



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2016 – 01:18 PM EDT

PDB ID : 5B86
Title : Crystal structure of M-Sec
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Deposited on : 2016-06-12
Resolution : 3.02 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

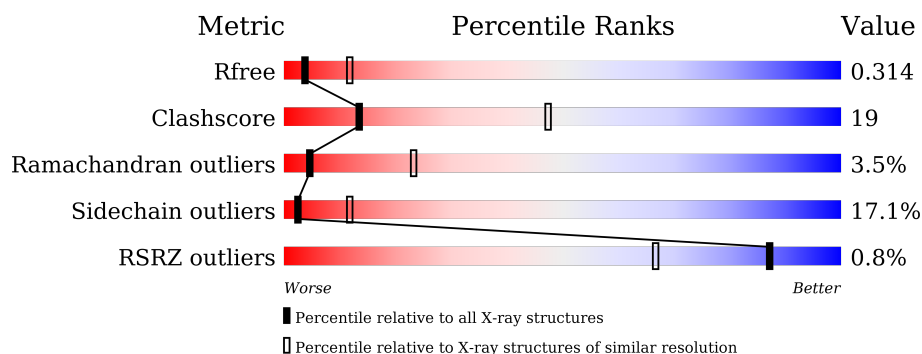
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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X-RAY DIFFRACTION

A.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

Mol	Chain	Length	Quality of chain
1	A	600	<div> <div></div> <div>52%</div> <div>38%</div> <div>6%</div> <div></div> <div></div> </div>
1	B	600	<div> <div></div> <div>49%</div> <div>39%</div> <div>9%</div> <div></div> <div></div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9312 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 Tumor necrosis factor alpha-induced protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	Se	0	0	0
			4638	2948	814	859	8	9			
1	B	578	Total	C	N	O	S	Se	0	0	0
			4628	2942	811	858	8	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLY	-	expression tag	UNP Q61333
A	52	PRO	-	expression tag	UNP Q61333
B	51	GLY	-	expression tag	UNP Q61333
B	52	PRO	-	expression tag	UNP Q61333

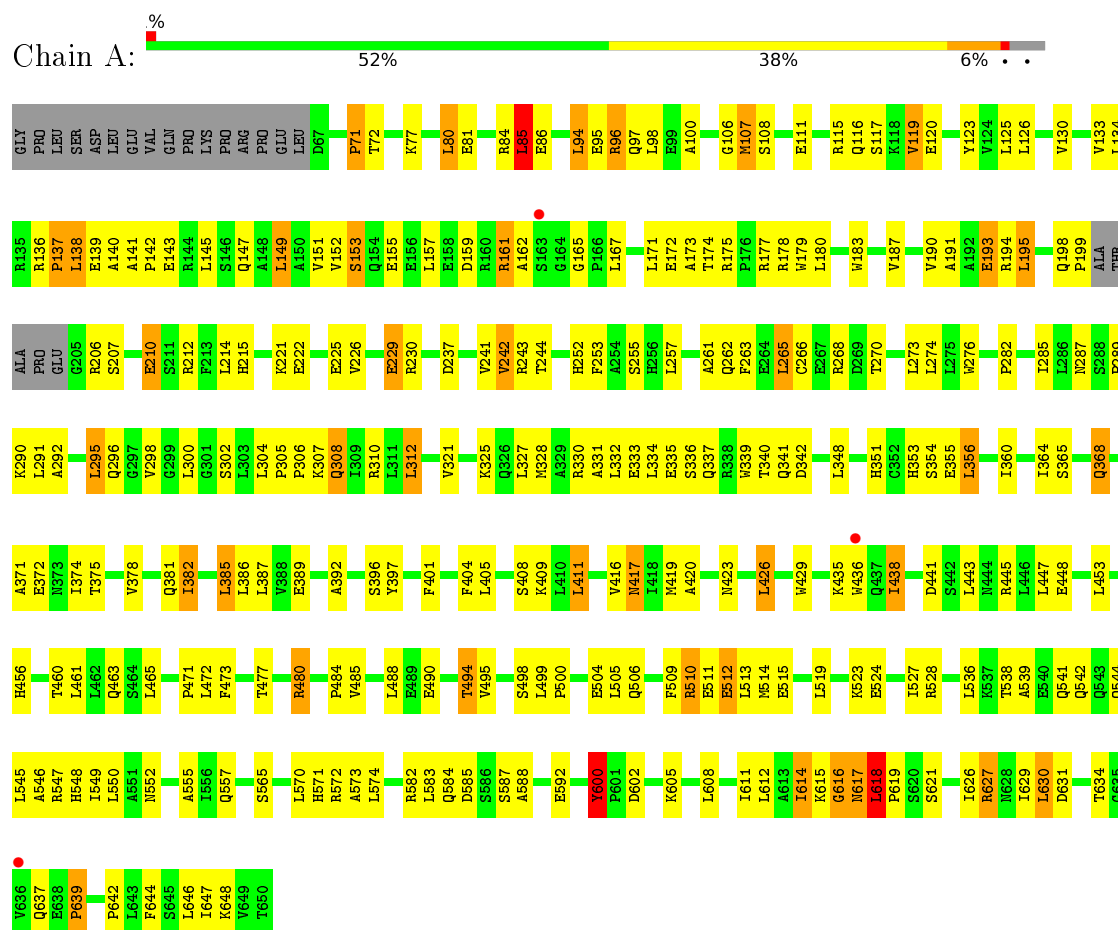
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		
2	B	30	Total	O	0	0
			30	30		

