



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:01 PM UTC

PDB ID : 3GGR / pdb_00003ggr
Title : Crystal Structure of the Human Rad9-Hus1-Rad1 complex
Authors : Xu, M.; Bai, L.; Hang, H.Y.; Jiang, T.
Deposited on : 2009-03-02
Resolution : 3.20 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

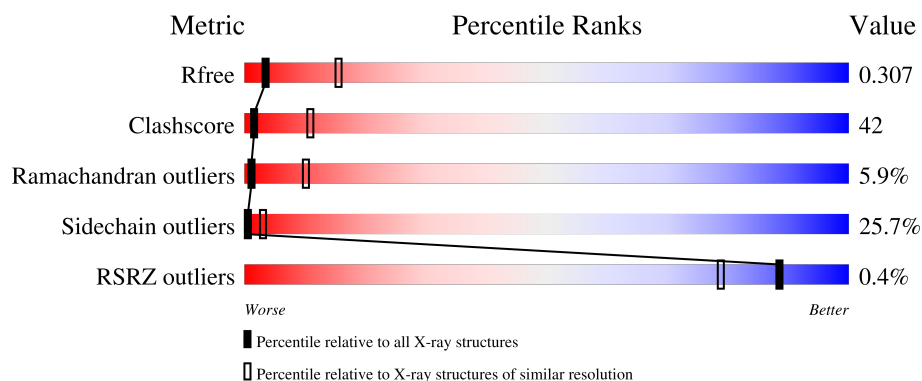
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	270	32%50%15%..
2	B	286	% 31%46%18%..
3	C	282	26%46%19%•6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6325 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 Cell cycle checkpoint control protein RAD9A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2038	1296	355	372	15			

- Molecule 2 is a protein called Checkpoint protein HUS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	278	Total	C	N	O	S	0	0	0
			2203	1399	377	412	15			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	MET	-	expression tag	UNP O60921
B	-4	HIS	-	expression tag	UNP O60921
B	-3	HIS	-	expression tag	UNP O60921
B	-2	HIS	-	expression tag	UNP O60921
B	-1	HIS	-	expression tag	UNP O60921
B	0	HIS	-	expression tag	UNP O60921
B	1	HIS	-	expression tag	UNP O60921

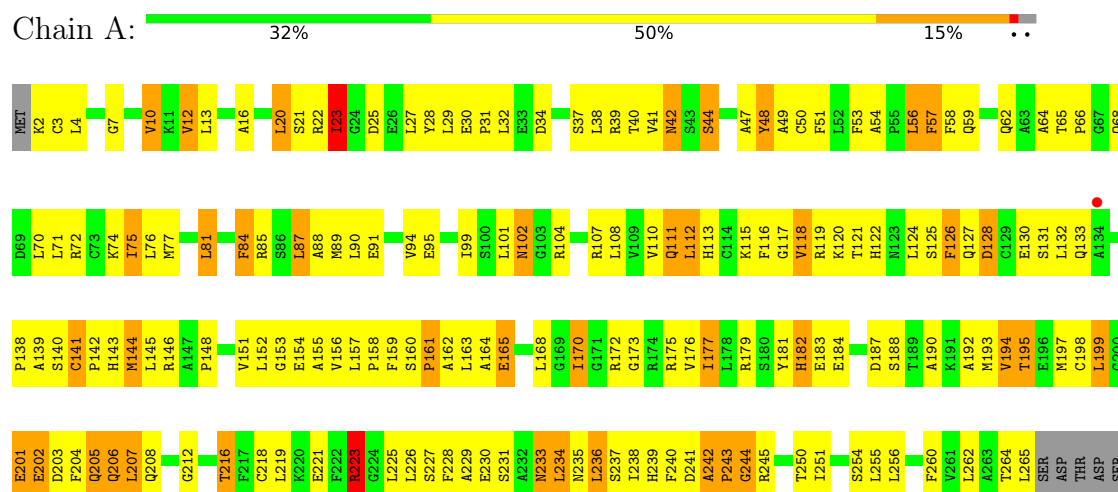
- Molecule 3 is a protein called Cell cycle checkpoint protein RAD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	264	Total	C	N	O	S	0	0	0
			2084	1320	342	404	18			

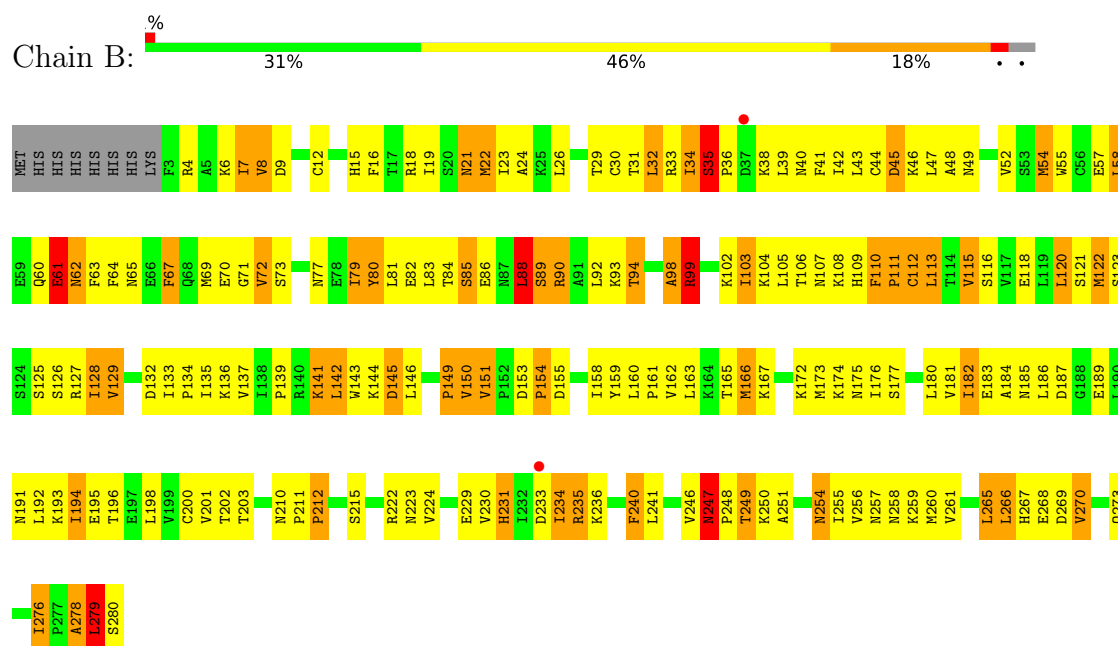
3 Residue-property plots

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 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: Cell cycle checkpoint control protein RAD9A



