



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 11:13 PM EDT

PDB ID : 5B86  
Title : Crystal structure of M-Sec  
Authors : Yamashita, M.; Sato, Y.; Yamagata, A.; Fukai, S.  
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](mailto: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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

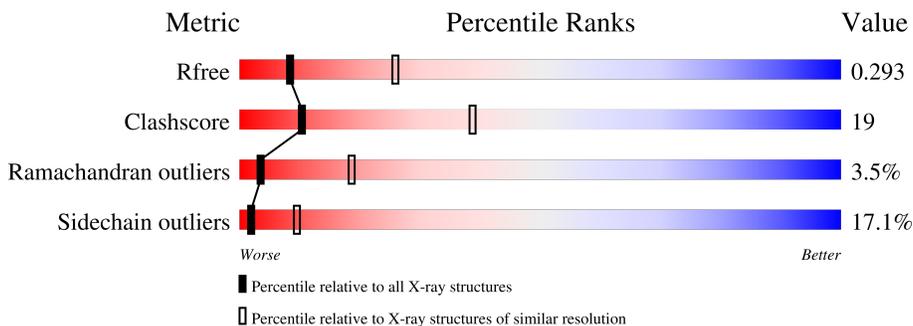
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.02 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))
$R_{free}$	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	600	 52% 38% 6% .
1	B	600	 49% 38% 9% .

## 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
			Total	C	N	O	S	Se			
1	A	579	4638	2948	814	859	8	9	0	0	0
1	B	578	4628	2942	811	858	8	9	0	0	0

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

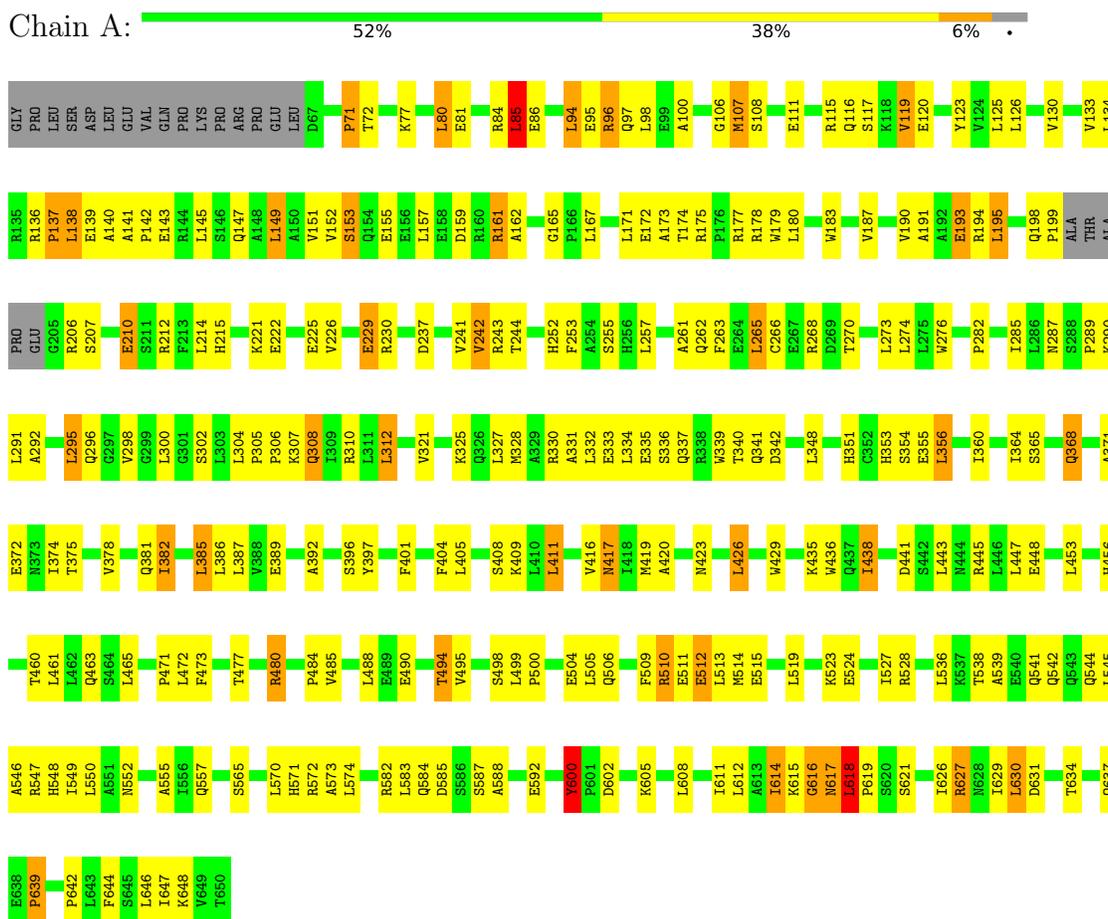
- Molecule 2 is water.