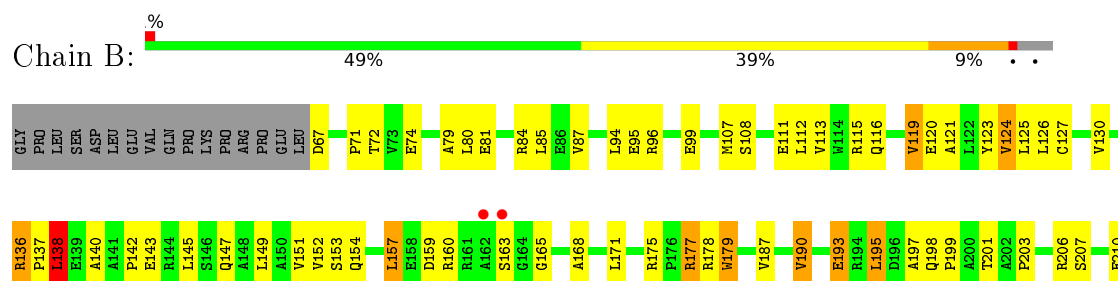
3 Residue-property plots

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

- Molecule 1: Tumor necrosis factor alpha-induced protein 2



- Molecule 1: Tumor necrosis factor alpha-induced protein 2



G616	L519	R445	I358	Y281	S211
M617	K523	L446	D859	F282	R212
L618	K524	L447	I360	M283	F213
P619	E524	E448	L361	D284	L214
S620	I527	P449	Q362	I285	H215
S621	R528	L450	I363	L286	M216
E622	L529	L453	I364	M287	M217
V623	R533	K454	Q368	S288	R218
R624	L534	F458	E372	P289	T219
S625	R535	L461	N373	K290	M220
I626	L536	L462	I374	L291	K221
R627	K537	Q463	T375	E294	L224
N628	T538	S464	D376	I303	V227
L629	A539	L465	S377	L304	V228
D631	E540	F466	V378	P305	E229
ILE	Q541	L467	Q381	P306	R230
ASN	Q542	D468	I382	K307	L231
THR	Q543	L469	K383	Q308	L234
GLY	Q544	K470	Q384	I309	L236
VAL	L550	P471	L385	R310	F235
GLN	A551	L472	L386	L311	P236
E638	N552	F473	L387	L312	D237
P639	Q557	K474	I393	E313	E238
P642	G558	K475	L394	F316	F239
L643	F559	F476	R395	L317	M240
F644	F562	L477	Q398	L318	V241
S645	A567	Q478	S408	S318	V242
L646	T568	T479	K409	N319	R243
I647	M576	E489	L410	F320	T244
R648	E579	F490	L411	V321	E247
V649	I580	L491	R415	T322	Y251
T650	I581	L492	V416	S323	H252
	R582	T493	M419	V324	P253
	L583	T494	A420	Q325	A254
	A588	V495	M423	L326	S255
	I589	S496	M424	L327	H256
	K590	E501	C425	M328	L257
	V593	F502	L426	A329	C258
	D602	S503	F427	R330	A259
		E504	F428	L334	L260
		L505	M429	E335	F263
		H506	W436	W339	E264
	K605	D507	Q437	D342	L265
	G606	C508	I438	V343	C266
	H607	F509	S439	A344	D269
	L608	R510	H440	P345	L272
	L612	L513	D441	W436	L273
	A613	H514	S442	I438	L274
	I614	E515	L443	H351	L275
	K615		R444	C352	L276
				H353	H276
				S354	N279
				E355	L280
				L356	
				A357	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.41Å 107.83Å 229.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.44 – 3.02 46.44 – 3.02	Depositor EDS
% Data completeness (in resolution range)	86.1 (46.44-3.02) 87.3 (46.44-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.229 , 0.292 0.250 , 0.314	Depositor DCC
R_{free} test set	2148 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9312	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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	0.50	0/4717	0.71	2/6380 (0.0%)
1	B	0.46	0/4708	0.69	2/6369 (0.0%)
All	All	0.48	0/9425	0.70	4/12749 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	LEU	CA-CB-CG	7.45	132.44	115.30
1	B	265	LEU	CA-CB-CG	6.26	129.70	115.30
1	A	618	LEU	CA-CB-CG	6.03	129.17	115.30
1	A	85	LEU	CA-CB-CG	5.41	127.74	115.30

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	4638	0	4693	166	1
1	B	4628	0	4679	183	1
2	A	16	0	0	3	0
2	B	30	0	0	9	0
All	All	9312	0	9372	349	1

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 19.