• Molecule 2: Checkpoint protein HUS1



• Molecule 3: Cell cycle checkpoint protein RAD1

MET	P165	P166	P167	P168	P169	P170	P171	P172	P173	P174	P175	P176	P177	P178	P179	P180	P181	P182	P183	P184	P185	P186	P187	P188	P189	P190	P191	P192	P193	P194	P195	P196	P197	P198	P199	P200	P201	P202	P203	P204	P205	P206	P207	P208	P209	P210	P211	P212	P213	P214	P215	P216	P217	P218	P219	P220	P221	P222	P223	P224	P225	P226	P227	P228	P229	P230	P231	P232	P233	P234	P235	P236	P237	P238	P239	P240	P241	P242	P243	P244	P245	P246	P247	P248	P249	P250	P251	P252	P253	P254	P255	P256	P257	P258	P259	P260	P261	P262	P263	P264	P265	P266	P267	P268	P269	P270	P271	P272	P273	P274	P275	P276	P277	P278	P279	P280	P281	P282	P283	P284	P285	P286	P287	P288	P289	P290	P291	P292	P293	P294	P295	P296	P297	P298	P299	P300	P301	P302	P303	P304	P305	P306	P307	P308	P309	P310	P311	P312	P313	P314	P315	P316	P317	P318	P319	P320	P321	P322	P323	P324	P325	P326	P327	P328	P329	P330	P331	P332	P333	P334	P335	P336	P337	P338	P339	P340	P341	P342	P343	P344	P345	P346	P347	P348	P349	P350	P351	P352	P353	P354	P355	P356	P357	P358	P359	P360	P361	P362	P363	P364	P365	P366	P367	P368	P369	P370	P371	P372	P373	P374	P375	P376	P377	P378	P379	P380	P381	P382	P383	P384	P385	P386	P387	P388	P389	P390	P391	P392	P393	P394	P395	P396	P397	P398	P399	P400	P401	P402	P403	P404	P405	P406	P407	P408	P409	P410	P411	P412	P413	P414	P415	P416	P417	P418	P419	P420	P421	P422	P423	P424	P425	P426	P427	P428	P429	P430	P431	P432	P433	P434	P435	P436	P437	P438	P439	P440	P441	P442	P443	P444	P445	P446	P447	P448	P449	P450	P451	P452	P453	P454	P455	P456	P457	P458	P459	P460	P461	P462	P463	P464	P465	P466	P467	P468	P469	P470	P471	P472	P473	P474	P475	P476	P477	P478	P479	P480	P481	P482	P483	P484	P485	P486	P487	P488	P489	P490	P491	P492	P493	P494	P495	P496	P497	P498	P499	P500	P501	P502	P503	P504	P505	P506	P507	P508	P509	P510	P511	P512	P513	P514	P515	P516	P517	P518	P519	P520	P521	P522	P523	P524	P525	P526	P527	P528	P529	P530	P531	P532	P533	P534	P535	P536	P537	P538	P539	P540	P541	P542	P543	P544	P545	P546	P547	P548	P549	P550	P551	P552	P553	P554	P555	P556	P557	P558	P559	P560	P561	P562	P563	P564	P565	P566	P567	P568	P569	P570	P571	P572	P573	P574	P575	P576	P577	P578	P579	P580	P581	P582	P583	P584	P585	P586	P587	P588	P589	P590	P591	P592	P593	P594	P595	P596	P597	P598	P599	P600	P601	P602	P603	P604	P605	P606	P607	P608	P609	P610	P611	P612	P613	P614	P615	P616	P617	P618	P619	P620	P621	P622	P623	P624	P625	P626	P627	P628	P629	P630	P631	P632	P633	P634	P635	P636	P637	P638	P639	P640	P641	P642	P643	P644	P645	P646	P647	P648	P649	P650	P651	P652	P653	P654	P655	P656	P657	P658	P659	P660	P661	P662	P663	P664	P665	P666	P667	P668	P669	P670	P671	P672	P673	P674	P
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.03Å 67.16Å 83.41Å 90.00° 97.58° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (15.00-3.20) 98.4 (15.00-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.289 , 0.306 (Not available) , 0.307	Depositor DCC
R_{free} test set	1280 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	84.2	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6325	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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

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	0.64	0/2075	1.09	8/2800 (0.3%)
2	B	0.73	1/2242 (0.0%)	1.19	22/3035 (0.7%)
3	C	0.72	0/2122	1.10	11/2870 (0.4%)
All	All	0.70	1/6439 (0.0%)	1.13	41/8705 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	276	ILE	CA-C	5.29	1.57	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	HIS	N-CA-C	8.12	120.93	108.42
3	C	272	CYS	N-CA-C	7.42	126.21	109.81
2	B	88	LEU	N-CA-C	-7.30	102.50	111.40
2	B	276	ILE	CA-C-N	7.21	127.13	120.21
2	B	276	ILE	C-N-CA	7.21	127.13	120.21
2	B	276	ILE	N-CA-C	7.11	115.73	107.77
3	C	152	VAL	N-CA-C	7.10	119.10	111.58
3	C	151	ASN	N-CA-C	6.72	119.07	108.79
2	B	125	SER	N-CA-C	6.70	121.06	113.02
2	B	35	SER	CA-C-N	-6.51	111.70	119.84
2	B	35	SER	C-N-CA	-6.51	111.70	119.84
2	B	270	VAL	N-CA-C	6.46	116.70	106.88
3	C	98	SER	N-CA-C	-6.46	105.44	113.38
2	B	278	ALA	N-CA-C	6.43	121.79	113.88
2	B	99	ARG	N-CA-C	6.33	124.29	110.80
3	C	126	GLY	N-CA-C	6.28	122.64	113.48
1	A	208	GLN	CB-CA-C	6.06	119.74	109.80
2	B	112	CYS	N-CA-C	6.02	118.22	109.07
2	B	258	ASN	N-CA-C	5.94	120.10	112.86
1	A	216	THR	N-CA-C	5.92	117.94	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	229	GLU	N-CA-C	5.85	117.92	107.80
2	B	154	PRO	N-CA-C	5.80	124.42	112.47
3	C	189	ARG	N-CA-C	5.78	118.37	109.07
1	A	144	MET	CB-CA-C	-5.66	98.55	109.37
1	A	132	LEU	N-CA-C	5.59	116.90	108.46
3	C	251	LEU	N-CA-C	5.55	117.70	108.99
1	A	208	GLN	N-CA-C	-5.48	100.37	109.46
2	B	98	ALA	N-CA-C	5.40	122.30	110.80
1	A	23	ILE	N-CA-C	-5.40	108.58	113.71
1	A	203	ASP	N-CA-C	-5.39	106.67	113.20
3	C	113	GLN	N-CA-C	5.38	122.27	110.80
2	B	47	LEU	N-CA-C	-5.35	99.48	109.32
2	B	279	LEU	N-CA-C	5.26	117.55	109.07
2	B	128	ILE	CA-C-N	-5.25	115.64	122.94
2	B	128	ILE	C-N-CA	-5.25	115.64	122.94
3	C	180	THR	N-CA-C	5.25	117.64	110.55
2	B	125	SER	N-CA-CB	-5.24	102.87	110.47
2	B	198	LEU	CB-CA-C	5.16	120.04	109.67
3	C	237	LEU	N-CA-C	-5.07	106.88	113.16
3	C	173	THR	N-CA-C	5.03	118.83	111.34
2	B	38	LYS	N-CA-C	5.02	119.13	112.30

There are no chirality outliers.

There are no planarity outliers.

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	2038	0	2069	173	0
2	B	2203	0	2250	197	0
3	C	2084	0	2056	181	0
All	All	6325	0	6375	535	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 42.

