



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:06 AM UTC

PDB ID : 8QJA / pdb_00008qja
Title : T6SS-linked Rhs repeat protein - Advenella mimigardefordensis VgrG-Rhs core
Authors : Kielkopf, C.S.; Shneider, M.M.; Leiman, P.G.; Taylor, N.M.I.
Deposited on : 2023-09-13
Resolution : 3.36 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

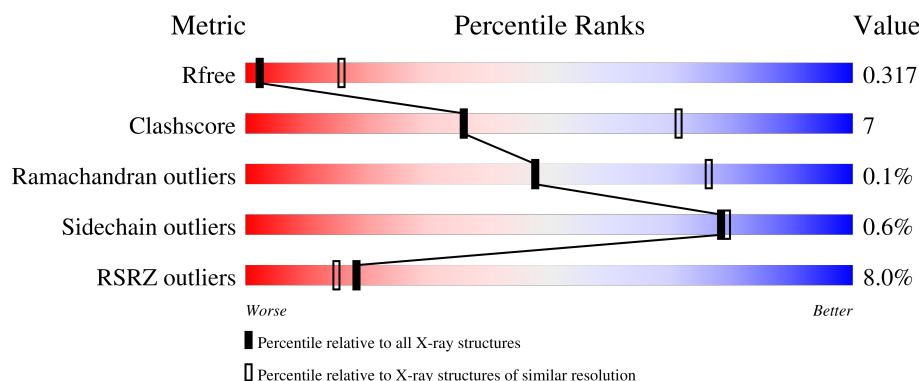
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	1879	5% 43% 11% 46%
1	B	1879	4% 44% 11% 45%
1	C	1879	4% 44% 11% 46%
1	D	1879	4% 44% 10% 46%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33470 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 Putative type VI secretion system YD repeat-containing Rhs element Vgr protein.

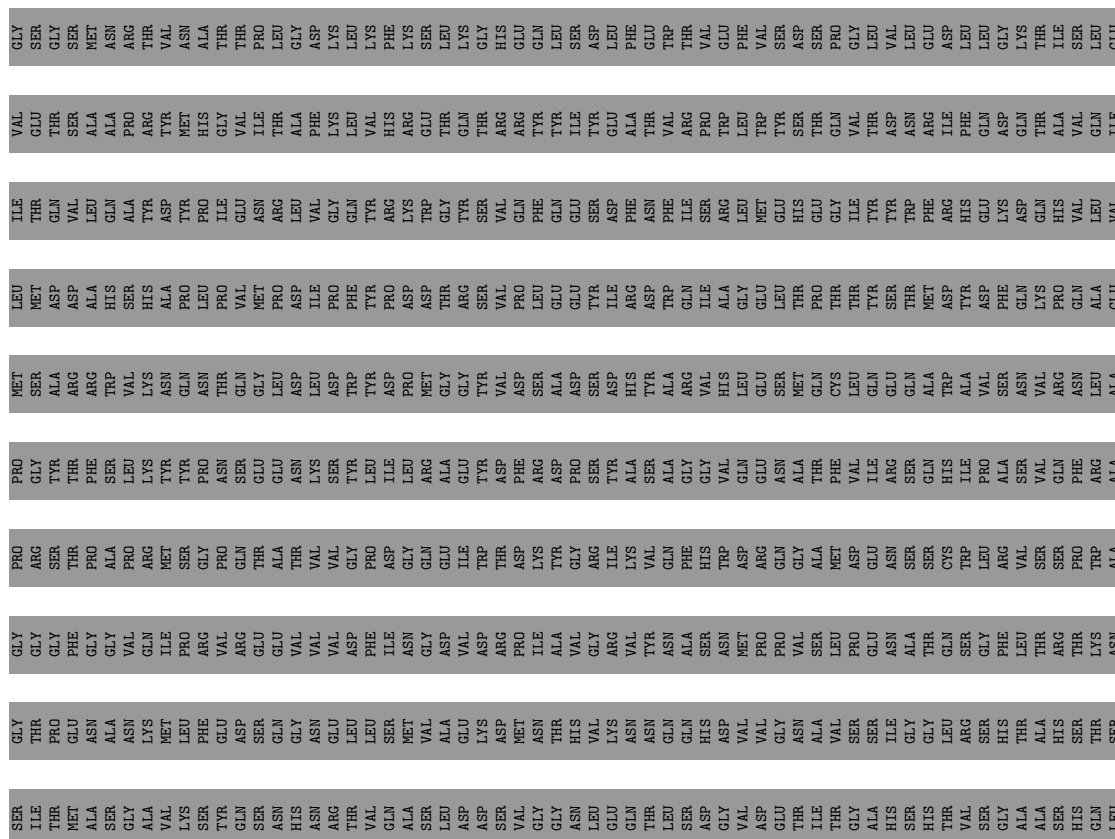
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1021	Total	C	N	O	S	0	0	0
			8365	5240	1479	1631	15			
1	B	1026	Total	C	N	O	S	0	0	0
			8390	5255	1484	1636	15			
1	C	1020	Total	C	N	O	S	0	0	0
			8355	5233	1478	1629	15			
1	D	1021	Total	C	N	O	S	0	0	0
			8360	5236	1479	1630	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-802	GLY	-	expression tag	UNP W0PIA9
A	-801	SER	-	expression tag	UNP W0PIA9
A	-800	GLY	-	expression tag	UNP W0PIA9
A	-799	SER	-	expression tag	UNP W0PIA9
B	-802	GLY	-	expression tag	UNP W0PIA9
B	-801	SER	-	expression tag	UNP W0PIA9
B	-800	GLY	-	expression tag	UNP W0PIA9
B	-799	SER	-	expression tag	UNP W0PIA9
C	-802	GLY	-	expression tag	UNP W0PIA9
C	-801	SER	-	expression tag	UNP W0PIA9
C	-800	GLY	-	expression tag	UNP W0PIA9
C	-799	SER	-	expression tag	UNP W0PIA9
D	-802	GLY	-	expression tag	UNP W0PIA9
D	-801	SER	-	expression tag	UNP W0PIA9
D	-800	GLY	-	expression tag	UNP W0PIA9
D	-799	SER	-	expression tag	UNP W0PIA9







F1036	R1037	E926	D831	E799	Y667	D499	R362	Y202	R44	ILE
P1041	D831	D804	P881	E500	R681	E500	A363	H203	R44	LYS
D1050	Y940	A806	P883	G502	G502	G502	V368	G207	L48	THR
P1051	F945	R812	S684	R503	S684	R503	D383	D208	F50	ALA
T1052	F1055	F1056	G685	A518	G685	A518	P384	D209	V51	GLY
G1053	F1055	F1056	E686	R527	E686	R527	N387	P212	E59	ARG
F1054	F1055	F1056	S689	K543	S689	K543	P405	R214	R62	ASN
F1055	F1055	F1056	Y693	L546	Y693	L546	H408	T216	T63	GLY
G1056	F1055	F1056	G694	L549	G694	L549	Q413	L217	Y64	VAL
F1060	F1055	F1056	A695	Q556	A695	Q556	Q413	A218	L77	ALA
A1064	P1065	P1066	V698	D562	V698	D562	E417	R219	L77	LYS
P1065	P1066	P1067	L702	D562	L702	D562	Q422	Y220	R80	THR
T1067	P1067	P1068	E707	D562	E707	D562	Q422	Q221	T83	ALA
A1068	P1068	P1069	R721	R566	R721	R566	S423	A230	G95	GLY
N1069	P1069	P1070	K722	R566	K722	R566	V424	Q234	R105	THR
N1070	P1070	P1071	R723	V571	R723	V571	N425	Y235	R105	GLY
D1071	P1071	P1072	R723	V571	R723	V571	P426	E236	Q116	VAL
P1072	P1072	P1073	L729	D574	L729	D574	V430	H246	E117	ALA
P1073	P1073	P1074	D735	D574	D735	D574	S431	L247	E117	ASP
F1074	P1074	P1075	V736	A595	V736	A595	T432	W118	Y119	GLY
G1075	P1075	P1076	S738	R597	S738	R597	L433	D120	Y119	ALA
F1076	P1076	P1077	R739	R597	R739	R597	S434	R121	D120	THR
F1077	P1077	P1078	N746	E602	N746	E602	L441	T122	GLY	ASN
F1078	P1078	P1079	L747	Y603	L747	Y603	T442	E123	ALA	VAL
F1079	P1079	P1080	A748	D604	A748	D604	R443	E124	ALA	ALA
F1080	P1080	P1081	Q749	L610	Q749	L610	S448	I126	ALA	THR
F1081	P1081	P1082	L755	K611	L755	K611	N448	E136	ALA	THR
F1082	P1082	P1083	R756	R612	R756	R612	K450	V137	ALA	THR
F1083	P1083	P1084	S757	R613	S757	R613	E455	S138	ALA	THR
F1084	P1084	P1085	R758	N634	R758	N634	Y456	Q139	ALA	THR
F1085	P1085	P1086	D765	C637	D765	C637	D457	Q142	ALA	THR
F1086	P1086	P1087	G766	E642	G766	E642	L458	R143	ALA	THR
F1087	P1087	P1088	S767	Y643	S767	Y643	L459	T144	ALA	THR
F1088	P1088	P1089	L768	D644	L768	D644	K464	E148	ALA	THR
F1089	P1089	P1090	I771	N647	I771	N647	D467	S150	ALA	THR
F1090	P1090	P1091	D772	I650	D772	I650	M471	R155	ALA	THR
F1091	P1091	P1092	S774	R651	S774	R651	M479	A160	ALA	THR
F1092	P1092	P1093	R788	N657	R788	N657	N484	D161	ALA	THR
F1093	P1093	P1094	L789	N662	L789	N662	E485	R162	ALA	THR
F1094	P1094	P1095	A792	R663	A792	R663	F354	V181	ALA	THR
F1095	P1095	P1096	T793	E664	T793	E664	L358	V188	ALA	THR
F1096	P1096	P1097	A794	Y665	A794	Y665	T361	D191	ALA	THR