All (349) 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:605:LYS:HE3	1:B:630:LEU:HB2	1.52	0.92
1:B:179:TRP:NE1	2:B:701:HOH:O	2.00	0.91
1:A:608:LEU:HD23	1:A:626:ILE:HG12	1.51	0.91
1:A:328:MSE:HE2	1:A:360:ILE:HG23	1.53	0.90
1:B:615:LYS:HB3	1:B:618:LEU:HD21	1.55	0.89
1:B:157:LEU:HD11	1:B:177:ARG:HB2	1.53	0.88
1:B:353:HIS:HB2	1:B:420:ALA:HB1	1.55	0.86
1:B:157:LEU:HD21	1:B:178:ARG:H	1.41	0.85
1:A:157:LEU:HD21	1:A:178:ARG:H	1.42	0.84
1:A:291:LEU:HB3	1:A:295:LEU:HD11	1.60	0.84
1:B:538:THR:HB	1:B:541:GLN:HG2	1.58	0.82
1:B:503:SER:HA	1:B:510:ARG:HH21	1.44	0.81
1:B:197:ALA:O	1:B:212:ARG:NH2	2.17	0.77
1:B:335:GLU:OE1	1:B:353:HIS:NE2	2.18	0.76
1:B:351:HIS:HD2	1:B:419:MSE:HB2	1.50	0.75
1:A:472:LEU:HD13	1:A:490:GLU:HG2	1.68	0.74
1:A:130:VAL:HG21	1:A:149:LEU:HD11	1.69	0.73
1:A:642:PRO:HB3	1:A:646:LEU:HD21	1.71	0.72
1:B:195:LEU:HG	1:B:216:MSE:HG2	1.70	0.72
1:B:536:LEU:HD23	1:B:542:GLN:HA	1.71	0.72
1:B:426:LEU:HB2	1:B:509:PHE:HE1	1.55	0.71
1:A:328:MSE:HG2	1:A:360:ILE:HD12	1.73	0.70
1:B:317:LEU:HB3	1:B:382:ILE:HD11	1.71	0.70
1:A:335:GLU:HG3	1:A:356:LEU:HG	1.72	0.70
1:B:215:HIS:O	1:B:219:THR:OG1	2.09	0.70
1:A:130:VAL:HG22	1:A:149:LEU:HD21	1.72	0.70
1:A:544:GLN:OE1	1:A:547:ARG:NH2	2.25	0.70
1:A:615:LYS:O	1:A:617:ASN:N	2.24	0.69
1:B:442:SER:HA	1:B:445:ARG:HE	1.58	0.69
1:B:328:MSE:HE2	1:B:360:ILE:HG23	1.74	0.69
1:B:335:GLU:HG3	1:B:356:LEU:HD23	1.74	0.69
1:A:484:PRO:HB3	1:A:552:ASN:HD21	1.58	0.69
1:B:474:LYS:HG2	1:B:528:ARG:NH2	2.08	0.69
1:B:318:SER:O	1:B:322:THR:OG1	2.11	0.68
1:A:465:LEU:HD21	1:A:495:VAL:HG23	1.74	0.67
1:A:157:LEU:HD11	1:A:177:ARG:HB2	1.77	0.67
1:B:216:MSE:HE1	1:B:256:HIS:CD2	2.30	0.67
1:A:335:GLU:HB3	1:A:353:HIS:CE1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:HIS:O	1:A:460:THR:OG1	2.12	0.66
1:B:274:LEU:HD11	1:B:313:GLU:HA	1.75	0.66
1:A:157:LEU:HD21	1:A:178:ARG:N	2.10	0.66
1:B:489:GLU:O	1:B:493:THR:OG1	2.13	0.65
1:B:289:PRO:HA	2:B:706:HOH:O	1.96	0.65
1:A:408:SER:HB3	1:A:411:LEU:HG	1.79	0.65
1:A:557:GLN:HG3	1:A:571:HIS:CE1	2.31	0.65
1:B:642:PRO:HB2	1:B:646:LEU:HD21	1.77	0.65
1:A:335:GLU:HB3	1:A:353:HIS:NE2	2.12	0.65
1:B:602:ASP:OD2	1:B:644:PHE:N	2.30	0.64
1:A:371:ALA:HB1	1:A:378:VAL:HG12	1.80	0.64
1:A:321:VAL:HG21	1:A:385:LEU:HD22	1.80	0.64
1:B:96:ARG:NH1	1:B:159:ASP:OD1	2.30	0.64
1:B:364:ILE:HG23	1:B:386:LEU:HD13	1.81	0.63
1:B:168:ALA:HB3	1:B:171:LEU:HG	1.80	0.62
1:A:108:SER:HB3	1:A:111:GLU:HB2	1.81	0.62
1:A:426:LEU:HD13	1:A:506:GLN:HG2	1.80	0.62
1:B:153:SER:O	1:B:157:LEU:HD13	2.00	0.62
1:B:142:PRO:HA	1:B:145:LEU:HD12	1.80	0.62
1:B:615:LYS:HD2	1:B:618:LEU:HD11	1.81	0.61
1:B:207:SER:HB3	1:B:210:GLU:H	1.65	0.60
1:B:67:ASP:N	1:B:67:ASP:OD2	2.34	0.60
1:B:375:THR:HB	1:B:378:VAL:H	1.66	0.60
1:A:126:LEU:O	1:A:130:VAL:HG23	2.02	0.60
1:A:302:SER:OG	1:A:304:LEU:O	2.09	0.60
1:A:140:ALA:HB3	1:A:142:PRO:HD3	1.82	0.60
1:A:510:ARG:HH12	1:A:514:MSE:HE3	1.67	0.60
1:B:538:THR:HG22	1:B:540:GLU:H	1.66	0.59
1:B:72:THR:HG22	1:B:74:GLU:H	1.67	0.59
1:A:157:LEU:HD11	1:A:177:ARG:H	1.66	0.59
1:A:356:LEU:HD22	1:A:360:ILE:HG12	1.84	0.59
1:B:429:TRP:HZ3	1:B:443:LEU:HD13	1.67	0.59
1:A:307:LYS:HA	1:A:310:ARG:HH11	1.68	0.58
1:B:475:LYS:HA	1:B:478:GLN:HB2	1.85	0.58
1:B:510:ARG:NH1	2:B:702:HOH:O	2.16	0.58
1:B:276:TRP:HZ3	1:B:285:ILE:HD11	1.69	0.58
1:A:602:ASP:OD1	1:A:644:PHE:N	2.33	0.57
1:B:321:VAL:HG21	1:B:385:LEU:HD13	1.86	0.57
1:A:527:ILE:HG12	1:A:647:ILE:HG23	1.86	0.57
1:B:157:LEU:HD21	1:B:178:ARG:N	2.17	0.57
1:A:300:LEU:HD12	1:A:300:LEU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LYS:HG3	1:A:647:ILE:HG12	1.85	0.57
1:B:288:SER:OG	1:B:289:PRO:HD3	2.05	0.57
1:B:121:ALA:O	1:B:124:VAL:HG13	2.05	0.57
1:B:335:GLU:CD	1:B:353:HIS:HE2	2.07	0.57
1:A:605:LYS:HE2	1:A:630:LEU:HA	1.87	0.56
1:A:538:THR:O	1:A:541:GLN:HG2	2.05	0.56
1:A:265:LEU:HD22	1:A:265:LEU:H	1.70	0.56
