



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:42 PM UTC

PDB ID : 1CN4 / pdb_00001cn4
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

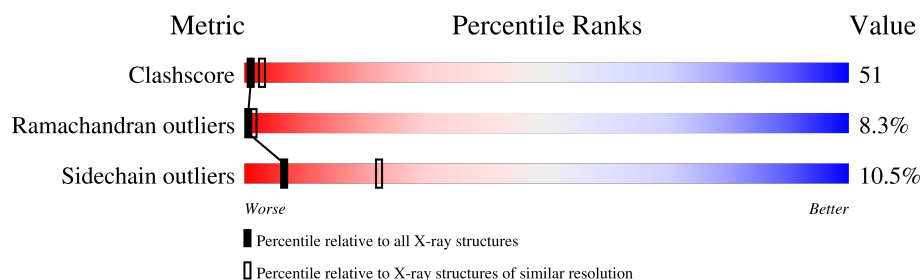
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	228	29% 54% 11% • 5%
1	B	228	28% 56% 12% •
2	C	166	22% 55% 14% • 7%

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 mutation	UNP P19235
B	52	GLN	ASN	engineered mutation	UNP P19235
A	164	GLN	ASN	engineered mutation	UNP P19235
B	164	GLN	ASN	engineered mutation	UNP P19235
A	211	GLU	ALA	engineered mutation	UNP P19235
B	211	GLU	ALA	engineered mutation	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 mutation	UNP P01588
C	38	LYS	ASN	engineered mutation	UNP P01588
C	83	LYS	ASN	engineered mutation	UNP P01588

- Molecule 3 is water.

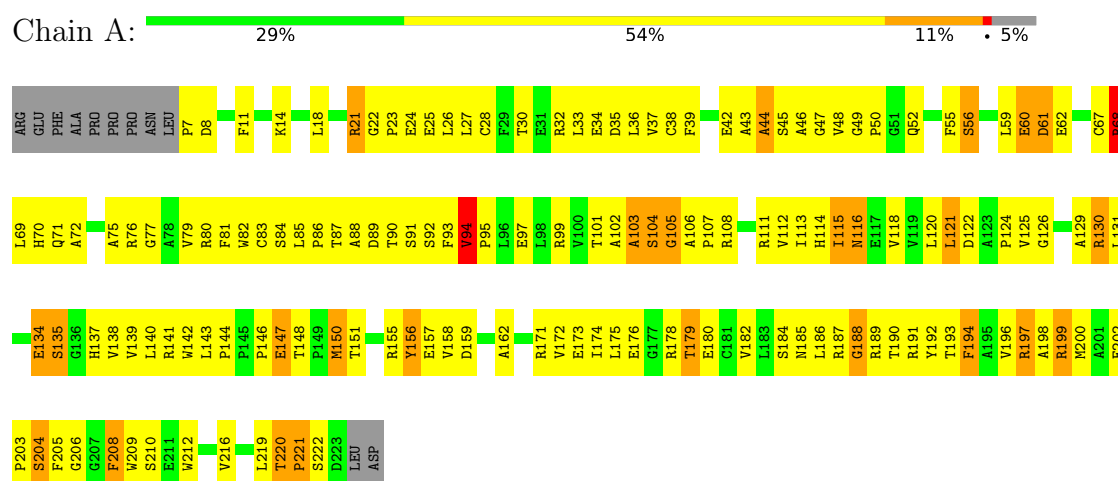
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	O 4	0	0
3	B	5	Total 5	O 5	0	0
3	C	6	Total 6	O 6	0	0

3 Residue-property plots

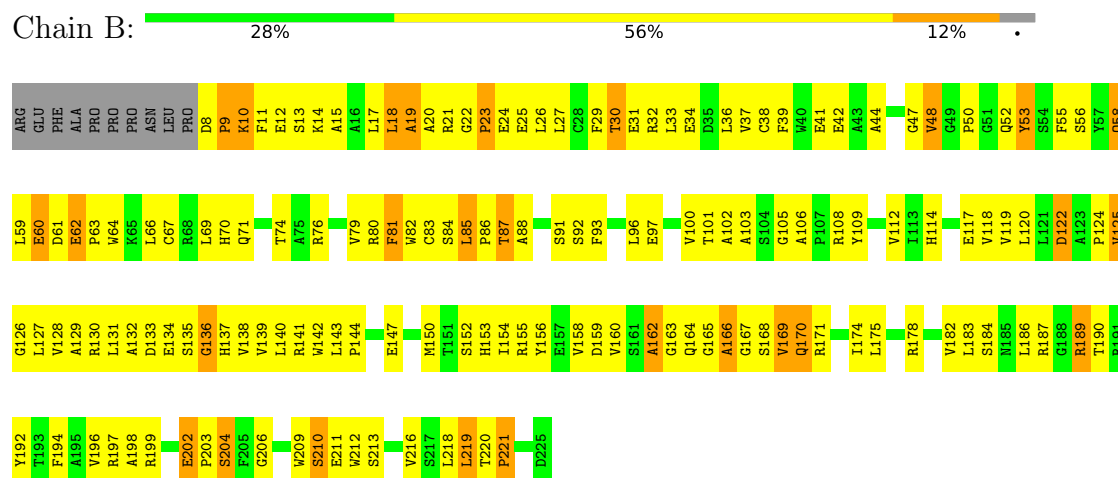
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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)