F1097	P1097	P1098	F795	V666	F795	V666			ALA	THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.24Å 97.78Å 215.01Å 85.69° 89.99° 76.89°	Depositor
Resolution (Å)	48.48 – 3.36 48.48 – 3.36	Depositor EDS
% Data completeness (in resolution range)	91.2 (48.48-3.36) 93.9 (48.48-3.36)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.20.1_4487, BUSTER	Depositor
R, R_{free}	0.257 , 0.317 0.257 , 0.317	Depositor DCC
R_{free} test set	3510 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.874	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	33470	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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 [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	0.10	0/8565	0.34	0/11607
1	B	0.10	0/8590	0.34	0/11641
1	C	0.11	0/8555	0.33	0/11593
1	D	0.11	0/8560	0.34	0/11600
All	All	0.10	0/34270	0.33	0/46441

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	8365	0	7857	127	0
1	B	8390	0	7882	121	0
1	C	8355	0	7844	118	0
1	D	8360	0	7849	115	0
All	All	33470	0	31432	475	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 7.

All (475) 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:B:29:ARG:NH2	1:B:121:ARG:O	2.09	0.85
1:B:55:VAL:HG11	1:B:417:GLU:HB3	1.57	0.84
1:D:299:ASP:HB2	1:D:543:LYS:HE3	1.59	0.83
1:A:219:ARG:HH22	1:A:236:GLU:HG2	1.47	0.80
1:C:117:GLU:HG2	1:C:128:ARG:HG2	1.65	0.79
1:C:29:ARG:NH2	1:C:121:ARG:O	2.16	0.77
1:B:257:ARG:NH1	1:B:520:ASP:O	2.18	0.77
1:B:692:ARG:HG2	1:B:698:VAL:HA	1.66	0.77
1:A:257:ARG:NH1	1:A:520:ASP:O	2.18	0.76
1:C:257:ARG:NH1	1:C:520:ASP:O	2.18	0.76
1:D:144:THR:HB	1:D:160:ALA:HB3	1.66	0.76
1:C:635:GLU:HG3	1:D:571:VAL:HG21	1.67	0.76
1:C:143:ARG:NH1	1:C:145:GLU:OE2	2.18	0.76
1:B:994:ARG:HE	1:B:1003:ASP:HB2	1.48	0.75
1:C:219:ARG:HB2	1:C:232:VAL:HB	1.66	0.75
1:A:144:THR:HB	1:A:160:ALA:HB3	1.68	0.75
1:B:26:LYS:HD2	1:B:105:ARG:HH21	1.52	0.74
1:B:729:LEU:HB2	1:B:748:ALA:HB2	1.68	0.74
1:A:1065:PRO:HD3	1:A:1076:LEU:HD11	1.70	0.73
1:A:213:LEU:HB3	1:A:215:ARG:HH12	1.53	0.73
1:A:348:LYS:HB3	1:A:361:THR:HB	1.71	0.72
1:B:579:LYS:NZ	1:B:581:ASN:OD1	2.23	0.71
1:D:972:GLN:HB3	1:D:981:LEU:HB2	1.72	0.71
1:B:656:TYR:HB2	1:B:663:ARG:HB2	1.73	0.70
1:C:758:ARG:HH21	1:C:771:ILE:HD13	1.54	0.70
1:A:364:ASP:OD1	1:A:366:THR:OG1	2.09	0.70
1:B:652:GLU:HB2	1:B:667:TRP:HB2	1.72	0.69
1:B:692:ARG:HD2	1:B:696:GLY:O	1.93	0.69
1:A:1021:GLN:HB3	1:A:1073:PRO:HD3	1.73	0.69
1:B:185:ILE:HG13	1:B:186:GLN:HG2	1.73	0.69
1:D:644:ASP:HB3	1:D:650:ILE:HD11	1.75	0.69
1:C:616:HIS:HD2	1:D:556:GLN:HB2	1.56	0.68
1:B:208:ASP:HA	1:B:211:THR:HG22	1.75	0.68
1:D:602:GLU:OE2	1:D:613:ARG:NH1	2.26	0.68
1:C:871:ARG:NH1	1:C:896:ASP:OD1	2.26	0.68
1:D:597:ARG:NH1	1:D:867:ASP:O	2.26	0.68
1:C:363:ALA:HB3	1:C:606:MET:HE3	1.76	0.67
1:C:62:ARG:HD2	1:C:77:LEU:HD13	1.75	0.67
1:A:62:ARG:HD2	1:A:77:LEU:HD13	1.77	0.66
1:B:865:GLU:HB2	1:B:874:LYS:HB3	1.78	0.66
1:C:996:SER:HB3	1:C:1002:LEU:HD21	1.78	0.66
1:D:518:ALA:HB3	1:D:527:ARG:HB3	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:HG13	1:A:186:GLN:HG3	1.76	0.66
1:B:787:ASP:O	1:B:1066:ASN:HB3	1.96	0.66
1:B:1069:ASN:OD1	1:B:1070:TRP:N	2.30	0.65
1:B:677:ARG:C	1:B:692:ARG:HH22	2.03	0.65
1:C:729:LEU:HB2	1:C:748:ALA:HB2	1.76	0.65
1:A:121:ARG:NH1	1:A:353:GLU:O	2.29	0.65
1:C:26:LYS:HD3	1:C:123:GLU:HG2	1.79	0.65
1:C:616:HIS:CD2	1:D:556:GLN:HB2	2.32	0.65
1:A:433:LEU:HD22	1:A:441:LEU:HD11	1.79	0.64
1:C:185:ILE:HG13	1:C:186:GLN:HG3	1.80	0.64
1:C:945:PHE:HB2	1:C:1021:GLN:HG2	1.80	0.64
1:C:1067:THR:HA	1:C:1071:ILE:HD11	1.79	0.64
1:C:144:THR:HB	1:C:160:ALA:HB3	1.80	0.64
1:B:408:HIS:HB3	1:B:426:PRO:HB3	1.80	0.64
1:A:112:LEU:HD11	1:A:127:TRP:HB3	1.79	0.63
1:B:62:ARG:HD2	1:B:77:LEU:HD13	1.80	0.63
1:D:484:ASN:OD1	1:D:485:GLU:N	2.32	0.63
1:D:221:GLN:HB3	1:D:230:ALA:HB3	1.80	0.63
1:A:1067:THR:HA	1:A:1071:ILE:HD11	1.81	0.63
1:C:602:GLU:OE1	1:D:837:LYS:NZ	2.32	0.62
1:C:1021:GLN:HB3	1:C:1073:PRO:HG3	1.79	0.62
1:C:597:ARG:NH1	1:C:867:ASP:O	2.33	0.62
1:A:221:GLN:HB3	1:A:230:ALA:HB3	1.81	0.62
1:D:368:VAL:HG22	1:D:384:PRO:HD3	1.80	0.62
1:D:422:GLN:HE21	1:D:430:VAL:HG13	1.63	0.62
1:D:142:GLN:HA	1:D:162:ARG:HD3	1.81	0.62
1:D:26:LYS:HG3	1:D:105:ARG:NH2	2.15	0.62
1:C:245:ASN:ND2	1:C:266:ASP:O	2.30	0.62
1:A:729:LEU:HB2	1:A:748:ALA:HB2	1.82	0.61
