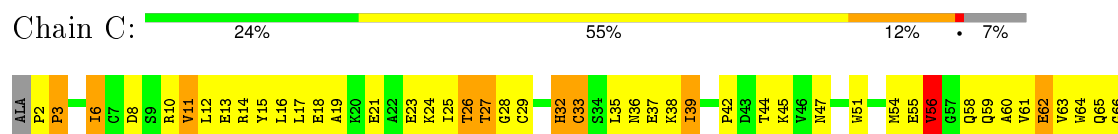
• Molecule 1: PROTEIN (ERYTHROPOIETIN RECEPTOR)



• Molecule 1: PROTEIN (ERYTHROPOIETIN RECEPTOR)



• Molecule 2: PROTEIN (ERYTHROPOIETIN)



L67	A68	L69	L70	S71	E72	A73	V74	L75	R76	A79	L80	L81	V82	K83	S84	S85	Q86	P87	W88	E89	P90	L91	Q92	V95	V99	S100	G101	L102	L105	T106	T107	L108	L109	R110	A111	L112	Q115	K116	E117	A118	I119	S120	P121	D122	D123	ALA	ALA	SER	ALA	ALA	ALA	PRO	LEU	R131	T132
L133	D136	T137	F138	R139	K140	L141	F142	R143	V144	V145	S146	N147	F148	L149	R150	G151	R152	L153	K154	L155	V156	T157	A160	C161	R162	THR	GLY	ASP	ARG																										

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.34Å 80.34Å 134.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	83.4 (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.280 , 0.336	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4604	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	0/1735	0.69	0/2368
1	B	0.43	0/1741	0.69	1/2375 (0.0%)
2	C	0.49	0/1227	0.71	1/1661 (0.1%)
All	All	0.44	0/4703	0.70	2/6404 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	133	ILE	N-CA-C	-5.61	95.87	111.00
1	B	23	PRO	N-CA-C	5.11	125.39	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	15	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	1688	0	1635	154	0
1	B	1695	0	1640	161	0
2	C	1206	0	1226	128	0
3	A	4	0	0	0	0
3	B	5	0	0	1	0
3	C	6	0	0	2	0
All	All	4604	0	4501	435	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 48.

All (435) 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:115:ILE:HD12	1:A:115:ILE:H	1.09	1.07
1:B:25:GLU:HG2	1:B:26:LEU:H	1.26	1.01
2:C:6:ILE:HG21	2:C:112:LEU:HD11	1.47	0.95
1:A:49:GLY:H	1:A:52:GLN:HG3	1.31	0.95
1:B:55:PHE:HD2	1:B:67:CYS:HB3	1.29	0.94
2:C:26:THR:HB	2:C:139:ARG:HA	1.52	0.91
1:A:115:ILE:CD1	1:A:115:ILE:H	1.89	0.83
1:B:162:ALA:H	1:B:168:SER:HB2	1.45	0.82
1:A:115:ILE:N	1:A:115:ILE:HD12	1.94	0.81
2:C:132:THR:C	2:C:133:ILE:HD12	2.00	0.80
1:A:44:ALA:HB3	1:A:48:VAL:HG21	1.63	0.80
1:A:191:ARG:HB3	1:A:219:LEU:HD12	1.64	0.79
1:B:186:LEU:HB3	1:B:192:TYR:HE2	1.45	0.78
1:A:91:SER:O	1:A:115:ILE:HD13	1.82	0.78
1:B:162:ALA:H	1:B:168:SER:CB	1.96	0.77
1:B:129:ALA:HB2	1:B:140:LEU:HG	1.64	0.77
1:B:190:THR:O	1:B:219:LEU:HA	1.85	0.77
1:B:189:ARG:HA	1:B:220:THR:O	1.83	0.77
1:B:8:ASP:N	1:B:9:PRO:HD2	2.00	0.76
1:A:99:ARG:HG3	1:A:99:ARG:HH11	1.49	0.76
2:C:61:VAL:HG22	2:C:118:ALA:HA	1.68	0.75
1:A:158:VAL:HB	1:A:172:VAL:CG1	2.16	0.75
1:A:120:LEU:HD13	1:A:208:PHE:HB2	1.70	0.74
1:A:55:PHE:HD1	1:A:56:SER:N	1.86	0.73
1:B:30:THR:HG22	1:B:118:VAL:HG23	1.71	0.73
1:A:137:HIS:CG	1:A:184:SER:HA	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:CYS:SG	1:A:68:ARG:NH1	2.62	0.72
1:B:50:PRO:HD3	1:B:71:GLN:NE2	2.04	0.72