All (535) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:ILE:C	2:B:79:ILE:HD12	1.53	1.29
2:B:109:HIS:O	2:B:110:PHE:CD1	1.88	1.26
1:A:71:LEU:O	1:A:72:ARG:HD3	1.33	1.21
1:A:71:LEU:C	1:A:72:ARG:HD3	1.66	1.18
2:B:110:PHE:HD1	2:B:110:PHE:O	1.25	1.17
2:B:110:PHE:CD1	2:B:110:PHE:O	1.97	1.16
3:C:153:ILE:HG22	3:C:154:ASN:H	1.01	1.16
2:B:79:ILE:HD12	2:B:79:ILE:O	1.48	1.14
3:C:153:ILE:CG2	3:C:154:ASN:H	1.66	1.08
2:B:106:THR:CG2	2:B:107:ASN:H	1.62	1.08
3:C:237:LEU:HB2	3:C:258:ARG:HH22	1.18	1.07
2:B:106:THR:HG22	2:B:107:ASN:N	1.63	1.03
2:B:35:SER:HB3	2:B:39:LEU:HB2	1.38	1.01
2:B:79:ILE:C	2:B:79:ILE:CD1	2.30	1.00
2:B:106:THR:HG22	2:B:107:ASN:H	0.86	1.00
2:B:12:CYS:HB3	2:B:63:PHE:HB2	1.44	0.99
2:B:113:LEU:O	2:B:134:PRO:HD2	1.61	0.99
1:A:71:LEU:O	1:A:72:ARG:CD	2.08	0.99
3:C:156:ILE:HD11	3:C:179:ILE:HD13	1.44	0.99
1:A:87:LEU:HD13	1:A:88:ALA:H	1.29	0.98
3:C:101:MET:HB2	3:C:102:PRO:HD2	1.43	0.98
2:B:55:TRP:CD1	2:B:149:PRO:HG2	2.00	0.96
2:B:234:ILE:HG22	2:B:235:ARG:H	1.32	0.94
3:C:153:ILE:HG22	3:C:154:ASN:N	1.79	0.93
1:A:254:SER:HB3	1:A:255:LEU:HD12	1.50	0.93
2:B:18:ARG:HA	2:B:21:ASN:ND2	1.84	0.92
1:A:74:LYS:C	1:A:75:ILE:HG12	1.94	0.91
2:B:69:MET:HE1	2:B:79:ILE:HG23	1.52	0.91
2:B:250:LYS:HD2	2:B:266:LEU:HG	1.50	0.91
2:B:35:SER:OG	2:B:36:PRO:CD	2.20	0.90
2:B:35:SER:OG	2:B:36:PRO:HD2	1.70	0.89
3:C:113:GLN:HE21	3:C:115:TYR:HE2	1.21	0.89
1:A:146:ARG:HG3	1:A:236:LEU:HD23	1.56	0.87
2:B:30:CYS:HB2	2:B:42:ILE:HG23	1.57	0.85
3:C:186:PRO:O	3:C:187:TYR:CD2	2.29	0.85
3:C:24:VAL:CG1	3:C:105:LEU:HB3	2.06	0.84
3:C:209:LEU:HD23	3:C:209:LEU:H	1.42	0.82
2:B:69:MET:CE	2:B:79:ILE:HG23	2.10	0.82
3:C:42:CYS:HB3	3:C:51:VAL:HG23	1.60	0.81
1:A:187:ASP:H	1:A:190:ALA:HB3	1.44	0.81
2:B:112:CYS:HB2	2:B:134:PRO:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:237:LEU:HB2	3:C:258:ARG:NH2	1.95	0.81
3:C:221:ASN:ND2	3:C:244:ARG:HD2	1.96	0.80
2:B:234:ILE:HD11	2:B:280:SER:OXT	1.80	0.80
3:C:236:VAL:HG13	3:C:236:VAL:O	1.82	0.80
2:B:46:LYS:O	2:B:46:LYS:HG3	1.78	0.80
1:A:159:PHE:HB3	1:A:195:THR:HB	1.64	0.79
3:C:178:GLN:HB3	3:C:189:ARG:HB3	1.63	0.79
3:C:158:LEU:HA	3:C:211:GLU:HG3	1.65	0.79
1:A:155:ALA:HA	1:A:197:MET:HG2	1.64	0.79
3:C:27:LEU:O	3:C:31:LEU:HB2	1.83	0.78
1:A:41:VAL:HG22	1:A:48:TYR:HB2	1.66	0.78
2:B:109:HIS:O	2:B:110:PHE:HD1	1.62	0.78
2:B:141:LYS:HG3	2:B:142:LEU:N	1.99	0.77
3:C:156:ILE:CD1	3:C:179:ILE:HD13	2.14	0.77
3:C:224:LYS:NZ	3:C:276:GLU:HG3	1.99	0.77
2:B:71:GLY:C	2:B:73:SER:H	1.92	0.76
2:B:81:LEU:HB2	2:B:136:LYS:HD2	1.67	0.76
2:B:184:ALA:HB3	2:B:255:ILE:HD12	1.68	0.76
2:B:112:CYS:SG	2:B:133:ILE:HG23	2.25	0.76
2:B:107:ASN:CG	2:B:108:LYS:H	1.92	0.76
3:C:101:MET:HB2	3:C:102:PRO:CD	2.17	0.75
1:A:193:MET:HG3	2:B:133:ILE:O	1.87	0.75
1:A:242:ALA:HB1	1:A:243:PRO:HD3	1.69	0.75
2:B:155:ASP:HB3	2:B:256:VAL:HA	1.69	0.74
3:C:153:ILE:CG2	3:C:154:ASN:N	2.38	0.74
3:C:240:LYS:HB3	3:C:256:MET:HG3	1.68	0.73
1:A:119:ARG:HB3	3:C:201:LEU:CD1	2.18	0.73
3:C:24:VAL:HG12	3:C:105:LEU:HB3	1.68	0.73
3:C:26:ASN:ND2	3:C:260:GLU:HB3	2.04	0.73
1:A:242:ALA:HB1	1:A:243:PRO:CD	2.18	0.73
2:B:64:PHE:CD2	2:B:67:PHE:HB3	2.24	0.73
2:B:230:VAL:O	2:B:231:HIS:HB3	1.89	0.72
2:B:110:PHE:HD1	2:B:110:PHE:C	1.97	0.72
3:C:274:ASP:CG	3:C:275:GLU:H	1.96	0.72
1:A:30:GLU:HB2	1:A:37:SER:OG	1.89	0.72
3:C:223:TYR:CZ	3:C:252:SER:HB2	2.24	0.72
1:A:99:ILE:HG13	1:A:110:VAL:HG13	1.70	0.72
1:A:119:ARG:HB3	3:C:201:LEU:HD13	1.71	0.71
1:A:240:PHE:HD1	1:A:241:ASP:H	1.36	0.71
1:A:65:THR:N	1:A:66:PRO:HD2	2.06	0.70
2:B:18:ARG:HA	2:B:21:ASN:HD22	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:LEU:HD11	3:C:70:PHE:CD1	2.26	0.70
2:B:72:VAL:HG12	2:B:72:VAL:O	1.92	0.70
1:A:148:PRO:HA	1:A:234:LEU:HD12	1.74	0.70
2:B:36:PRO:HD2	2:B:39:LEU:HD13	1.72	0.70
2:B:35:SER:CB	2:B:39:LEU:HB2	2.18	0.70
2:B:79:ILE:HD12	2:B:80:TYR:N	2.04	0.70
1:A:159:PHE:HB3	1:A:195:THR:CB	2.22	0.70
2:B:167:LYS:HB2	2:B:241:LEU:HG	1.73	0.69
2:B:19:ILE:HD11	2:B:270:VAL:HG21	1.75	0.69
2:B:240:PHE:HE1	2:B:265:LEU:HD21	1.58	0.69
2:B:4:ARG:HB3	2:B:105:LEU:HD13	1.75	0.69
3:C:227:LEU:HD11	3:C:273:PRO:HG3	1.75	0.68
1:A:22:ARG:O	1:A:22:ARG:HG3	1.94	0.68
1:A:87:LEU:HD23	1:A:112:LEU:HG	1.76	0.68
2:B:4:ARG:O	2:B:104:LYS:HB2	1.94	0.68
2:B:48:ALA:O	2:B:49:ASN:OD1	2.11	0.68
2:B:26:LEU:HD11	2:B:54:MET:SD	2.33	0.68
2:B:106:THR:HG21	2:B:109:HIS:CD2	2.29	0.67
1:A:74:LYS:O	1:A:75:ILE:HG12	1.95	0.67
3:C:24:VAL:HG11	3:C:105:LEU:HB3	1.77	0.66
3:C:46:LYS:HA	3:C:75:VAL:HG11	1.77	0.66
1:A:218:CYS:SG	1:A:221:GLU:OE1	2.54	0.66
2:B:79:ILE:O	2:B:79:ILE:CD1	2.33	0.65
2:B:6:LYS:HE2	2:B:8:VAL:HG22	1.78	0.65
2:B:107:ASN:CG	2:B:108:LYS:N	2.52	0.65
2:B:18:ARG:O	2:B:22:MET:HB2	1.95	0.65
1:A:21:SER:HB2	1:A:81:LEU:HD22	1.77	0.65
1:A:71:LEU:C	1:A:72:ARG:CD	2.57	0.65
2:B:259:LYS:CE	2:B:279:LEU:HD21	2.27	0.65
3:C:228:LEU:O	3:C:231:SER:HB3	1.97	0.65
1:A:141:CYS:HB3	1:A:239:HIS:C	2.22	0.65
3:C:179:ILE:CD1	3:C:244:ARG:HE	2.09	0.65
1:A:228:PHE:O	1:A:233:ASN:ND2	2.30	0.65
2:B:247:ASN:OD1	2:B:247:ASN:N	2.28	0.65
2:B:35:SER:O	2:B:69:MET:HG2	1.97	0.64
1:A:117:GLY:H	3:C:204:PRO:HD2	1.62	0.64
1:A:170:ILE:HD11	1:A:172:ARG:HD2	1.78	0.64
3:C:124:GLU:HB2	3:C:129:VAL:HG13	1.79	0.64
1:A:74:LYS:C	1:A:75:ILE:CG1	2.70	0.64
2:B:259:LYS:HE2	2:B:279:LEU:HD21	1.79	0.64
3:C:208:ASP:HB2	3:C:211:GLU:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:MET:O	3:C:118:PRO:HD2	1.99	0.63
2:B:71:GLY:C	2:B:73:SER:N	2.55	0.63
2:B:180:LEU:HD21	2:B:182:ILE:CD1	2.28	0.63
2:B:19:ILE:O	2:B:23:ILE:HG12	1.98	0.63
3:C:159:GLN:OE1	3:C:161:GLU:HB3	1.98	0.63
1:A:56:LEU:HB3	1:A:255:LEU:HD23	1.81	0.62
1:A:141:CYS:HB3	1:A:240:PHE:N	2.14	0.62
2:B:201:VAL:HG13	3:C:134:ILE:HD12	1.81	0.62
2:B:259:LYS:HE2	2:B:279:LEU:HD11	1.80	0.62
2:B:234:ILE:HG22	2:B:235:ARG:N	2.11	0.62
1:A:28:TYR:HB2	1:A:39:ARG:HB3	1.80	0.62