ALA	P2	P3	R4	L5	I6	C7	D8	S9	R10	V11	L12	E13	R14	Y15	L16	L17	E18	A19	K20	E21	A22	E23	K24	I25	T26	T27	G28	C29	A30	E31	H32	C33	S34	L35	N36	E37	K38	I39	P42	D43	T44	K45	V46	N47	W51	M54	E55	V56	G57	Q58	Q59	A60	V61	E62	V63	W64		
R131	T132	I133	T134	A135	D136	T137	F138	R139	K140	L141	F142	R143	V144	Y145	S146	N147	F148	L149	R150	G151	K152	L153	K154	L155	Y156	T157	A160	C161	R162	THR	GLY	ASP	ARG	L105	T106	T107	L108	L109	R110	A111	L112	Q115	K116	E117	A118	I119	S120	P121	P122	D123	ALA	ALA	SER	A60	ALA	ALA	PRO	LEU

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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

5.1 Standard geometry

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	0.51	0/1735	1.01	10/2368 (0.4%)
1	B	0.51	0/1741	1.05	10/2375 (0.4%)
2	C	0.62	0/1227	1.02	5/1661 (0.3%)
All	All	0.54	0/4703	1.03	25/6404 (0.4%)

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 (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	GLY	CA-C-N	8.55	130.53	119.84
1	B	22	GLY	C-N-CA	8.55	130.53	119.84
2	C	4	ARG	N-CA-C	-8.46	97.78	109.71
1	B	202	GLU	N-CA-C	-8.32	100.32	110.31
2	C	133	ILE	N-CA-C	-8.11	95.87	108.44
1	A	94	VAL	CA-C-N	7.00	128.10	119.98
1	A	94	VAL	C-N-CA	7.00	128.10	119.98
1	A	121	LEU	N-CA-C	6.84	121.01	110.20
1	A	68	ARG	N-CA-C	-6.40	102.05	110.43
2	C	33	CYS	N-CA-C	-6.29	104.41	113.21
1	A	22	GLY	CA-C-N	6.28	125.50	118.97
1	A	22	GLY	C-N-CA	6.28	125.50	118.97
1	B	23	PRO	N-CA-C	6.27	125.39	112.47
2	C	143	ARG	N-CA-C	-6.26	103.38	111.02
1	B	162	ALA	N-CA-C	-6.17	106.43	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ALA	N-CA-C	-6.10	101.45	110.48
1	B	24	GLU	N-CA-C	5.81	120.06	113.15
1	A	44	ALA	N-CA-C	5.79	115.67	108.19
2	C	20	LYS	N-CA-C	-5.77	105.07	111.71
1	B	34	GLU	N-CA-C	-5.69	104.75	112.26
1	B	62	GLU	CA-C-N	5.46	125.77	119.93
1	B	62	GLU	C-N-CA	5.46	125.77	119.93
1	A	46	ALA	N-CA-C	-5.28	105.94	112.38
1	A	188	GLY	N-CA-C	5.04	120.78	112.30
1	B	53	TYR	N-CA-C	5.04	118.28	110.17

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 ⓘ

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	161	0
1	B	1695	0	1640	170	0
2	C	1206	0	1226	144	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	468	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 51.