2:C:162:ARG:HA	2:C:162:ARG:CZ	2.19	0.72
2:C:64:TRP:HZ3	2:C:109:LEU:HB2	1.56	0.71
1:B:55:PHE:CD2	1:B:67:CYS:HB3	2.21	0.71
1:A:150:MET:CE	2:C:11:VAL:HA	2.21	0.70
1:A:68:ARG:NH2	1:A:84:SER:HB2	2.04	0.70
1:A:120:LEU:CD1	1:A:208:PHE:HB2	2.22	0.70
1:B:25:GLU:HG2	1:B:26:LEU:N	2.04	0.69
2:C:142:PHE:O	2:C:145:TYR:HB3	1.92	0.69
2:C:23:GLU:O	2:C:25:ILE:N	2.25	0.69
2:C:140:LYS:O	2:C:144:VAL:HG23	1.92	0.69
1:B:132:ALA:O	1:B:134:GLU:N	2.27	0.68
1:A:156:TYR:O	1:A:174:ILE:HG12	1.93	0.68
2:C:74:VAL:HG21	2:C:102:LEU:HD12	1.75	0.68
1:A:7:PRO:HD2	1:A:11:PHE:HD2	1.58	0.67
1:B:100:VAL:HB	1:B:109:TYR:HB2	1.76	0.67
1:B:74:THR:CG2	1:B:76:ARG:HG2	2.24	0.67
1:B:140:LEU:HD21	1:B:194:PHE:HB3	1.76	0.67
1:A:68:ARG:HD2	1:A:68:ARG:C	2.15	0.67
1:B:17:LEU:HG	1:B:21:ARG:HH21	1.59	0.67
1:A:158:VAL:HB	1:A:172:VAL:HG12	1.76	0.67
1:B:91:SER:HA	2:C:47:ASN:OD1	1.95	0.66
1:A:32:ARG:O	1:A:34:GLU:N	2.28	0.66
1:A:139:VAL:HA	1:A:182:VAL:HG22	1.77	0.66
1:A:137:HIS:ND1	1:A:184:SER:HA	2.10	0.66
1:A:68:ARG:NH2	1:A:84:SER:H	1.93	0.66
1:A:92:SER:HB3	1:A:116:ASN:HB3	1.77	0.66
2:C:160:ALA:C	2:C:162:ARG:H	2.01	0.65
1:A:49:GLY:N	1:A:52:GLN:HG3	2.10	0.65
1:B:129:ALA:HA	1:B:139:VAL:O	1.96	0.65
1:B:163:GLY:C	1:B:165:GLY:H	2.00	0.65
1:A:42:GLU:OE1	1:A:108:ARG:NH1	2.30	0.65
1:A:68:ARG:O	1:A:68:ARG:HD2	1.97	0.65
1:B:189:ARG:O	1:B:189:ARG:HG3	1.96	0.64
1:A:187:ARG:HH11	1:A:187:ARG:HG3	1.63	0.64
1:B:55:PHE:HD1	1:B:100:VAL:HG22	1.61	0.64
1:A:59:LEU:O	1:A:60:GLU:O	2.16	0.64
2:C:153:LEU:O	2:C:157:THR:HG23	1.98	0.63
1:A:129:ALA:O	1:A:130:ARG:HB2	1.98	0.63
1:B:30:THR:HG23	1:B:119:VAL:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ARG:O	1:B:33:LEU:HB2	1.97	0.63
1:B:55:PHE:HD2	1:B:67:CYS:CB	2.07	0.63
1:A:68:ARG:HH22	1:A:84:SER:N	1.96	0.63
2:C:35:LEU:HD23	2:C:137:THR:C	2.19	0.63
1:B:128:VAL:HG23	1:B:141:ARG:HB2	1.80	0.63
1:A:118:VAL:HG23	1:A:118:VAL:O	1.98	0.62
1:A:150:MET:HE3	2:C:11:VAL:HA	1.81	0.62
1:B:187:ARG:HG3	1:B:187:ARG:HH11	1.64	0.62
1:B:153:HIS:HE1	2:C:154:LYS:HE3	1.63	0.62
1:B:25:GLU:CG	1:B:26:LEU:H	2.07	0.62
1:A:194:PHE:O	1:A:216:VAL:HG12	1.99	0.62
1:B:218:LEU:HD12	1:B:219:LEU:H	1.66	0.61
2:C:38:LYS:HG3	2:C:39:ILE:N	2.16	0.61
1:B:189:ARG:N	1:B:220:THR:OG1	2.34	0.61
1:B:189:ARG:N	1:B:221:PRO:O	2.34	0.61
1:A:156:TYR:CD1	1:A:156:TYR:N	2.68	0.61
2:C:14:ARG:O	2:C:18:GLU:HG3	2.00	0.61
1:A:35:ASP:HA	1:A:90:THR:HG21	1.82	0.60
1:A:199:ARG:HB3	1:A:199:ARG:HH11	1.65	0.60
1:A:187:ARG:O	1:A:220:THR:HG21	2.00	0.60
1:A:68:ARG:HH22	1:A:84:SER:H	1.50	0.60
1:A:140:LEU:O	1:A:180:GLU:HA	2.00	0.60
2:C:38:LYS:CG	2:C:39:ILE:H	2.14	0.60
2:C:26:THR:O	2:C:29:CYS:HB3	2.02	0.60
1:A:175:LEU:HG	1:A:178:ARG:HB3	1.84	0.60
1:B:59:LEU:HD23	1:B:96:LEU:HD13	1.84	0.59