1:A:701:ILE:HD12	1:A:709:LEU:HD11	1.83	0.61
1:C:34:GLY:HA2	1:C:38:LEU:HG	1.82	0.61
1:D:478:ASN:HB3	1:D:484:ASN:HB3	1.82	0.60
1:A:972:GLN:HB3	1:A:981:LEU:HB2	1.82	0.60
1:A:545:ARG:NH1	1:A:565:ASP:OD1	2.34	0.60
1:B:255:THR:HG22	1:B:500:GLU:HB2	1.82	0.60
1:C:722:LYS:HB2	1:C:730:ALA:HB3	1.83	0.60
1:A:66:SER:O	1:A:80:ARG:NH1	2.33	0.60
1:A:1072:ASP:HB2	1:A:1073:PRO:HD2	1.82	0.60
1:D:945:PHE:HB2	1:D:1021:GLN:HG2	1.82	0.60
1:A:794:ALA:O	1:A:797:GLU:HG2	2.02	0.60
1:D:905:GLN:OE1	1:D:908:SER:OG	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:TYR:HE1	1:B:360:LEU:HD13	1.67	0.60
1:C:129:ARG:NH2	1:C:132:VAL:O	2.33	0.60
1:B:1032:HIS:HB2	1:B:1039:TYR:HB3	1.84	0.60
1:C:793:THR:HG22	1:C:798:THR:HG23	1.83	0.59
1:C:692:ARG:NH2	1:C:942:GLU:OE2	2.35	0.59
1:B:726:ASN:OD1	1:B:987:GLY:N	2.34	0.59
1:A:602:GLU:HB2	1:A:611:LYS:HB2	1.83	0.59
1:C:99:TYR:HB3	1:C:107:VAL:HB	1.85	0.59
1:D:735:ASP:OD1	1:D:736:VAL:N	2.36	0.59
1:B:689:SER:HB2	1:B:702:LEU:HB2	1.83	0.59
1:C:1023:GLN:HB3	1:C:1032:HIS:HB3	1.84	0.58
1:C:383:ASP:OD1	1:C:387:ASN:N	2.36	0.58
1:D:62:ARG:HA	1:D:83:THR:HG22	1.85	0.58
1:B:34:GLY:HA2	1:B:38:LEU:HG	1.85	0.58
1:C:710:SER:HB3	1:C:723:ARG:HG2	1.84	0.58
1:A:331:ASP:OD1	1:A:332:GLU:N	2.36	0.58
1:B:604:ASP:HB3	1:B:610:LEU:HD11	1.85	0.58
1:B:457:ASP:OD1	1:B:458:LEU:N	2.36	0.58
1:B:1052:ILE:HD12	1:B:1076:LEU:HB3	1.86	0.58
1:C:181:VAL:HG22	1:C:188:VAL:HB	1.85	0.58
1:A:556:GLN:HB2	1:B:616:HIS:ND1	2.18	0.58
1:C:606:MET:HA	1:C:606:MET:HE2	1.86	0.58
1:A:368:VAL:HG22	1:A:384:PRO:HD3	1.86	0.57
1:D:181:VAL:HG22	1:D:188:VAL:HB	1.87	0.57
1:D:348:LYS:HB2	1:D:361:THR:HB	1.87	0.57
1:C:348:LYS:HB3	1:C:361:THR:HB	1.87	0.57
1:A:424:VAL:HG22	1:A:430:VAL:HG12	1.87	0.57
1:C:1050:ASP:H	1:C:1060:PHE:HB3	1.70	0.57
1:C:62:ARG:HA	1:C:83:THR:HG22	1.86	0.57
1:A:213:LEU:HB3	1:A:215:ARG:NH1	2.18	0.56
1:A:457:ASP:OD1	1:A:458:LEU:N	2.38	0.56
1:B:465:GLN:HG2	1:B:473:GLU:HB3	1.87	0.56
1:B:562:ASP:OD1	1:B:566:ARG:N	2.36	0.56
1:B:1050:ASP:H	1:B:1060:PHE:HB3	1.69	0.56
1:C:845:GLU:HB3	1:C:854:ARG:HB3	1.86	0.56
1:C:972:GLN:HB3	1:C:981:LEU:HB2	1.88	0.56
1:A:707:GLU:OE2	1:A:710:SER:OG	2.22	0.56
1:D:975:HIS:CD2	1:D:976:ILE:HG23	2.41	0.56
1:D:413:GLN:NE2	1:D:422:GLN:OE1	2.38	0.56
1:C:331:ASP:OD1	1:C:332:GLU:N	2.39	0.56
1:B:80:ARG:HE	1:B:246:HIS:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ASP:OD1	1:A:471:ASN:N	2.37	0.55
1:B:68:MET:HE3	1:B:104:GLY:HA2	1.88	0.55
1:B:1037:ARG:HA	1:B:1048:GLN:NE2	2.21	0.55
1:A:121:ARG:HH12	1:A:353:GLU:C	2.14	0.55
1:D:34:GLY:HA2	1:D:38:LEU:HG	1.88	0.55
1:C:779:THR:HG23	1:C:794:ALA:HB2	1.88	0.55
1:D:116:GLN:HE21	1:D:118:TRP:NE1	2.05	0.55
1:D:457:ASP:OD1	1:D:458:LEU:N	2.39	0.55
1:A:34:GLY:HA2	1:A:38:LEU:HG	1.88	0.55
1:A:945:PHE:CD2	1:A:1073:PRO:HG3	2.42	0.55
1:D:248:ILE:HG23	1:D:261:LEU:HD12	1.88	0.55
1:A:289:ASP:HB2	1:A:296:TYR:HE1	1.71	0.55
1:A:29:ARG:NH2	1:A:121:ARG:O	2.39	0.55
1:A:62:ARG:HA	1:A:83:THR:HG22	1.88	0.55
1:D:1037:ARG:NH2	1:D:1060:PHE:O	2.38	0.55
1:A:408:HIS:HB3	1:A:426:PRO:HB3	1.87	0.55
1:D:408:HIS:HB3	1:D:426:PRO:HB3	1.87	0.55
1:D:756:ARG:HD2	1:D:774:SER:HB3	1.87	0.54
1:D:116:GLN:HE21	1:D:118:TRP:HE1	1.55	0.54
1:D:842:MET:HE3	1:D:857:LYS:HD3	1.88	0.54
1:B:45:PHE:HE1	1:B:248:ILE:HG13	1.72	0.54
1:B:488:ARG:HH12	1:B:494:LEU:HG	1.72	0.54
1:B:851:ASN:HB3	1:B:866:TRP:CE2	2.42	0.54
1:D:851:ASN:HB3	1:D:866:TRP:CE2	2.43	0.54
1:A:804:ASP:OD1	1:A:808:ASN:N	2.33	0.54
1:C:107:VAL:HG13	1:C:123:GLU:OE1	2.07	0.54
1:D:48:LEU:HD21	1:D:51:VAL:HG23	1.88	0.54
1:D:254:LYS:HB2	1:D:501:GLU:HG2	1.90	0.54
1:D:255:THR:OG1	1:D:503:ARG:NH2	2.41	0.54
1:A:289:ASP:HB3	1:A:294:LYS:HB2	1.90	0.54
1:B:852:LEU:O	1:B:866:TRP:NE1	2.29	0.54
1:A:213:LEU:HD13	1:A:215:ARG:HH22	1.72	0.54
1:C:51:VAL:HG13	1:C:59:GLU:HG2	1.89	0.54
1:D:768:LEU:HD21	1:D:771:ILE:HD11	1.90	0.54
1:C:467:ASP:OD1	1:C:471:ASN:N	2.40	0.54
1:C:744:LYS:HE2	1:C:746:ASN:HD22	1.71	0.54
1:B:126:ILE:HB	1:B:138:SER:HB3	1.90	0.53
1:C:55:VAL:HG11	1:C:417:GLU:HB3	1.90	0.53
1:D:666:VAL:H	1:D:683:PRO:HB3	1.72	0.53
1:D:1050:ASP:H	1:D:1060:PHE:HB3	1.72	0.53
1:C:676:ASN:HB3	1:C:692:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:THR:HG21	1:C:384:PRO:HB3	1.91	0.53
1:D:148:GLU:O	1:D:155:ARG:N	2.42	0.53
1:A:26:LYS:HE3	1:A:123:GLU:O	2.09	0.53