All (468) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:MET:HE1	2:C:11:VAL:HA	1.27	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
2:C:132:THR:C	2:C:133:ILE:HD12	2.00	0.85
1:A:115:ILE:H	1:A:115:ILE:CD1	1.89	0.83
1:B:162:ALA:H	1:B:168:SER:HB2	1.45	0.82
1:A:115:ILE:HD12	1:A:115:ILE:N	1.94	0.81
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:129:ALA:HB2	1:B:140:LEU:HG	1.64	0.77
1:B:162:ALA:H	1:B:168:SER:CB	1.96	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:HH11	1:A:99:ARG:HG3	1.49	0.76
1:A:158:VAL:HB	1:A:172:VAL:CG1	2.16	0.75
2:C:61:VAL:HG22	2:C:118:ALA:HA	1.68	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:67:CYS:SG	1:A:68:ARG:NH1	2.62	0.72
1:A:137:HIS:CG	1:A:184:SER:HA	2.24	0.72
1:B:50:PRO:HD3	1:B:71:GLN:NE2	2.04	0.72
1:A:68:ARG:C	1:A:68:ARG:HD2	2.15	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: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
1:B:163:GLY:C	1:B:165:GLY:H	2.00	0.69
2:C:23:GLU:O	2:C:25:ILE:N	2.25	0.69
2:C:142:PHE:O	2:C:145:TYR:HB3	1.92	0.69
2:C:140:LYS:O	2:C:144:VAL:HG23	1.92	0.69
2:C:160:ALA:C	2:C:162:ARG:H	2.01	0.68
1:B:132:ALA:O	1:B:134:GLU:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:35:LEU:HD23	2:C:137:THR:C	2.19	0.68
1:A:7:PRO:HD2	1:A:11:PHE:HD2	1.58	0.67
1:B:74:THR:CG2	1:B:76:ARG:HG2	2.24	0.67
1:B:100:VAL:HB	1:B:109:TYR:HB2	1.76	0.67
1:B:17:LEU:HG	1:B:21:ARG:HH21	1.59	0.67
1:B:140:LEU:HD21	1:B:194:PHE:HB3	1.76	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
1:A:42:GLU:OE1	1:A:108:ARG:NH1	2.30	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:A:68:ARG:HD2	1:A:68:ARG:O	1.97	0.65
1:B:189:ARG:O	1:B:189:ARG:HG3	1.96	0.64
1:A:187:ARG:HG3	1:A:187:ARG:HH11	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
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
1:B:128:VAL:HG23	1:B:141:ARG:HB2	1.80	0.63
1:A:118:VAL:O	1:A:118:VAL:HG23	1.98	0.62
1:B:153:HIS:HE1	2:C:154:LYS:HE3	1.63	0.62
1:B:187:ARG:HG3	1:B:187:ARG:HH11	1.64	0.62
1:A:194:PHE:O	1:A:216:VAL:HG12	1.99	0.62
1:B:25:GLU:CG	1:B:26:LEU:H	2.07	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:A:156:TYR:CD1	1:A:156:TYR:N	2.68	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
2:C:14:ARG:O	2:C:18:GLU:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASP:HA	1:A:90:THR:HG21	1.82	0.60
1:A:199:ARG:HH11	1:A:199:ARG:HB3	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
1:A:175:LEU:HG	1:A:178:ARG:HB3	1.84	0.60
2:C:26:THR:O	2:C:29:CYS:HB3	2.02	0.60
1:B:59:LEU:HD23	1:B:96:LEU:HD13	1.84	0.59
1:B:50:PRO:C	1:B:52:GLN:H	2.10	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:59:LEU:O	1:B:60:GLU:C	2.46	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:27:THR:C	2:C:29:CYS:H	2.09	0.59
1:A:18:LEU:HB3	1:A:27:LEU:HD13	1.84	0.59
2:C:149:LEU:O	2:C:153:LEU:HB3	2.02	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:135:SER:O	1:B:137:HIS:N	2.35	0.58
1:B:199:ARG:HB2	1:B:209:TRP:CZ3	2.38	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
1:A:197:ARG:HG3	1:A:209:TRP:CE3	2.38	0.58
2:C:150:ARG:O	2:C:154:LYS:HB3	2.04	0.58
1:B:158:VAL:HG22	1:B:196:VAL:HG22	1.84	0.58
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:A:60:GLU:HB2	1:A:95:PRO:HD2	1.85	0.57