2:C:55:GLU:O	2:C:59:GLN:HG3	2.02	0.59
1:B:136:GLY:O	1:B:184:SER:HA	2.01	0.59
1:B:155:ARG:NH2	1:B:199:ARG:HH11	1.99	0.59
1:B:142:TRP:O	1:B:143:LEU:HD23	2.03	0.59
2:C:149:LEU:O	2:C:153:LEU:HB3	2.02	0.59
1:A:18:LEU:HB3	1:A:27:LEU:HD13	1.84	0.59
1:A:44:ALA:HB3	1:A:48:VAL:CG2	2.30	0.59
1:A:131:LEU:HD22	1:A:221:PRO:HD3	1.83	0.59
1:B:199:ARG:HB2	1:B:209:TRP:CZ3	2.38	0.58
1:B:135:SER:O	1:B:137:HIS:N	2.35	0.58
1:B:197:ARG:HD2	1:B:212:TRP:CH2	2.37	0.58
2:C:85:SER:O	2:C:87:PRO:HD3	2.03	0.58
2:C:150:ARG:O	2:C:154:LYS:HB3	2.04	0.58
1:A:197:ARG:HG3	1:A:209:TRP:CE3	2.38	0.58
1:B:158:VAL:HG22	1:B:196:VAL:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:SER:HB3	1:A:94:VAL:HG21	1.85	0.57
1:A:99:ARG:HG3	1:A:99:ARG:NH1	2.19	0.57
2:C:2:PRO:N	2:C:3:PRO:CD	2.68	0.57
1:B:168:SER:O	1:B:169:VAL:HG13	2.05	0.57
1:A:60:GLU:HB2	1:A:95:PRO:HD2	1.85	0.57
2:C:38:LYS:HG3	2:C:39:ILE:H	1.70	0.57
1:A:202:GLU:N	1:A:202:GLU:OE1	2.31	0.57
2:C:76:ARG:HE	2:C:76:ARG:HA	1.69	0.57
2:C:136:ASP:OD1	2:C:137:THR:HG23	2.05	0.57
1:A:121:LEU:O	1:A:210:SER:HB2	2.04	0.57
1:B:155:ARG:HH11	1:B:155:ARG:HG3	1.69	0.56
1:B:79:VAL:HG22	1:B:80:ARG:N	2.20	0.56
1:B:32:ARG:N	1:B:32:ARG:HD2	2.20	0.56
2:C:89:GLU:HB2	2:C:90:PRO:HD3	1.86	0.56
1:A:70:HIS:O	1:A:81:PHE:HA	2.05	0.56
1:A:141:ARG:HG3	1:A:141:ARG:HH11	1.71	0.56
1:A:139:VAL:HG22	1:A:182:VAL:CG2	2.34	0.56
1:B:169:VAL:O	1:B:170:GLN:HB2	2.06	0.56
1:B:131:LEU:HD11	1:B:221:PRO:HD3	1.88	0.56
2:C:119:ILE:N	2:C:119:ILE:HD12	2.21	0.56
1:B:171:ARG:NH2	1:B:212:TRP:HZ2	2.03	0.56
1:A:139:VAL:HG22	1:A:182:VAL:HG22	1.88	0.56
1:B:8:ASP:N	1:B:9:PRO:CD	2.68	0.55
1:A:7:PRO:HG2	1:A:8:ASP:H	1.71	0.55
2:C:86:GLN:HE21	2:C:86:GLN:HA	1.70	0.55
2:C:12:LEU:HD12	2:C:12:LEU:O	2.06	0.55
1:B:44:ALA:HB1	1:B:47:GLY:O	2.06	0.55
1:A:26:LEU:O	1:A:111:ARG:NH1	2.40	0.55
1:B:10:LYS:O	1:B:13:SER:HB2	2.06	0.55
1:B:209:TRP:HB2	3:B:228:HOH:O	2.06	0.55
1:B:50:PRO:C	1:B:52:GLN:H	2.10	0.55
2:C:38:LYS:CG	2:C:39:ILE:N	2.68	0.55
2:C:67:LEU:HD11	2:C:102:LEU:HD22	1.89	0.55
1:A:175:LEU:HG	1:A:178:ARG:CB	2.37	0.55
2:C:27:THR:C	2:C:29:CYS:H	2.09	0.54
2:C:131:ARG:CZ	2:C:132:THR:HG22	2.36	0.54
1:B:59:LEU:O	1:B:60:GLU:C	2.46	0.54
1:A:21:ARG:O	1:A:21:ARG:HG3	2.06	0.54
2:C:2:PRO:N	2:C:3:PRO:HD3	2.21	0.54
1:B:27:LEU:O	1:B:38:CYS:HA	2.06	0.54
1:B:55:PHE:HB2	1:B:69:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:119:ILE:H	2:C:119:ILE:CD1	2.21	0.54
2:C:101:GLY:O	2:C:105:LEU:HG	2.07	0.54
1:A:36:LEU:HD13	1:A:115:ILE:HG23	1.87	0.54
2:C:59:GLN:O	2:C:62:GLU:HB2	2.08	0.54
2:C:8:ASP:O	2:C:11:VAL:HG12	2.07	0.54
1:B:144:PRO:HB3	1:B:156:TYR:OH	2.07	0.54
1:B:48:VAL:CG2	1:B:79:VAL:HG11	2.38	0.54
2:C:119:ILE:H	2:C:119:ILE:HD12	1.72	0.54
1:B:130:ARG:HD2	1:B:130:ARG:O	2.07	0.54