1:A:62:ARG:NH2	1:A:241:TYR:OH	2.41	0.53
1:A:604:ASP:HB3	1:A:610:LEU:HD11	1.91	0.53
1:D:455:GLU:HB2	1:D:464:LYS:HB3	1.91	0.52
1:D:161:ASP:OD1	1:D:162:ARG:N	2.40	0.52
1:D:352:ASP:HB3	1:D:358:LEU:HD11	1.91	0.52
1:D:432:THR:OG1	1:D:443:ARG:NH2	2.38	0.52
1:B:144:THR:HB	1:B:160:ALA:HB3	1.91	0.52
1:D:684:SER:HB2	1:D:686:GLU:OE1	2.09	0.52
1:D:29:ARG:NH1	1:D:124:GLU:OE2	2.36	0.52
1:D:604:ASP:HB3	1:D:610:LEU:HD11	1.92	0.52
1:D:1066:ASN:HD21	1:D:1070:TRP:HD1	1.55	0.52
1:C:756:ARG:HD3	1:C:981:LEU:HD21	1.91	0.52
1:C:851:ASN:HB3	1:C:866:TRP:CE2	2.44	0.52
1:B:48:LEU:HD21	1:B:51:VAL:HG23	1.92	0.52
1:C:83:THR:H	1:C:86:THR:HG1	1.56	0.52
1:D:324:THR:HB	1:D:342:PRO:HG2	1.91	0.52
1:C:476:GLU:HB3	1:C:485:GLU:HG2	1.90	0.51
1:B:872:LEU:O	1:B:892:TYR:OH	2.24	0.51
1:A:476:GLU:HB3	1:A:485:GLU:HG2	1.92	0.51
1:B:1016:ASN:ND2	1:B:1018:LEU:O	2.42	0.51
1:C:457:ASP:OD1	1:C:458:LEU:N	2.39	0.51
1:A:562:ASP:OD1	1:A:566:ARG:N	2.38	0.51
1:B:1052:ILE:HG13	1:B:1076:LEU:HD22	1.93	0.51
1:B:219:ARG:NH2	1:B:236:GLU:OE1	2.26	0.51
1:B:392:ASP:OD2	1:B:401:ARG:NH2	2.40	0.51
1:B:1037:ARG:NH2	1:B:1060:PHE:O	2.41	0.51
1:D:26:LYS:HD2	1:D:123:GLU:HG3	1.93	0.51
1:A:689:SER:HB2	1:A:702:LEU:HB2	1.91	0.51
1:B:476:GLU:HB3	1:B:485:GLU:HG2	1.93	0.51
1:B:331:ASP:OD1	1:B:332:GLU:N	2.44	0.51
1:B:974:ASP:OD1	1:B:978:THR:N	2.41	0.51
1:B:410:SER:HB3	1:B:426:PRO:HD3	1.93	0.50
1:B:413:GLN:OE1	1:B:422:GLN:NE2	2.42	0.50
1:C:53:PRO:O	1:C:186:GLN:NE2	2.44	0.50
1:B:383:ASP:OD1	1:B:387:ASN:N	2.43	0.50
1:B:488:ARG:HD2	1:B:737:MET:HE1	1.94	0.50
1:A:978:THR:HG23	1:A:1020:TYR:H	1.76	0.50
1:A:1052:ILE:HG12	1:A:1055:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:ARG:HB3	1:C:296:TYR:HB2	1.94	0.50
1:C:562:ASP:OD1	1:C:566:ARG:N	2.42	0.50
1:A:546:LEU:HD21	1:A:549:LEU:HD21	1.94	0.50
1:B:348:LYS:HB2	1:B:361:THR:HB	1.94	0.50
1:B:893:ASP:OD1	1:B:894:THR:N	2.43	0.50
1:D:897:ARG:HD3	1:D:1035:ARG:HH21	1.76	0.50
1:D:120:ASP:C	1:D:122:THR:H	2.20	0.50
1:D:353:GLU:HG3	1:D:354:PHE:HD1	1.77	0.49
1:D:681:ARG:NH1	1:D:685:GLY:O	2.43	0.49
1:B:794:ALA:O	1:B:797:GLU:HG2	2.12	0.49
1:C:847:ASP:OD1	1:C:848:ALA:N	2.44	0.49
1:D:799:GLU:OE2	1:D:812:ARG:NH2	2.45	0.49
1:A:842:MET:HE3	1:A:857:LYS:HD3	1.94	0.49
1:C:768:LEU:HD21	1:C:771:ILE:HD11	1.94	0.49
1:D:203:HIS:CD2	1:D:217:LEU:HD13	2.46	0.49
1:D:1000:LYS:HB2	1:D:1041:PRO:HB2	1.95	0.49
1:A:26:LYS:HD2	1:A:123:GLU:HG3	1.92	0.49
1:A:133:ASP:OD1	1:A:149:ARG:NH1	2.44	0.49
1:B:368:VAL:HG22	1:B:384:PRO:HD3	1.94	0.49
1:D:847:ASP:OD1	1:D:848:ALA:N	2.45	0.49
1:D:126:ILE:HB	1:D:138:SER:HB2	1.95	0.49
1:D:434:SER:HB2	1:D:443:ARG:HG2	1.94	0.49
1:A:656:TYR:HB2	1:A:663:ARG:HB2	1.94	0.49
1:C:998:LEU:O	1:C:1039:TYR:OH	2.26	0.49
1:A:122:THR:HG23	1:A:334:HIS:CE1	2.47	0.49
1:A:595:ALA:O	1:A:849:GLN:NE2	2.44	0.49
1:C:1019:CYS:O	1:C:1023:GLN:HB2	2.13	0.49
1:A:768:LEU:HD21	1:A:771:ILE:HD11	1.95	0.49
1:A:926:GLU:HB2	1:A:935:LYS:HD3	1.93	0.49
1:D:26:LYS:HD3	1:D:28:CYS:SG	2.53	0.49
1:D:1072:ASP:HB3	1:D:1076:LEU:HG	1.94	0.49
1:A:89:VAL:HB	1:A:154:PHE:HB2	1.94	0.48
1:A:235:TYR:OH	1:A:461:ARG:NH1	2.45	0.48
1:A:352:ASP:HB3	1:A:358:LEU:HD11	1.95	0.48
1:B:994:ARG:HB3	1:B:1003:ASP:HB2	1.95	0.48
1:C:780:THR:HB	1:C:793:THR:OG1	2.13	0.48
1:D:139:GLN:O	1:D:142:GLN:HG2	2.12	0.48
1:D:707:GLU:OE1	1:D:723:ARG:NH2	2.45	0.48
1:A:773:ASP:OD1	1:A:774:SER:N	2.45	0.48
1:B:1037:ARG:HA	1:B:1048:GLN:HE21	1.78	0.48
1:D:999:GLY:HA3	1:D:1020:TYR:HE1	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASP:OD1	1:A:162:ARG:N	2.45	0.48
1:B:285:ARG:NH1	1:B:286:PHE:O	2.47	0.48
1:A:847:ASP:OD1	1:A:848:ALA:N	2.44	0.48
1:B:26:LYS:HD2	1:B:105:ARG:NH2	2.24	0.48
1:C:532:LEU:HD12	1:C:786:LEU:HD12	1.96	0.48
1:D:739:ARG:HH11	1:D:766:GLY:HA2	1.78	0.48
1:C:308:THR:HB	1:C:317:HIS:HB2	1.96	0.48
1:B:308:THR:HB	1:B:317:HIS:HB2	1.94	0.48
1:C:455:GLU:HB2	1:C:464:LYS:HB2	1.96	0.48
1:D:467:ASP:OD1	1:D:471:ASN:N	2.46	0.48
1:C:99:TYR:N	1:C:107:VAL:O	2.35	0.48
1:A:746:ASN:ND2	1:A:755:LEU:HB3	2.28	0.47
1:B:676:ASN:HB3	1:B:692:ARG:NH2	2.28	0.47
1:A:851:ASN:HB3	1:A:866:TRP:CE2	2.48	0.47
1:B:928:THR:HG22	1:B:933:VAL:HG22	1.96	0.47
1:C:461:ARG:HB3	1:C:477:TYR:CZ	2.49	0.47
1:A:105:ARG:NH1	1:A:107:VAL:HG22	2.30	0.47
1:A:799:GLU:HG2	1:A:814:LYS:HB3	1.96	0.47
1:B:121:ARG:NH2	1:B:353:GLU:HB2	2.29	0.47