2:B:201:VAL:HG13	3:C:134:ILE:CD1	2.30	0.62
2:B:6:LYS:HG3	2:B:7:ILE:N	2.13	0.62
3:C:16:SER:HB3	3:C:80:VAL:HG13	1.81	0.62
3:C:34:ILE:O	3:C:53:VAL:HG21	2.00	0.62
1:A:57:PHE:CZ	1:A:255:LEU:HD13	2.34	0.61
2:B:43:LEU:HD11	2:B:149:PRO:HG3	1.82	0.61
3:C:15:TYR:HD1	3:C:112:TYR:HB3	1.66	0.61
3:C:223:TYR:CE1	3:C:252:SER:HB2	2.36	0.61
1:A:156:VAL:O	1:A:160:SER:HB3	2.00	0.61
1:A:236:LEU:HB2	1:A:250:THR:OG1	2.00	0.61
2:B:110:PHE:O	2:B:111:PRO:C	2.43	0.61
2:B:102:LYS:HB2	2:B:116:SER:HB3	1.81	0.61
2:B:106:THR:HG21	2:B:109:HIS:NE2	2.16	0.61
3:C:53:VAL:HB	3:C:61:ALA:HB3	1.83	0.61
3:C:259:ASN:N	3:C:259:ASN:HD22	1.99	0.61
1:A:107:ARG:HD2	1:A:125:SER:HB3	1.81	0.61
2:B:141:LYS:HG3	2:B:142:LEU:H	1.65	0.61
2:B:180:LEU:HD21	2:B:182:ILE:HD13	1.82	0.61
3:C:244:ARG:NH1	3:C:244:ARG:HB2	2.15	0.61
2:B:80:TYR:CZ	2:B:144:LYS:HB3	2.36	0.61
2:B:109:HIS:O	2:B:110:PHE:CE1	2.53	0.60
3:C:30:ILE:HD13	3:C:265:CYS:SG	2.41	0.60
1:A:170:ILE:HD11	1:A:172:ARG:HB3	1.82	0.60
3:C:251:LEU:CB	3:C:272:CYS:HB3	2.30	0.60
1:A:120:LYS:HE2	1:A:122:HIS:HE1	1.65	0.60
1:A:126:PHE:CG	1:A:127:GLN:N	2.67	0.60
2:B:71:GLY:O	2:B:73:SER:N	2.25	0.60
2:B:106:THR:CG2	2:B:107:ASN:N	2.34	0.60
3:C:84:ILE:HD12	3:C:89:LEU:HD22	1.84	0.60
3:C:224:LYS:HZ1	3:C:276:GLU:HG3	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:158:LEU:O	3:C:239:CYS:HB2	2.02	0.60
1:A:161:PRO:HG3	2:B:90:ARG:HH21	1.67	0.60
3:C:275:GLU:O	3:C:276:GLU:HG2	2.02	0.60
1:A:223:ARG:CG	1:A:223:ARG:HH11	2.15	0.59
1:A:205:GLN:NE2	1:A:234:LEU:HD11	2.18	0.59
3:C:171:ASP:C	3:C:172:MET:HG2	2.27	0.59
3:C:186:PRO:O	3:C:187:TYR:HD2	1.82	0.59
3:C:246:ASP:HA	3:C:249:GLY:O	2.02	0.59
2:B:109:HIS:C	2:B:110:PHE:CD1	2.78	0.59
3:C:101:MET:CB	3:C:102:PRO:HD2	2.27	0.59
1:A:41:VAL:CG2	1:A:48:TYR:HB2	2.33	0.59
2:B:55:TRP:CD1	2:B:149:PRO:CG	2.83	0.59
2:B:249:THR:OG1	2:B:267:HIS:ND1	2.26	0.59
2:B:183:GLU:HG2	2:B:230:VAL:HG12	1.85	0.58
1:A:64:ALA:C	1:A:66:PRO:HD2	2.28	0.58
1:A:223:ARG:HH11	1:A:223:ARG:HG3	1.68	0.58
3:C:274:ASP:CG	3:C:275:GLU:N	2.61	0.58
2:B:191:ASN:HA	2:B:203:THR:O	2.03	0.58
2:B:4:ARG:HH22	2:B:60:GLN:HE22	1.52	0.57
1:A:146:ARG:HG3	1:A:236:LEU:CD2	2.31	0.57
3:C:179:ILE:HD12	3:C:244:ARG:HE	1.68	0.57
1:A:95:GLU:HB2	1:A:113:HIS:O	2.04	0.57
3:C:112:TYR:CD2	3:C:113:GLN:N	2.72	0.57
1:A:38:LEU:O	1:A:50:CYS:HA	2.03	0.57
1:A:193:MET:HA	2:B:135:ILE:HD11	1.85	0.57
2:B:4:ARG:HH12	2:B:67:PHE:HD1	1.53	0.57
1:A:13:LEU:HD23	1:A:84:PHE:CZ	2.39	0.57
1:A:168:LEU:O	1:A:170:ILE:HG22	2.05	0.57
3:C:44:ALA:HB3	3:C:80:VAL:HB	1.87	0.57
3:C:92:CYS:SG	3:C:134:ILE:HG21	2.45	0.57
1:A:172:ARG:HG2	1:A:173:GLY:N	2.19	0.57
2:B:15:HIS:O	2:B:19:ILE:HG12	2.03	0.56
1:A:23:ILE:HD13	1:A:260:PHE:CE2	2.40	0.56
3:C:235:LEU:HD23	3:C:256:MET:SD	2.45	0.56
1:A:148:PRO:HA	1:A:234:LEU:CD1	2.35	0.56
3:C:264:ILE:HG12	3:C:264:ILE:O	2.05	0.56
2:B:64:PHE:HD2	2:B:67:PHE:HB3	1.69	0.56
3:C:22:ASP:H	3:C:71:GLN:HE21	1.52	0.56
2:B:121:SER:HB2	2:B:128:ILE:HG13	1.87	0.56
2:B:62:ASN:ND2	2:B:63:PHE:HD1	2.04	0.56
1:A:175:ARG:HH21	1:A:207:LEU:HD23	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ASN:HD22	2:B:63:PHE:N	2.03	0.56
2:B:81:LEU:HA	2:B:139:PRO:HD3	1.88	0.56
2:B:259:LYS:HD3	2:B:278:ALA:HB3	1.87	0.56
3:C:21:LEU:HA	3:C:71:GLN:HG2	1.88	0.56
1:A:112:LEU:HB2	1:A:119:ARG:HG2	1.87	0.55
3:C:37:ARG:NH1	3:C:55:ASN:O	2.37	0.55
1:A:121:THR:HG22	3:C:199:SER:HB2	1.88	0.55
1:A:160:SER:C	1:A:162:ALA:H	2.14	0.55
2:B:61:GLU:HG3	2:B:62:ASN:N	2.22	0.55
1:A:168:LEU:HD12	1:A:216:THR:OG1	2.07	0.55
3:C:253:LEU:HG	3:C:253:LEU:O	2.07	0.55
2:B:24:ALA:HA	2:B:85:SER:HB3	1.86	0.55
1:A:42:ASN:HB2	1:A:47:ALA:H	1.72	0.55
2:B:222:ARG:HG2	2:B:223:ASN:H	1.72	0.55
2:B:185:ASN:HB2	2:B:189:GLU:HB3	1.89	0.55
1:A:4:LEU:HD22	1:A:59:GLN:HB3	1.89	0.55
1:A:117:GLY:N	3:C:204:PRO:HD2	2.21	0.55
3:C:89:LEU:HD11	3:C:93:LEU:HD21	1.88	0.55
3:C:39:HIS:HB2	3:C:83:ARG:NH1	2.22	0.55
3:C:245:THR:OG1	3:C:251:LEU:HG	2.07	0.55
2:B:31:THR:N	2:B:43:LEU:O	2.37	0.55
1:A:243:PRO:O	1:A:244:GLY:C	2.50	0.54
2:B:106:THR:HG22	2:B:107:ASN:OD1	2.07	0.54
2:B:110:PHE:HE1	2:B:112:CYS:SG	2.30	0.54
1:A:160:SER:HB2	1:A:223:ARG:HH22	1.72	0.54
3:C:222:ARG:HD3	3:C:275:GLU:OE2	2.06	0.54
2:B:103:ILE:O	2:B:103:ILE:HG13	2.08	0.54
3:C:209:LEU:H	3:C:209:LEU:CD2	2.18	0.54
2:B:234:ILE:HD13	2:B:236:LYS:HE2	1.89	0.54
3:C:59:VAL:HG21	3:C:227:LEU:CB	2.38	0.54
3:C:165:GLU:O	3:C:168:SER:HB2	2.08	0.54
3:C:227:LEU:CD1	3:C:273:PRO:HG3	2.38	0.54
3:C:251:LEU:HB2	3:C:272:CYS:HB3	1.90	0.54
3:C:264:ILE:HD13	3:C:264:ILE:H	1.73	0.54
1:A:158:PRO:HA	2:B:94:THR:HG21	1.89	0.54
3:C:251:LEU:HB3	3:C:272:CYS:CB	2.38	0.54
3:C:155:LYS:HG2	3:C:214:HIS:HB2	1.90	0.54
3:C:187:TYR:HB3	3:C:202:ASP:OD1	2.08	0.54
2:B:86:GLU:O	2:B:89:SER:N	2.41	0.53
3:C:30:ILE:HG13	3:C:258:ARG:HD2	1.90	0.53
2:B:63:PHE:O	2:B:63:PHE:CD2	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:TYR:HA	3:C:112:TYR:HB3	1.91	0.53
1:A:172:ARG:CG	1:A:173:GLY:N	2.71	0.53
2:B:106:THR:CG2	2:B:107:ASN:OD1	2.57	0.53
1:A:160:SER:O	1:A:162:ALA:N	2.41	0.53
2:B:55:TRP:HB2	2:B:149:PRO:HB2	1.89	0.53
1:A:254:SER:CB	1:A:255:LEU:HD12	2.31	0.53
2:B:144:LYS:CG	2:B:145:ASP:N	2.72	0.53
3:C:229:LYS:HB3	3:C:230:PRO:CD	2.38	0.53
3:C:236:VAL:O	3:C:236:VAL:CG1	2.53	0.53
1:A:160:SER:HB2	1:A:223:ARG:NH2	2.24	0.52
2:B:69:MET:HE3	2:B:77:ASN:O	2.08	0.52
1:A:144:MET:HE1	1:A:146:ARG:HH21	1.74	0.52
2:B:112:CYS:SG	2:B:133:ILE:CG2	2.97	0.52
3:C:122:PHE:CD1	3:C:122:PHE:C	2.87	0.52
3:C:224:LYS:HZ2	3:C:276:GLU:HG3	1.73	0.52
2:B:173:MET:HB3	2:B:194:ILE:HD12	1.91	0.52
2:B:186:LEU:HG	2:B:187:ASP:OD2	2.09	0.52
1:A:148:PRO:HB2	1:A:151:VAL:HG13	1.92	0.52
1:A:154:GLU:O	1:A:158:PRO:HD3	2.09	0.52
1:A:226:LEU:O	1:A:229:ALA:HB2	2.09	0.52
3:C:29:THR:O	3:C:32:LYS:N	2.43	0.52
1:A:159:PHE:O	1:A:161:PRO:HD2	2.10	0.51
1:A:164:ALA:O	1:A:219:LEU:HB3	2.10	0.51
1:A:142:PRO:HG2	1:A:143:HIS:CD2	2.45	0.51