1:A:199:ARG:HG2	1:A:200:MET:N	2.21	0.54
2:C:95:VAL:O	2:C:99:VAL:HG23	2.08	0.54
1:B:186:LEU:HB3	1:B:192:TYR:CE2	2.35	0.54
1:A:203:PRO:HG2	1:A:204:SER:H	1.72	0.54
2:C:19:ALA:HB1	2:C:146:SER:HB3	1.89	0.53
1:B:216:VAL:HG13	1:B:216:VAL:O	2.08	0.53
1:B:53:TYR:CD1	1:B:102:ALA:HA	2.42	0.53
1:A:92:SER:O	1:A:93:PHE:HB2	2.08	0.53
1:B:32:ARG:HH21	1:B:147:GLU:HB2	1.74	0.53
1:A:14:LYS:CG	1:A:120:LEU:HD23	2.39	0.53
1:B:127:LEU:HA	1:B:141:ARG:O	2.08	0.53
1:B:187:ARG:NH1	1:B:187:ARG:HG3	2.24	0.53
1:A:193:THR:HA	1:A:216:VAL:O	2.07	0.53
1:A:146:PRO:O	1:A:148:THR:N	2.41	0.53
1:A:55:PHE:HB2	1:A:69:LEU:HD21	1.90	0.53
1:A:199:ARG:CB	1:A:199:ARG:HH11	2.22	0.53
2:C:8:ASP:OD1	2:C:10:ARG:HG2	2.09	0.53
1:A:68:ARG:HH22	1:A:84:SER:HB2	1.72	0.52
1:B:198:ALA:H	1:B:210:SER:HB3	1.73	0.52
1:B:186:LEU:HD22	1:B:192:TYR:CE2	2.44	0.52
1:B:44:ALA:CB	1:B:48:VAL:HB	2.40	0.52
1:B:101:THR:HG23	1:B:106:ALA:O	2.09	0.52
1:B:204:SER:HA	2:C:150:ARG:HD2	1.90	0.52
1:A:131:LEU:CD2	1:A:221:PRO:HD3	2.39	0.52
1:B:84:SER:O	1:B:85:LEU:C	2.48	0.52
2:C:115:GLN:O	2:C:118:ALA:HB3	2.10	0.52
2:C:56:VAL:HG12	2:C:156:TYR:CE1	2.44	0.52
1:B:47:GLY:O	1:B:48:VAL:HB	2.08	0.52
1:A:72:ALA:O	1:A:80:ARG:N	2.32	0.52
1:A:24:GLU:OE2	1:A:108:ARG:NH2	2.43	0.52
1:A:135:SER:OG	1:A:137:HIS:CD2	2.63	0.52
1:A:45:SER:O	1:A:48:VAL:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PRO:HD2	1:A:11:PHE:CD2	2.42	0.51
1:B:92:SER:O	1:B:93:PHE:HB2	2.10	0.51
2:C:26:THR:CB	2:C:139:ARG:HA	2.31	0.51
2:C:33:CYS:O	2:C:138:PHE:N	2.38	0.51
1:A:156:TYR:HD1	1:A:156:TYR:N	2.09	0.51
1:B:53:TYR:HD1	1:B:102:ALA:HA	1.75	0.51
1:A:104:SER:OG	1:A:105:GLY:N	2.43	0.51
1:B:219:LEU:HD12	1:B:219:LEU:H	1.76	0.51
2:C:58:GLN:NE2	2:C:58:GLN:HA	2.25	0.51
2:C:81:LEU:HD22	2:C:95:VAL:HG21	1.91	0.51
2:C:139:ARG:HB3	2:C:139:ARG:NH1	2.26	0.51
2:C:133:ILE:N	2:C:133:ILE:HD12	2.26	0.51
2:C:79:ALA:O	2:C:81:LEU:N	2.43	0.51
1:A:142:TRP:NE1	1:A:179:THR:HB	2.25	0.51
1:B:138:VAL:O	1:B:182:VAL:HA	2.11	0.51
1:B:48:VAL:HA	1:B:52:GLN:OE1	2.10	0.51
1:B:175:LEU:HB2	1:B:178:ARG:HG3	1.93	0.51
2:C:23:GLU:C	2:C:25:ILE:H	2.14	0.51
1:B:125:VAL:HG12	1:B:126:GLY:H	1.76	0.51
1:A:125:VAL:O	1:A:143:LEU:HB2	2.11	0.50
1:B:130:ARG:HD2	1:B:130:ARG:C	2.31	0.50
1:A:68:ARG:HH22	1:A:84:SER:CA	2.24	0.50
1:B:108:ARG:HD2	1:B:109:TYR:CE1	2.46	0.50
2:C:160:ALA:C	2:C:162:ARG:N	2.65	0.50
1:A:129:ALA:HA	1:A:140:LEU:HD23	1.92	0.50
2:C:36:ASN:O	2:C:37:GLU:HB2	2.12	0.50
2:C:105:LEU:O	2:C:107:THR:N	2.45	0.50
1:B:18:LEU:O	1:B:19:ALA:C	2.49	0.50
1:A:30:THR:HG21	1:A:115:ILE:O	2.11	0.50
2:C:87:PRO:O	2:C:89:GLU:N	2.45	0.50
1:A:197:ARG:HD2	1:A:212:TRP:CH2	2.47	0.50
1:B:129:ALA:HB3	1:B:194:PHE:CD2	2.47	0.50
1:A:130:ARG:CZ	1:A:130:ARG:HB3	2.41	0.50
1:B:62:GLU:HB3	1:B:63:PRO:HD2	1.92	0.50