1:B:161:ASP:OD1	1:B:162:ARG:N	2.46	0.47
1:C:44:ARG:HA	1:C:64:TYR:O	2.15	0.47
1:A:742:GLU:HG3	1:A:759:GLN:HG3	1.96	0.47
1:A:928:THR:HG22	1:A:933:VAL:HG22	1.96	0.47
1:B:779:THR:HG23	1:B:794:ALA:HB2	1.96	0.47
1:B:148:GLU:HG2	1:B:157:LYS:HB2	1.96	0.47
1:B:1052:ILE:HG23	1:B:1055:PHE:HB2	1.97	0.47
1:D:433:LEU:HD22	1:D:441:LEU:HD11	1.95	0.47
1:A:434:SER:HB3	1:A:443:ARG:HG2	1.96	0.47
1:B:112:LEU:HD11	1:B:127:TRP:HB3	1.96	0.47
1:B:920:HIS:HA	1:B:1035:ARG:HH11	1.79	0.47
1:A:852:LEU:O	1:A:866:TRP:NE1	2.35	0.47
1:B:202:TRP:CE3	1:B:214:ARG:HB3	2.50	0.47
1:A:36:ILE:HG13	1:A:37:GLY:N	2.30	0.47
1:A:202:TRP:HA	1:A:215:ARG:O	2.15	0.46
1:A:665:TYR:HB3	1:A:683:PRO:HG2	1.96	0.46
1:C:147:PHE:HB3	1:C:154:PHE:HB3	1.97	0.46
1:C:161:ASP:OD1	1:C:162:ARG:N	2.47	0.46
1:C:676:ASN:HB3	1:C:692:ARG:HH11	1.79	0.46
1:C:975:HIS:CD2	1:C:976:ILE:HG23	2.51	0.46
1:A:213:LEU:HB3	1:A:215:ARG:HH22	1.80	0.46
1:C:335:ASN:HB3	1:C:351:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ARG:NH1	1:B:124:GLU:OE2	2.38	0.46
1:B:1020:TYR:HB2	1:B:1023:GLN:HG3	1.97	0.46
1:C:721:ARG:HG2	1:C:729:LEU:HD11	1.98	0.46
1:A:248:ILE:HD11	1:A:251:TYR:HB3	1.98	0.46
1:B:36:ILE:HG13	1:B:37:GLY:N	2.31	0.46
1:C:488:ARG:HH12	1:C:494:LEU:HG	1.80	0.46
1:C:804:ASP:OD1	1:C:808:ASN:N	2.38	0.46
1:B:799:GLU:OE2	1:B:812:ARG:NH1	2.49	0.46
1:C:443:ARG:HG3	1:C:451:THR:HG23	1.98	0.46
1:A:946:VAL:HG22	1:A:977:GLY:HA3	1.98	0.46
1:A:329:ILE:HB	1:A:338:GLU:HB3	1.98	0.46
1:B:62:ARG:HA	1:B:83:THR:HG22	1.97	0.45
1:A:612:ARG:HG2	1:A:869:PHE:CZ	2.51	0.45
1:D:383:ASP:HB2	1:D:384:PRO:HD2	1.98	0.45
1:D:546:LEU:HD21	1:D:549:LEU:HD21	1.97	0.45
1:A:845:GLU:HB3	1:A:854:ARG:HB3	1.98	0.45
1:B:72:ASP:HA	1:B:79:PRO:HA	1.98	0.45
1:C:201:ILE:HB	1:C:218:ALA:HB3	1.99	0.45
1:A:183:THR:HG22	1:A:184:ALA:H	1.82	0.45
1:A:974:ASP:OD1	1:A:978:THR:N	2.47	0.45
1:C:36:ILE:HG13	1:C:37:GLY:N	2.32	0.45
1:C:584:LYS:HB3	1:C:585:PRO:HD3	1.99	0.45
1:A:945:PHE:HE2	1:A:1035:ARG:HG3	1.82	0.45
1:C:405:PRO:HB2	1:C:645:VAL:HG21	1.98	0.45
1:A:105:ARG:CZ	1:A:107:VAL:HG22	2.47	0.45
1:A:528:LYS:NZ	1:A:530:ASP:OD1	2.49	0.45
1:B:756:ARG:HD2	1:B:774:SER:OG	2.16	0.45
1:B:975:HIS:CD2	1:B:976:ILE:HG23	2.51	0.45
1:C:488:ARG:HD2	1:C:737:MET:HE1	1.97	0.45
1:D:1071:ILE:HG22	1:D:1073:PRO:HD3	1.98	0.45
1:B:1019:CYS:O	1:B:1023:GLN:HB2	2.17	0.45
1:D:80:ARG:HE	1:D:246:HIS:HB2	1.82	0.45
1:C:604:ASP:HB3	1:C:610:LEU:HD11	1.99	0.45
1:D:36:ILE:HG13	1:D:37:GLY:N	2.32	0.45
1:A:112:LEU:O	1:A:129:ARG:NH1	2.50	0.45
1:B:581:ASN:HB2	1:B:591:SER:OG	2.17	0.45
1:D:308:THR:HB	1:D:317:HIS:HB2	1.99	0.45
1:B:768:LEU:O	1:B:783:TYR:OH	2.33	0.45
1:D:27:GLU:OE2	1:D:44:ARG:NH1	2.50	0.45
1:D:657:ASN:ND2	1:D:662:ASN:OD1	2.50	0.45
1:C:221:GLN:HB3	1:C:230:ALA:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:692:ARG:HG2	1:C:698:VAL:HG22	1.98	0.44
1:A:105:ARG:HH12	1:A:123:GLU:HG2	1.82	0.44
1:A:335:ASN:HB3	1:A:351:TYR:CZ	2.52	0.44
1:B:1037:ARG:NH1	1:B:1075:GLY:O	2.46	0.44
1:C:201:ILE:O	1:C:217:LEU:N	2.40	0.44
1:D:634:ASN:OD1	1:D:637:CYS:N	2.51	0.44
1:A:156:LEU:O	1:A:169:LEU:HD12	2.16	0.44
1:C:29:ARG:HD2	1:C:334:HIS:C	2.42	0.44
1:D:804:ASP:OD1	1:D:805:PRO:HD2	2.18	0.44
1:C:40:VAL:O	1:C:271:LYS:HG2	2.18	0.44
1:A:80:ARG:HH12	1:A:247:LEU:HD23	1.83	0.44
1:B:271:LYS:HD3	1:B:288:TRP:CD1	2.52	0.44
1:C:76:GLU:OE1	1:C:86:THR:HG22	2.18	0.44
1:D:387:ASN:HB3	1:D:405:PRO:HG2	2.00	0.44
1:D:788:ARG:HA	1:D:1065:PRO:O	2.18	0.44
1:A:83:THR:H	1:A:86:THR:HG1	1.66	0.44
1:D:597:ARG:HH21	1:D:849:GLN:HG3	1.81	0.44
1:D:663:ARG:NH1	1:D:926:GLU:OE1	2.50	0.44
1:B:262:GLU:OE1	1:B:274:ARG:NH2	2.46	0.44
1:B:329:ILE:HB	1:B:338:GLU:HB3	2.00	0.44
1:D:562:ASP:OD1	1:D:566:ARG:N	2.41	0.44
1:A:383:ASP:OD1	1:A:387:ASN:N	2.49	0.44
1:A:658:ALA:HB1	1:A:891:ILE:HD12	1.99	0.44
1:C:408:HIS:HB3	1:C:426:PRO:HB3	2.00	0.44
1:D:422:GLN:HE22	1:D:424:VAL:CG2	2.31	0.44
1:A:461:ARG:HB3	1:A:477:TYR:CZ	2.53	0.43
1:B:541:ASP:OD1	1:B:545:ARG:N	2.51	0.43
1:B:972:GLN:HB3	1:B:981:LEU:HB2	1.99	0.43
1:D:215:ARG:NH1	1:D:459:LEU:HD22	2.33	0.43
1:A:455:GLU:HB2	1:A:464:LYS:HB3	1.99	0.43
1:A:557:PHE:CD2	1:A:572:GLY:HA2	2.54	0.43
1:B:847:ASP:OD1	1:B:848:ALA:N	2.52	0.43
1:C:546:LEU:HD21	1:C:549:LEU:HD21	2.01	0.43
1:B:1035:ARG:HE	1:B:1036:PHE:HE1	1.67	0.43
1:A:121:ARG:HH22	1:A:353:GLU:HA	1.84	0.43