1:A:202:GLU:OE1	1:A:202:GLU:N	2.31	0.57
1:B:168:SER:O	1:B:169:VAL:HG13	2.05	0.57
2:C:38:LYS:HG3	2:C:39:ILE:H	1.70	0.57
2:C:76:ARG:HE	2:C:76:ARG:HA	1.69	0.57
1:B:84:SER:O	1:B:85:LEU:C	2.48	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:HG3	1:B:155:ARG:HH11	1.69	0.56
1:A:70:HIS:O	1:A:81:PHE:HA	2.05	0.56
1:B:32:ARG:HD2	1:B:32:ARG:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:TRP:CD1	2:C:59:GLN:HE22	2.23	0.56
2:C:89:GLU:HB2	2:C:90:PRO:HD3	1.86	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:79:VAL:HG22	1:B:80:ARG:N	2.20	0.56
1:B:131:LEU:HD11	1:B:221:PRO:HD3	1.88	0.56
2:C:119:ILE:HD12	2:C:119:ILE:N	2.21	0.56
1:A:139:VAL:HG22	1:A:182:VAL:HG22	1.88	0.56
1:B:171:ARG:NH2	1:B:212:TRP:HZ2	2.03	0.56
1:A:7:PRO:HG2	1:A:8:ASP:H	1.71	0.55
1:B:8:ASP:N	1:B:9:PRO:CD	2.68	0.55
2:C:86:GLN:HA	2:C:86:GLN:HE21	1.70	0.55
2:C:12:LEU:O	2:C:12:LEU:HD12	2.06	0.55
2:C:23:GLU:C	2:C:25:ILE:H	2.14	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:44:ALA:HB1	1:B:47:GLY:O	2.06	0.55
1:B:130:ARG:HD2	1:B:130:ARG:C	2.31	0.55
1:B:209:TRP:HB2	3:B:228:HOH:O	2.06	0.55
2:C:160:ALA:C	2:C:162:ARG:N	2.65	0.55
2:C:38:LYS:CG	2:C:39:ILE:N	2.68	0.55
1:A:175:LEU:HG	1:A:178:ARG:CB	2.37	0.55
1:B:18:LEU:O	1:B:19:ALA:C	2.49	0.55
2:C:67:LEU:HD11	2:C:102:LEU:HD22	1.89	0.55
1:B:150:MET:HE3	1:B:153:HIS:CD2	2.42	0.55
2:C:131:ARG:CZ	2:C:132:THR:HG22	2.36	0.54
1:A:21:ARG:O	1:A:21:ARG:HG3	2.06	0.54
1:B:27:LEU:O	1:B:38:CYS:HA	2.06	0.54
2:C:2:PRO:N	2:C:3:PRO:HD3	2.21	0.54
1:A:59:LEU:O	1:A:60:GLU:C	2.50	0.54
1:B:55:PHE:HB2	1:B:69:LEU:HD11	1.90	0.54
2:C:119:ILE:CD1	2:C:119:ILE:H	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
1:B:144:PRO:HB3	1:B:156:TYR:OH	2.07	0.54
2:C:8:ASP:O	2:C:11:VAL:HG12	2.07	0.54
2:C:59:GLN:O	2:C:62:GLU:HB2	2.08	0.54
1:B:48:VAL:CG2	1:B:79:VAL:HG11	2.38	0.54
2:C:119:ILE:HD12	2:C:119:ILE:H	1.72	0.54
1:A:199:ARG:HG2	1:A:200:MET:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ARG:HD2	1:B:130:ARG:O	2.07	0.54
2:C:95:VAL:O	2:C:99:VAL:HG23	2.08	0.54
1:A:203:PRO:HG2	1:A:204:SER:H	1.72	0.54
1:B:186:LEU:HB3	1:B:192:TYR:CE2	2.35	0.54
2:C:109:LEU:C	2:C:111:ALA:N	2.65	0.54
1:B:53:TYR:CD1	1:B:102:ALA:HA	2.42	0.53
1:B:216:VAL:HG13	1:B:216:VAL:O	2.08	0.53
2:C:19:ALA:HB1	2:C:146:SER:HB3	1.89	0.53
1:A:23:PRO:C	1:A:25:GLU:H	2.17	0.53
1:A:92:SER:O	1:A:93:PHE:HB2	2.08	0.53
2:C:32:HIS:C	2:C:33:CYS:SG	2.91	0.53
1:A:75:ALA:C	1:A:77:GLY:H	2.17	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:HG3	1:B:187:ARG:NH1	2.24	0.53
1:A:146:PRO:O	1:A:148:THR:N	2.41	0.53
1:A:193:THR:HA	1:A:216:VAL:O	2.07	0.53
1:A:55:PHE:HB2	1:A:69:LEU:HD21	1.90	0.53
1:A:103:ALA:O	1:A:104:SER:C	2.51	0.53
1:A:199:ARG:HH11	1:A:199:ARG:CB	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:A:131:LEU:CD2	1:A:221:PRO:HD3	2.39	0.52
1:B:204:SER:HA	2:C:150:ARG:HD2	1.90	0.52
1:A:155:ARG:C	1:A:156:TYR:CD1	2.88	0.52
1:B:166:ALA:O	1:B:167:GLY:C	2.52	0.52
2:C:56:VAL:HG12	2:C:156:TYR:CE1	2.44	0.52
2:C:115:GLN:O	2:C:118:ALA:HB3	2.10	0.52
1:A:72:ALA:O	1:A:80:ARG:N	2.32	0.52
1:B:47:GLY:O	1:B:48:VAL:HB	2.08	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:TYR:N	1:A:156:TYR:HD1	2.09	0.51