1:A:91:SER:HB3	1:A:94:VAL:CG2	2.41	0.49
1:B:60:GLU:O	1:B:61:ASP:HB2	2.12	0.49
1:A:59:LEU:O	1:A:60:GLU:C	2.50	0.49
2:C:6:ILE:HD13	2:C:6:ILE:O	2.12	0.49
1:B:138:VAL:HB	1:B:183:LEU:HB2	1.94	0.49
1:A:202:GLU:HB3	1:A:203:PRO:HA	1.93	0.49
1:A:28:CYS:HA	1:A:37:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:79:ALA:O	2:C:82:VAL:N	2.43	0.49
1:B:174:ILE:HG22	1:B:175:LEU:N	2.27	0.49
1:B:163:GLY:O	1:B:165:GLY:N	2.45	0.49
1:A:196:VAL:HG12	1:A:197:ARG:N	2.28	0.49
1:B:55:PHE:CD1	1:B:100:VAL:HG22	2.47	0.49
2:C:109:LEU:C	2:C:111:ALA:N	2.65	0.49
2:C:81:LEU:CD2	2:C:95:VAL:HG21	2.43	0.49
1:A:36:LEU:HD23	1:A:85:LEU:HD12	1.95	0.49
1:A:135:SER:OG	1:A:137:HIS:NE2	2.44	0.49
1:B:74:THR:HG21	1:B:76:ARG:HG2	1.95	0.49
2:C:138:PHE:O	2:C:141:LEU:N	2.46	0.48
2:C:32:HIS:C	2:C:33:CYS:SG	2.91	0.48
2:C:131:ARG:NH1	2:C:132:THR:HG22	2.28	0.48
1:B:44:ALA:HB1	1:B:48:VAL:HB	1.95	0.48
1:A:23:PRO:C	1:A:25:GLU:H	2.17	0.48
2:C:108:LEU:O	2:C:111:ALA:HB3	2.13	0.48
1:B:58:GLN:HG2	1:B:58:GLN:O	2.11	0.48
1:A:75:ALA:C	1:A:77:GLY:H	2.17	0.48
1:B:154:ILE:HG23	1:B:199:ARG:O	2.13	0.48
1:B:29:PHE:O	1:B:36:LEU:HD12	2.12	0.48
2:C:82:VAL:HG12	2:C:83:LYS:N	2.28	0.48
1:A:162:ALA:HB2	1:A:192:TYR:CE1	2.47	0.48
1:B:155:ARG:HH22	1:B:199:ARG:HH11	1.60	0.48
1:B:163:GLY:C	1:B:165:GLY:N	2.66	0.48
1:A:103:ALA:O	1:A:104:SER:C	2.51	0.48
2:C:42:PRO:N	2:C:69:LEU:HD23	2.27	0.48
1:A:158:VAL:HG23	1:A:174:ILE:HD11	1.95	0.48
2:C:13:GLU:O	2:C:17:LEU:HG	2.14	0.48
1:A:150:MET:HE1	2:C:11:VAL:HA	1.96	0.47
2:C:123:ASP:OD1	2:C:123:ASP:N	2.33	0.47
2:C:67:LEU:CD1	2:C:102:LEU:HD22	2.44	0.47
1:A:125:VAL:O	1:A:143:LEU:N	2.43	0.47
2:C:67:LEU:HD23	2:C:109:LEU:HD12	1.97	0.47
1:A:86:PRO:HG2	1:A:89:ASP:OD2	2.14	0.47
1:A:155:ARG:C	1:A:156:TYR:CD1	2.88	0.47
2:C:154:LYS:HD2	2:C:154:LYS:O	2.13	0.47
2:C:88:TRP:CD1	2:C:90:PRO:HD2	2.50	0.47
1:B:166:ALA:O	1:B:167:GLY:C	2.52	0.47
1:A:36:LEU:HD23	1:A:85:LEU:CD1	2.44	0.47
1:A:70:HIS:HB3	1:A:82:TRP:CE2	2.49	0.47
1:A:142:TRP:CZ2	1:A:179:THR:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:32:HIS:N	2:C:32:HIS:ND1	2.61	0.47
2:C:21:GLU:O	2:C:25:ILE:HG12	2.15	0.47
1:A:121:LEU:HD11	1:A:200:MET:SD	2.54	0.47
1:A:175:LEU:HD12	1:A:176:GLU:O	2.14	0.47
1:B:158:VAL:HG12	1:B:159:ASP:N	2.29	0.47
1:B:59:LEU:O	1:B:62:GLU:HB2	2.15	0.47
1:B:37:VAL:HA	1:B:83:CYS:O	2.15	0.47
1:B:62:GLU:CB	1:B:63:PRO:HD2	2.45	0.47
1:A:38:CYS:O	1:A:82:TRP:HA	2.15	0.47
1:B:58:GLN:HB2	1:B:64:TRP:HA	1.96	0.47
1:A:178:ARG:HH11	1:A:178:ARG:HG2	1.80	0.46
1:B:174:ILE:HG22	1:B:178:ARG:HB2	1.96	0.46
1:A:86:PRO:CG	1:A:89:ASP:OD2	2.63	0.46
1:A:137:HIS:CE1	1:A:184:SER:OG	2.68	0.46
2:C:71:SER:O	2:C:74:VAL:HG23	2.15	0.46
2:C:118:ALA:C	2:C:120:SER:H	2.17	0.46
1:A:18:LEU:O	1:A:21:ARG:HB3	2.14	0.46
2:C:79:ALA:C	2:C:81:LEU:N	2.69	0.46