1:A:147:GLN:O	1:A:151:VAL:HG23	2.04	0.56
1:A:351:HIS:CE1	1:A:416:VAL:HG13	2.41	0.56
1:B:203:PRO:HD2	1:B:206:ARG:NE	2.20	0.56
1:B:289:PRO:HD2	1:B:291:LEU:HB2	1.88	0.56
1:A:546:ALA:CB	1:A:582:ARG:HB2	2.37	0.55
1:A:332:LEU:HD11	1:A:397:TYR:HA	1.88	0.55
1:B:207:SER:HB3	1:B:210:GLU:HB2	1.88	0.55
1:B:147:GLN:O	1:B:151:VAL:HG23	2.06	0.55
1:B:408:SER:HB3	1:B:411:LEU:HD12	1.88	0.55
1:A:342:ASP:HB2	1:A:411:LEU:HD13	1.89	0.55
1:B:465:LEU:HD11	1:B:495:VAL:HA	1.88	0.55
1:A:484:PRO:HG2	1:A:548:HIS:CG	2.42	0.54
1:B:177:ARG:HG2	1:B:179:TRP:CZ3	2.42	0.54
1:B:625:SER:O	1:B:628:ASN:HB2	2.07	0.54
1:A:401:PHE:O	1:A:404:PHE:HB3	2.08	0.54
1:B:615:LYS:HD2	1:B:618:LEU:HD21	1.89	0.54
1:A:420:ALA:O	1:A:423:ASN:HB2	2.08	0.54
1:B:175:ARG:O	1:B:177:ARG:N	2.41	0.54
1:B:534:LEU:O	1:B:614:ILE:HG22	2.08	0.53
1:B:157:LEU:HG	1:B:177:ARG:H	1.73	0.53
1:B:419:MSE:O	1:B:423:ASN:ND2	2.41	0.53
1:B:426:LEU:HB2	1:B:509:PHE:CE1	2.41	0.53
1:A:542:GLN:OE1	1:A:584:GLN:NE2	2.41	0.53
1:B:274:LEU:HD13	1:B:374:ILE:HD13	1.89	0.53
1:A:473:PHE:CE2	1:A:524:GLU:HB3	2.44	0.53
1:B:617:ASN:H	1:B:618:LEU:HD22	1.74	0.53
1:A:96:ARG:NE	2:A:702:HOH:O	2.42	0.53
1:A:167:LEU:HD22	1:A:173:ALA:HA	1.90	0.52
1:B:108:SER:HB2	1:B:111:GLU:HB2	1.91	0.52
1:B:608:LEU:O	1:B:612:LEU:HG	2.09	0.52
1:B:615:LYS:HB3	1:B:618:LEU:CD2	2.35	0.52
1:B:115:ARG:O	1:B:119:VAL:HG12	2.09	0.52
1:A:583:LEU:HD22	1:A:588:ALA:HB1	1.90	0.52
1:B:462:LEU:HD21	1:B:513:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:HG12	1:A:134:LEU:HD23	1.90	0.52
1:B:157:LEU:HD11	1:B:177:ARG:CB	2.35	0.52
1:B:583:LEU:HD13	1:B:588:ALA:HB1	1.91	0.52
1:B:353:HIS:O	1:B:355:GLU:N	2.42	0.52
1:A:95:GLU:OE2	1:A:175:ARG:NH1	2.43	0.52
1:B:81:GLU:HG3	1:B:125:LEU:HD21	1.91	0.52
1:B:95:GLU:OE1	1:B:175:ARG:NH1	2.43	0.52
1:A:261:ALA:HB2	1:A:304:LEU:HD11	1.92	0.51
1:B:263:PHE:O	1:B:265:LEU:HD22	2.10	0.51
1:A:96:ARG:NH1	1:A:159:ASP:OD2	2.42	0.51
1:A:337:GLN:HA	1:A:340:THR:HB	1.92	0.51
1:A:546:ALA:HB2	1:A:582:ARG:HB2	1.93	0.51
1:A:84:ARG:CD	1:A:86:GLU:H	2.23	0.51
1:B:354:SER:O	1:B:358:ILE:HG12	2.10	0.51
1:B:515:GLU:HG2	1:B:567:ALA:HB2	1.93	0.51
1:B:126:LEU:O	1:B:130:VAL:HG23	2.10	0.51
1:B:224:LEU:O	1:B:228:VAL:HG23	2.11	0.51
1:A:222:GLU:O	1:A:226:VAL:HG23	2.11	0.51
1:A:509:PHE:HA	1:A:512:GLU:HB2	1.92	0.51
1:B:154:GLN:HA	1:B:157:LEU:HD22	1.91	0.51
1:A:339:TRP:HA	1:A:417:ASN:OD1	2.10	0.51
1:B:542:GLN:NE2	1:B:615:LYS:O	2.44	0.51
1:B:187:VAL:HG11	1:B:244:THR:HG22	1.92	0.50
1:B:607:HIS:HE2	1:B:647:ILE:HG22	1.76	0.50
1:A:96:ARG:NH2	1:A:159:ASP:OD2	2.44	0.50
1:B:523:LYS:O	1:B:527:ILE:HG13	2.11	0.50
1:A:295:LEU:HA	1:A:298:VAL:HG23	1.93	0.50
1:B:519:LEU:O	1:B:523:LYS:HB2	2.12	0.50
1:A:605:LYS:NZ	1:A:630:LEU:HD13	2.26	0.50
1:A:221:LYS:HE3	1:A:225:GLU:OE2	2.11	0.49
1:B:120:GLU:O	1:B:124:VAL:HG12	2.12	0.49
1:B:429:TRP:NE1	2:B:703:HOH:O	2.34	0.49
1:A:153:SER:O	1:A:157:LEU:HD13	2.12	0.49
1:B:279:ASN:O	1:B:283:ASN:HB2	2.12	0.49
1:A:180:LEU:O	1:A:183:TRP:HB3	2.12	0.49
1:B:351:HIS:CD2	1:B:419:MSE:HB2	2.40	0.49
1:A:365:SER:HB3	1:A:435:LYS:NZ	2.27	0.49
1:A:573:ALA:HA	1:A:600:TYR:CE1	2.48	0.49
1:B:136:ARG:HH11	1:B:136:ARG:HB2	1.78	0.49
1:B:190:VAL:HA	1:B:193:GLU:HG2	1.95	0.49
1:B:214:LEU:HD22	1:B:276:TRP:HZ2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:VAL:HG11	1:B:294:GLU:HG3	1.95	0.49
1:B:543:GLN:HG3	1:B:582:ARG:HG2	1.95	0.49
1:A:193:GLU:HG3	1:A:194:ARG:N	2.29	0.48
1:A:536:LEU:O	1:A:616:GLY:HA3	2.13	0.48
1:B:126:LEU:HD23	2:B:701:HOH:O	2.14	0.48
1:B:328:MSE:HB3	1:B:393:LEU:HD13	1.94	0.48
1:A:206:ARG:HD2	1:A:206:ARG:H	1.78	0.48
1:A:229:GLU:HB3	1:A:230:ARG:HG3	1.96	0.48
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.65	0.48
1:B:623:VAL:HA	1:B:626:ILE:HB	1.96	0.48
1:A:524:GLU:HA	1:A:527:ILE:HD12	1.96	0.48
1:A:133:VAL:HA	1:A:139:GLU:OE1	2.14	0.48
1:B:257:LEU:HB3	1:B:304:LEU:HD21	1.96	0.48
1:A:107:MSE:HE1	1:A:115:ARG:CZ	2.44	0.48