2:B:259:LYS:NZ	2:B:279:LEU:HD21	2.25	0.51
3:C:62:ASN:HB2	3:C:268:GLU:HB3	1.92	0.51
2:B:55:TRP:HD1	2:B:149:PRO:HG2	1.65	0.51
1:A:89:MET:HG3	1:A:90:LEU:HD12	1.92	0.51
1:A:199:LEU:CD1	2:B:128:ILE:HG23	2.40	0.51
2:B:81:LEU:HD22	2:B:136:LYS:HD2	1.92	0.51
2:B:177:SER:HB3	2:B:194:ILE:HD13	1.93	0.51
1:A:31:PRO:O	1:A:72:ARG:NH2	2.43	0.51
1:A:177:ILE:HG12	1:A:204:PHE:CZ	2.45	0.51
3:C:175:GLU:HB2	3:C:225:ILE:HG13	1.92	0.51
3:C:224:LYS:H	3:C:273:PRO:HG2	1.76	0.51
1:A:102:ASN:HD21	1:A:104:ARG:HE	1.59	0.51
1:A:161:PRO:HB2	1:A:163:LEU:H	1.76	0.51
2:B:133:ILE:O	2:B:133:ILE:HG22	2.11	0.51
3:C:112:TYR:HD2	3:C:113:GLN:N	2.08	0.51
3:C:257:ILE:HG22	3:C:257:ILE:O	2.10	0.51
1:A:20:LEU:O	1:A:23:ILE:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLU:O	1:A:218:CYS:HA	2.11	0.51
3:C:52:THR:OG1	3:C:62:ASN:ND2	2.39	0.51
2:B:150:VAL:O	2:B:151:VAL:HG13	2.10	0.51
3:C:89:LEU:CD1	3:C:93:LEU:HD21	2.41	0.51
3:C:152:VAL:HG13	3:C:243:ILE:HG23	1.93	0.50
1:A:119:ARG:HB3	3:C:201:LEU:HD11	1.93	0.50
2:B:113:LEU:O	2:B:134:PRO:CD	2.46	0.50
2:B:110:PHE:CE1	2:B:112:CYS:SG	3.04	0.50
2:B:120:LEU:HD23	2:B:122:MET:HG2	1.93	0.50
1:A:13:LEU:HA	1:A:16:ALA:HB3	1.92	0.50
3:C:42:CYS:CB	3:C:51:VAL:HG23	2.37	0.50
2:B:9:ASP:HB2	2:B:65:ASN:HD21	1.77	0.50
2:B:180:LEU:CD2	2:B:182:ILE:HD13	2.42	0.50
2:B:185:ASN:CB	2:B:189:GLU:HB3	2.41	0.50
3:C:245:THR:O	3:C:250:PHE:HA	2.10	0.50
1:A:102:ASN:ND2	1:A:104:ARG:HE	2.09	0.50
2:B:4:ARG:NE	2:B:34:ILE:HG12	2.26	0.50
2:B:19:ILE:HG21	2:B:58:LEU:HD22	1.93	0.50
3:C:199:SER:C	3:C:200:HIS:HD2	2.20	0.50
1:A:160:SER:CB	1:A:223:ARG:HH22	2.25	0.49
1:A:187:ASP:N	1:A:190:ALA:HB3	2.22	0.49
3:C:171:ASP:O	3:C:173:THR:HG23	2.12	0.49
3:C:176:VAL:HG22	3:C:222:ARG:HG3	1.94	0.49
3:C:178:GLN:CB	3:C:189:ARG:HB3	2.38	0.49
1:A:230:GLU:H	1:A:233:ASN:HD21	1.61	0.49
2:B:144:LYS:HG2	2:B:145:ASP:H	1.76	0.49
3:C:232:THR:O	3:C:233:LYS:C	2.55	0.49
3:C:255:TYR:HB3	3:C:268:GLU:HG3	1.94	0.49
2:B:110:PHE:CD1	2:B:110:PHE:C	2.69	0.49
3:C:208:ASP:HB2	3:C:211:GLU:O	2.12	0.49
2:B:155:ASP:CG	2:B:257:ASN:H	2.20	0.49
1:A:168:LEU:HD23	1:A:170:ILE:CG2	2.43	0.49
1:A:176:VAL:HG23	1:A:199:LEU:O	2.12	0.49
2:B:183:GLU:HB2	2:B:191:ASN:HB2	1.93	0.49
1:A:75:ILE:CD1	1:A:108:LEU:HD22	2.43	0.49
2:B:12:CYS:CB	2:B:63:PHE:HB2	2.30	0.49
2:B:256:VAL:HB	2:B:260:MET:CB	2.42	0.49
1:A:182:HIS:HD2	1:A:194:VAL:HG11	1.78	0.49
2:B:144:LYS:CG	2:B:145:ASP:H	2.25	0.49
3:C:152:VAL:O	3:C:244:ARG:O	2.31	0.48
3:C:203:TYR:N	3:C:203:TYR:CD2	2.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:MET:HE3	2:B:192:LEU:HD21	1.94	0.48
1:A:28:TYR:CE1	1:A:131:SER:HB2	2.48	0.48
1:A:228:PHE:HE2	1:A:256:LEU:HD21	1.79	0.48
3:C:59:VAL:HG21	3:C:227:LEU:HB2	1.96	0.48
3:C:175:GLU:HB3	3:C:223:TYR:HB2	1.94	0.48
1:A:235:ASN:C	1:A:236:LEU:HG	2.39	0.48
2:B:115:VAL:HG23	2:B:132:ASP:HB2	1.95	0.48
3:C:152:VAL:HG12	3:C:153:ILE:O	2.13	0.48
2:B:69:MET:HE3	2:B:79:ILE:HG23	1.94	0.48
2:B:80:TYR:OH	2:B:144:LYS:HB3	2.13	0.48
2:B:81:LEU:HD13	2:B:136:LYS:HD2	1.96	0.48
2:B:160:LEU:HD13	2:B:163:LEU:HD11	1.96	0.48
1:A:160:SER:C	1:A:162:ALA:N	2.71	0.47
2:B:181:VAL:HB	2:B:193:LYS:HB3	1.95	0.47
2:B:233:ASP:OD1	2:B:234:ILE:N	2.41	0.47
3:C:232:THR:O	3:C:236:VAL:HG12	2.13	0.47
1:A:13:LEU:HD23	1:A:84:PHE:CE2	2.49	0.47
1:A:87:LEU:CD1	1:A:88:ALA:H	2.14	0.47
1:A:242:ALA:CB	1:A:243:PRO:CD	2.91	0.47
2:B:248:PRO:HA	2:B:267:HIS:HB2	1.96	0.47
3:C:21:LEU:O	3:C:106:THR:OG1	2.32	0.47
1:A:39:ARG:NH2	1:A:133:GLN:O	2.48	0.47
1:A:53:PHE:CE1	1:A:256:LEU:CD1	2.98	0.47
1:A:205:GLN:HE22	1:A:234:LEU:HD11	1.78	0.47
2:B:35:SER:OG	2:B:36:PRO:HD3	2.11	0.47
3:C:84:ILE:HG22	3:C:136:THR:HG22	1.95	0.47
1:A:230:GLU:O	1:A:231:SER:HB2	2.14	0.47
2:B:55:TRP:HD1	2:B:149:PRO:CG	2.26	0.47
2:B:259:LYS:HE2	2:B:279:LEU:CD1	2.45	0.47
1:A:88:ALA:C	1:A:90:LEU:N	2.73	0.47
1:A:152:LEU:HD22	1:A:179:ARG:HH21	1.80	0.47
2:B:233:ASP:CG	2:B:234:ILE:H	2.23	0.47
3:C:180:THR:HG23	3:C:181:MET:N	2.28	0.47
1:A:117:GLY:HA2	3:C:202:ASP:O	2.15	0.47
1:A:206:GLN:HE21	1:A:206:GLN:HB2	1.56	0.47
2:B:72:VAL:O	2:B:72:VAL:CG1	2.62	0.47
3:C:117:TYR:HB3	3:C:136:THR:O	2.15	0.47
3:C:49:ILE:HD13	3:C:109:ARG:HH22	1.80	0.47
2:B:181:VAL:HG11	2:B:193:LYS:NZ	2.30	0.47
2:B:184:ALA:CB	2:B:255:ILE:HD12	2.42	0.47
3:C:150:THR:HB	3:C:247:ASN:ND2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LEU:HD22	1:A:88:ALA:N	2.30	0.47
3:C:31:LEU:O	3:C:34:ILE:HG13	2.15	0.47
3:C:166:ALA:HB1	3:C:201:LEU:HG	1.97	0.47
1:A:107:ARG:NH1	1:A:125:SER:OG	2.42	0.46
1:A:182:HIS:CG	1:A:183:GLU:N	2.83	0.46
2:B:19:ILE:CD1	2:B:270:VAL:HG21	2.42	0.46
1:A:201:GLU:HG3	1:A:202:GLU:H	1.81	0.46
2:B:103:ILE:HD13	2:B:113:LEU:HD11	1.97	0.46
3:C:24:VAL:HG12	3:C:105:LEU:CB	2.42	0.46
1:A:111:GLN:HB3	1:A:120:LYS:HG3	1.98	0.46
2:B:6:LYS:NZ	2:B:60:GLN:HG2	2.31	0.46
2:B:136:LYS:HG2	2:B:137:VAL:N	2.31	0.46
2:B:256:VAL:HB	2:B:260:MET:HB3	1.98	0.46
3:C:21:LEU:HD11	3:C:70:PHE:HD1	1.75	0.46
3:C:59:VAL:HG21	3:C:227:LEU:HB3	1.98	0.46
1:A:145:LEU:HB3	1:A:237:SER:HB2	1.98	0.46
1:A:225:LEU:CD2	1:A:235:ASN:HD21	2.29	0.46
2:B:23:ILE:HG13	2:B:42:ILE:HD13	1.98	0.46
2:B:35:SER:HB3	2:B:39:LEU:CB	2.28	0.46
3:C:21:LEU:N	3:C:107:ALA:O	2.34	0.46
3:C:235:LEU:CD2	3:C:267:VAL:CG2	2.94	0.46
1:A:7:GLY:O	1:A:10:VAL:HB	2.16	0.46
3:C:83:ARG:HB3	3:C:139:PRO:HG2	1.97	0.46
1:A:126:PHE:CD2	1:A:127:GLN:N	2.85	0.45
2:B:153:ASP:OD1	2:B:153:ASP:N	2.48	0.45
3:C:155:LYS:CG	3:C:214:HIS:HB2	2.46	0.45
1:A:54:ALA:HB3	1:A:255:LEU:HB3	1.97	0.45
3:C:145:PHE:CD2	3:C:147:PHE:HE2	2.34	0.45
1:A:51:PHE:HE2	1:A:260:PHE:CE1	2.34	0.45
1:A:227:SER:C	1:A:229:ALA:H	2.24	0.45
2:B:12:CYS:O	2:B:16:PHE:N	2.46	0.45
2:B:55:TRP:CZ2	2:B:57:GLU:HB2	2.52	0.45
3:C:19:ALA:HA	3:C:72:GLU:O	2.17	0.45
2:B:30:CYS:CB	2:B:42:ILE:HG23	2.37	0.45
3:C:46:LYS:HG3	3:C:78:GLU:OE1	2.15	0.45
1:A:141:CYS:CB	1:A:239:HIS:C	2.89	0.45