1:B:29:PHE:HA	1:B:118:VAL:HB	1.98	0.46
2:C:27:THR:C	2:C:29:CYS:N	2.69	0.46
2:C:147:ASN:O	2:C:151:GLY:HA3	2.15	0.46
1:A:158:VAL:HG12	1:A:159:ASP:N	2.30	0.46
1:A:138:VAL:O	1:A:182:VAL:HA	2.15	0.46
1:A:188:GLY:HA3	1:A:222:SER:O	2.16	0.46
1:A:194:PHE:N	1:A:194:PHE:CD1	2.84	0.46
1:A:35:ASP:OD1	1:A:35:ASP:C	2.54	0.46
2:C:81:LEU:O	2:C:84:SER:HB3	2.15	0.46
2:C:42:PRO:CD	2:C:69:LEU:HD23	2.46	0.46
1:B:81:PHE:CD1	1:B:81:PHE:N	2.83	0.46
1:A:60:GLU:O	1:A:61:ASP:C	2.55	0.46
2:C:105:LEU:C	2:C:107:THR:N	2.68	0.46
2:C:29:CYS:SG	2:C:32:HIS:O	2.73	0.46
1:B:131:LEU:HD11	1:B:221:PRO:CG	2.46	0.46
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.77	0.46
1:B:91:SER:HB3	2:C:45:LYS:HB2	1.98	0.46
1:B:70:HIS:O	1:B:81:PHE:HA	2.16	0.46
1:A:71:GLN:HB2	1:A:81:PHE:HE1	1.81	0.46
1:B:162:ALA:N	1:B:168:SER:OG	2.49	0.45
2:C:140:LYS:HG3	2:C:143:ARG:NH2	2.30	0.45
1:A:114:HIS:C	1:A:116:ASN:H	2.19	0.45
1:A:198:ALA:O	1:A:210:SER:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLY:HA2	1:A:220:THR:CG2	2.46	0.45
1:A:71:GLN:HA	1:A:80:ARG:O	2.16	0.45
2:C:12:LEU:HD11	2:C:16:LEU:HD11	1.98	0.45
2:C:42:PRO:HD3	2:C:69:LEU:HD23	1.99	0.45
1:B:162:ALA:HB3	1:B:168:SER:HB3	1.99	0.45
2:C:73:ALA:O	2:C:74:VAL:C	2.55	0.45
1:A:82:TRP:CD1	1:A:82:TRP:N	2.85	0.45
1:B:138:VAL:CG2	1:B:186:LEU:HD12	2.46	0.45
2:C:162:ARG:HH11	2:C:162:ARG:HB2	1.82	0.45
1:B:117:GLU:C	1:B:206:GLY:O	2.55	0.45
2:C:51:TRP:CE2	2:C:59:GLN:NE2	2.85	0.45
1:A:32:ARG:C	1:A:34:GLU:H	2.20	0.45
1:B:42:GLU:OE2	1:B:53:TYR:HE2	2.00	0.45
1:A:135:SER:HG	1:A:137:HIS:CD2	2.34	0.45
1:B:74:THR:C	1:B:76:ARG:N	2.69	0.45
1:B:52:GLN:O	1:B:103:ALA:N	2.46	0.45
1:B:210:SER:OG	1:B:211:GLU:N	2.50	0.45
1:A:157:GLU:O	1:A:196:VAL:HG13	2.17	0.44
2:C:23:GLU:C	2:C:25:ILE:N	2.71	0.44
1:A:125:VAL:HG22	1:A:126:GLY:N	2.33	0.44
2:C:73:ALA:O	2:C:76:ARG:N	2.51	0.44
1:B:174:ILE:HG22	1:B:175:LEU:H	1.82	0.44
1:A:55:PHE:CB	1:A:69:LEU:HD21	2.47	0.44
2:C:74:VAL:HG21	2:C:102:LEU:CD1	2.44	0.44
2:C:88:TRP:O	2:C:91:LEU:N	2.51	0.44
1:B:14:LYS:NZ	1:B:122:ASP:OD1	2.41	0.44
2:C:55:GLU:OE1	2:C:58:GLN:CB	2.66	0.44
1:B:36:LEU:HG	1:B:37:VAL:N	2.33	0.44
1:B:132:ALA:HB2	1:B:139:VAL:HG23	1.98	0.44
1:B:55:PHE:CE2	1:B:83:CYS:SG	3.11	0.44
2:C:63:VAL:O	2:C:64:TRP:C	2.57	0.44
1:B:138:VAL:HG23	1:B:186:LEU:HD12	1.99	0.43
1:B:129:ALA:HB2	1:B:140:LEU:CG	2.42	0.43
1:B:130:ARG:NH1	1:B:139:VAL:HG21	2.32	0.43
1:A:45:SER:C	1:A:47:GLY:N	2.71	0.43
1:B:131:LEU:HD11	1:B:221:PRO:CD	2.47	0.43
1:B:97:GLU:HG3	1:B:112:VAL:HG22	1.99	0.43
1:A:55:PHE:C	1:A:55:PHE:CD1	2.91	0.43
1:A:102:ALA:O	1:A:103:ALA:C	2.56	0.43
1:B:102:ALA:O	1:B:105:GLY:N	2.51	0.43
1:B:19:ALA:O	1:B:20:ALA:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:PHE:C	1:B:39:PHE:CD1	2.91	0.43