1:B:53:TYR:HD1	1:B:102:ALA:HA	1.75	0.51
2:C:33:CYS:O	2:C:138:PHE:N	2.38	0.51
2:C:118:ALA:C	2:C:120:SER:H	2.17	0.51
1:A:104:SER:OG	1:A:105:GLY:N	2.43	0.51
1:B:219:LEU:H	1:B:219:LEU:HD12	1.76	0.51
2:C:58:GLN:HA	2:C:58:GLN:NE2	2.25	0.51
2:C:81:LEU:HD22	2:C:95:VAL:HG21	1.91	0.51
1:A:142:TRP:NE1	1:A:179:THR:HB	2.25	0.51
2:C:79:ALA:O	2:C:81:LEU:N	2.43	0.51
2:C:133:ILE:HD12	2:C:133:ILE:N	2.26	0.51
2:C:139:ARG:NH1	2:C:139:ARG:HB3	2.26	0.51
1:B:48:VAL:HA	1:B:52:GLN:OE1	2.10	0.51
1:B:138:VAL:O	1:B:182:VAL:HA	2.11	0.51
1:B:175:LEU:HB2	1:B:178:ARG:HG3	1.93	0.51
1:A:60:GLU:O	1:A:61:ASP:C	2.55	0.51
1:B:125:VAL:HG12	1:B:126:GLY:H	1.76	0.51
2:C:105:LEU:C	2:C:107:THR:N	2.68	0.51
1:A:125:VAL:O	1:A:143:LEU:HB2	2.11	0.50
1:A:35:ASP:OD1	1:A:35:ASP:C	2.54	0.50
1:A:68:ARG:HH22	1:A:84:SER:CA	2.24	0.50
1:A:129:ALA:HA	1:A:140:LEU:HD23	1.92	0.50
1:B:108:ARG:HD2	1:B:109:TYR:CE1	2.46	0.50
2:C:36:ASN:O	2:C:37:GLU:HB2	2.12	0.50
1:A:114:HIS:C	1:A:116:ASN:H	2.19	0.50
2:C:105:LEU:O	2:C:107:THR:N	2.45	0.50
1:A:30:THR:HG21	1:A:115:ILE:O	2.11	0.50
1:A:197:ARG:HD2	1:A:212:TRP:CH2	2.47	0.50
2:C:79:ALA:C	2:C:81:LEU:N	2.69	0.50
2:C:87:PRO:O	2:C:89:GLU:N	2.45	0.50
1:A:130:ARG:HB3	1:A:130:ARG:CZ	2.41	0.50
1:B:129:ALA:HB3	1:B:194:PHE:CD2	2.47	0.50
1:A:32:ARG:C	1:A:34:GLU:H	2.20	0.50
1:B:62:GLU:HB3	1:B:63:PRO:HD2	1.92	0.50
2:C:73:ALA:O	2:C:74:VAL:C	2.55	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:B:117:GLU:C	1:B:206:GLY:O	2.55	0.49
2:C:6:ILE:O	2:C:6:ILE:HD13	2.12	0.49
1:A:28:CYS:HA	1:A:37:VAL:O	2.13	0.49
1:A:202:GLU:HB3	1:A:203:PRO:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:VAL:HB	1:B:183:LEU:HB2	1.94	0.49
1:B:174:ILE:HG22	1:B:175:LEU:N	2.27	0.49
2:C:79:ALA:O	2:C:82:VAL:N	2.43	0.49
1:A:196:VAL:HG12	1:A:197:ARG:N	2.28	0.49
1:B:163:GLY:O	1:B:165:GLY:N	2.45	0.49
1:B:55:PHE:CD1	1:B:100:VAL:HG22	2.47	0.49
2:C:23:GLU:C	2:C:25:ILE:N	2.71	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
1:B:44:ALA:HB1	1:B:48:VAL:HB	1.95	0.48
1:B:74:THR:C	1:B:76:ARG:N	2.69	0.48
2:C:131:ARG:NH1	2:C:132:THR:HG22	2.28	0.48
2:C:138:PHE:O	2:C:141:LEU:N	2.46	0.48
1:B:58:GLN:O	1:B:58:GLN:HG2	2.11	0.48
2:C:108:LEU:O	2:C:111:ALA:HB3	2.13	0.48
1:B:154:ILE:HG23	1:B:199:ARG:O	2.13	0.48
2:C:63:VAL:O	2:C:64:TRP:C	2.57	0.48
1:A:162:ALA:HB2	1:A:192:TYR:CE1	2.47	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:B:155:ARG:HH22	1:B:199:ARG:HH11	1.60	0.48
1:A:55:PHE:CD1	1:A:55:PHE:C	2.91	0.48
1:A:102:ALA:O	1:A:103:ALA:C	2.56	0.48
1:B:19:ALA:O	1:B:20:ALA:C	2.56	0.48
1:B:39:PHE:CD1	1:B:39:PHE:C	2.91	0.48
1:A:113:ILE:C	1:A:114:HIS:ND1	2.72	0.48
2:C:27:THR:C	2:C:29:CYS:N	2.69	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
2:C:59:GLN:O	2:C:60:ALA:C	2.56	0.48
2:C:123:ASP:OD1	2:C:123:ASP:N	2.33	0.47
1:A:125:VAL:O	1:A:143:LEU:N	2.43	0.47
2:C:67:LEU:CD1	2:C:102:LEU:HD22	2.44	0.47
1:A:86:PRO:HG2	1:A:89:ASP:OD2	2.14	0.47
2:C:67:LEU:HD23	2:C:109:LEU:HD12	1.97	0.47
2:C:88:TRP:CD1	2:C:90:PRO:HD2	2.50	0.47
2:C:88:TRP:O	2:C:89:GLU:C	2.57	0.47
2:C:154:LYS:HD2	2:C:154:LYS:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:32:HIS:ND1	2:C:32:HIS:N	2.61	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:9:PRO:C	1:B:11:PHE:N	2.73	0.47