1:A:519:LEU:HD13	1:A:570:LEU:HD21	1.96	0.47
1:B:281:TYR:CE1	1:B:286:LEU:HD13	2.48	0.47
1:A:207:SER:HB3	1:A:210:GLU:H	1.79	0.47
1:A:488:LEU:HD21	1:A:555:ALA:HB3	1.96	0.47
1:B:354:SER:HA	1:B:424:ASN:OD1	2.14	0.47
1:B:199:PRO:HB3	1:B:215:HIS:HB2	1.96	0.47
1:B:351:HIS:NE2	1:B:416:VAL:HG12	2.28	0.47
1:A:331:ALA:O	1:A:335:GLU:HG2	2.13	0.47
1:B:476:PHE:CE2	1:B:487:THR:HB	2.49	0.47
1:A:270:THR:O	1:A:274:LEU:HB2	2.15	0.47
1:A:85:LEU:HD12	1:A:145:LEU:HB2	1.97	0.47
1:A:514:MSE:HG3	1:A:565:SER:HB2	1.96	0.47
1:B:528:ARG:HA	1:B:528:ARG:HD3	1.60	0.47
1:A:419:MSE:HG2	1:A:505:LEU:HD13	1.96	0.47
1:A:353:HIS:C	1:A:355:GLU:N	2.68	0.47
1:B:454:LYS:HD3	1:B:509:PHE:HE2	1.79	0.47
1:A:225:GLU:N	1:A:291:LEU:HD21	2.30	0.46
1:B:236:PRO:HG2	1:B:239:PHE:CD2	2.50	0.46
1:B:618:LEU:HD22	1:B:618:LEU:N	2.31	0.46
1:A:545:LEU:O	1:A:548:HIS:HB2	2.16	0.46
1:A:195:LEU:HD23	1:A:252:HIS:HB3	1.98	0.46
1:A:257:LEU:HB3	1:A:304:LEU:CD2	2.45	0.46
1:B:618:LEU:HD22	1:B:618:LEU:H	1.81	0.46
1:B:605:LYS:HE2	1:B:626:ILE:HG22	1.97	0.46
1:B:606:GLY:HA3	1:B:649:VAL:HG11	1.96	0.46
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.65	0.46
1:B:221:LYS:HB3	1:B:221:LYS:HE2	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:VAL:HG21	1:B:385:LEU:HD22	1.98	0.46
1:B:342:ASP:HB3	1:B:411:LEU:HD13	1.98	0.46
1:B:619:PRO:HG2	1:B:621:SER:HB2	1.98	0.46
1:A:149:LEU:CD1	1:A:179:TRP:HZ3	2.29	0.46
1:B:269:ASP:HA	1:B:272:LEU:HG	1.98	0.46
1:A:195:LEU:HA	1:A:195:LEU:HD12	1.81	0.45
1:A:510:ARG:NH1	1:A:514:MSE:HE3	2.30	0.45
1:A:282:PRO:O	1:A:287:ASN:HB2	2.15	0.45
1:B:343:VAL:O	1:B:345:PRO:HD3	2.16	0.45
1:B:345:PRO:HB2	1:B:351:HIS:CE1	2.51	0.45
1:B:429:TRP:CD2	1:B:447:LEU:HD12	2.51	0.45
1:A:276:TRP:HZ3	1:A:285:ILE:HD11	1.81	0.45
1:A:490:GLU:O	1:A:494:THR:OG1	2.34	0.45
1:A:506:GLN:HB3	1:A:509:PHE:HD1	1.82	0.45
1:B:438:ILE:HG22	1:B:439:SER:H	1.81	0.45
1:B:450:LEU:HA	1:B:450:LEU:HD23	1.77	0.45
1:B:473:PHE:CE1	1:B:491:ILE:HD13	2.52	0.45
1:B:507:ASP:HA	1:B:510:ARG:HG2	1.96	0.45
1:B:470:LYS:HB2	1:B:471:PRO:HD3	1.99	0.45
1:B:590:LYS:HZ3	1:B:624:ARG:HB3	1.81	0.45
1:A:142:PRO:HB2	1:A:145:LEU:HD12	1.99	0.45
1:A:167:LEU:HD13	1:A:173:ALA:HB2	1.99	0.45
1:B:203:PRO:HD2	1:B:206:ARG:HE	1.81	0.45
1:B:280:LEU:O	1:B:284:ASP:HB2	2.16	0.45
1:B:289:PRO:HB2	1:B:290:LYS:H	1.58	0.45
1:B:607:HIS:NE2	1:B:647:ILE:HG22	2.32	0.45
1:B:605:LYS:HG2	1:B:626:ILE:HG23	1.99	0.45
1:A:137:PRO:HB3	1:A:143:GLU:OE1	2.16	0.45
1:A:263:PHE:O	1:A:265:LEU:HD13	2.16	0.45
1:B:272:LEU:HA	1:B:275:LEU:HB3	1.99	0.45
1:A:140:ALA:HB3	1:A:142:PRO:CD	2.47	0.45
1:A:353:HIS:HB2	1:A:420:ALA:HB1	1.98	0.45
1:B:231:LEU:HD22	1:B:231:LEU:HA	1.77	0.44
1:A:221:LYS:HB2	1:A:285:ILE:HG23	1.99	0.44
1:A:165:GLY:O	1:A:167:LEU:HD12	2.17	0.44
1:B:627:ARG:HA	1:B:627:ARG:HD3	1.64	0.44
1:A:84:ARG:HD3	1:A:86:GLU:H	1.82	0.44
1:B:136:ARG:NH1	1:B:136:ARG:HB2	2.32	0.44
1:B:163:SER:C	1:B:165:GLY:H	2.20	0.44
1:B:488:LEU:HD22	1:B:552:ASN:HB3	2.00	0.44
1:A:536:LEU:HD23	1:A:542:GLN:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:ARG:HA	1:A:572:ARG:HD3	1.64	0.44
1:A:583:LEU:HD11	1:A:592:GLU:HG3	1.99	0.44
1:B:442:SER:HA	1:B:445:ARG:NE	2.29	0.44
1:A:330:ARG:NH1	1:A:333:GLU:OE1	2.51	0.44
1:A:401:PHE:CD2	1:A:453:LEU:HG	2.53	0.44
1:B:398:GLN:NE2	2:B:707:HOH:O	2.41	0.44
1:B:79:ALA:O	1:B:84:ARG:HG3	2.16	0.44
1:A:98:LEU:HD21	1:A:171:LEU:HD21	1.99	0.44
1:A:305:PRO:HG2	1:A:308:GLN:HB2	1.98	0.44
1:B:127:CYS:HA	2:B:701:HOH:O	2.18	0.44
1:B:136:ARG:HH11	1:B:138:LEU:HD22	1.83	0.44
1:B:175:ARG:CZ	1:B:177:ARG:HD2	2.48	0.44
1:B:481:TRP:CZ2	1:B:529:LEU:HD12	2.53	0.44
1:A:438:ILE:H	1:A:438:ILE:HG13	1.58	0.44
1:A:488:LEU:HD22	1:A:552:ASN:OD1	2.18	0.44
1:A:190:VAL:HA	1:A:193:GLU:HG2	1.98	0.43
1:B:157:LEU:CD2	1:B:178:ARG:H	2.22	0.43
1:A:375:THR:HB	1:A:378:VAL:HG23	2.00	0.43
1:B:415:ARG:HD3	1:B:501:GLU:OE2	2.17	0.43