2:B:211:PRO:HA	2:B:212:PRO:HD3	1.79	0.45
2:B:234:ILE:CG2	2:B:235:ARG:H	2.12	0.45
3:C:118:PRO:HB2	3:C:120:MET:HE2	1.99	0.45
3:C:167:PHE:O	3:C:167:PHE:CG	2.69	0.45
1:A:127:GLN:O	1:A:128:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ARG:HB2	1:A:212:GLY:HA2	1.97	0.45
1:A:199:LEU:HD12	1:A:199:LEU:HA	1.77	0.45
2:B:195:GLU:HB2	2:B:200:CYS:SG	2.57	0.45
1:A:161:PRO:O	1:A:162:ALA:HB3	2.17	0.45
2:B:249:THR:HG1	2:B:267:HIS:HD1	1.55	0.45
3:C:67:ALA:HA	3:C:70:PHE:CD2	2.52	0.45
1:A:113:HIS:HA	1:A:118:VAL:HG22	1.97	0.45
2:B:54:MET:HE2	2:B:54:MET:HB3	1.80	0.45
3:C:18:VAL:HG13	3:C:74:LYS:HB3	1.99	0.45
3:C:93:LEU:H	3:C:93:LEU:HG	1.61	0.45
3:C:246:ASP:CG	3:C:246:ASP:O	2.60	0.45
2:B:246:VAL:O	2:B:247:ASN:C	2.60	0.44
1:A:57:PHE:CD2	1:A:255:LEU:HB2	2.53	0.44
1:A:57:PHE:CD1	1:A:255:LEU:HD22	2.52	0.44
3:C:202:ASP:OD2	3:C:202:ASP:C	2.61	0.44
1:A:243:PRO:HA	1:A:264:THR:HG22	2.00	0.44
2:B:113:LEU:HD22	2:B:113:LEU:HA	1.76	0.44
3:C:235:LEU:HD22	3:C:267:VAL:CG2	2.48	0.44
3:C:157:ILE:HG21	3:C:210:MET:O	2.17	0.44
2:B:88:LEU:HD22	2:B:88:LEU:HA	1.82	0.44
3:C:31:LEU:HB3	3:C:90:LEU:HD21	2.00	0.44
3:C:166:ALA:C	3:C:168:SER:H	2.25	0.44
2:B:181:VAL:HG11	2:B:193:LYS:HZ1	1.82	0.44
3:C:35:HIS:HB2	3:C:90:LEU:HD11	2.00	0.44
1:A:153:GLY:O	1:A:154:GLU:C	2.61	0.44
3:C:221:ASN:ND2	3:C:221:ASN:N	2.65	0.44
1:A:57:PHE:CG	1:A:255:LEU:HD22	2.53	0.43
1:A:88:ALA:C	1:A:90:LEU:H	2.26	0.43
2:B:40:ASN:HB2	2:B:60:GLN:OE1	2.18	0.43
3:C:15:TYR:CD1	3:C:112:TYR:HB3	2.49	0.43
3:C:64:PHE:N	3:C:64:PHE:CD1	2.85	0.43
1:A:51:PHE:HB3	1:A:53:PHE:CE2	2.53	0.43
1:A:115:LYS:HB3	1:A:116:PHE:H	1.75	0.43
2:B:55:TRP:HB2	2:B:149:PRO:CB	2.48	0.43
3:C:231:SER:HB2	3:C:269:TYR:CD1	2.54	0.43
3:C:244:ARG:HB2	3:C:244:ARG:CZ	2.48	0.43
1:A:81:LEU:O	1:A:85:ARG:N	2.51	0.43
1:A:152:LEU:HD22	1:A:179:ARG:NH2	2.33	0.43
1:A:221:GLU:HB3	1:A:262:LEU:HD22	2.01	0.43
2:B:155:ASP:CB	2:B:256:VAL:HA	2.41	0.43
3:C:67:ALA:HA	3:C:70:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:PHE:CE1	1:A:255:LEU:HD13	2.54	0.43
1:A:65:THR:N	1:A:66:PRO:CD	2.80	0.43
1:A:170:ILE:CD1	1:A:172:ARG:HB3	2.49	0.43
2:B:158:ILE:HG12	2:B:159:TYR:O	2.18	0.43
2:B:254:ASN:OD1	2:B:254:ASN:N	2.51	0.43
3:C:180:THR:HG22	3:C:186:PRO:HA	2.00	0.43
2:B:118:GLU:HG2	2:B:129:VAL:CG1	2.49	0.43
3:C:118:PRO:HA	3:C:134:ILE:O	2.19	0.43
1:A:138:PRO:C	1:A:140:SER:H	2.27	0.42
1:A:145:LEU:HA	1:A:206:GLN:O	2.19	0.42
1:A:170:ILE:CG1	1:A:172:ARG:HB3	2.49	0.42
1:A:72:ARG:HB2	1:A:130:GLU:OE1	2.19	0.42
2:B:163:LEU:HD21	2:B:251:ALA:HB1	2.01	0.42
1:A:16:ALA:HB1	1:A:53:PHE:HZ	1.85	0.42
1:A:107:ARG:HD2	1:A:125:SER:CB	2.49	0.42
3:C:173:THR:HG21	3:C:194:GLY:CA	2.50	0.42
1:A:4:LEU:C	1:A:58:PHE:HD1	2.27	0.42
1:A:143:HIS:HD2	1:A:239:HIS:O	2.02	0.42
2:B:18:ARG:HA	2:B:21:ASN:HD21	1.75	0.42
3:C:24:VAL:HG12	3:C:105:LEU:O	2.19	0.42
2:B:180:LEU:O	2:B:233:ASP:N	2.53	0.42
3:C:83:ARG:O	3:C:139:PRO:HD2	2.19	0.42
3:C:162:GLY:O	3:C:165:GLU:HB2	2.19	0.42
1:A:12:VAL:O	1:A:16:ALA:HB2	2.20	0.42
2:B:99:ARG:HA	2:B:99:ARG:NE	2.33	0.42
3:C:208:ASP:HA	3:C:211:GLU:HB3	2.02	0.42
3:C:219:GLN:HE22	3:C:250:PHE:HE1	1.68	0.42
1:A:102:ASN:HD21	1:A:104:ARG:NE	2.18	0.42
1:A:117:GLY:H	3:C:204:PRO:CD	2.29	0.42
1:A:157:LEU:N	1:A:158:PRO:CD	2.82	0.42
1:A:29:LEU:HD12	1:A:38:LEU:CD2	2.50	0.42
2:B:63:PHE:O	2:B:63:PHE:CG	2.72	0.42
3:C:181:MET:HB2	3:C:218:THR:HB	2.01	0.42
1:A:124:LEU:O	3:C:196:ALA:HB1	2.20	0.42
2:B:172:LYS:O	2:B:175:ASN:HB2	2.20	0.42
3:C:122:PHE:HA	3:C:130:THR:O	2.20	0.42
3:C:178:GLN:O	3:C:188:PHE:HA	2.19	0.42
1:A:42:ASN:HD22	1:A:44:SER:CB	2.33	0.41
2:B:92:LEU:HD23	2:B:92:LEU:HA	1.89	0.41
3:C:29:THR:HA	3:C:32:LYS:HB3	2.02	0.41
3:C:51:VAL:HG12	3:C:63:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:158:LEU:HD22	3:C:163:LEU:HD12	2.02	0.41
3:C:257:ILE:HG12	3:C:266:PHE:CE2	2.54	0.41
1:A:240:PHE:CD1	1:A:241:ASP:N	2.85	0.41
2:B:19:ILE:HG21	2:B:58:LEU:CD2	2.50	0.41
2:B:31:THR:HG23	2:B:82:GLU:HB3	2.02	0.41
2:B:98:ALA:HB1	2:B:99:ARG:H	1.65	0.41
1:A:219:LEU:O	1:A:219:LEU:HG	2.21	0.41
1:A:223:ARG:CG	1:A:223:ARG:NH1	2.79	0.41
3:C:150:THR:HB	3:C:247:ASN:HB3	2.03	0.41
1:A:27:LEU:HD13	1:A:77:MET:HE1	2.01	0.41
1:A:75:ILE:O	1:A:76:LEU:C	2.61	0.41
2:B:210:ASN:HA	2:B:211:PRO:HD3	1.90	0.41
2:B:279:LEU:O	2:B:280:SER:OXT	2.39	0.41
1:A:51:PHE:HE2	1:A:260:PHE:HE1	1.69	0.41
1:A:182:HIS:HD2	1:A:194:VAL:CG1	2.33	0.41
1:A:202:GLU:C	1:A:204:PHE:H	2.27	0.41
2:B:81:LEU:HB2	2:B:136:LYS:CD	2.45	0.41
3:C:154:ASN:HD22	3:C:179:ILE:HB	1.84	0.41
3:C:188:PHE:O	3:C:202:ASP:HA	2.20	0.41
3:C:236:VAL:HB	3:C:256:MET:HE2	2.03	0.41
2:B:259:LYS:HE2	2:B:279:LEU:CD2	2.47	0.41
3:C:75:VAL:HG23	3:C:80:VAL:HG21	2.03	0.41
1:A:225:LEU:HD12	1:A:260:PHE:CD1	2.56	0.41
2:B:32:LEU:HG	2:B:33:ARG:N	2.35	0.41
2:B:256:VAL:HB	2:B:260:MET:HB2	2.03	0.41
2:B:268:GLU:HG3	2:B:269:ASP:H	1.84	0.41
3:C:179:ILE:HD12	3:C:244:ARG:NE	2.34	0.41
1:A:40:THR:O	1:A:49:ALA:N	2.52	0.41
2:B:4:ARG:HD2	2:B:105:LEU:CD1	2.51	0.40
2:B:247:ASN:HA	2:B:248:PRO:HD2	1.92	0.40
3:C:31:LEU:CD1	3:C:86:LEU:HD11	2.51	0.40
3:C:251:LEU:HB3	3:C:272:CYS:HB3	1.98	0.40
1:A:56:LEU:HB3	1:A:255:LEU:CD2	2.49	0.40
2:B:4:ARG:HH11	2:B:4:ARG:HG2	1.85	0.40
2:B:6:LYS:CD	2:B:60:GLN:HE21	2.34	0.40
2:B:44:CYS:O	2:B:45:ASP:HB2	2.20	0.40
3:C:14:GLN:HE21	3:C:14:GLN:HB2	1.63	0.40
2:B:58:LEU:HB3	2:B:270:VAL:HG12	2.03	0.40
3:C:118:PRO:HA	3:C:135:ASN:HA	2.04	0.40
1:A:4:LEU:HD22	1:A:59:GLN:CB	2.52	0.40
1:A:205:GLN:H	1:A:205:GLN:HG2	1.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:ASN:O	3:C:267:VAL:HB	2.22	0.40
3:C:170:LEU:H	3:C:170:LEU:HG	1.70	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	262/270 (97%)	200 (76%)	50 (19%)	12 (5%)	2	15
2	B	276/286 (96%)	207 (75%)	52 (19%)	17 (6%)	1	9
3	C	262/282 (93%)	203 (78%)	41 (16%)	18 (7%)	1	7
All	All	800/838 (96%)	610 (76%)	143 (18%)	47 (6%)	1	10