2:C:21:GLU:O	2:C:25:ILE:HG12	2.15	0.47
2:C:85:SER:C	2:C:87:PRO:HD3	2.40	0.47
1:B:59:LEU:O	1:B:62:GLU:HB2	2.15	0.47
1:B:158:VAL:HG12	1:B:159:ASP:N	2.29	0.47
1:A:38:CYS:O	1:A:82:TRP:HA	2.15	0.47
1:A:55:PHE:HD1	1:A:55:PHE:C	2.23	0.47
1:B:37:VAL:HA	1:B:83:CYS:O	2.15	0.47
1:B:58:GLN:HB2	1:B:64:TRP:HA	1.96	0.47
1:B:62:GLU:CB	1:B:63:PRO:HD2	2.45	0.47
1:A:86:PRO:CG	1:A:89:ASP:OD2	2.63	0.46
1:A:178:ARG:HG2	1:A:178:ARG:HH11	1.80	0.46
1:B:86:PRO:O	1:B:87:THR:C	2.57	0.46
1:B:174:ILE:HG22	1:B:178:ARG:HB2	1.96	0.46
2:C:156:TYR:O	2:C:157:THR:C	2.58	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
1:A:18:LEU:O	1:A:21:ARG:HB3	2.14	0.46
1:B:14:LYS:NZ	1:B:122:ASP:OD1	2.41	0.46
1:B:29:PHE:HA	1:B:118:VAL:HB	1.98	0.46
2:C:147:ASN:O	2:C:151:GLY:HA3	2.15	0.46
1:A:138:VAL:O	1:A:182:VAL:HA	2.15	0.46
1:A:158:VAL:HG12	1:A:159:ASP:N	2.30	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
2:C:42:PRO:CD	2:C:69:LEU:HD23	2.46	0.46
2:C:81:LEU:O	2:C:84:SER:HB3	2.15	0.46
1:B:81:PHE:CD1	1:B:81:PHE:N	2.83	0.46
2:C:109:LEU:O	2:C:110:ARG:C	2.58	0.46
1:B:131:LEU:HD11	1:B:221:PRO:CG	2.46	0.46
2:C:29:CYS:SG	2:C:32:HIS:O	2.73	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:A:71:GLN:HB2	1:A:81:PHE:HE1	1.81	0.46
1:A:114:HIS:C	1:A:116:ASN:N	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:HIS:O	1:B:81:PHE:HA	2.16	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
2:C:82:VAL:C	2:C:84:SER:H	2.24	0.45
1:A:198:ALA:O	1:A:210:SER:HB3	2.17	0.45
1:A:71:GLN:HA	1:A:80:ARG:O	2.16	0.45
1:A:188:GLY:HA2	1:A:220:THR:CG2	2.46	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:A:82:TRP:CD1	1:A:82:TRP:N	2.85	0.45
1:B:74:THR:C	1:B:76:ARG:H	2.25	0.45
1:B:162:ALA:HB3	1:B:168:SER:HB3	1.99	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:42:GLU:OE2	1:B:53:TYR:HE2	2.00	0.45
2:C:51:TRP:CE2	2:C:59:GLN:NE2	2.85	0.45
1:A:135:SER:HG	1:A:137:HIS:CD2	2.34	0.45
1:A:86:PRO:O	1:A:87:THR:C	2.60	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
1:B:50:PRO:C	1:B:52:GLN:N	2.75	0.44
1:B:135:SER:O	1:B:136:GLY:C	2.59	0.44
2:C:138:PHE:C	2:C:140:LYS:N	2.75	0.44
1:B:122:ASP:O	1:B:210:SER:OG	2.30	0.44
1:A:121:LEU:C	1:A:122:ASP:O	2.56	0.44
1:A:125:VAL:HG22	1:A:126:GLY:N	2.33	0.44
1:B:163:GLY:C	1:B:165:GLY:N	2.66	0.44
1:B:174:ILE:HG22	1:B:175:LEU:H	1.82	0.44
2:C:73:ALA:O	2:C:76:ARG:N	2.51	0.44
2:C:138:PHE:O	2:C:139:ARG:C	2.60	0.44
1:A:55:PHE:CB	1:A:69:LEU:HD21	2.47	0.44
1:B:202:GLU:N	1:B:202:GLU:CD	2.76	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
2:C:55:GLU:OE1	2:C:58:GLN:CB	2.66	0.44
1:B:26:LEU:C	1:B:27:LEU:HD23	2.43	0.44
1:B:31:GLU:C	1:B:33:LEU:H	2.25	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
2:C:89:GLU:H	2:C:89:GLU:CD	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:PHE:CE2	1:B:83:CYS:SG	3.11	0.44
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:B:138:VAL:HG23	1:B:186:LEU:HD12	1.99	0.43
1:A:45:SER:C	1:A:47:GLY:N	2.71	0.43
1:B:97:GLU:HG3	1:B:112:VAL:HG22	1.99	0.43
1:B:131:LEU:HD11	1:B:221:PRO:CD	2.47	0.43
2:C:12:LEU:HD12	2:C:12:LEU:C	2.43	0.43
1:B:11:PHE:O	1:B:12:GLU:C	2.61	0.43
1:B:102:ALA:O	1:B:105:GLY:N	2.51	0.43
1:B:196:VAL:HG12	1:B:197:ARG:N	2.34	0.43