1:A:854:ARG:NH1	1:A:863:GLU:OE2	2.52	0.43
1:B:155:ARG:HD3	1:B:155:ARG:HA	1.88	0.43
1:B:177:PHE:HB3	1:B:192:HIS:CE1	2.54	0.43
1:B:227:ASP:CG	1:B:246:HIS:HD1	2.26	0.43
1:B:576:LYS:NZ	1:B:849:GLN:O	2.38	0.43
1:C:39:ASP:OD1	1:C:40:VAL:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ASP:HB3	1:D:333:PHE:H	1.83	0.43
1:D:689:SER:HB2	1:D:702:LEU:HB2	2.00	0.43
1:D:999:GLY:HA3	1:D:1020:TYR:CE1	2.54	0.43
1:B:1046:PHE:CZ	1:B:1075:GLY:HA2	2.54	0.43
1:C:689:SER:HB2	1:C:702:LEU:HB2	2.01	0.43
1:D:49:ASP:OD2	1:D:62:ARG:NH1	2.52	0.43
1:D:746:ASN:OD1	1:D:755:LEU:HA	2.17	0.43
1:A:29:ARG:HD2	1:A:334:HIS:C	2.43	0.42
1:B:215:ARG:CZ	1:B:459:LEU:HD11	2.50	0.42
1:C:668:GLU:HB2	1:C:681:ARG:HB2	2.01	0.42
1:C:721:ARG:HG3	1:C:731:VAL:HG22	2.00	0.42
1:D:150:SER:HB3	1:D:155:ARG:HG2	2.02	0.42
1:D:219:ARG:HH22	1:D:236:GLU:HG2	1.83	0.42
1:B:68:MET:HE1	1:B:82:ILE:HB	2.00	0.42
1:B:211:THR:OG1	1:B:212:PRO:HD3	2.19	0.42
1:A:739:ARG:HD2	1:A:762:TYR:CG	2.54	0.42
1:A:898:ARG:HH12	1:A:1026:ASP:CG	2.28	0.42
1:B:183:THR:HG22	1:B:184:ALA:H	1.83	0.42
1:D:1020:TYR:HB3	1:D:1021:GLN:H	1.60	0.42
1:A:27:GLU:OE2	1:A:44:ARG:NH1	2.52	0.42
1:A:40:VAL:O	1:A:271:LYS:HG2	2.18	0.42
1:C:693:TYR:OH	1:C:713:ARG:HD2	2.19	0.42
1:C:1035:ARG:HG2	1:C:1036:PHE:CD2	2.55	0.42
1:D:721:ARG:HB3	1:D:729:LEU:HD11	2.01	0.42
1:A:201:ILE:O	1:A:217:LEU:N	2.49	0.42
1:B:461:ARG:HB3	1:B:477:TYR:CZ	2.54	0.42
1:A:537:HIS:HB2	1:A:550:GLN:HB3	2.01	0.42
1:A:749:GLN:O	1:D:749:GLN:NE2	2.53	0.42
1:B:677:ARG:O	1:B:692:ARG:NH2	2.48	0.42
1:D:44:ARG:HA	1:D:64:TYR:O	2.20	0.42
1:D:996:SER:HB3	1:D:1002:LEU:HD21	2.01	0.42
1:B:83:THR:H	1:B:86:THR:HG1	1.68	0.42
1:B:1052:ILE:CD1	1:B:1076:LEU:HB3	2.49	0.42
1:C:411:GLU:OE2	1:C:413:GLN:NE2	2.53	0.42
1:D:421:ILE:HD13	1:D:421:ILE:HA	1.90	0.42
1:A:169:LEU:HD23	1:A:181:VAL:HG13	2.01	0.42
1:A:756:ARG:HD2	1:A:774:SER:HB2	2.02	0.42
1:B:574:ASP:OD1	1:B:574:ASP:N	2.53	0.42
1:D:612:ARG:HG2	1:D:869:PHE:CZ	2.55	0.42
1:B:557:PHE:HB2	1:B:573:PHE:CE1	2.55	0.42
1:C:758:ARG:HE	1:C:771:ILE:HG21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:758:ARG:NH1	1:D:773:ASP:OD2	2.50	0.42
1:B:531:PRO:HB2	1:B:785:ALA:HB1	2.02	0.41
1:C:227:ASP:HB3	1:C:243:TYR:CE1	2.55	0.41
1:C:710:SER:HB3	1:C:723:ARG:CG	2.49	0.41
1:A:39:ASP:OD1	1:A:40:VAL:N	2.52	0.41
1:A:624:ASP:HB3	1:A:630:ILE:HG13	2.03	0.41
1:A:1034:ASN:ND2	1:A:1039:TYR:HB2	2.35	0.41
1:A:36:ILE:HD12	1:A:272:CYS:HB3	2.01	0.41
1:C:215:ARG:HH12	1:C:234:GLN:HB2	1.85	0.41
1:C:950:GLN:HB2	1:C:971:TYR:CE2	2.55	0.41
1:A:26:LYS:NZ	1:A:28:CYS:HB3	2.35	0.41
1:A:314:TYR:HB3	1:A:330:ARG:CZ	2.50	0.41
1:B:350:GLU:O	1:B:358:LEU:N	2.49	0.41
1:D:448:SER:HB2	1:D:450:LYS:HG2	2.02	0.41
1:A:788:ARG:HG2	1:A:1065:PRO:HB3	2.02	0.41
1:D:383:ASP:OD1	1:D:387:ASN:N	2.48	0.41
1:C:112:LEU:HD22	1:C:116:GLN:HB3	2.02	0.41
1:C:156:LEU:O	1:C:169:LEU:HD12	2.21	0.41
1:C:285:ARG:HB3	1:C:298:THR:HB	2.03	0.41
1:A:488:ARG:HD2	1:A:737:MET:HE1	2.03	0.41
1:B:44:ARG:HA	1:B:64:TYR:O	2.20	0.41
1:B:389:TRP:CE2	1:B:405:PRO:HD3	2.55	0.41
1:C:255:THR:OG1	1:C:503:ARG:NH2	2.54	0.41
1:D:642:GLU:HB2	1:D:651:ARG:HB3	2.02	0.41
1:B:479:ARG:NH1	1:B:480:TYR:OH	2.54	0.41
1:B:543:LYS:HA	1:B:543:LYS:HD2	1.84	0.41
1:B:746:ASN:ND2	1:B:755:LEU:HB3	2.36	0.41
1:C:724:GLN:HB3	1:C:970:HIS:CE1	2.56	0.41
1:C:971:TYR:CE1	1:C:982:LEU:HD13	2.55	0.41
1:A:142:GLN:HA	1:A:162:ARG:HG2	2.03	0.41
1:A:252:SER:HA	1:A:258:GLY:HA2	2.03	0.41
1:A:945:PHE:HD2	1:A:1022:GLY:HA3	1.86	0.41
1:A:1032:HIS:CE1	1:A:1041:PRO:HG3	2.56	0.41
1:B:557:PHE:CD2	1:B:572:GLY:HA2	2.56	0.41
1:B:569:ARG:HG3	1:B:578:LYS:O	2.21	0.41
1:B:897:ARG:HD3	1:B:1035:ARG:NH1	2.35	0.41
1:C:773:ASP:OD1	1:C:774:SER:N	2.54	0.41
1:C:854:ARG:NH1	1:C:863:GLU:OE2	2.54	0.41
1:D:51:VAL:HG13	1:D:59:GLU:HG2	2.02	0.41
1:D:789:LEU:HD11	1:D:792:ALA:HB2	2.03	0.41
1:D:854:ARG:NH1	1:D:863:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ILE:HD12	1:B:272:CYS:HB3	2.03	0.41
1:B:729:LEU:N	1:B:746:ASN:O	2.42	0.41
1:C:205:VAL:HG12	1:C:208:ASP:H	1.86	0.41
1:C:488:ARG:NH1	1:C:494:LEU:HG	2.36	0.41
1:C:557:PHE:CD2	1:C:572:GLY:HA2	2.56	0.41
1:D:913:THR:HA	1:D:926:GLU:O	2.21	0.41
1:A:27:GLU:CD	1:A:44:ARG:HH12	2.30	0.40
1:D:950:GLN:HB2	1:D:971:TYR:CE2	2.56	0.40
1:C:27:GLU:OE2	1:C:44:ARG:NH1	2.53	0.40
1:C:258:GLY:N	1:C:278:ASP:OD2	2.52	0.40