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	243	PRO
2	B	35	SER
2	B	45	ASP
2	B	72	VAL
2	B	99	ARG
3	C	101	MET
1	A	94	VAL
1	A	128	ASP
1	A	242	ALA
2	B	52	VAL
2	B	143	TRP
2	B	149	PRO
2	B	231	HIS
3	C	113	GLN

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Mol	Chain	Res	Type
3	C	140	GLU
1	A	139	ALA
1	A	223	ARG
2	B	70	GLU
2	B	111	PRO
2	B	123	SER
3	C	78	GLU
3	C	153	ILE
3	C	231	SER
3	C	233	LYS
1	A	126	PHE
1	A	188	SER
1	A	192	ALA
2	B	61	GLU
2	B	154	PRO
2	B	212	PRO
3	C	55	ASN
3	C	85	ASN
3	C	142	THR
3	C	195	ASN
3	C	272	CYS
2	B	161	PRO
2	B	235	ARG
3	C	261	ASP
1	A	244	GLY
2	B	247	ASN
3	C	100	PRO
1	A	161	PRO
3	C	186	PRO
3	C	197	GLY
3	C	114	GLY
3	C	139	PRO

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	212/229 (93%)	163 (77%)	49 (23%)	1	5
2	B	255/263 (97%)	195 (76%)	60 (24%)	1	4
3	C	238/256 (93%)	166 (70%)	72 (30%)	0	1
All	All	705/748 (94%)	524 (74%)	181 (26%)	0	3