2:C:82:VAL:C	2:C:84:SER:N	2.77	0.43
1:A:32:ARG:C	1:A:34:GLU:N	2.76	0.43
1:A:39:PHE:HA	1:A:81:PHE:O	2.17	0.43
1:A:193:THR:HG23	1:A:216:VAL:O	2.18	0.43
1:B:141:ARG:HB3	1:B:141:ARG:CZ	2.49	0.43
2:C:35:LEU:HD12	2:C:39:ILE:HD11	2.00	0.43
2:C:70:LEU:O	2:C:73:ALA:N	2.51	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:55:GLU:O	2:C:56:VAL:C	2.62	0.43
1:A:157:GLU:HB3	1:A:197:ARG:CD	2.49	0.43
1:B:150:MET:HE3	1:B:153:HIS:HD2	1.82	0.43
2:C:27:THR:OG1	2:C:28:GLY:N	2.52	0.43
2:C:35:LEU:HD23	2:C:137:THR:CA	2.49	0.43
2:C:56:VAL:HG23	3:C:172:HOH:O	2.18	0.43
2:C:116:LYS:HG3	2:C:117:GLU:N	2.34	0.43
1:A:101:THR:HG22	1:A:102:ALA:N	2.32	0.43
1:A:159:ASP:OD1	1:A:171:ARG:NH1	2.52	0.43
1:B:189:ARG:O	1:B:189:ARG:CG	2.65	0.43
2:C:59:GLN:O	2:C:63:VAL:HG23	2.19	0.43
2:C:38:LYS:O	2:C:39:ILE:CB	2.67	0.42
1:B:114:HIS:O	1:B:117:GLU:N	2.38	0.42
2:C:61:VAL:O	2:C:62:GLU:C	2.62	0.42
2:C:70:LEU:O	2:C:73:ALA:HB3	2.18	0.42
1:B:36:LEU:HD12	1:B:36:LEU:HA	1.82	0.42
1:B:69:LEU:HD23	1:B:82:TRP:O	2.18	0.42
1:B:71:GLN:OE1	1:B:81:PHE:CE2	2.72	0.42
1:B:79:VAL:HG22	1:B:80:ARG:H	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLY:O	1:A:48:VAL:C	2.63	0.42
2:C:79:ALA:C	2:C:81:LEU:H	2.28	0.42
1:A:150:MET:HE1	2:C:11:VAL:CA	2.20	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
2:C:105:LEU:O	2:C:106:THR:C	2.63	0.42
1:A:146:PRO:C	1:A:148:THR:N	2.78	0.42
1:A:203:PRO:HG2	1:A:204:SER:N	2.35	0.42
1:B:86:PRO:O	1:B:88:ALA:N	2.53	0.42
2:C:31:GLU:CD	2:C:31:GLU:H	2.28	0.42
2:C:88:TRP:C	2:C:90:PRO:HD2	2.45	0.42
1:A:175:LEU:O	1:A:176:GLU:C	2.61	0.42
1:B:171:ARG:CZ	1:B:212:TRP:HZ2	2.32	0.42
2:C:79:ALA:O	2:C:80:LEU:C	2.63	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:105:LEU:C	2:C:107:THR:H	2.28	0.41
1:A:106:ALA:HA	1:A:107:PRO:HD3	1.81	0.41
1:A:157:GLU:HB3	1:A:197:ARG:HD2	2.01	0.41
1:B:60:GLU:OE2	2:C:143:ARG:NH2	2.52	0.41
2:C:55:GLU:HB3	3:C:172:HOH:O	2.21	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:186:LEU:HD22	1:A:192:TYR:CE2	2.56	0.41
1:A:208:PHE:CD1	1:A:208:PHE:N	2.88	0.41
2:C:51:TRP:NE1	2:C:59:GLN:HE22	2.18	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: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:HG2	1:A:86:PRO:O	2.21	0.41
1:A:188:GLY:C	1:A:190:THR:N	2.78	0.41
1:B:117:GLU:HA	1:B:206:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ARG:CZ	1:B:212:TRP:CZ2	3.04	0.41
1:B:82:TRP:CD1	1:B:82:TRP:N	2.89	0.40
2:C:38:LYS:C	2:C:39:ILE:HG12	2.46	0.40
2:C:86:GLN:HE21	2:C:86:GLN:CA	2.30	0.40
1:A:205:PHE:HB3	1:A:206:GLY:H	1.76	0.40
1:B:159:ASP:OD1	1:B:160:VAL:N	2.54	0.40
1:B:56:SER:HA	1:B:66:LEU:HA	2.04	0.40
1:B:202:GLU:HB3	1:B:203:PRO:HA	2.02	0.40
2:C:51:TRP:NE1	2:C:59:GLN:NE2	2.70	0.40
2:C:133:ILE:C	2:C:134:THR:CG2	2.95	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:A:97:GLU:HA	1:A:112:VAL:HG22	2.04	0.40
1:B:11:PHE:CE1	1:B:15:ALA:HB2	2.56	0.40
1:B:124:PRO:HG2	1:B:213:SER:HB3	2.03	0.40
1:B:186:LEU:HD22	1:B:192:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/228 (94%)	162 (75%)	34 (16%)	19 (9%)	0	1
1	B	216/228 (95%)	159 (74%)	41 (19%)	16 (7%)	1	2
2	C	150/166 (90%)	94 (63%)	43 (29%)	13 (9%)	0	1
All	All	581/622 (93%)	415 (71%)	118 (20%)	48 (8%)	0	1