1:A:242:VAL:HG23	1:A:243:ARG:H	1.83	0.43
1:A:389:GLU:O	1:A:392:ALA:HB3	2.19	0.43
1:A:648:LYS:HA	1:A:648:LYS:HD3	1.56	0.43
1:A:151:VAL:O	1:A:155:GLU:HG2	2.19	0.43
1:A:557:GLN:HG3	1:A:571:HIS:ND1	2.33	0.43
1:A:136:ARG:HB3	1:A:138:LEU:HD23	2.01	0.43
1:A:545:LEU:O	1:A:549:ILE:HG12	2.17	0.43
1:A:81:GLU:HG2	1:A:125:LEU:HD21	2.01	0.43
1:B:458:PHE:HA	1:B:461:LEU:HD11	2.01	0.43
1:B:623:VAL:O	1:B:627:ARG:HG2	2.19	0.43
1:B:468:ASP:O	1:B:472:LEU:HG	2.18	0.43
1:B:473:PHE:CE2	1:B:524:GLU:HB3	2.54	0.43
1:A:199:PRO:HB3	1:A:215:HIS:HB2	2.00	0.42
1:B:227:VAL:O	1:B:231:LEU:HB2	2.19	0.42
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.71	0.42
1:A:637:GLN:C	1:A:639:PRO:HD3	2.40	0.42
1:B:237:ASP:N	1:B:237:ASP:OD2	2.50	0.42
1:B:398:GLN:HA	1:B:453:LEU:HD12	2.01	0.42
1:B:467:LEU:HA	1:B:470:LYS:HG3	2.00	0.42
1:B:480:ARG:NH2	2:B:704:HOH:O	2.37	0.42
1:B:212:ARG:HD2	2:B:729:HOH:O	2.19	0.42
1:A:351:HIS:CE1	1:A:504:GLU:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HD12	1:B:175:ARG:HE	1.85	0.42
1:B:357:ALA:HA	1:B:428:PHE:CE1	2.54	0.42
1:B:559:PHE:HA	1:B:562:GLU:OE2	2.20	0.42
1:B:602:ASP:N	1:B:602:ASP:OD1	2.39	0.42
1:B:615:LYS:O	1:B:617:ASN:N	2.53	0.42
1:A:157:LEU:CD1	1:A:177:ARG:H	2.29	0.42
1:B:254:ALA:O	1:B:258:CYS:HB2	2.20	0.42
1:B:281:TYR:CE1	1:B:303:LEU:HD21	2.55	0.42
1:A:405:LEU:HA	1:A:405:LEU:HD23	1.88	0.42
1:B:140:ALA:H	1:B:142:PRO:HD2	1.84	0.42
1:A:71:PRO:HD3	2:A:704:HOH:O	2.20	0.42
1:B:247:GLU:HB3	1:B:251:TYR:CE2	2.54	0.42
1:A:328:MSE:HE3	1:A:364:ILE:HG13	2.02	0.42
1:A:515:GLU:HB2	2:A:710:HOH:O	2.19	0.41
1:A:574:LEU:HD23	1:A:574:LEU:HA	1.78	0.41
1:A:97:GLN:O	1:A:100:ALA:HB3	2.19	0.41
1:B:330:ARG:O	1:B:334:LEU:HB2	2.20	0.41
1:A:611:ILE:O	1:A:614:ILE:HG12	2.20	0.41
1:B:527:ILE:HG12	1:B:647:ILE:HG12	2.02	0.41
1:A:274:LEU:HD11	1:A:312:LEU:HB3	2.03	0.41
1:A:523:LYS:HG2	1:A:527:ILE:HD11	2.02	0.41
1:B:160:ARG:HB2	1:B:175:ARG:HG2	2.01	0.41
1:B:420:ALA:HA	1:B:423:ASN:HD22	1.85	0.41
1:A:187:VAL:HG11	1:A:244:THR:HG22	2.03	0.41
1:A:416:VAL:H	1:A:416:VAL:HG23	1.64	0.41
1:A:441:ASP:O	1:A:445:ARG:HB2	2.20	0.41
1:A:506:GLN:HB3	1:A:509:PHE:CD1	2.55	0.41
1:B:168:ALA:O	1:B:171:LEU:HB2	2.21	0.41
1:A:191:ALA:O	1:A:195:LEU:HB2	2.21	0.41
1:A:360:ILE:HD13	1:A:360:ILE:HA	1.76	0.41
1:A:353:HIS:CB	1:A:420:ALA:HB1	2.51	0.41
1:A:84:ARG:HD3	1:A:85:LEU:N	2.36	0.41
1:A:94:LEU:HD12	1:A:94:LEU:HA	1.84	0.41
1:B:441:ASP:O	1:B:445:ARG:HG3	2.21	0.41
1:B:618:LEU:HA	1:B:619:PRO:HD2	1.73	0.41
1:A:368:GLN:O	1:A:372:GLU:HB2	2.20	0.41
1:A:435:LYS:HB3	1:A:436:TRP:CE3	2.56	0.41
1:B:252:HIS:O	1:B:255:SER:HB3	2.20	0.41
1:B:353:HIS:C	1:B:355:GLU:N	2.74	0.41
1:B:381:GLN:O	1:B:385:LEU:HB2	2.21	0.41
1:A:119:VAL:HG12	1:A:120:GLU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ARG:HB3	1:A:162:ALA:H	1.74	0.41
1:A:617:ASN:O	1:A:618:LEU:HD23	2.21	0.41
1:A:583:LEU:CD1	1:A:592:GLU:HG3	2.51	0.41
1:B:576:MSE:O	1:B:580:ILE:HG13	2.20	0.41
1:B:501:GLU:HG2	1:B:502:PHE:CD1	2.56	0.40
1:A:602:ASP:N	1:A:602:ASP:OD2	2.46	0.40
1:A:612:LEU:O	1:A:615:LYS:HB2	2.21	0.40
1:A:84:ARG:HD2	1:A:86:GLU:H	1.84	0.40
1:B:358:ILE:O	1:B:362:GLN:HB2	2.21	0.40
1:A:327:LEU:HD23	1:A:327:LEU:HA	1.93	0.40
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.77	0.40
1:A:77:LYS:O	1:A:81:GLU:HG3	2.20	0.40
1:B:305:PRO:HG2	1:B:308:GLN:HB2	2.03	0.40
1:B:316:PHE:O	1:B:319:ASN:HB2	2.21	0.40
1:B:324:VAL:HG21	1:B:386:LEU:CD2	2.51	0.40
1:B:387:LEU:HD23	1:B:387:LEU:HA	1.67	0.40
1:B:358:ILE:HG22	1:B:427:PHE:CZ	2.56	0.40
1:A:157:LEU:HD12	1:A:175:ARG:HE	1.86	0.40
1:A:381:GLN:O	1:A:385:LEU:HB2	2.22	0.40
1:A:382:ILE:O	1:A:386:LEU:HG	2.21	0.40
1:A:471:PRO:O	1:A:473:PHE:N	2.54	0.40
1:B:228:VAL:CG1	1:B:294:GLU:HG3	2.51	0.40
1:B:393:LEU:HG	1:B:393:LEU:O	2.14	0.40
1:B:85:LEU:HD23	1:B:145:LEU:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ARG:NH1	1:B:264:GLU:OE2[4_455]	2.17	0.03