1:B:196:VAL:HG12	1:B:197:ARG:N	2.34	0.43
1:A:113:ILE:C	1:A:114:HIS:ND1	2.72	0.43
2:C:70:LEU:O	2:C:73:ALA:N	2.51	0.43
2:C:35:LEU:HD12	2:C:39:ILE:HD11	2.00	0.43
1:B:141:ARG:CZ	1:B:141:ARG:HB3	2.49	0.43
1:A:193:THR:HG23	1:A:216:VAL:O	2.18	0.43
1:A:39:PHE:HA	1:A:81:PHE:O	2.17	0.43
2:C:59:GLN:O	2:C:60:ALA:C	2.56	0.43
1:A:188:GLY:HA2	1:A:220:THR:OG1	2.19	0.43
1:B:199:ARG:HB2	1:B:209:TRP:CE3	2.53	0.43
2:C:27:THR:OG1	2:C:28:GLY:N	2.52	0.43
2:C:56:VAL:HG23	3:C:172:HOH:O	2.18	0.43
2:C:35:LEU:HD23	2:C:137:THR:CA	2.49	0.43
1:A:157:GLU:HB3	1:A:197:ARG:CD	2.49	0.43
2:C:116:LYS:HG3	2:C:117:GLU:N	2.34	0.43
1:B:189:ARG:O	1:B:189:ARG:CG	2.65	0.43
1:A:159:ASP:OD1	1:A:171:ARG:NH1	2.52	0.43
2:C:59:GLN:O	2:C:63:VAL:HG23	2.19	0.43
1:A:101:THR:HG22	1:A:102:ALA:N	2.32	0.43
2:C:38:LYS:O	2:C:39:ILE:CB	2.67	0.42
2:C:88:TRP:O	2:C:89:GLU:C	2.57	0.42
1:B:114:HIS:O	1:B:117:GLU:N	2.38	0.42
2:C:70:LEU:O	2:C:73:ALA:HB3	2.18	0.42
1:B:36:LEU:HA	1:B:36:LEU:HD12	1.82	0.42
1:B:69:LEU:HD23	1:B:82:TRP:O	2.18	0.42
1:B:158:VAL:CG1	1:B:159:ASP:N	2.82	0.42
1:B:197:ARG:HD2	1:B:212:TRP:CZ2	2.55	0.42
1:B:79:VAL:HG22	1:B:80:ARG:H	1.84	0.42
1:B:71:GLN:OE1	1:B:81:PHE:CE2	2.72	0.42
1:B:9:PRO:C	1:B:11:PHE:N	2.73	0.42
2:C:85:SER:C	2:C:87:PRO:HD3	2.40	0.42
1:B:9:PRO:O	1:B:11:PHE:N	2.52	0.42
1:B:41:GLU:HG2	1:B:80:ARG:HB2	2.00	0.42
1:B:198:ALA:O	1:B:209:TRP:CE3	2.73	0.42
1:A:115:ILE:O	1:A:115:ILE:HG22	2.20	0.42
1:A:134:GLU:O	1:A:135:SER:CB	2.67	0.42
1:B:48:VAL:HG21	1:B:79:VAL:HG11	2.01	0.42
2:C:19:ALA:CB	2:C:146:SER:HB3	2.50	0.42
2:C:91:LEU:O	2:C:95:VAL:HG23	2.20	0.42
1:A:203:PRO:HG2	1:A:204:SER:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:PRO:O	1:B:88:ALA:N	2.53	0.42
2:C:156:TYR:O	2:C:157:THR:C	2.58	0.42
1:B:86:PRO:O	1:B:87:THR:C	2.57	0.42
1:B:171:ARG:CZ	1:B:212:TRP:HZ2	2.32	0.42
1:B:160:VAL:HG22	1:B:194:PHE:HD1	1.84	0.41
2:C:44:THR:HG21	2:C:144:VAL:HG13	2.02	0.41
2:C:66:GLY:HA3	2:C:148:PHE:CZ	2.54	0.41
2:C:55:GLU:HB3	3:C:172:HOH:O	2.21	0.41
1:B:60:GLU:OE2	2:C:143:ARG:NH2	2.52	0.41
1:A:157:GLU:HB3	1:A:197:ARG:HD2	2.01	0.41
1:A:106:ALA:HA	1:A:107:PRO:HD3	1.81	0.41
1:A:68:ARG:HH22	1:A:84:SER:CB	2.31	0.41
2:C:109:LEU:O	2:C:111:ALA:N	2.54	0.41
1:A:134:GLU:N	1:A:134:GLU:OE1	2.53	0.41
1:A:208:PHE:CD1	1:A:208:PHE:N	2.88	0.41
2:C:109:LEU:O	2:C:110:ARG:C	2.58	0.41
1:A:186:LEU:HD22	1:A:192:TYR:CE2	2.56	0.41
1:B:20:ALA:O	1:B:23:PRO:HD3	2.21	0.41
1:A:87:THR:O	1:A:89:ASP:N	2.54	0.41
1:A:114:HIS:C	1:A:116:ASN:N	2.74	0.41
1:A:59:LEU:O	1:A:62:GLU:HB2	2.21	0.41
1:A:141:ARG:HG3	1:A:141:ARG:NH1	2.35	0.41
1:A:86:PRO:O	1:A:86:PRO:HG2	2.21	0.41
1:B:171:ARG:CZ	1:B:212:TRP:CZ2	3.04	0.41
1:B:117:GLU:HA	1:B:206:GLY:O	2.20	0.41
1:B:82:TRP:N	1:B:82:TRP:CD1	2.89	0.40
2:C:86:GLN:CA	2:C:86:GLN:HE21	2.30	0.40