1:D:116:GLN:NE2	1:D:118:TRP:HE1	2.17	0.40
1:A:364:ASP:OD1	1:A:364:ASP:C	2.65	0.40
1:A:676:ASN:HB3	1:A:692:ARG:NH1	2.36	0.40
1:C:739:ARG:HD2	1:C:762:TYR:CD2	2.57	0.40
1:D:27:GLU:CD	1:D:44:ARG:HH12	2.30	0.40
1:A:44:ARG:HA	1:A:64:TYR:O	2.21	0.40
1:A:349:TYR:CE1	1:A:360:LEU:HD13	2.57	0.40
1:A:801:PHE:HZ	1:A:997:ALA:HB3	1.86	0.40
1:B:488:ARG:HH12	1:B:494:LEU:CG	2.35	0.40
1:C:788:ARG:HA	1:C:1065:PRO:O	2.21	0.40
1:C:795:PHE:CG	1:C:796:ASN:N	2.85	0.40
1:D:39:ASP:OD1	1:D:40:VAL:N	2.54	0.40
1:D:665:TYR:HB3	1:D:683:PRO:HG3	2.03	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	1013/1879 (54%)	969 (96%)	44 (4%)	0	100	100
1	B	1018/1879 (54%)	971 (95%)	47 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1012/1879 (54%)	966 (96%)	45 (4%)	1 (0%)	48	76
1	D	1013/1879 (54%)	968 (96%)	43 (4%)	2 (0%)	43	70
All	All	4056/7516 (54%)	3874 (96%)	179 (4%)	3 (0%)	48	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	694	GLY
1	D	694	GLY
1	D	95	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	889/1607 (55%)	883 (99%)	6 (1%)	76	77
1	B	890/1607 (55%)	886 (100%)	4 (0%)	84	82
1	C	887/1607 (55%)	881 (99%)	6 (1%)	76	77
1	D	887/1607 (55%)	883 (100%)	4 (0%)	81	80
All	All	3553/6428 (55%)	3533 (99%)	20 (1%)	78	79

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	VAL
1	A	200	THR
1	A	366	THR
1	A	430	VAL
1	A	442	ILE
1	A	1021	GLN
1	B	69	THR
1	B	366	THR
1	B	790	VAL

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Mol	Chain	Res	Type
1	B	1052	ILE
1	C	199	THR
1	C	205	VAL
1	C	216	THR
1	C	255	THR
1	C	442	ILE
1	C	1021	GLN
1	D	121	ARG
1	D	255	THR
1	D	421	ILE
1	D	1021	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	ASN
1	A	408	HIS
1	A	422	GLN
1	A	537	HIS
1	A	539	ASN
1	A	648	ASN
1	A	697	HIS
1	A	724	GLN
1	A	733	ASN
1	A	862	GLN
1	A	972	GLN
1	A	1017	ASN
1	A	1021	GLN
1	A	1023	GLN
1	A	1048	GLN
1	B	387	ASN
1	B	633	HIS
1	B	648	ASN
1	B	972	GLN
1	B	1048	GLN
1	C	168	GLN
1	C	377	GLN
1	C	408	HIS
1	C	537	HIS
1	C	724	GLN
1	C	754	ASN
1	C	970	HIS

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Mol	Chain	Res	Type
1	C	972	GLN
1	C	1001	GLN
1	D	116	GLN
1	D	165	ASN
1	D	335	ASN
1	D	657	ASN
1	D	676	ASN
1	D	724	GLN
1	D	796	ASN
1	D	851	ASN
1	D	972	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [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	1021/1879 (54%)	0.84	95 (9%)	14 13	30, 56, 98, 228	0
1	B	1026/1879 (54%)	0.80	80 (7%)	19 15	30, 56, 99, 175	0
1	C	1020/1879 (54%)	0.80	70 (6%)	23 18	39, 68, 108, 156	0
1	D	1021/1879 (54%)	0.82	81 (7%)	18 15	38, 69, 111, 201	0
All	All	4088/7516 (54%)	0.82	326 (7%)	18 15	30, 62, 107, 228	0

All (326) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1035	ARG	6.6
1	D	1067	THR	5.7
1	D	1020	TYR	5.5
1	A	1073	PRO	5.3
1	A	574	ASP	4.7
1	A	1020	TYR	4.7
1	C	1068	ALA	4.7
1	D	735	ASP	4.6
1	A	213	LEU	4.6
1	B	206	THR	4.5
1	D	1054	LEU	4.5
1	D	594	ASP	4.4
1	A	1034	ASN	4.4
1	A	903	ASN	4.4
1	D	202	TRP	4.3
1	B	1020	TYR	4.3
1	C	1067	THR	4.2
1	D	574	ASP	4.2
1	B	1064	ALA	4.2
1	C	460	GLY	4.1
1	B	1075	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	693	TYR	3.9
1	A	530	ASP	3.9
1	A	95	GLY	3.8
1	A	1067	THR	3.8
1	B	1035	ARG	3.8
1	B	1067	THR	3.8
1	B	210	GLY	3.8
1	B	275	GLU	3.7
1	C	76	GLU	3.7
1	D	1052	ILE	3.7
1	D	793	THR	3.7
1	D	597	ARG	3.7
1	C	79	PRO	3.6
1	D	1019	CYS	3.6
1	D	95	GLY	3.5
1	A	1022	GLY	3.5
1	A	1066	ASN	3.5
1	B	163	ALA	3.5
1	A	266	ASP	3.5
1	A	1036	PHE	3.4
1	A	1070	TRP	3.4
1	A	1019	CYS	3.4
1	C	1019	CYS	3.4
1	D	1066	ASN	3.4
1	A	704	ASP	3.4
1	D	1070	TRP	3.4
1	D	236	GLU	3.4
1	A	94	THR	3.4
1	D	815	THR	3.4
1	A	215	ARG	3.3
1	D	794	ALA	3.3
1	A	46	SER	3.3
1	B	966	LEU	3.3
1	C	173	ALA	3.2
1	D	499	ASP	3.2
1	D	363	ALA	3.2
1	A	906	GLU	3.2
1	B	1076	LEU	3.2
1	D	1073	PRO	3.2
1	D	23	ALA	3.2
1	C	1076	LEU	3.2
1	D	707	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	1068	ALA	3.2
1	B	904	GLN	3.1
1	B	767	SER	3.1
1	B	1065	PRO	3.1
1	D	795	PHE	3.1
1	C	1073	PRO	3.1
1	A	1064	ALA	3.1
1	B	710	SER	3.1
1	A	417	GLU	3.1
1	A	985	ASP	3.1
1	D	347	GLU	3.0
1	A	705	ASP	3.0
1	C	574	ASP	3.0
1	B	695	ALA	3.0
1	D	1064	ALA	3.0
1	B	1012	ALA	3.0
1	B	28	CYS	3.0
1	C	186	GLN	3.0
1	D	1053	GLY	3.0
1	A	292	GLU	3.0
1	C	28	CYS	3.0
1	A	1063	TYR	3.0
1	A	1072	ASP	3.0
1	B	208	ASP	3.0