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 [i](#)

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

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



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



R212	R282	R359	L446	K523	N617
F213	M283	I360	L447	L618	L618
L214	D284	L361	E448	E524	P619
H215	I285	Q362	F449	S620	S620
M216	I363	L363	L450	I527	S621
Q217	M287	L364	L453	R528	E622
R218	S288	Q368	K454	L529	V623
T219	P289	E372	F458	R533	R624
M220	K290	N373	L461	L534	S625
K221	L291	I374	L462	L628	I626
L224	E294	T375	Q463	S538	R627
V227	L303	S376	S464	A539	N628
V228	L304	V378	L465	E540	I629
E229	P305	D377	L466	L550	L630
R230	P306	V378	F467	A551	D631
L231	K307	Q381	L468	Q541	I631
L234	I309	I382	D468	Q542	ILE
F235	R310	K383	L469	Q543	ASN
P236	L311	Q384	P471	Q544	THR
D237	L312	L385	L472	A552	GLY
E238	E313	L386	F473	N552	VAL
F239	F316	L387	K474	Q557	GLN
M240	L317	L393	K475	G558	P642
V241	S318	L394	F476	F559	L643
V242	N319	R395	T477	Q478	F644
R243	E320	Q398	Q479	E562	S645
T244	V321	S408	R480	A567	L646
E247	T322	K409	W481	T588	I647
Y251	V324	L410	T487	M576	K648
H252	K325	L411	L488	E579	V649
F253	Q326	R415	E489	I580	F650
A254	I327	W416	I491	S581	T650
S255	M328	M419	T492	L582	
H256	A329	A420	T493	L583	
C258	R330	M423	V494	A588	
L260	E335	M424	S496	K590	
F263	W339	C425	E501	F593	
E264	D342	L426	F502	D602	
L265	V343	F427	S503	K605	
C266	A344	F428	E504	G606	
D269	P345	W429	L505	H607	
L272	G350	W436	G506	L608	
L273	H351	Q437	C508	L612	
L274	C352	I438	F509	A613	
L275	H353	S439	R510	I614	
W276	S354	H440	L513	K615	
N279	E355	D441	W514	O616	
L280	L356	S442	E515		
A357	A357	L443	L519		
Y281	I358	R444			
		R445			

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.229 , 0.292 0.230 , 0.293	Depositor DCC
$R_{free}$ test set	1981 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.3	Xtrriage
Anisotropy	0.178	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 64.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	9312	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

*Continued on next page...*

*Continued from previous page...*

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:OD2	1:B:67:ASP:N	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:H	1:A:300:LEU:HD12	1.69	0.57

*Continued on next page...*

*Continued from previous page...*

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:147:GLN:O	1:A:151:VAL:HG23	2.04	0.56
1:A:265:LEU:HD22	1:A:265:LEU:H	1.70	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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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:H	1:A:206:ARG:HD2	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:85:LEU:HD12	1:A:145:LEU:HB2	1.97	0.47
1:A:270:THR:O	1:A:274:LEU:HB2	2.15	0.47
1:A:419:MSE:HG2	1:A:505:LEU:HD13	1.96	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: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: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:B:618:LEU:HD22	1:B:618:LEU:H	1.81	0.46
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.65	0.46
1:B:221:LYS:HE2	1:B:221:LYS:HB3	1.78	0.46

*Continued on next page...*

*Continued from previous page...*

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:HD12	1:A:195:LEU:HA	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:605:LYS:HG2	1:B:626:ILE:HG23	1.99	0.45
1:B:607:HIS:NE2	1:B:647:ILE:HG22	2.32	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:HB2	1:B:136:ARG:NH1	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

*Continued on next page...*

*Continued from previous page...*

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:79:ALA:O	1:B:84:ARG:HG3	2.16	0.44
1:B:398:GLN:NE2	2:B:707:HOH:O	2.41	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

*Continued on next page...*

*Continued from previous page...*

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:OD1	1:B:602:ASP:N	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:97:GLN:O	1:A:100:ALA:HB3	2.19	0.41
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: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: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:A:353:HIS:CB	1:A:420:ALA:HB1	2.51	0.41
1:A:360:ILE:HD13	1:A:360:ILE:HA	1.76	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:119:VAL:HG12	1:A:120:GLU:N	2.36	0.41
1:A:161:ARG:HB3	1:A:162:ALA:H	1.74	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:A:617:ASN:O	1:A:618:LEU:HD23	2.21	0.41
1:B:252:HIS:O	1:B:255:SER:HB3	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:84:ARG:HD2	1:A:86:GLU:H	1.84	0.40
1:A:602:ASP:OD2	1:A:602:ASP:N	2.46	0.40
1:A:612:LEU:O	1:A:615:LYS:HB2	2.21	0.40
1:B:358:ILE:O	1:B:362:GLN:HB2	2.21	0.40
1:A:77:LYS:O	1:A:81:GLU:HG3	2.20	0.40
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.77	0.40
1:A:327:LEU:HD23	1:A:327:LEU:HA	1.93	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:358:ILE:HG22	1:B:427:PHE:CZ	2.56	0.40
1:B:387:LEU:HA	1:B:387:LEU:HD23	1.67	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:85:LEU:HD23	1:B:145:LEU:HB2	2.04	0.40
1:B:228:VAL:CG1	1:B:294:GLU:HG3	2.51	0.40
1:B:393:LEU:O	1:B:393:LEU:HG	2.14	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%)	2	14
1	B	574/600 (96%)	496 (86%)	63 (11%)	15 (3%)	5	26
All	All	1149/1200 (96%)	979 (85%)	130 (11%)	40 (4%)	3	18

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

*Continued on next page...*

*Continued from previous page...*

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 [i](#)

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%)	<b>3</b> <b>13</b>
1	B	502/513 (98%)	405 (81%)	97 (19%)	<b>1</b> <b>7</b>
All	All	1006/1026 (98%)	834 (83%)	172 (17%)	<b>2</b> <b>9</b>

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

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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

*Continued on next page...*

*Continued from previous page...*

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

Sometimes 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.