1:B:159:ASP:OD1	1:B:160:VAL:N	2.54	0.40
1:A:205:PHE:HB3	1:A:206:GLY:H	1.76	0.40
2:C:51:TRP:NE1	2:C:59:GLN:NE2	2.70	0.40
1:B:74:THR:C	1:B:76:ARG:H	2.25	0.40
1:B:202:GLU:HB3	1:B:203:PRO:HA	2.02	0.40
1:B:56:SER:HA	1:B:66:LEU:HA	2.04	0.40
2:C:38:LYS:O	2:C:39:ILE:HB	2.21	0.40
2:C:146:SER:O	2:C:150:ARG:HG2	2.22	0.40
1:B:186:LEU:HD22	1:B:192:TYR:CZ	2.56	0.40
1:B:11:PHE:CE1	1:B:15:ALA:HB2	2.56	0.40
2:C:82:VAL:C	2:C:84:SER:H	2.24	0.40
1:A:97:GLU:HA	1:A:112:VAL:HG22	2.04	0.40
1:B:124:PRO:HG2	1:B:213:SER:HB3	2.03	0.40

There are no symmetry-related clashes.

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	215/228 (94%)	162 (75%)	34 (16%)	19 (9%)	1	2
1	B	216/228 (95%)	159 (74%)	41 (19%)	16 (7%)	1	3
2	C	150/166 (90%)	94 (63%)	43 (29%)	13 (9%)	1	2
All	All	581/622 (93%)	415 (71%)	118 (20%)	48 (8%)	1	2

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	60	GLU
1	A	104	SER
1	A	147	GLU
1	A	221	PRO
1	B	9	PRO
1	B	19	ALA
1	B	48	VAL
1	B	133	ASP
1	B	136	GLY
1	B	166	ALA
1	B	170	GLN
2	C	24	LYS
2	C	88	TRP
1	A	76	ARG
1	A	103	ALA
1	B	87	THR
1	B	122	ASP
1	B	164	GLN
1	B	189	ARG
2	C	54	MET
2	C	79	ALA
2	C	119	ILE
1	A	50	PRO

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Mol	Chain	Res	Type
1	A	61	ASP
1	A	130	ARG
1	A	135	SER
1	B	10	LYS
1	B	152	SER
1	B	221	PRO
2	C	80	LEU
2	C	121	PRO
2	C	151	GLY
1	A	88	ALA
1	A	105	GLY
1	A	189	ARG
1	B	60	GLU
2	C	106	THR
1	A	21	ARG
1	A	150	MET
1	A	204	SER
2	C	39	ILE
2	C	68	ALA
1	A	185	ASN
2	C	92	GLN
2	C	56	VAL
1	A	144	PRO
1	B	169	VAL

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	179/190 (94%)	158 (88%)	21 (12%)	7	20
1	B	179/190 (94%)	169 (94%)	10 (6%)	26	59
2	C	129/138 (94%)	110 (85%)	19 (15%)	4	11
All	All	487/518 (94%)	437 (90%)	50 (10%)	9	26

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	56	SER
1	A	68	ARG
1	A	79	VAL
1	A	82	TRP
1	A	83	CYS
1	A	115	ILE
1	A	116	ASN
1	A	122	ASP
1	A	134	GLU
1	A	147	GLU
1	A	151	THR
1	A	156	TYR
1	A	173	GLU
1	A	181	CYS
1	A	191	ARG
1	A	194	PHE
1	A	197	ARG
1	A	199	ARG
1	A	208	PHE
1	A	220	THR
1	B	30	THR
1	B	81	PHE
1	B	82	TRP
1	B	83	CYS
1	B	120	LEU
1	B	181	CYS
1	B	204	SER
1	B	210	SER
1	B	219	LEU
1	B	224	LEU
2	C	3	PRO
2	C	6	ILE
2	C	11	VAL
2	C	26	THR
2	C	27	THR
2	C	32	HIS
2	C	33	CYS
2	C	56	VAL
2	C	62	GLU
2	C	65	GLN
2	C	74	VAL
2	C	76	ARG

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Mol	Chain	Res	Type
2	C	86	GLN
2	C	100	SER
2	C	119	ILE
2	C	123	ASP
2	C	147	ASN
2	C	157	THR
2	C	162	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	110	HIS
1	A	164	GLN
1	B	71	GLN
1	B	137	HIS
1	B	153	HIS
1	B	164	GLN
1	B	170	GLN
2	C	78	GLN
2	C	86	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](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.