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	575/600 (96%)	483 (84%)	67 (12%)	25 (4%)	3	18
1	B	574/600 (96%)	496 (86%)	63 (11%)	15 (3%)	7	31
All	All	1149/1200 (96%)	979 (85%)	130 (11%)	40 (4%)	4	23

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	A	463	GLN
1	A	639	PRO
1	B	286	LEU
1	B	616	GLY
1	B	619	PRO
1	A	292	ALA
1	A	480	ARG
1	A	500	PRO
1	A	616	GLY
1	A	627	ARG
1	A	629	ILE
1	B	113	VAL
1	B	201	THR
1	B	288	SER
1	B	289	PRO
1	A	161	ARG
1	A	172	GLU
1	A	306	PRO
1	A	409	LYS
1	A	619	PRO
1	A	630	LEU
1	A	634	THR
1	B	112	LEU
1	B	639	PRO
1	A	106	GLY
1	A	289	PRO
1	A	618	LEU
1	A	137	PRO
1	A	539	ALA
1	B	71	PRO
1	B	306	PRO
1	B	137	PRO
1	B	350	GLY

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Mol	Chain	Res	Type
1	B	354	SER
1	A	141	ALA
1	B	374	ILE
1	A	374	ILE
1	A	600	TYR
1	A	614	ILE