1	B	849	GLN	3.0
1	A	206	THR	3.0
1	A	1076	LEU	2.9
1	B	1038	TYR	2.9
1	B	1052	ILE	2.9
1	A	103	VAL	2.9
1	D	138	SER	2.9
1	A	191	ASP	2.9
1	D	931	ASP	2.9
1	B	1069	ASN	2.9
1	C	944	SER	2.9
1	A	594	ASP	2.9
1	B	726	ASN	2.9
1	D	806	ALA	2.9
1	D	118	TRP	2.9
1	D	1055	PHE	2.9
1	A	597	ARG	2.9
1	B	1063	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	993	GLY	2.9
1	D	1075	GLY	2.9
1	A	1021	GLN	2.8
1	B	1023	GLN	2.8
1	B	815	THR	2.8
1	A	37	GLY	2.8
1	D	1074	PHE	2.8
1	B	267	HIS	2.8
1	A	806	ALA	2.8
1	B	211	THR	2.8
1	C	60	TRP	2.8
1	A	1005	ILE	2.8
1	B	1016	ASN	2.8
1	D	952	GLN	2.8
1	D	1035	ARG	2.8
1	B	712	GLU	2.8
1	B	945	PHE	2.8
1	A	1037	ARG	2.8
1	D	950	GLN	2.8
1	B	36	ILE	2.8
1	B	1070	TRP	2.7
1	B	847	ASP	2.7
1	B	1066	ASN	2.7
1	B	79	PRO	2.7
1	C	36	ILE	2.7
1	A	672	ASP	2.7
1	D	596	ASP	2.7
1	D	765	ASP	2.7
1	A	218	ALA	2.7
1	B	1068	ALA	2.7
1	A	780	THR	2.7
1	B	884	HIS	2.7
1	B	1019	CYS	2.7
1	C	1074	PHE	2.7
1	D	667	TRP	2.7
1	C	137	VAL	2.7
1	C	903	ASN	2.7
1	A	35	SER	2.7
1	A	66	SER	2.7
1	B	848	ALA	2.7
1	A	207	GLY	2.6
1	D	136	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	35	SER	2.6
1	C	363	ALA	2.6
1	C	1052	ILE	2.6
1	D	36	ILE	2.6
1	C	877	ASN	2.6
1	B	127	TRP	2.6
1	D	213	LEU	2.6
1	B	940	TYR	2.6
1	D	940	TYR	2.6
1	B	903	ASN	2.6
1	A	69	THR	2.6
1	A	291	SER	2.6
1	C	829	SER	2.6
1	A	120	ASP	2.6
1	B	1021	GLN	2.6
1	A	1056	GLY	2.6
1	A	596	ASP	2.6
1	B	37	GLY	2.6
1	C	1069	ASN	2.6
1	C	1070	TRP	2.5
1	C	82	ILE	2.5
1	C	267	HIS	2.5
1	D	965	HIS	2.5
1	A	710	SER	2.5
1	A	36	ILE	2.5
1	A	409	THR	2.5
1	D	695	ALA	2.5
1	A	686	GLU	2.5
1	C	136	GLU	2.5
1	A	344	ASP	2.5
1	A	847	ASP	2.5
1	C	248	ILE	2.5
1	C	1065	PRO	2.5
1	A	1023	GLN	2.5
1	D	234	GLN	2.5
1	D	209	ASP	2.5
1	B	23	ALA	2.4
1	A	63	THR	2.4
1	A	735	ASP	2.4
1	C	280	GLY	2.4
1	D	422	GLN	2.4
1	D	949	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	72	ASP	2.4
1	B	266	ASP	2.4
1	A	204	GLU	2.4
1	A	942	GLU	2.4
1	A	966	LEU	2.4
1	C	199	THR	2.4
1	B	530	ASP	2.4
1	B	596	ASP	2.4
1	C	847	ASP	2.4
1	C	1020	TYR	2.4
1	B	860	SER	2.4
1	D	698	VAL	2.4
1	D	647	ASN	2.4
1	D	657	ASN	2.4
1	D	1034	ASN	2.4
1	B	251	TYR	2.4
1	C	442	ILE	2.4
1	C	917	TRP	2.4
1	A	581	ASN	2.3
1	D	737	MET	2.3
1	A	77	LEU	2.3
1	D	1076	LEU	2.3
1	C	181	VAL	2.3
1	A	725	SER	2.3
1	C	384	PRO	2.3
1	B	215	ARG	2.3
1	A	184	ALA	2.3
1	B	441	LEU	2.3
1	C	154	PHE	2.3
1	D	77	LEU	2.3
1	A	236	GLU	2.3
1	C	712	GLU	2.3
1	C	415	THR	2.3
1	C	725	SER	2.3
1	D	875	THR	2.3
1	B	1018	LEU	2.3
1	A	711	PHE	2.3
1	B	1036	PHE	2.3
1	B	993	GLY	2.3
1	C	163	ALA	2.3
1	C	202	TRP	2.3
1	B	35	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	767	SER	2.3
1	A	657	ASN	2.3
1	A	931	ASP	2.3
1	B	942	GLU	2.3
1	B	1014	GLY	2.3
1	A	680	THR	2.3
1	B	791	SER	2.3
1	C	967	SER	2.3
1	A	175	ASN	2.3
1	D	681	ARG	2.3
1	C	499	ASP	2.3
1	B	460	GLY	2.2
1	C	621	PHE	2.2
1	C	66	SER	2.2
1	C	234	GLN	2.2
1	A	27	GLU	2.2
1	D	212	PRO	2.2
1	A	795	PHE	2.2
1	D	220	TYR	2.2
1	A	323	GLY	2.2
1	B	125	LEU	2.2
1	D	191	ASP	2.2
1	C	220	TYR	2.2
1	B	1047	ILE	2.2
1	A	648	ASN	2.2
1	B	77	LEU	2.2
1	B	906	GLU	2.2
1	A	787	ASP	2.2
1	C	155	ARG	2.2
1	A	202	TRP	2.2
1	D	63	THR	2.2
1	C	885	VAL	2.2
1	D	315	ILE	2.2
1	D	966	LEU	2.2
1	A	1069	ASN	2.2
1	B	910	ALA	2.2
1	D	903	ASN	2.2
1	D	491	GLY	2.2
1	A	1074	PHE	2.2
1	B	893	ASP	2.2
1	C	789	LEU	2.1
1	B	281	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	723	ARG	2.1
1	A	845	GLU	2.1
1	C	184	ALA	2.1
1	C	411	GLU	2.1
1	C	761	ALA	2.1
1	C	865	GLU	2.1
1	C	696	GLY	2.1
1	D	33	GLY	2.1
1	B	1074	PHE	2.1
1	D	859	ASP	2.1
1	B	202	TRP	2.1
1	C	99	TYR	2.1
1	A	755	LEU	2.1
1	C	950	GLN	2.1
1	B	696	GLY	2.1
1	A	908	SER	2.1
1	D	1069	ASN	2.1
1	B	990	VAL	2.1
1	B	483	ILE	2.1
1	D	747	LEU	2.1
1	A	214	ARG	2.1
1	D	495	THR	2.1
1	C	905	GLN	2.1
1	D	909	GLY	2.1
1	B	346	PHE	2.1
1	C	32	VAL	2.1
1	A	1002	LEU	2.1
1	B	859	ASP	2.1
1	B	30	GLY	2.1
1	D	207	GLY	2.1
1	A	98	GLU	2.1
1	B	212	PRO	2.1
1	D	767	SER	2.0
1	B	201	ILE	2.0
1	C	1016	ASN	2.0
1	A	70	ALA	2.0
1	A	778	THR	2.0
1	A	1068	ALA	2.0
1	C	191	ASP	2.0
1	D	1056	GLY	2.0
1	A	990	VAL	2.0
1	A	677	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	998	LEU	2.0
1	D	1071	ILE	2.0
1	B	158	THR	2.0
1	C	187	THR	2.0
1	A	499	ASP	2.0
1	C	859	ASP	2.0
1	D	417	GLU	2.0
1	C	31	ARG	2.0
1	A	217	LEU	2.0
1	C	198	ILE	2.0
1	D	976	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.