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	CYS
1	A	10	VAL
1	A	12	VAL
1	A	20	LEU
1	A	23	ILE
1	A	25	ASP
1	A	32	LEU
1	A	34	ASP
1	A	44	SER
1	A	48	TYR
1	A	56	LEU
1	A	57	PHE
1	A	62	GLN
1	A	68	GLN
1	A	70	LEU
1	A	75	ILE
1	A	81	LEU
1	A	84	PHE
1	A	87	LEU
1	A	91	GLU
1	A	101	LEU
1	A	102	ASN
1	A	111	GLN
1	A	112	LEU
1	A	118	VAL
1	A	141	CYS
1	A	165	GLU
1	A	170	ILE
1	A	177	ILE
1	A	181	TYR
1	A	184	GLU
1	A	194	VAL
1	A	195	THR

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Mol	Chain	Res	Type
1	A	198	CYS
1	A	199	LEU
1	A	201	GLU
1	A	202	GLU
1	A	205	GLN
1	A	206	GLN
1	A	207	LEU
1	A	223	ARG
1	A	233	ASN
1	A	234	LEU
1	A	236	LEU
1	A	238	ILE
1	A	245	ARG
1	A	251	ILE
1	A	265	LEU
2	B	7	ILE
2	B	8	VAL
2	B	21	ASN
2	B	22	MET
2	B	29	THR
2	B	32	LEU
2	B	34	ILE
2	B	41	PHE
2	B	54	MET
2	B	58	LEU
2	B	61	GLU
2	B	62	ASN
2	B	67	PHE
2	B	79	ILE
2	B	80	TYR
2	B	83	LEU
2	B	84	THR
2	B	85	SER
2	B	88	LEU
2	B	89	SER
2	B	90	ARG
2	B	93	LYS
2	B	94	THR
2	B	103	ILE
2	B	110	PHE
2	B	113	LEU
2	B	115	VAL

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Mol	Chain	Res	Type
2	B	120	LEU
2	B	122	MET
2	B	126	SER
2	B	127	ARG
2	B	129	VAL
2	B	141	LYS
2	B	142	LEU
2	B	145	ASP
2	B	146	LEU
2	B	150	VAL
2	B	151	VAL
2	B	162	VAL
2	B	165	THR
2	B	166	MET
2	B	174	LYS
2	B	176	ILE
2	B	182	ILE
2	B	194	ILE
2	B	196	THR
2	B	202	THR
2	B	215	SER
2	B	224	VAL
2	B	234	ILE
2	B	240	PHE
2	B	247	ASN
2	B	249	THR
2	B	254	ASN
2	B	261	VAL
2	B	265	LEU
2	B	266	LEU
2	B	273	GLN
2	B	276	ILE
2	B	279	LEU
3	C	14	GLN
3	C	17	LEU
3	C	18	VAL
3	C	28	SER
3	C	30	ILE
3	C	31	LEU
3	C	34	ILE
3	C	37	ARG
3	C	42	CYS

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Mol	Chain	Res	Type
3	C	49	ILE
3	C	52	THR
3	C	64	PHE
3	C	65	ILE
3	C	71	GLN
3	C	72	GLU
3	C	75	VAL
3	C	81	THR
3	C	83	ARG
3	C	84	ILE
3	C	88	VAL
3	C	93	LEU
3	C	96	PHE
3	C	98	SER
3	C	101	MET
3	C	111	CYS
3	C	112	TYR
3	C	123	LEU
3	C	125	GLU
3	C	128	VAL
3	C	129	VAL
3	C	136	THR
3	C	140	GLU
3	C	141	GLU
3	C	146	ASP
3	C	150	THR
3	C	153	ILE
3	C	158	LEU
3	C	163	LEU
3	C	164	ARG
3	C	169	GLU
3	C	170	LEU
3	C	172	MET
3	C	180	THR
3	C	181	MET
3	C	184	ASP
3	C	189	ARG
3	C	203	TYR
3	C	208	ASP
3	C	209	LEU
3	C	215	CYS
3	C	220	VAL

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Mol	Chain	Res	Type
3	C	221	ASN
3	C	222	ARG
3	C	225	ILE
3	C	227	LEU
3	C	228	LEU
3	C	236	VAL
3	C	237	LEU
3	C	240	LYS
3	C	241	VAL
3	C	242	SER
3	C	251	LEU
3	C	253	LEU
3	C	254	GLN
3	C	255	TYR
3	C	257	ILE
3	C	259	ASN
3	C	260	GLU
3	C	263	GLN
3	C	264	ILE
3	C	267	VAL
3	C	275	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	18	HIS
1	A	42	ASN
1	A	102	ASN
1	A	122	HIS
1	A	182	HIS
1	A	205	GLN
1	A	206	GLN
1	A	210	GLN
1	A	235	ASN
1	A	259	HIS
2	B	21	ASN
2	B	60	GLN
2	B	62	ASN
2	B	65	ASN
2	B	96	GLN
2	B	254	ASN

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Mol	Chain	Res	Type
2	B	258	ASN
3	C	14	GLN
3	C	26	ASN
3	C	71	GLN
3	C	135	ASN
3	C	214	HIS
3	C	217	GLN
3	C	219	GLN
3	C	221	ASN
3	C	247	ASN
3	C	259	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	264/270 (97%)	-0.06	1 (0%) 88 79	40, 69, 79, 79	0
2	B	278/286 (97%)	0.04	2 (0%) 84 69	39, 68, 79, 80	0
3	C	264/282 (93%)	-0.04	0 100 100	38, 71, 79, 79	0
All	All	806/838 (96%)	-0.02	3 (0%) 88 79	38, 69, 79, 80	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	37	ASP	4.4
1	A	134	ALA	2.3
2	B	233	ASP	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.