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	504/513 (98%)	429 (85%)	75 (15%)	4	16
1	B	502/513 (98%)	405 (81%)	97 (19%)	2	9
All	All	1006/1026 (98%)	834 (83%)	172 (17%)	2	12

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	THR
1	A	80	LEU
1	A	85	LEU
1	A	94	LEU
1	A	96	ARG
1	A	107	MSE
1	A	116	GLN
1	A	117	SER
1	A	119	VAL
1	A	123	TYR
1	A	138	LEU
1	A	149	LEU
1	A	152	VAL
1	A	153	SER
1	A	174	THR
1	A	193	GLU
1	A	195	LEU

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Mol	Chain	Res	Type
1	A	198	GLN
1	A	210	GLU
1	A	212	ARG
1	A	229	GLU
1	A	237	ASP
1	A	241	VAL
1	A	242	VAL
1	A	253	PHE
1	A	255	SER
1	A	262	GLN
1	A	265	LEU
1	A	266	CYS
1	A	268	ARG
1	A	273	LEU
1	A	290	LYS
1	A	295	LEU
1	A	296	GLN
1	A	308	GLN
1	A	312	LEU
1	A	325	LYS
1	A	334	LEU
1	A	336	SER
1	A	341	GLN
1	A	348	LEU
1	A	354	SER
1	A	356	LEU
1	A	368	GLN
1	A	382	ILE
1	A	385	LEU
1	A	396	SER
1	A	411	LEU
1	A	417	ASN
1	A	426	LEU
1	A	429	TRP
1	A	438	ILE
1	A	443	LEU
1	A	447	LEU
1	A	448	GLU
1	A	461	LEU
1	A	477	THR
1	A	485	VAL
1	A	494	THR

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Mol	Chain	Res	Type
1	A	498	SER
1	A	499	LEU
1	A	510	ARG
1	A	511	GLU
1	A	512	GLU
1	A	513	LEU
1	A	528	ARG
1	A	550	LEU
1	A	585	ASP
1	A	587	SER
1	A	600	TYR
1	A	617	ASN
1	A	618	LEU
1	A	621	SER
1	A	627	ARG
1	A	631	ASP
1	B	80	LEU
1	B	87	VAL
1	B	94	LEU
1	B	99	GLU
1	B	107	MSE
1	B	116	GLN
1	B	119	VAL
1	B	123	TYR
1	B	124	VAL
1	B	136	ARG
1	B	138	LEU
1	B	143	GLU
1	B	149	LEU
1	B	152	VAL
1	B	157	LEU
1	B	177	ARG
1	B	179	TRP
1	B	190	VAL
1	B	193	GLU
1	B	195	LEU
1	B	198	GLN
1	B	212	ARG
1	B	218	ARG
1	B	219	THR
1	B	229	GLU
1	B	231	LEU

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Mol	Chain	Res	Type
1	B	234	LEU
1	B	241	VAL
1	B	242	VAL
1	B	253	PHE
1	B	257	LEU
1	B	258	CYS
1	B	260	LEU
1	B	264	GLU
1	B	265	LEU
1	B	266	CYS
1	B	274	LEU
1	B	284	ASP
1	B	290	LYS
1	B	308	GLN
1	B	309	ILE
1	B	311	LEU
1	B	312	LEU
1	B	316	PHE
1	B	322	THR
1	B	323	SER
1	B	326	GLN
1	B	339	TRP
1	B	342	ASP
1	B	351	HIS
1	B	354	SER
1	B	361	LEU
1	B	368	GLN
1	B	372	GLU
1	B	375	THR
1	B	376	SER
1	B	383	LYS
1	B	385	LEU
1	B	394	LEU
1	B	395	ARG
1	B	398	GLN
1	B	409	LYS
1	B	410	LEU
1	B	415	ARG
1	B	416	VAL
1	B	436	TRP
1	B	443	LEU
1	B	447	LEU

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Mol	Chain	Res	Type
1	B	448	GLU
1	B	453	LEU
1	B	461	LEU
1	B	462	LEU
1	B	463	GLN
1	B	464	SER
1	B	465	LEU
1	B	489	GLU
1	B	493	THR
1	B	495	VAL
1	B	496	SER
1	B	505	LEU
1	B	510	ARG
1	B	533	ARG
1	B	536	LEU
1	B	543	GLN
1	B	544	GLN
1	B	550	LEU
1	B	557	GLN
1	B	568	THR
1	B	579	GLU
1	B	593	VAL
1	B	605	LYS
1	B	614	ILE
1	B	615	LYS
1	B	618	LEU
1	B	621	SER
1	B	623	VAL
1	B	646	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	413	ASN
1	A	417	ASN
1	A	520	HIS
1	A	552	ASN
1	B	250	HIS
1	B	256	HIS
1	B	518	HIS
1	B	541	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [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	570/600 (95%)	-0.06	3 (0%)	91 76	28, 74, 126, 185	0
1	B	569/600 (94%)	-0.05	6 (1%)	82 57	36, 77, 132, 184	0
All	All	1139/1200 (94%)	-0.06	9 (0%)	87 67	28, 76, 130, 185	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	636	VAL	7.0
1	B	162	ALA	4.4
1	B	415	ARG	3.6
1	B	354	SER	3.1
1	A	163	SER	3.1
1	A	436	TRP	2.8
1	B	163	SER	2.6
1	B	631	ASP	2.0
1	B	628	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.