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	LEU

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	160 (89%)	19 (11%)	6	22
1	B	179/190 (94%)	169 (94%)	10 (6%)	19	50
2	C	129/138 (94%)	107 (83%)	22 (17%)	2	7
All	All	487/518 (94%)	436 (90%)	51 (10%)	6	22

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	68	ARG
1	A	79	VAL
1	A	83	CYS
1	A	94	VAL
1	A	115	ILE
1	A	116	ASN
1	A	124	PRO
1	A	134	GLU
1	A	147	GLU
1	A	151	THR
1	A	156	TYR
1	A	173	GLU
1	A	179	THR
1	A	194	PHE
1	A	197	ARG
1	A	199	ARG

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Mol	Chain	Res	Type
1	A	208	PHE
1	A	220	THR
1	B	18	LEU
1	B	30	THR
1	B	58	GLN
1	B	81	PHE
1	B	85	LEU
1	B	120	LEU
1	B	125	VAL
1	B	204	SER
1	B	210	SER
1	B	219	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	63	VAL
2	C	65	GLN
2	C	67	LEU
2	C	74	VAL
2	C	76	ARG
2	C	86	GLN
2	C	100	SER
2	C	106	THR
2	C	119	ILE
2	C	123	ASP
2	C	149	LEU
2	C	157	THR
2	C	162	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	70	HIS
1	A	71	GLN
1	A	110	HIS

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Mol	Chain	Res	Type
1	A	164	GLN
1	B	58	GLN
1	B	71	GLN
1	B	153	HIS
1	B	164	GLN
1	B	170	GLN
2	C	58	GLN
2	C	59	GLN
2	C	78	GLN
2	C	86	GLN
2	C	92	GLN
2	C	94	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.